Mathematical Optimization for Optimal Decision-Making in Practice:
Energy Systems and Political Districting

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Abstract

Decision-making can be a complex task. For example, there are an enormous number of possibilities to route vehicles of a logistics company, to define timetables at a university, or to determine locations of charging stations for electric cars. For a given problem, more decision alternatives can exist than particles in the whole universe. This combinatorial explosion is not only due to the large amount of data that can be involved. Manifold dependencies between (sub-)decisions, different conditions, and criteria also influence the complexity. In most cases and especially if one is interested in a best possible decision, it is hopeless to solve complex decision problems by hand or by simple enumeration using a computer.
Mathematics and in particular its subfield mathematical optimization provides concepts, methods, and a research environment to master complex decision-making problems. Mathematics enables the decision-maker to identify a verifiably best possible solution which can then be implemented in practice. This leads to a growing number of success stories of applying mathematical optimization: E.g., in saving money, in improving environmental protection, in ensuring fairness, and in saving lives.

In this thesis, two application areas are investigated with regard to optimal decision-making. They are representatives of the wide range of application areas in which mathematics leads to decisions that are better, more transparent, and/or more objective.

The first application deals with optimal decentralized energy systems. The task is to design a system of various energy conversion technologies capable of meeting the demand of different forms of energy. An optimally designed decentralized energy system can be beneficial for large industrial plants, hospitals, research facilities, or even housing estates. In addition, ecological advantages can be achieved. The contribution of this thesis encompasses the development of a solution method that incorporates non-linear and non-convex technology models. This characteristic distinguishes the proposed method from most of the literature. The vast majority of approaches proposed in the literature neglects that physical, chemical, and technical interrelations are naturally non-linear. The proposed solution method is based on a developed adaptive discretization approach and provides high-quality solutions on real-world inspired data instances. As a further contribution, the first-ever results on the problem's computational complexity are presented. The results justify the development of solution methods with potentially exponential runtime. Such a well-founded justification has been missing until today.

The second application deals with optimal delimitation of electoral districts. The task is to partition a territory into a given number of electoral districts, meeting several requirements and criteria given by law and jurisprudence. The terminology "optimal" here means the greatest possible compliance with the legal criteria. The thesis focuses on the problem

variant for German federal elections. In Germany, the revision of the electoral districts is on the agenda before every election. In addition, the topic is currently being discussed in the context of reforming the electoral law. The contribution of this thesis encompasses a comprehensive review of solution methods and districting software proposed in the literature. Then, a definition of the political districting problem meeting the German specifications is given. The presented mixed-integer linear programming formulation is based on a novel consideration of administrative conformity and continuity. Both criteria turned out to be most important in German practice and are not appropriately incorporated in the literature yet. Based on the model, primal heuristics and exact preprocessing techniques are proposed. To enable a practical application of the findings, all research is packed into a ready-to-use decision support system. The software is based on a geographical information system and includes current and detailed data. Last but not least, the thesis documented how the developed software was successfully applied in practice. On behalf of the German Federal Returning Officer optimization-based delimitations of electoral districts were computed in order to support a parliamentary commission working on a reform of the electoral law.

Zusammenfassung

Das Treffen von Entscheidungen kann eine komplexe Aufgabe sein. So gibt es beispielsweise eine enorme Anzahl an Möglichkeiten, Fahrzeuge eines Logistikunternehmens zu routen, Stundenpläne für eine Universität festzulegen oder Standorte für Ladestationen für Elektroautos zu definieren. Für eine Problemstellung können mehr Entscheidungsalternativen existieren als Partikel im gesamten Universum. Diese kombinatorische Explosion ist nicht nur auf die großen Datenmengen zurückzuführen, die beteiligt sein können. Vielfältige Abhängigkeiten zwischen (Teil-)Entscheidungen, unterschiedliche Bedingungen und Kriterien beeinflussen ebenfalls die Komplexität. In den meisten Fällen und insbesondere, wenn man an einer bestmöglichen Entscheidung interessiert ist, ist es hoffnungslos, komplexe Entscheidungsprobleme von Hand oder durch einfache Enumeration mit dem Computer zu lösen.
Die Mathematik und insbesondere ihr Teilgebiet die mathematische Optimierung bieten Konzepte, Methoden und eine Forschungsumgebung zur Bewältigung komplexer Entscheidungsprobleme. Die Mathematik ermöglicht es den Entscheidungstragenden, eine nachweislich bestmögliche Lösung zu finden, die dann in der Praxis umgesetzt werden kann. Dies führt zu einer wachsenden Anzahl von Erfolgsgeschichten durch Anwendung mathematischer Optimierung: Zum Beispiel, um Geld zu sparen, den Umweltschutz zu verbessern, Fairness zu gewährleisten oder Leben zu retten.

In dieser Dissertation werden zwei Anwendungsfelder mit dem Ziel einer optimalen Entscheidungsfindung bearbeitet. Die beiden Anwendungen repräsentieren das breite Spektrum der Gebiete, in denen Mathematik zu besseren, transparenteren und/oder objektiveren Entscheidungen führen kann.

Die erste Anwendung beinhaltet die Optimierung von dezentralen Energiesystemen. Die Aufgabe besteht darin, ein System aus verschiedenen Energieumwandlungstechnologien zu bestimmen, das in der Lage ist, einen Bedarf an verschiedenen Energieformen zu erfüllen. Ein optimal ausgelegtes dezentrales Energiesystem kann für große Industrieanlagen, Krankenhäuser, Forschungseinrichtungen oder auch Wohnsiedlungen vorteilhaft sein. Darüber hinaus können auch ökologische Vorteile erzielt werden. Der Beitrag dieser Arbeit umfasst die Entwicklung einer Lösungsmethode, die nicht-lineare und nicht-konvexe Technologiemodelle berücksichtigt. Dieses Merkmal unterscheidet die vorgeschlagene Methode von den meisten in der Literatur vorgeschlagenen. Die überwiegende Mehrheit der in der Literatur präsentierten Ansätze vernachlässigt, dass physikalische, chemische und technische Zusammenhänge natürlicherweise nicht-linear sind. Die vorgeschlagene Lösungsmethode basiert auf einem entwickelten adaptiven Diskretisierungsansatz und liefert qualitativ hochwertige Lösungen für auf realen Daten basierende Instanzen. Als weiterer Beitrag werden die ersten Ergebnisse zur Komplexität des Problems bewiesen. Die Resultate rechtfertigen die Entwicklung von Lösungsmethoden mit potentiell exponentieller Laufzeit. Eine solche fundierte Begründung fehlt bis heute.

Die zweite Anwendung beinhaltet die optimale Einteilung von Wahlkreisen. Die Aufgabe besteht darin, ein Gebiet in eine bestimmte Anzahl an Wahlkreisen aufzuteilen, sodass mehrere Anforderungen und Kriterien erfüllt werden, die durch das Gesetz und Rechtsprechungen vorgegeben sind. Die Terminologie “optimal” bedeutet hier eine bestmögliche Erfüllung der gesetzlichen Einteilungskriterien. Im Mittelpunkt der Arbeit steht die Problemvariante bei der deutschen Bundestagswahl. In Deutschland wird vor jeder Wahl eine Revision der Wahlkreise durchgeführt. Darüber hinaus wird das Thema derzeit im Rahmen einer Reform des Wahlrechts diskutiert. Der Beitrag dieser Dissertation umfasst eine ausführliche Darstellung der Lösungsmethoden, die in der Literatur vorgeschlagen werden, sowie verfügbare Software, die das Einteilen von Wahlkreisen unterstützt. Anschließend wird eine formale Definition der Problemstellung der Wahlkreiseinteilung präsentiert, die die deutschen Vorgaben berücksichtigt. Die entwickelte gemischt-ganzzahlige lineare Formulierung basiert auf einer neuartigen Bemessung von administrativer Konformität und Kontinuität. Beide Kriterien haben sich in der deutschen Praxis aus besonderes wichtig erwiesen und sind in der Literatur noch nicht ausreichend berücksichtigt worden. Basierend auf dem Modell werden primale Heuristiken und exakte Preprocessing-Verfahren vorgestellt. Um eine praktische Anwendung der Methoden zu ermöglichen, ist die gesamte Forschung in ein einsatzbereites Entscheidungsunterstützungssystem integriert. Die Software basiert auf einem geografischen Informationssystem und beinhaltet detaillierte, aktuelle Daten. Abschließend dokumentiert die Dissertation, wie die entwickelte Software erfolgreich in der Praxis eingesetzt wurde. Im Auftrag des Bundeswahlleiters wurden optimierungsbasierte Wahlkreiseinteilungen berechnet, um eine parlamentarische Kommission bei den Bemühungen um eine Reform des Wahlrechts zu unterstützen.

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1 Introduction

Decision-making is a crucial component of today's modern society. The growing interconnection of people and also of objects, newly emerging consumer needs, and innovative technologies as well as (digital) services — all this does not only lead to *Big Data*. In fact, it rather results in *Big Decision-Making*.

Data is an important factor today and also in the future. But data and also forecasts based on collected information provide only answers to questions like *"What happened?"* and *"What will (probably) happen?"*. Data essentially documents the past. The much more crucial factor, however, is to make decisions on the basis of data and to derive recommendations for action for the present and future: *"What to do? And when?"*. Decision-making describes the process of translating data into decisions, under consideration of constraints and evaluation criteria.

In many cases, decision-making *can not* be performed manually. The reason is that an underlying task can be time-sensitive or too complex.

Logistics On a typical day, the logistics provider UPS delivers 16,000,000 million packages in the United States. Each of the 55,000 drivers serves about 160 customers.[1] The timely fulfillment of these orders is an enormous task. Decisions include the design of the logistics network including locations of warehouses and transshipment points as well as transport vehicles. Daily decisions include the planning of employee shifts, allocation of consignments to vehicles, and the routing of the delivering vehicles fleet.

Even taking advantage of a computer and its processing speed does not necessarily have to be successful in such planning tasks. When simply working through decision options, it can still take several years to identify an alternative considering all requirements. For example, there are vastly more possible sequences to deliver 60 packages than the estimated number of fundamental partices in the entire universe.[2] And there is still much more to be decided in logistics than just one delivery sequence. Such a *combinatorial explosion* cannot even be mastered by rapid and computer-aided trial and error.

Besides the complexity aspect, many decisions *should not* be made by hand or according to instinct, as potential consequences are too serious.

Large crowds of people Every year up to 4,000,000 Muslims perform their religious duty in form of a pilgrimage to the region of Mecca, Saudi Arabia.[3] Most of them approach the holy

[1] Source: Holland et al. (2017)
[2] Source: Numerphile, `https://www.youtube.com/watch?v=lpj0E0a0mlU` (last access: April 14, 2019).
[3] Source: Haase et al. (2016, 2019)

sites on four specific consecutive days of the year. This makes the Hajj, as the pilgrimage is called, to one of the largest annually pedestrian events in the world. Unfortunately, several sad crowd disasters with thousands of victims occurred. Decisions include the design and operation of the infrastructure, directing flows of pilgrims, scheduling of rituals at focal sites, and planning reactions to dangerous situations.

> *The Science of Better.*
>
> **— a campaign to market operations research**
> (INFORMS, www.informs.org, www.scienceofbetter.org,
> see also www.scienceofbetter.co.uk of The OR Society)

Operations Research (OR) is the discipline of applying advanced analytical methods to support complex and sensetive decision-making. In fact, OR helps to make better and even provably best possible decisions in real-world applications. The field uses computer science and mathematics. Especially, **Mathematical Optimization** provides techniques, concepts, methods, and all in all a research environment to tackle combinatorial explosions of today's complex decision-making problems. The combination of mathematics and computer science enables the consideration of *all* decision alternatives and to identify an optimal one. This is exactly what sets OR apart from other types of decision-making processes.

Given examples in logistics and crowd events are successfully mastered using OR methods and techniques of mathematical optimization.

Optimized delivery routes – with OR In order to master the increasing number of small package orders, UPS starts a research project in 2003 with the goal to modernize its pickup and delivery operations. As a result, an implemented on-road integrated optimization and navigation system provides the drivers with an optimized route based on the packages to be picked up and delivered. The deployment of the system for all 55,000 US drivers was achieved in 2016. UPS reported that the use of OR saves costs of up to 400 million US dollar per year. The annual CO_2 emissions have been reduced by 100,000 tons. In addition, UPS quotes drivers who point out that the system allows them to focus more on driving safety than determining their route. This success story is documented by Holland et al. (2017).

Safe and effective crowd control – with OR In the aftermath of a crowd disaster at the Islamic pilgrimage to Mecca in 2006, authorities initiated a comprehensive project to prevent crowd disasters in the future. A problem-specific and OR-based decision support system was developed. A real-time video tracking system and an optimization-based scheduling tool was implemented. This enables uncongested and smooth pilgrim flows. From then on the system was an integral part of the Hajj planning. OR helped to reduce operation and maintenance costs. But most importantly: No crowd disaster occurred under the systems usage. OR significantly contributed to saving lives in mass gatherings. The conducted research and a detailed documentation of the achievements is presented by Haase et al. (2016, 2019).

Ethics, Transparency, and Objectivity: Increasingly Important Aspects in Decision-Making

Today's world is characterized by the fact that every day more information is available within seconds. At the same time, information and decisions are increasingly being questioned, triggered by the spread of misinformation and falsification. In addition, more and more complex and time-sensitive decision-making problems arise, which are handled more frequently automatically.

In this setting, following aspects are gaining more and more significance – also in decision-making: transparency and objectivity.

Autonomous driving The board system of a self-driving car records at any time a vast amount of data of its environment. The data is interpreted and decisions on the proceeding movement are derived within milliseconds. However, even such a system is not able to prevent all critical situations. At the moment an accident is unavoidable, it may be necessary to decide whether to protect the car's passengers or pedestrians outside the vehicle. How does the system make this decision?
Certainly, this topic encompasses questions which still have to be clarified legally and are not to be addressed mathematically in the first place. However, such a serious decision-making process should be transparent. It should be disclosed which specifications and assessments are used to automatically determine a decision. At least this is necessary to legally evaluate the process and to compare it with laws that still have to be developed. In addition, this will also be necessary to obtain acceptance in society.

Fairness as a criterion Several everyday applications exist, where fairness or justice is (or should be) a major criteria for assessment of a decision: E.g., organ allocation for transplantation (Bertsimas et al., 2013), work/staff scheduling (Rocha et al., 2012), flow allocation in communication networks (Amaldi et al., 2013).
To ensure best possible fairness in such complex decision-making problems, one practically is forced to apply OR methods like mathematical optimization.

It is certain that there is no unique definition of how fairness or justice is to be measured. Also legal requirements often leave room for interpretation. Mathematics and algorithms, being a sequence of operations, are inherently unbiased. The decisive factor is how they are applied. For each decision made on the basis of OR methods, the decision-making process can be presented transparently. This can be done in the form of the underlying mathematical model or algorithm. It can be judged (by humans) which data, specifications or measurement influence the decision. Furthermore, the decision-making process can be verified.

Mathematical optimization enables transparency and can even promote and create this as well as objectivity. However, this only holds if the authority of the machine, i.e. the human being, allows that.

The Process of Operations Research

In order to tackle a decision-making problem with the research toolbox provided by OR, the following phases have to be considered. Although, a list of fundamental aspects is presented, the process should not be viewed as linear. In reality there are many loops between the phases, since they influence each other and are closely related. For all phases holds that a look into the literature and building on what is already known is helpful.

Orientation A specific decision-making context has to be identified and delimited. It is necessary to clarify what decision(s) one is faced with. Conditions that restrict decision alternatives or limit resources as well as dependencies between decisions have to be identified. Specific factors that effect the assessment of valid decisions have to be determined, e.g., costs or environmental aspects. Last but not least, involved data and parameters has to be deduced.

Practice Practical knowledge should be acquired and taken into account. However, statements from practice should also be questioned in a first step. Frozen procedures may be unfounded and may hinder improvement. Furthermore, its is interesting how the decisions have been made so far and how they have worked out. It may even be possible to identify what characteristic has been lacking in previous decisions.

Definition The considered problem has to defined formally, i.e., converted into mathematics. A formal definition encompasses decisions and their domain as well as constraints and objectives with numerical measurements. Furthermore, type and format of input data has to be specified. This phase can also include the preparation of simplifications of the problem.

Complexity The problem's computational complexity should be investigated. This is essential for making a preselection of suitable solution techniques and its justification.

Decision Model In general, a model is an abstract representation (of selected characteristics) of the original problem. While a problem's definition is unique, there are many possibilities to model a given problem. Finding a good model is one key issue for a successful application of OR. Concepts like mixed-integer (non)-linear programming can be used. A model describes all possible solutions. An evaluation of solution alternatives is done via a (multi-criteria) objective. Besides, maybe the problem can be modeled as a variant of well-known problem classes like network flow, combinatorial graph problems, etc.

Data In order to evolve a model from mathematical theory to practical relevance, data is necessary. Data used as input for decision models is often different to (unstructured) data collected by (and used in) companies. The effort to obtain suitable data that is complete, accurate and representative should not be underestimated. Data may also be subject to uncertainty. This can be taken into account in the model of the problem. If no real-world data can be used, data as close to reality as possible has to be artificially generated. One set of data that covers the model's parameters is called a problem instance. Instances of different sizes should be available for the development of solution methods.

Solution A model and problem's complexity at hand, a solution method has to be developed. For most problems it is impracticable to enumerate all possible solutions. Methods of mathematical optimization are characterized by the fact that through theory and detected structure whole classes of decision alternatives can be excluded. To achieve this for new problem variants, research is necessary. Developed solution methods have to be implemented and tested. Some first determined solutions should be interpreted and validated immediately. If possible, also in practical application. At this point weaknesses and inadequacies in the applied model or even problem definition are often identified. An iteration to previous steps and adjustments may be necessary.

Decision Support To make developed and tested solution methods usable in practice, a comprehensive decision support system can be created. In addition to the OR-based computation of suitable decision recommendations, such a software system can also offer visualizations, monitoring, and solution analysis. Depending on the application, it can also be useful for the operator of the software to be able to manually adjust calculated solutions.

Structure of this Thesis: Energy Systems and Political Districting

In this thesis, research and contributions on two different fields of decision-making are documented. The considered practical applications are based on different motivations: The first one is driven by technical, engineering, economical, and ecological aspects. The second application is motivated by social, legal, and political issues. Thereby, the almost unlimited range of application areas of operations research and mathematical optimization is emphasized. Furthermore, the contrary motivations reveal the versatility of the terms *better* and *optimal*.

Following this introductory chapter, the thesis is structured in two parts. Part I deals with energy systems and part II with political districting. Both parts are surrounded by chapters with application specific introducing as well as concluding remarks. All other chapters of this cumulative dissertation are based on articles which are published in peer-reviewed journals or conference proceedings, are in revision in peer-reviewed journals, or in preparation for submission (cf. overview on page iii).

Part I: Energy Systems (Chapters 3 and 4)

Chapter 3 is based on joint work with colleagues and PhD candidates Martin Comis and Felix J.L. Willamowski. The paper "The Synthesis Problem of Decentralized Energy Systems is strongly NP-hard" is published in Computers & Chemical Engineering 124, pp. 343–349, May 2019 (Goderbauer et al., 2019).
Contribution of the thesis' author: principal author, literature review, problem definition, contributions to the development of the three proofs of complexity.

In addition to the published paper, the thesis includes the detailed presentation of an alternative proof of strong NP-hardness (cf. Sec. 3.5). In the published paper, this proof is only outlined.

Chapter 4 is based on joint work with colleague and PhD candidate Björn Bahl, colleagues Dr. Philip Voll and Prof. Dr. André Bardow, as well as supervisors Prof. Dr. Marco Lübbecke and Prof. Dr. Arie M.C.A. Koster. The paper "An adaptive discretization MINLP algorithm for optimal synthesis of decentralized energy supply systems" is published in Computers & Chemical Engineering 95, pp. 38–48, December 2016 (Goderbauer et al., 2016).
The work was presented by the thesis' author at 22nd International Symposium on Mathematical Programming, Pittsburgh, USA, July 2015 and at International Conference on Operations Research, Vienna, Austria, September 2015.
Contribution of the thesis' author: principal author, conceptual development of the method and models, technical implementation, calculation and evaluation of computational results. In addition to the published paper, the thesis includes further variants of the presented method and related theoretical results (cf. Sec. 4.6).

Part II: Political Districting (Chapters 7 – 11)

Chapter 7 is based on joint work with student assistant Martin Wicke. The paper "Constituencies for German Federal Elections: Legal Requirements and Their Observance" is in the review process (first revision) of German Politics and Society (Goderbauer and Wicke, 2017).
Contribution of the thesis' author: principal author, conceptual development of research questions, embedding in existing literature, conceptual development of measurement functions, mentoring of the implementation for data preparation and evaluation, evaluation of results.

Chapter 8 is based on joint work with student assistant Jeff Winandy. The paper "Political Districting Problem: Literature Review and Discussion with regard to Federal Elections in Germany" is in the review process (second revision) of Computers & Operations Research (Goderbauer and Winandy, 2017).
Contribution of the thesis' author: principal author, defining the volume of literature to be considered, development of the definition of the political districting problem and its German variant, evaluation and presentation of literature.

Chapter 9 is based on joint work with supervisor Prof. Dr. Marco Lübbecke. The working paper "A Geovisual Decision Support System for Optimal Political Districting" is in preparation for submission (Goderbauer and Lübbecke, 2019a).
The work was presented by the thesis' author at International Conference on Operations Research, Brussels, Belgium, September 2018.

Chapter 10 is based on joint work with student assistant Leonie Ermert. The paper "Proportional Apportionment for Connected Coalitions" is published (in print) in Operations Research Proceedings 2018 (Goderbauer and Ermert, 2019).
Contribution of the thesis' author: principal author, conceptual development of the method

and models, development of complexity proof, assistance by the implementation, calculation and evaluation of results.

Chapter 11 is based on joint work with supervisor Prof. Dr. Marco Lübbecke. The paper "Reform der Bundestagswahlkreise: Unterstützung durch mathematische Optimierung" is published in Zeitschrift für Parlamentsfragen 50(1), pp. 3–21, April 2019 (Goderbauer and Lübbecke, 2019b).
In addition to the published paper, the thesis' version is much more detailed and includes further results and evaluations.

Part I

ENERGY SYSTEMS

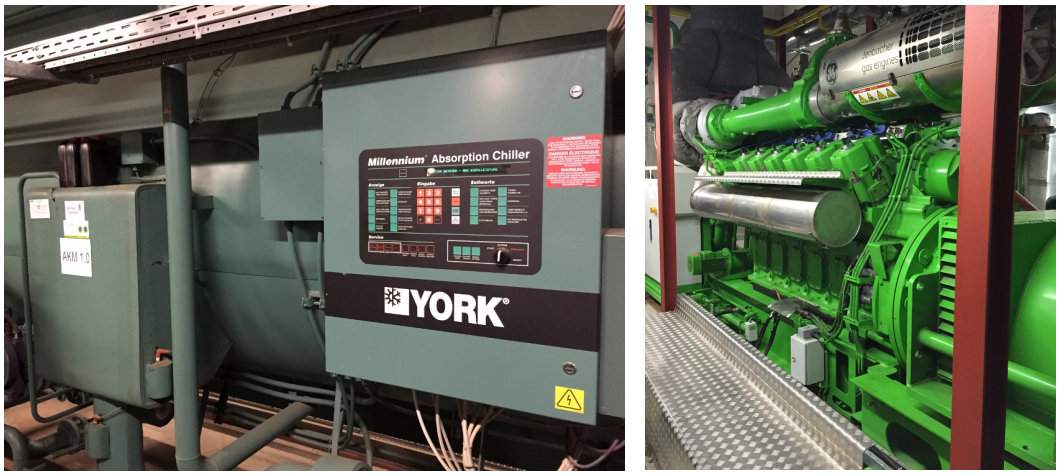
Optimal Design, Dimension, and Operation of Energy Supply Systems

2 Introducing Remarks and Contribution of this Thesis

2.1 Optimal Design, Dimension, and Operation of Decentralized Energy Supply Systems

Conventionally, energy such as electricity or heat is generated at large and centralized facilities. This kind of *centralized energy systems* include cogeneration plants, wind farms, biomass-fuelled power plants, and hydroelectric dams. These facilities are usually far away from the final consumer and are connected to energy transmission networks to distribute energy flows to multiple end-users of an entire region.

Institutions such as hospitals, chemical parks, industrial production facilities, individual urban districts, and research complexes are increasingly choosing a different strategy to meet their energy needs. Next to electricity and heating energy, these institutions may request for steam or pressurized air to conduct production steps and cold to compensate the heat caused by certain processes. In order to satisfy these high demands for different forms of energy, it is often the case that customized energy supply systems are installed *on site*. The energy required is generated in the direct vicinity of the final energy user. This leads to a massive reduction of energy transportation losses. *On-site* (also *decentralized*, or *distributed*) *energy systems* supply multiple flows of energy simultaneously and incorporate different small-capacity energy conversion technologies. The efficiency of an decentralized energy



(a) Absorption chiller.

(b) Combined heat and power engine.

Fig. 2.1: Decentralized energy supply system at RWTH Aachen University providing energy in form of cold (Fig. 2.1a), heat and electricity (Fig. 2.1b) (Technikzentrale Hörn on January 28, 2015).

supply system is not so much determined by its individual components but the synergy of all technologies forming the system and addressing specific local demands for energy (Alanne and Saari, 2006; Altmann et al., 2010; Bouffard and Kirschen, 2008).

Example of a Decentralized Energy Supply System At RWTH Aachen, a technology-driven University in Germany with more than $45\,000$ students and almost $9\,500$ employees (RWTH Aachen University, 2018b), the majority of consumed energy is generated by the university's own decentralized supply systems. Three combined heat and power (CHP) engines (Fig. 2.1b) cover one third of the total electricity demand (36 million kWh of a total of 108 million kWh). The heat generated by the latest CHP, put into operation in September 2017, is fed directly into the heating network of the university. The heat from the other two CHPs is used by absorption chillers (Fig. 2.1a) to supply the cold water networks which cover the cooling demand of, e.g., the RWTH Compute Cluster. In the future, RWTH Aachen University will continue to expand the decentralized energy supply systems within its master plan "Energy 2025". The university's aim is to continue to exert a controlling and sustainable influence on internal energy demand and consumption (RWTH Aachen University, 2018a).

Decentralized energy supply systems situated close to final energy consumers can be very beneficial – economically for the operating institution and ecologically for the whole environment. Alanne and Saari (2006), and Karger and Hennings (2009) concluded in their studies that distributed energy systems are a good option with respect to sustainable development and climate protection. Efficient decentralized energy generation does not only lead to environmental benefits like the reduction of greenhouse gas emissions or primary energy savings, but it also results in significant cost savings as shown by various authors, e.g., Keirstead et al. (2012), Onishi et al. (2017), and Ren et al. (2010).

Both, **economical advantages** and **ecological advantages**, indisputably lead to the motivation **to research on mathematical methods to ensure optimal energy supply systems**.

Optimal Synthesis of Decentralized Energy Supply Systems

When energy needs of a group of consumers and details of their locations are identified (*problem instance*), we address the integrated problem of (Frangopoulos et al., 2002)

(i) selecting energy conversion technologies and the interconnections between these components (*synthesis level*),

(ii) deciding the technical specifications such as capacities or operating limits of selected components and the properties of the substances entering and exiting each component at the nominal load (*design level*), and simultaneously

(iii) specifying operating properties of the system's components and substances, e.g., on/off status, energy output, pressures, temperatures, for each instant of time of a planning horizon to meet the energy demands (*operation level*).

Together, this integrated problem is referred to as the (conceptual) *synthesis problem of decentralized energy supply systems*.

Combining these tasks with an *objective*, e.g., a multi-criteria approach incorporating the minimization of the total cost and the minimization of environmental effects, Frangopoulos (2003) summarized the complete optimization question to be answered as follows: "What is the synthesis of the system, the design characteristics of the components and the operation strategy that lead to an overall optimum?"

Parameters such as energy demands and purchase prices are subject to *uncertainties* as they naturally vary over time. Neglecting the variability of uncertain problem data in solution approaches may lead to energy systems that perform well in the most likely scenario but perform badly under different circumstances. At worst, such simplification can lead to infeasible demand configurations. Under consideration of uncertainties in the operation level, it is common to formulate the considered synthesis problem as a *two-stage stochastic programming model* (Birge and Louveaux, 2011; Grossmann and Guillén-Gosálbez, 2010; Wakui et al., 2018; Zhou et al., 2013b). Its structure and the assignment of presented problem levels to the two stages are depicted in Figure 2.2.

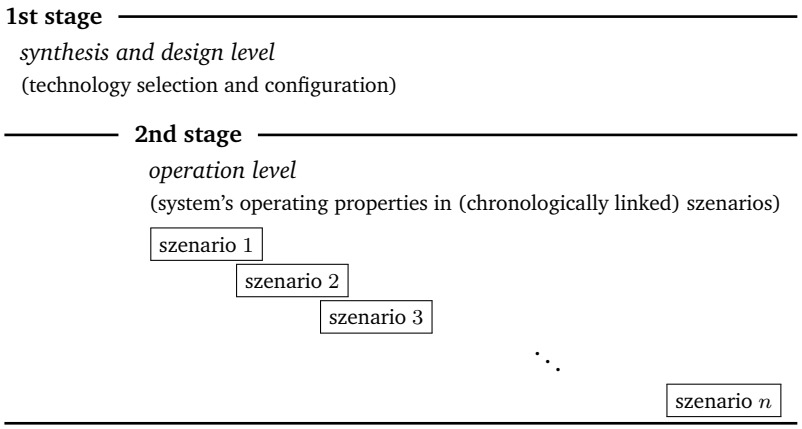


Fig. 2.2: Two-stage stochastic model of the synthesis problem of decentralized energy supply systems. The objective function to be optimized consists of the objective function of the first stage and expectation of the objective function of the second-stage scenarios.

First-stage decisions involve the synthesis and design level, i.e., the one-time investment decisions of conversion units and system infrastructure. The *second stage* consists of a set of szenarios, i.e., realizations of the uncertain parameters. For example, scenario parameters for energy demands can be derived from large (real-world) time series via identification of patterns, selection of data points, or aggregation to representative periods (Bahl et al., 2018). For each szenario, the second stage consists of the operation level decisions. Scenarios can nevertheless depend on each other, for instance because they are chronologically linked by storage technologies or ramping constraints. The special structure of two-stage stochastic models (with and without linked scenarios) can be exploited by applying decomposition approaches such as Lagrange relaxation (Fisher, 1981; Geoffrion, 1974) or Dantzig-Wolfe reformulation (Dantzig and Wolfe, 1960; Lübbecke and Desrosiers, 2005).
Besides stochastic programming, *robust optimization* (Ben-Tal and Nemirovski, 1998; Bertsi-

mas and Sim, 2004; Büsing, Goderbauer, et al., 2019) is another major approach to handle uncertainties for optimal decision-making. Majewski et al. (2017) employed a concept of robust optimization to synthesis of decentralized energy systems.

Identified open research challenges and issues

Based on the literature (cf. latest surveys of Wang et al. (2018), Andiappan (2017), Mancarella (2014), and Liu et al. (2011)), the following open research topics have been identified.

Mainly neglect of non-linear and non-convex properties Due to physical, chemical, and technical interrelations, part-load performance models of energy conversion units, i.e., the relationship between input and output energy, are naturally *non-linear*. In addition, taking into account the cost of the system, the investment cost curves of the technologies are non-linear because of the economies of scale (Papoulias and Grossmann, 1983). However, the vast majority of solution methods proposed in the literature for synthesis of energy systems neglects these key characteristics. It is common (cf. latest surveys of Andiappan (2017) and Wang et al. (2018)) to simplify these non-linearities in technology models and investment curves and to *(piece-wise) linearize* them. This practice is usually justified by the fact that common solution algorithms for linear problems, e.g., modeled as MILP, are faster, more effective, and able to handle larger problem instances than algorithms that solve non-linear and thereby often non-convex problems, e.g., modeled as non-convex MINLP. Only few authors consider non-linearties for the synthesis of energy systems, e.g., Bruno et al. (1998), Chen and Lin (2011), Elsido et al. (2017), and Varbanov et al. (2005).
In an extensive overview article on applying mathematical programming techniques in process engineering, Grossmann (2012) identified the *integration of non-linear* and non-convex characteristics as a *major open research issue* for optimal and practically relevant decision-making.

Missing collections of problem instances for benchmarking In general, each paper that proposes a new optimization-based solution approach for the synthesis of energy systems comes with a *case study* in which the developed method is applied. Latest works of, e.g., Wakui et al. (2018), Elsido et al. (2017), Bracco et al. (2016), Yokoyama et al. (2015), Bischi et al. (2014), and Zhou et al. (2013b) incorporate case studies with *between one and four test problems*. The considered test instances are usually practically motivated and based on real-world data. The authors report in detail about the energy systems computed by proposed solution approach and interpret implications for practice. In rather few works the performance of the developed method is compared to state-of-the-art approaches. Despite very small considered test sets and rare benchmarks, however, statements are made about the *(computational) performance* of the developed methods for the synthesis problem of energy systems.
These aspects are *contrary to much-noticed guidelines* on the design and reporting of computational experiments to benchmark solution approaches (Johnson, 2002; Beiranvand et al., 2017; Barr et al., 1995). Beiranvand et al. (2017) states that “an appropriate test set should generally seek to avoid the deficiency of too few problems”. Barr et al. (1995) adds that to

enable a comparison with other published results, a new approach “should be tested on all standard problems [...] for which it was designed”.

„Conjectures“ on computational complexity Regarding the complexity, the comprehensive literature on the synthesis problem of decentralized energy systems *shows a consensus* that the optimization problem, in some sense, is *hard to solve*. However, explanations given are generally not sufficient to follow any statement on the problem’s complexity. The authors use arguments like the number of decisions to be taken, combinatorial options or amount of input data: “many different feasible configurations” (Lozano et al., 2009), “wide variety of technology options [...], great fluctuations in energy consumption, and temporal variations in energy prices” (Carvalho et al., 2012), “number of periods considered” and “number of components considered in the superstructure” (Voll, 2013; Wang et al., 2018), “number of integer variables” (Yokoyama et al., 2015),“number of different technologies considered and the number of buildings served by the system” (Bracco et al., 2016).
In fact, there is a *crucial lack of formal proofs* of the claims stated in literature. While a variety of solution approaches and models have been proposed for different configurations of the synthesis problem of energy systems, there have been *no results on the problem’s computational complexity*. The discussion of such theoretical questions, however, is an active area of inquiry in the field of optimization-based process engineering, cf. work of Letsios et al. (2018), Dey and Gupte (2015), Alfaki and Haugland (2013), Furman and Sahinidis (2004), Ahmed and Sahinidis (2000).

2.2 Contribution of this Thesis

The thesis’ major contribution on the synthesis problem of decentralized energy systems is threefold. All open research issues revealed above are addressed: The first is of theoretical nature with high significance for scientific research. The second is based on the practical motivation to integrate technical and physical interrelations more realistically into solution approaches. Besides, a large set of problem instances obtained by real-world data and best known solutions is provided to enable benchmarking.

① **First-ever results on the problem’s computational complexity** A formal proof that the synthesis problem of decentralized energy supply systems is *NP-hard in the strong sense* is contributed. It is shown that this result even holds for synthesis settings restricted to one type of conversion technology with two forms of output energy, e.g., a CHP engine. It is proven that already the operation problem is *weakly NP-hard* and thus no polynomial time solution algorithm can exist for the operation subproblem, unless $P = NP$. Furthermore, a proof of *inapproximability* for the considered synthesis problem is conducted: It is proven to be *NP-hard* to even *approximate* an optimal solution within a constant approximation factor. These results are relevant for previous and upcoming research as they mathematically justify the development of methods with potentially exponential runtime to compute feasible solutions or even to solve the synthesis problem of decentralized energy systems optimally or approximately. This well-founded justification has been missing until today.

② **Effective solution method for non-linear and non-convex technology models** A solution algorithm for the synthesis of energy systems under consideration of *non-linear technology models* is proposed. By including non-linear part-load performance and investment cost functions the considered optimization problem gets unavoidably *non-convex*. The solution method proposed obtains non-linear feasible solutions within short computation time. The developed approach is based on a coordinated interaction between approximate binary linear programs and small-size decomposable non-linear programs with only continuous variables. Essential is that the linear approximation is consistently improved by an *iterative adaptation of the underlying discretization*. However, the discretized problem is not enlarged in each iteration, but rather the discretization grid is *concentrated purposefully*. Next to this adaptive discretization approach, the original *non-convex MINLP* formulation is contributed. Besides and to benchmark the proposed algorithm with (piece-wise) linearized models as commonly used in literature, a method is proposed to *transfer a linear feasible solution to a "nearest" non-linear feasible one*. A *comprehensive computational study* based on a collection of 320 test instances obtained from real-world industrial data shows that the proposed method outperforms state-of-the-art solvers and previous approaches in terms of solution quality and computation time.
This contribution deals with an issue that is largely neglected in the literature, namely the integration of reality-related non-linearities. It is shown that the incorporation of non-linearities does not impede to compute efficient energy systems. Furthermore, the approach presented, including the adaptive discretization, reveals the possibility of being generalized or at least applied to other hard-to-solve and possibly non-convex (synthesis) problems.

③ **Online available collection of benchmark instances** A set of 320 *problem instances* for the optimization-based synthesis of decentralized energy supply systems (DESS) is provided. Under the name *DESSLib*, the collection of same-formatted instances is freely available online. Based on raw data given in hourly demand levels of a real-world problem from the pharmaceutical industry, the problem instances are categorized by two dimensions: the number of considered energy conversion components and the number of considered representative load cases, i.e., demand szenarios. In addition, part-load performance and investment cost functions as well as general parameters like purchase and selling prices are given. The DESSLib is used to evaluate the performance of the non-linear solution algorithm proposed in Chapter 4 in comparison to previous and common approaches. All received *primal bounds, dual bounds, and computation times* are available at DESSLib.
Providing the data of the test instances used as well as the best solutions found and its computation times is a first step in order to be able to compare proposed solution methods fairly in terms of efficiency and effectiveness.

These three aspects of the thesis' contribution are documented in the following Chapters 3 and 4.

3 The Synthesis Problem of Decentralized Energy Systems is strongly NP-hard

Abstract We analyze the computational complexity of the synthesis problem of decentralized energy systems. This synthesis problem consists of combining various types of energy conversion units and determining their sizing as well as operations in order to meet time-varying energy demands while maximizing an objective function, e.g., the net present value. In this paper, we prove that the synthesis problem of decentralized energy systems is strongly NP-hard. Furthermore, we prove a strong inapproximability result. This paper provides the first complexity findings in the long scientific history of the synthesis problem of decentralized energy systems.

3.1 Introduction

Decentralized energy is converted in the vicinity of its consumers rather than at a larger centralized plant and sent through a national grid or pipelines. This local generation allows reductions in transmission losses and carbon emissions as well as an increase in supply security. In energy systems, different forms of consumable energy are provided by various supplier technologies. The application of decentralized energy systems (DES) encompasses, e.g., chemical parks (Maréchal and Kalitventzeff, 2003), urban districts (Jennings et al., 2014; Maréchal et al., 2008), hospitals and research complexes (Arcuri et al., 2007; Lozano et al., 2009). DES are highly integrated systems due to a multitude of technical units providing different energy forms, energy distribution infrastructure, and connection to the energy market. Energy cost usually match company's profits in magnitude (Drumm et al., 2013). Thus, optimally designed decentralized energy systems not only save primary energy, but also considerably increase the system's profitability. An example for a DES is shown in Figure 3.1.

The goal of the synthesis problem of DES is the identification of an (economically) optimal energy system, i.e., a best possible selection of energy conversion technologies with optimal unit dimensions, while simultaneously considering its optimal operation. Thus, three types of decisions can be identified (Frangopoulos et al., 2002):

1. *Synthesis:* How many energy conversion units of what technology should be built?
2. *Design:* How should the technical specifications, e.g., capacities, of these units be chosen?
3. *Operation:* How should units be operated in each load case?

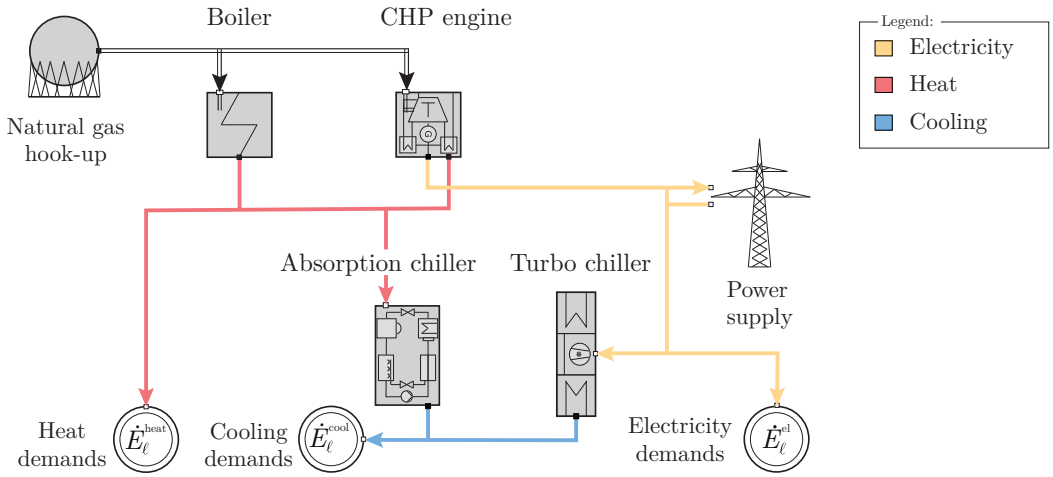


Fig. 3.1: Example of a decentralized energy system (Goderbauer et al., 2016).

These three decision levels influence each other and thus, global optimal solutions can only be obtained if all three levels are simultaneously considered in an integrated optimization approach.

Regarding the complexity of the synthesis problem of decentralized energy systems, the comprehensive literature shows a consensus that the problem is, in some sense, difficult to solve: It is "a complex and difficult problem" (Lozano et al., 2009), "a complex problem" (Carvalho et al., 2012; Maréchal et al., 2008), "an inherently difficult problem" (Voll et al., 2013b), "a complex and hard task" (Mehleri et al., 2013), "not a trivial task" (Zhou et al., 2013a), a problem "characterized by high complexity" (Bracco et al., 2016), and where it is "difficult to obtain the optimal solution" (Yokoyama et al., 2015). However, these complexity claims are not formally proven. Instead, argumentations are based on the number of decisions to be taken, combinatorial options, or amount of input data which is generally not sufficient. Above all, the simple fact that an (optimization) problem can be formulated as a, e.g., mixed-integer (non)linear program (MI(N)LP), does not allow any conclusion about the problem's computational complexity. Formulating and solving an optimization problem via MI(N)LP techniques is only *one* solution approach. However, to characterize a problem's computational complexity, we have to answer the question whether there is *any* solution approach that solves the problem efficiently.

Iyer and Grossmann (1998) emphasized that synthesis problems of energy systems "require specialized algorithms for their efficient solution". Elsido et al. (2017) underlined that "devising an efficient algorithm for tackling the [...] design optimization problem of complex networks of CHP units is still an open challenge". We answer this open challenge within our paper by proving the folklore result about the problem's difficulty in rigorous terms: There is no polynomial time algorithm, i.e., no efficient one, for solving the synthesis problem of decentralized energy systems unless P = NP. Moreover, we prove that no polynomial time algorithm exists which guarantees a constant approximation factor for the considered synthesis problem unless P = NP.

Complexity analyses are an active area of inquiry in the field of process system engineering. In a pioneering work, Ahmed and Sahinidis (2000) prove that the process planning problem is

weakly NP-hard. Shortly after, Furman and Sahinidis (2001) initiate the extensive complexity research on the problem of heat exchanger network synthesis by showing NP-hardness in the strong sense. In a follow-up work (Furman and Sahinidis, 2004) the same authors present approximation algorithms, i.e., polynomial time heuristics with guaranteed performance. Recently, Letsios et al. (2018) provide an alternative NP-hardness proof and additional approximation algorithms. In the wake of the upcoming interest in complexity analyses, also other problems received attention. The problem of sensor placement in water distribution networks is proven to be strongly NP-hard (Krause et al., 2008). The pooling problem is proven to be strongly NP-hard by Alfaki and Haugland (2013). Later, approximation algorithms and complexity results for special cases of the pooling problem are presented in (Dey and Gupte, 2015) and (Haugland, 2016). A rigorous analysis of the computational complexity of the synthesis problem of decentralized energy systems is missing to date. The following sections close that gap for this highly relevant and otherwise extensively studied synthesis problem.

For a detailed treatment of complexity theory including classes P and NP as well as the most-widely believed theoretical complexity assumption $P \neq NP$, we refer to (Garey and Johnson, 1979) and (Korte and Vygen, 2012, Chapter 15). In addition, we strongly recommend the three-page introduction into computational complexity theory in the paper of Furman and Sahinidis (2001, Section 2). Among other things, the authors introduce the concept of polynomial reductions and provide an illustrative example why a problem's computational complexity cannot be derived from a (MI(N)LP) formulation in general.

The paper is structured as follows: In Section 3.2, we formalize the synthesis problem of DES and present an exemplary setting. In Section 3.3, we prove three complexity results: NP-hardness in Section 3.3.1, NP-hardness in the strong sense in Section 3.3.2, and inapproximability in Section 3.3.3. The paper closes with a conclusion in Section 3.4.

3.2 Synthesis Problem of Decentralized Energy Systems

We formalize the synthesis problem of DES by describing given parameters, decisions to be taken, constraints to be fulfilled, and the objective to be optimized in Section 3.2.1. It is assumed that all parameters and data belong to the set of rational numbers. For a summarizing overview, we formulate the optimization problem as a mathematical program. The reason why we state a model is due to the fact that the formalism of mathematical programs ensures an unambiguous problem definition. In addition to the formal problem definition and mathematical model in Section 3.2.1, we present a practical setting in Section 3.2.2.

3.2.1 Problem Definition

We consider the widely used concept of superstructure-based synthesis (Liu et al., 2011). For the synthesis problem of DES, a superstructure includes all available conversion units

that can potentially be part of the energy system and can be operated to meet the energy demands (Buoro et al., 2013; Nishida et al., 1981; Westerberg, 1991). The energy demands of the DES vary over time. In order to take this into account, we consider a set of discrete load cases with individual durations and demands specified for each type of energy. These load cases can be derived from large (real-world) time series via selection of data points or via aggregation to typical periods. We assume a quasi-stationary system behavior, i.e., output energy is immediately available and units have no start-up time. Note, that the assumptions concerning system behavior ensure the independence of load cases, which is a simplification of reality. Coupling load cases through, e.g., storages or ramping constraints, leads to a more general setting to which all our complexity results can be directly transferred.

3.2.1.1 Parameters

A problem instance consists of a superstructure S, a set of load cases L, and a set of energy forms F. For a subset of the energy forms $F^{\text{mkt}} \subseteq F$ market access exists, i.e., they can be traded on the market. The selling and purchase price of energy form $f \in F^{\text{mkt}}$ is given by $p^{f,\text{sell}} \geq 0$ and $p^{f,\text{buy}} \geq 0$, respectively.

For each load case $\ell \in L$ its duration is denoted by $\Delta_\ell \geq 0$. Parameter $\dot{E}_\ell^f \geq 0$ specifies the demand of energy form $f \in F$ in load case $\ell \in L$.

Load cases	
$\Delta_\ell \geq 0$	duration of load case $\ell \in L$
$\dot{E}_\ell^f \geq 0$	demand of energy form $f \in F$ in load case $\ell \in L$
Conversion units: sizing and cost	
$\dot{\mathcal{V}}_s^{\text{N,set}} \subseteq \mathbb{Q}_{\geq 0}$	set of possible nominal output of energy f_s^{main} of unit $s \in S$
$I_s : \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0}$	investment cost function of unit $s \in S$
$m_s \in [0,1]$	maintenance cost factor of unit $s \in S$
Conversion units: part-load performance	
$\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}}) \subseteq [0, \dot{V}_s^{\text{N}}]$	set of possible output of energy form f_s^{main} of unit $s \in S$ with nominal output $\dot{V}_s^{\text{N}} \in \dot{\mathcal{V}}_s^{\text{N,set}}$
$\dot{V}_s^f : \dot{\mathcal{V}}_s^{\text{set}} \times \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0}$	function of output energy $f \in F_s^{\text{out}} \setminus \{f_s^{\text{main}}\}$ of unit $s \in S$
$\dot{U}_s^f : \dot{\mathcal{V}}_s^{\text{set}} \times \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0}$	function of input energy $f \in F_s^{\text{in}}$ of unit $s \in S$
Energy market	
$p^{f,\text{sell}} \geq 0$	market selling price of energy form $f \in F^{\text{mkt}}$
$p^{f,\text{buy}} \geq 0$	market purchase price of energy form $f \in F^{\text{mkt}}$
Net present value	
$\text{APVF} \geq 0$	annual present value factor

Tab. 3.1: Instance data for the synthesis problem of DES.

For each conversion unit $s \in S$ its forms of input energy $F_s^{\text{in}} \subseteq F$ and output energy $F_s^{\text{out}} \subseteq F$ are known. In order to model part-load performance of unit $s \in S$, a primary form of output energy $f_s^{\text{main}} \in F_s^{\text{out}}$ is specified. Note, a unique form of output energy, i.e., $|F_s^{\text{out}}| = 1$, implies $F_s^{\text{out}} = \{f_s^{\text{main}}\}$. For each unit $s \in S$ a set

$$\dot{\mathcal{V}}_s^{\text{N,set}} \subseteq \mathbb{Q}_{\geq 0}$$

of available capacities, i.e., maximum (nominal) output energy of form f_s^{main}, is given. For example, this set can be given in the form of a discrete set or an interval $\dot{\mathcal{V}}_s^{\text{N,set}} = [\dot{V}_s^{\text{N,min}}, \dot{V}_s^{\text{N,max}}]$ with $\dot{V}_s^{\text{N,max}} > \dot{V}_s^{\text{N,min}} \geq 0$.

The investment cost of unit $s \in S$ depends on its capacity and is determined by a given function $I_s : \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0}$. Annual maintenance costs of $s \in S$ are assumed to be a fixed fraction $m_s \in [0, 1]$ of the investment cost. To determine the net present value, being the objective function of the problem, the annual present value factor is given as parameter APVF ≥ 0.

The set of possible operation outputs of energy form f_s^{main} of unit $s \in S$ with nominal output $\dot{V}_s^{\text{N}} \in \dot{\mathcal{V}}_s^{\text{N,set}}$ is given as

$$\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}}) \subseteq [0, \dot{V}_s^{\text{N}}],$$

e.g., this set can be specified as a discrete set or an interval of the form $\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}}) = [\alpha_s^{\min} \cdot \dot{V}_s^{\text{N}}, \dot{V}_s^{\text{N}}]$ with minimum part-load factor $\alpha_s^{\min} \in [0, 1]$. In the following, $\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}})$ is regularly abbreviated with $\dot{\mathcal{V}}_s^{\text{set}}$. Based on the output of the main energy form f_s^{main}, the required input energy and other output energy is determined by specified functions

$$\dot{U}_s^f : \dot{\mathcal{V}}_s^{\text{set}} \times \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0} \text{ for } f \in F_s^{\text{in}} \text{ and}$$

$$\dot{V}_s^f : \dot{\mathcal{V}}_s^{\text{set}} \times \dot{\mathcal{V}}_s^{\text{N,set}} \to \mathbb{Q}_{\geq 0} \text{ for } f \in F_s^{\text{out}} \setminus \{f_s^{\text{main}}\}, \text{ respectively.}$$

All functions have to be polynomial time computable, such as discrete functions, polynomial fitted curves, or piecewise linear functions. A summary of all parameters can be found in Table 3.1.

3.2.1.2 Decisions

We previously identified three types of decisions: synthesis, design, and operation decisions. To formalize these decisions, we employ the notation of mathematical programming.

For every unit $s \in S$ of the superstructure, a binary decision variable $y_s \in \{0, 1\}$ denotes whether s is set up and thus part of the DES ($y_s = 1$) or not ($y_s = 0$). A decision variable $\dot{V}_s^{\text{N}} \in \dot{\mathcal{V}}_s^{\text{N,set}}$ signifies the (nominal) capacity of a set up unit $s \in S$.

A binary decision variable $\delta_{s\ell} \in \{0, 1\}$ denotes the on/off-status ($\delta_{s\ell} = 1$ means on) and a variable $\dot{V}_{s\ell} \in \dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}})$ represents the output of energy form f_s^{main} of unit $s \in S$ in load case $\ell \in L$. Note, by means of the functions $\dot{U}_s^f$ and $\dot{V}_s^f$ (cf. Section 3.2.1.1), the value of variable

$\dot{V}_{s\ell}$ determines the required input energy for all $f \in F_s^{\text{in}}$ and further output energy for all $f \in F_s^{\text{out}} \setminus \{f_s^{\text{main}}\}$ of unit $s \in S$, respectively.

Finally, continuous decision variables $\dot{U}_\ell^{f,\text{buy}} \geq 0$ and $\dot{V}_\ell^{f,\text{sell}} \geq 0$ denote the energy of form $f \in F^{\text{mkt}}$ bought from and sold on the market in load case $\ell \in L$, respectively.

3.2.1.3 Constraints

Logical, technical, environmental, and economical factors imply a set of constraints that have to be fulfilled by DES.

For each set up unit $s \in S$, its capacity $\dot{V}_s^{\text{N}}$ has to be chosen from the set of available capacities, i.e., $\dot{V}_s^{\text{N}} \in \dot{\mathcal{V}}_s^{\text{N,set}}$ (cf. Constraints (3.2)). Only set up conversion units can be operated in the load cases (cf. Constraints (3.3)). The output of energy form f^{main} of an operating unit $s \in S$ in load case $\ell \in L$, denoted by $\dot{V}_{s\ell}$, has to be chosen from the set $\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}})$ (cf. Constraints (3.4)). If $s \in S$ is not operated in load case $\ell \in L$, it must not generate output and does not require input energy (cf. Constraints (3.5) and factor $\delta_{s\ell}$ in (3.6)-(3.7)).

For each load case $\ell \in L$ and each energy form $f \in F$ the energy balance equation has to be met, i.e., output minus required input energy of operating units has to equal the energy demand $\dot{E}_\ell^f$ (cf. Constraints (3.6)). For energy forms $f \in F^{\text{mkt}}$ with market access, surplus energy can be sold and additional energy can be bought to equalize the energy balance (cf. Constraints (3.7)).

3.2.1.4 Objective

The net present value $\text{APVF} \cdot R^{\text{cf}} - I^{\text{tot}}$ is maximized, where I^{tot} denotes the total investments and R^{cf} denotes the net cash flow. The net cash flow R^{cf} is determined as the annual revenue from sold energy $\dot{V}_\ell^{f,\text{sell}} \geq 0$ for $f \in F^{\text{mkt}}$ minus the cost for energy $\dot{U}_\ell^{f,\text{buy}} \geq 0$ for $f \in F^{\text{mkt}}$ bought on the market as well as maintenance cost $m_s \cdot I_s(\dot{V}_s^{\text{N}})$ for all set up units $s \in S$.

3.2.1.5 Model

A mathematical model for the synthesis problem of DES is given by (3.1)–(3.12). The model adopts the previously introduced notation of the parameters and variables.

Note, in Objective (3.1) the negated net present value is minimized which is trivially equivalent to the maximization of the net present value as defined in Section 3.2.1.4. We present this equivalent version here, since a proof in our complexity analysis is based on an objective that has to be minimized (cf. Section 3.3.2). In Section 3.2.1.3, each description of constraints ends with a reference to mathematically formulated Constraints (3.2)–(3.7).

$$\min \quad (-1)\cdot\Bigg(\text{APVF}\cdot\Bigg[\sum_{\ell\in L}\Delta_\ell\cdot\Big(\sum_{f\in F^{\text{mkt}}} p^{f,\text{sell}}\cdot\dot{V}_\ell^{f,\text{sell}} - p^{f,\text{buy}}\cdot\dot{U}_\ell^{f,\text{buy}}\Big) - \sum_{s\in S} y_s\cdot m_s\cdot I_s(\dot{V}_s^{\text{N}})\Bigg] - \sum_{s\in S} y_s\cdot I_s(\dot{V}_s^{\text{N}})\Bigg) \tag{3.1}$$

$$\text{s.t.} \quad y_s = 1 \Longrightarrow \dot{V}_s^{\text{N}} \in \dot{\mathcal{V}}_s^{\text{N,set}} \qquad \forall\, s\in S \tag{3.2}$$

$$\delta_{s\ell} = 1 \Longrightarrow y_s = 1 \qquad \forall\, s\in S, \ell\in L \tag{3.3}$$

$$\delta_{s\ell} = 1 \Longrightarrow \dot{V}_{s\ell} \in \dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}}) \qquad \forall\, s\in S, \ell\in L \tag{3.4}$$

$$\delta_{s\ell} = 0 \Longrightarrow \dot{V}_{s\ell} = 0 \qquad \forall\, s\in S, \ell\in L \tag{3.5}$$

$$\sum_{s:f_s^{\text{main}}=f} \dot{V}_{s\ell} + \sum_{\substack{s:f\in F_s^{\text{out}},\\ f\neq f_s^{\text{main}}}} \delta_{s\ell}\cdot\dot{V}_s^f(\dot{V}_{s\ell},\dot{V}_s^{\text{N}}) = \dot{E}_\ell^f + \sum_{s:f\in F_s^{\text{in}}} \delta_{s\ell}\cdot\dot{U}_s^f(\dot{V}_{s\ell},\dot{V}_s^{\text{N}}) \qquad \forall\, \ell\in L, f\in F\setminus F^{\text{mkt}} \tag{3.6}$$

$$\dot{U}_\ell^{f,\text{buy}} + \sum_{s:f_s^{\text{main}}=f} \dot{V}_{s\ell} + \sum_{\substack{s:f\in F_s^{\text{out}},\\ f\neq f_s^{\text{main}}}} \delta_{s\ell}\cdot\dot{V}_s^f(\dot{V}_{s\ell},\dot{V}_s^{\text{N}}) = \dot{E}_\ell^f + \sum_{s:f\in F_s^{\text{in}}} \delta_{s\ell}\cdot\dot{U}_s^f(\dot{V}_{s\ell},\dot{V}_s^{\text{N}}) + \dot{V}_\ell^{f,\text{sell}} \qquad \forall\, \ell\in L, f\in F^{\text{mkt}} \tag{3.7}$$

$$y_s \in \{0,1\} \qquad \forall\, s\in S \tag{3.8}$$

$$\dot{V}_s^{\text{N}} \geq 0 \qquad \forall\, s\in S \tag{3.9}$$

$$\delta_{s\ell} \in \{0,1\} \qquad \forall\, s\in S, \ell\in L \tag{3.10}$$

$$\dot{V}_{s\ell} \geq 0 \qquad \forall\, s\in S, \ell\in L \tag{3.11}$$

$$\dot{U}_\ell^{f,\text{buy}}, \dot{V}_\ell^{f,\text{sell}} \geq 0 \qquad \forall\, \ell\in L, f\in F^{\text{mkt}} \tag{3.12}$$

This generic model (3.1)–(3.12) for the synthesis problem of DES can be used to formulate both, a MINLP or MILP. To do this, the (indicator) constraints (3.2) – (3.5) and the possibly non-linear investment cost functions I_s in (3.1) and part-load performance functions $\dot{V}_s^f, \dot{U}_s^f$ in (3.6) – (3.7) require an appropriate handling. A MINLP formulation, taking into account nonlinearities in the part-load performances and investment cost functions, is given in the work of Goderbauer et al. (2016). Using piecewise-linearized functions, Voll et al. (2013b) states a MILP formulation.

3.2.2 A Practical Setting

To put the general problem definition into more concrete terms, we present a practical setting based on the DES example illustrated in Figure 3.1. This DES setting is inspired by (Goderbauer et al., 2016; Voll et al., 2013b) and is used to concretize the constructed problem instances in the proofs of our complexity results in Section 3.3. Nevertheless, all complexity results presented in this paper hold for the general synthesis problem of DES as defined in Section 3.2.1.

We consider four energy conversion technologies in the supplier subsystem: The superstructure

$$S = B \dot\cup C \dot\cup T \dot\cup A$$

encompasses a set of boilers B, a set of combined heat and power (CHP) engines C, a set of turbo-driven compressor chillers T, and a set of absorption chillers A. Boilers and CHP engines burn gas. Boilers provide heat at high efficiency, and CHP engines generate electrical energy (el) and heat simultaneously.

$$\begin{aligned} \text{Boiler } s \in B \quad &: \quad F_s^{\text{in}} = \{\text{gas}\},\ F_s^{\text{out}} = \{\text{heat}\} \\ \text{CHP engine } s \in C \quad &: \quad F_s^{\text{in}} = \{\text{gas}\},\ F_s^{\text{out}} = \{\text{heat}, \text{el}\} \text{ with } f_s^{\text{main}} = \text{heat} \end{aligned}$$

Absorption chillers and turbo chillers provide cooling, requiring heat or electrical energy as input, respectively.

$$\begin{aligned} \text{Absorption chiller } s \in A \quad &: \quad F_s^{\text{in}} = \{\text{heat}\},\ F_s^{\text{out}} = \{\text{cool}\} \\ \text{Turbo chiller } s \in T \quad &: \quad F_s^{\text{in}} = \{\text{el}\},\ F_s^{\text{out}} = \{\text{cool}\} \end{aligned}$$

Market access exists for $F^{\text{mkt}} = \{\text{gas}, \text{el}\} \subset F = \{\text{gas}, \text{heat}, \text{cool}, \text{el}\}$.

3.3 Complexity

Let SDES be the decision problem whether a feasible solution to the synthesis problem of DES (cf. Section 3.2.1) with objective value $\beta \in \mathbb{Q}$ or less exists. We consider the minimization of the negated net present value as objective as indicated and explained in Section 3.2.1.5 in conjunction with Section 3.2.1.4.

3.3.1 NP-hardness

We prove NP-hardness of SDES via a reduction from SUBSET SUM which is known to be NP-complete (Garey and Johnson, 1979; Karp, 1972).

SUBSET SUM
Instance: Finite set D, size $w(d) \in \mathbb{Z}_{\geq 1}$ for each $d \in D$, and integer $k \geq 1$.
Question: Is there a subset $D' \subseteq D$ such that the sum of the sizes of elements in D' is exactly k, i.e., $\sum_{d \in D'} w(d) = k$?

Theorem 1 *SDES is NP-hard.*

Proof We perform a reduction from SUBSET SUM. Let $z := (D, w, k)$ be an instance of SUBSET SUM. In order to avoid the presentation of an overly abstract DES setting, we stick to the exemplary setting introduced in Section 3.2.2, including its conversion technologies and energy forms. In the following, we construct an instance $z'(z)$ of SDES. Figure 3.2 illustrates the construction.

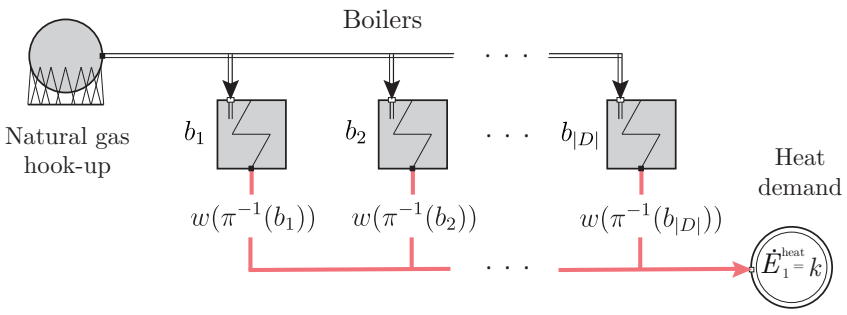


Fig. 3.2: Instance of SDES on basis of SUBSET SUM instance in proof of Theorem 1.

The set of considered energy forms is $F := \{\text{heat}, \text{gas}\}$ with market access $F^{\text{mkt}} := \{\text{gas}\}$. The superstructure $S := \{b_1, \ldots, b_{|D|}\}$ consists of $|D|$ boilers which convert gas into heat. Let $\pi : D \to S$ be a bijection between set D and superstructure S. For boiler $s \in S$ we define $\dot{\mathcal{V}}_s^{\text{N,set}} := \{w(\pi^{-1}(s))\}$ and $\dot{\mathcal{V}}_s^{\text{set}}(\dot{V}_s^{\text{N}}) := \{\dot{V}_s^{\text{N}}\}$. The instance contains only one load case, $L := \{1\}$, with demand $\dot{E}_1^{\text{heat}} := k$. There is no demand for gas, i.e., $\dot{E}_1^{\text{gas}} := 0$. We set investment cost $I_s := 0$ for $s \in S$ and annual present value factor APVF $:= 0$. Parameters $\Delta_1, m_s, \dot{U}_s^{\text{gas}}, p^{\text{gas,buy}}$, and $p^{\text{gas,sell}}$ can be chosen arbitrarily. By this choice, the objective equals 0 and we consequently set $\beta := 0$. Clearly, this instance can be constructed in polynomial time, and its encoding length is polynomially related to that of the input. Now we show that z is a YES-instance of SUBSET SUM if and only if $z'(z)$ is a YES-instance of SDES.

Let $z = (D, w, k)$ be a YES-instance of SUBSET SUM with feasible solution $D' \subseteq D$. Consider instance $z'(z)$ of SDES. Setting up boilers $S' := \{\pi(d) : d \in D'\} \subseteq S$ and operating all of them in load case $\ell = 1$ fulfills the energy demand with equality:

$$\sum_{s \in S'} \dot{V}_{s1} = \sum_{s \in S'} \dot{V}_s^{\text{N}} = \sum_{s \in S'} w(\pi^{-1}(s)) = \sum_{d \in D'} w(d) = k = \dot{E}_1^{\text{heat}}. \tag{3.13}$$

Thus, $z'(z)$ is a YES-instance of SDES.

For the other direction, let $z'(z)$ be a YES-instance of SDES. A feasible solution to $z'(z)$ contains a set of boilers $S' \subseteq S$ that are operated in load case $\ell = 1$ in order to meet the heat demand $\dot{E}_1^{\text{heat}} = k$. We define $D' := \{\pi^{-1}(s) : s \in S'\} \subseteq D$. Equation (3.13) holds again, thus we have $\sum_{s \in D'} w(s) = k$ by construction of D' which proves that z is a YES-instance of SUBSET SUM with feasible solution D'.

Thus, every solution to the SUBSET SUM instance transforms into a solution to the SDES instance, and vice versa. This completes the proof. ■

Corollary 2 *There can be no polynomial time algorithm solving the synthesis problem of decentralized energy systems unless $P = NP$.*

Corollary 3 *The optimization problem of SDES is NP-hard even for problem settings restricted to one load case and one type of conversion unit generating output form f with $f \notin F^{mkt}$.*

Actually, the reduction in the proof of Theorem 1 does not include decisions of the synthesis and design levels. This implies NP-hardness of the operation problem in each load case. In fact, the feasibility problem of the synthesis problem is considered, which implies that the decision problem whether any feasible solution with arbitrary objective value exists is already NP-hard.

Since SUBSET SUM can be solved in pseudo-polynomial time using, e.g., dynamic programming (Bellman, 1956), SUBSET SUM is weakly NP-complete. Thus, the above reduction proves that SDES is (at least) weakly NP-hard for one load case. In the following section, we consider multiple load cases and prove a stronger complexity result for the synthesis problem of DES: NP-hardness in the strong sense.

3.3.2 NP-hardness in the Strong Sense

To prove strong NP-hardness for the synthesis problem of DES we perform a reduction from SET COVER.

SET COVER
Instance: Finite set $U = \{1, \dots, n\}$, called universe, a collection $\mathcal{A} = \{A_1, \dots, A_m\}$ of subsets of U, i.e., $A_i \subseteq U$ for $i = 1, \dots, m$, and an integer $1 \leq k \leq |\mathcal{A}|$.
Question: Does $\mathcal{A}$ contain a cover for U of size k or less, i.e., a subset $\mathcal{A}' \subseteq \mathcal{A}$ with $|\mathcal{A}'| \leq k$ such that every element of U belongs to at least one set in $\mathcal{A}'$?

The decision problem SET COVER is known to be strongly NP-complete (Garey and Johnson, 1979). The corresponding optimization problem MIN SET COVER asks for a cover $\mathcal{A}' \subseteq \mathcal{A}$ of smallest size $|\mathcal{A}'|$.

Theorem 4 *SDES is strongly NP-hard.*

Proof Let $z \coloneqq (U, \mathcal{A}, k)$ with $U = \{1, \dots, n\}$, $n \in \mathbb{N}$, $\mathcal{A} = \{A_1, \dots, A_m\}$, and $k \leq |\mathcal{A}|$ be an instance of SET COVER. Again, we stick to the exemplary DES setting given in Section 3.2.2 to avoid too much abstraction. In the following, we construct an instance $z'(z)$ of SDES. Figure 3.3 illustrates the construction.

The set of considered energy forms is $F \coloneqq \{\text{heat}, \text{electricity (el)}, \text{gas}\}$ with $F^{\text{mkt}} \coloneqq \{\text{gas}, \text{el}\}$. Let $\varepsilon > 0$ with $|U| \cdot \varepsilon < 1$, e.g., $\varepsilon \coloneqq (|U|+1)^{-1}$. The set of load cases is $L \coloneqq U$ with demands

$$\dot{E}_\ell^{\text{heat}} \coloneqq \ell, \quad \dot{E}_\ell^{\text{el}} \coloneqq \ell^2 - \ell\varepsilon, \quad \dot{E}_\ell^{\text{gas}} \coloneqq 0,$$

and duration $\Delta_\ell \coloneqq 1$ for $\ell \in L$. The superstructure

$$S \coloneqq C \coloneqq \{c_A : A \in \mathcal{A}\}$$

consists of $|\mathcal{A}|$ CHP engines. Each CHP engine $c_A \in S$ corresponds to exactly one set $A \in \mathcal{A}$ and converts $F_{c_A}^{\text{in}} \coloneqq \{\text{gas}\}$ into $F_{c_A}^{\text{out}} \coloneqq \{\text{heat}, \text{el}\}$ with $f_{c_A}^{\text{main}} \coloneqq \text{heat}$. We define

$\dot{\mathcal{V}}_s^{\text{N,set}} := \{|U|\}$ for $s \in S$. The investment cost $I_s(\dot{V}_s^{\text{N}}) := 1$ of $s \in S$ is independent of the selected capacity $\dot{V}_s^N$. Maintenance costs are neglected, i.e., $m_s := 0$ for $s \in S$. For each CHP engine $c_A \in S$, $A \in \mathcal{A}$, we define $\dot{\mathcal{V}}_{c_A}^{\text{set}} := A$ as well as the part-load performance function

$$\dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}}) := \dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}) := \dot{V}_{c_A\ell},$$

and the electricity output

$$\dot{V}_{c_A}^{\text{el}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}}) := \dot{V}_{c_A}^{\text{el}}(\dot{V}_{c_A\ell}) := \dot{V}_{c_A\ell}^2.$$

The remaining parameters are defined as APVF $:= 1$,

$$p^{\text{gas,buy}} := \varepsilon, \quad p^{\text{gas,sell}} := 0, \quad p^{\text{el,buy}} := |\mathcal{A}|, \text{ and } \quad p^{\text{el,sell}} := 1.$$

Clearly, this instance can be constructed in polynomial time and its encoding length is polynomially related to that of the input. Now we show that there is a cover $\mathcal{A}'$ of size $\beta \leq k$ for SET COVER instance z if and only if there is a feasible solution with objective value β for SDES instance $z'(z)$.

Let $\mathcal{A}'$ be a cover of size $\beta \leq k \leq |\mathcal{A}|$ for SET COVER instance z. Setting up CHP engines $c_A \in S$ corresponding to cover members $A \in \mathcal{A}'$ and choosing their respective capacities as $\dot{V}_{c_A}^{\text{N}} = |U|$ leads to investment cost of β in the objective function of SDES. It remains to show that this energy system can satisfy all demands in all load cases with equality, without incurring extra cost. Consider an arbitrary load case $\ell^\star \in L$. Since $\mathcal{A}'$ is a cover of U, there exists $A^\star \in \mathcal{A}'$ with $\ell^\star \in A^\star$. Operating only CHP engine $c_{A^\star}$ in load case $\ell^\star$ with $\dot{V}_{c_{A^\star}\ell^\star} = \ell^\star$ satisfies the heat demand $\dot{E}_{\ell^\star}^{\text{heat}} = \ell^\star$. The operated CHP engine generates electricity $\dot{V}_{c_{A^\star}}^{\text{el}}(\ell^\star) = \ell^{\star 2}$. The demand $\dot{E}_{\ell^\star}^{\text{el}} = \ell^{\star 2} - \ell^\star\varepsilon$ is fulfilled and surplus electricity $\dot{V}_{\ell^\star}^{\text{el,sell}} = \ell^\star\varepsilon$ is sold. The revenue $\dot{V}_{\ell^\star}^{\text{el,sell}} p^{\text{el,sell}} = \ell^\star\varepsilon$ equals the operation cost $\dot{U}_{c_{A^\star}}^{\text{gas}}(\ell^\star) \cdot p^{\text{gas,buy}} = \ell^\star\varepsilon$. Since $\ell^\star \in L$ was chosen arbitrarily, this holds for every load case $\ell \in L$. It follows: We found a feasible solution with objective value β for SDES instance $z'(z)$.

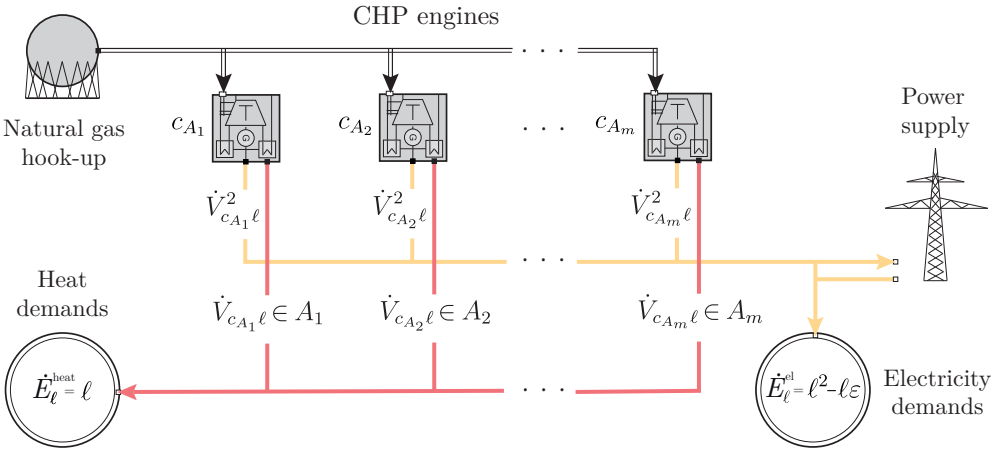


Fig. 3.3: SDES instance based on SET COVER instance in proof of Theorem 4.

Now, let a feasible solution for SDES instance $z'(z)$ with objective value $\beta \leq k \leq |S|$ be given. We show that this solution consists of exactly β set up CHP engines $\{c_{A_{i_1}}, \ldots, c_{A_{i_\beta}}\} \subseteq S$ and that the corresponding set $\{A_{i_1}, \ldots, A_{i_\beta}\} \subseteq \mathcal{A}$ forms a cover for U of cardinality β.

Let $S_\ell \subseteq S$ be the set of operated CHP engines in load case $\ell \in L$ (and thus a subset of all set up ones). We start by showing that the total operating cost in each load case $\ell \in L$ is non-negative, i.e., no profit can be generated by operating units. The only possible way to gain profit in a load case is by selling surplus electricity. Since $\dot{V}_s^{\text{el}} : \dot{\mathcal{V}}_s^{\text{set}} \to \mathbb{Q}_{\geq 0}, \dot{V}_{s\ell} \mapsto \dot{V}_{s\ell}^2$ is (i) a (strictly) superadditive function and (ii) $\dot{E}_\ell^{\text{heat}} = \ell = \sum_{s \in S_\ell} \dot{V}_{s\ell}$ holds, it follows that

$$\sum_{s \in S_\ell} \dot{V}_s^{\text{el}}(\dot{V}_{s\ell}) \overset{\text{(i)}}{\leq} \dot{V}_s^{\text{el}}\left(\sum_{s \in S_\ell} \dot{V}_{s\ell} \right) \overset{\text{(ii)}}{=} \dot{V}_s^{\text{el}}(\ell) = \ell^2. \tag{3.14}$$

Consequently, $\dot{V}_\ell^{\text{el,sell}} \leq \ell^2 - \dot{E}_\ell^{\text{el}} = \varepsilon\ell$ electrical energy can be sold with revenue $p^{\text{el,sell}} = 1$ per unit. Since operating all CHP engines in S_ℓ leads to gas cost of $p^{\text{gas,buy}} \cdot \ell = \varepsilon\ell$, the total operating costs for all $\ell \in L$ are non-negative.

We now show that $|S_\ell| = 1$ holds for all $\ell \in L$. To that end, assume the contrapositive, i.e., that there exists $\ell^\star \in L$ in which (at least) two set up CHP engines are operated ($|S_{\ell^\star}| \geq 2$). It holds that $\sum_{s \in S_{\ell^\star}} \dot{V}_{s\ell^\star} = \dot{E}_{\ell^\star}^{\text{heat}} = \ell^\star$. In combination with $|S_{\ell^\star}| \geq 2$ and $\dot{\mathcal{V}}_s^{\text{set}} \subset \mathbb{Z}_{\geq 1}$ for $s \in S$ this implies that $\ell^\star \geq 2$ and with Lemma 9 (Section 3.5) we can strengthen our previous estimation in Equation (3.14) to

$$\sum_{s \in S_{\ell^\star}} \dot{V}_s^{\text{el}}(\dot{V}_{s\ell^\star}) \overset{\text{Lem. 9}}{\leq} \dot{V}_s^{\text{el}}\left(\sum_{s \in S_{\ell^\star}} \dot{V}_{s\ell^\star} \right) - 2 = \dot{V}_s^{\text{el}}(\ell^\star) - 2 = \ell^{\star 2} - 2.$$

By construction, $|L|\varepsilon < 1$ and thus $\ell^\star\varepsilon < 1$, which implies $\sum_{s \in S_{\ell^\star}} \dot{V}_s^{\text{el}}(\dot{V}_{s\ell^\star}) \leq \ell^{\star 2} - 2 < \ell^{\star 2} - \ell^\star\varepsilon - 1 = \dot{E}_{\ell^\star}^{\text{el}} - 1$. Consequently, $\dot{U}_{\ell^\star}^{\text{el,buy}} > 1$ electricity has to be bought, implying cost $p^{\text{el,buy}} \cdot \dot{U}_{\ell^*}^{\text{el,buy}} > |\mathcal{A}| = |S| \geq k$ in the objective of SDES. As we have previously shown that no profit can be generated that could reduce this cost, this yields a contradiction to the fact that the given solution for the SDES instance $z'(z)$ has an objective value $\beta \leq k$.

It follows that for each load case $\ell \in L$ we have $|S_\ell| = 1$, say $S_\ell = \{s_\ell\}$. CHP engine s_ℓ must fulfill the heat demand, i.e., $\dot{V}_{s_\ell\ell} = \ell = \dot{E}_\ell^{\text{heat}}$, and $\ell \in \dot{\mathcal{V}}_{s_\ell}^{\text{set}}$. Consequently, s_ℓ generates electricity $\dot{V}_{s_\ell}^{\text{el}}(\ell) = \ell^2$. The demand $\dot{E}_\ell^{\text{el}} = \ell^2 - \ell\varepsilon$ is fulfilled and surplus electricity $\dot{V}_\ell^{\text{el,sell}} = \ell\varepsilon$ is sold. The revenue $\dot{V}_\ell^{\text{el,sell}} p^{\text{el,sell}} = \ell\varepsilon$ equals the operation cost $\dot{U}_{s_\ell}^{\text{gas}}(\ell) \cdot p^{\text{gas,buy}} = \ell\varepsilon$ and the total operation cost is 0.

Thus, we can conclude that the given solution for SDES instance $z'(z)$ with objective value $\beta \leq |S|$ must contain exactly β set up CHP engines $C^{z'(z)} \coloneqq \{c_{A_{i_1}}, \ldots, c_{A_{i_\beta}}\} \subseteq S$ causing investment costs β and operation cost 0. For all $\ell = 1, \ldots, |U|$ CHP engine $s_\ell = c_{A_{j_\ell}} \in C^{z'(z)}$ satisfies $\ell \in \dot{\mathcal{V}}_{c_{A_{j_\ell}}}^{\text{set}} = A_{j_\ell}$. Thus, $\{A_{j_\ell} : \ell \in L\} \subseteq \{A_{i_1}, \ldots, A_{i_\beta}\}$ is a set cover for U which implies that $\mathcal{A}' \coloneqq \{A_{i_1}, \ldots, A_{i_\beta}\}$ induced by $C^{z'(z)}$ is a set cover of size β for $z'(z)$.

In summary, a cover $\mathcal{A}'$ of size $\beta \leq |\mathcal{A}|$ for SET COVER instance z transforms into a feasible solution with objective value $\beta \leq |S|$ for SDES instance $z'(z)$, and vice versa. This completes the proof. ■

Corollary 5 *There can be no pseudo-polynomial time algorithm solving the synthesis problem of decentralized energy systems unless P = NP.*

Corollary 6 *The optimization problem of SDES is NP-hard even for problem settings restricted to one type of conversion unit with two different forms of output energy f_1, f_2 and $f_1 \in F^{mkt}$.*

Remark, that the SDES instance $z'(z)$ constructed in the proof of Theorem 4 does not obey the law of conservation of energy. Using the argumentation from the proof above, this can be circumvented by the following slight adjustment of the instance $z'(z)$:

$$\dot{E}_{\ell}^{\text{heat}} := \frac{\ell}{|U|}, \quad \dot{E}_{\ell}^{\text{el}} := \left(\frac{\ell}{|U|}\right)^2 - \frac{\ell\varepsilon}{|U|^2}, \quad \dot{\mathcal{V}}_{c_A}^{\text{N,set}} := \{1\}, \quad \dot{\mathcal{V}}_{c_A}^{\text{set}} := \bigcup_{a \in A} \frac{a}{|U|},$$

$$\dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}) := 2 \cdot \dot{V}_{c_A\ell}, \quad p^{\text{gas,buy}} := \frac{\varepsilon}{2}, \quad p^{\text{el,buy}} := |\mathcal{A}| \cdot |U|^2, \quad p^{\text{el,sell}} := |U|.$$

Since $0 < \dot{V}_{c_A\ell} \leq 1$ holds for all $\dot{V}_{c_A\ell} \in \dot{\mathcal{V}}_{c_A}^{\text{set}}, c_A \in S$, the inequality $2 \cdot \dot{V}_{c_A\ell} \geq \dot{V}_{c_A\ell} + \dot{V}_{c_A\ell}^2$ and therefore $\dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}}) \geq \dot{V}_{c_A\ell} + \dot{V}_{c_A}^{\text{el}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}})$ is fulfilled. A proof of Theorem 4 using this adjusted instance is conducted in detail in the Appendix on page 31.

3.3.3 Inapproximability

After proving that it is strongly NP-hard to compute an optimal solution for the synthesis problem of DES, the question regarding approximability arises: Is it possible that a polynomial time algorithm exists which guarantees a (constant) approximation factor for the considered synthesis problem? We show that under the assumption that P $\neq$ NP, the answer is: No.

The following corollary is a direct consequence from Theorem 4, i.e., from the fact that the considered synthesis problem is strongly NP-hard (Garey and Johnson, 1979).

Corollary 7 *For the synthesis problem of decentralized energy systems no fully polynomial time approximation scheme (FPTAS) exists, i.e., no algorithm exists that solves the problem for any $\varepsilon > 0$ within a factor of $(1+\varepsilon)$ of the optimal value in polynomial time with respect to the input size and $1/\varepsilon$, unless P = NP.*

The non-existence of an FPTAS itself does not exclude the existence of an efficient algorithm with, e.g., constant approximation guarantee. We strengthen the inapproximability result with the following theorem. Recall that $|L|$ denotes the number of load cases of an instance for the synthesis problem of DES.

Theorem 8 *Let $0 < \varepsilon < 1$. There can be no $\varepsilon \cdot \ln(|L|)$-approximation algorithm for the synthesis problem of decentralized energy systems unless P = NP.*

Proof Moshkovitz (2012) and Dinur and Steurer (2014) showed that for $0 < \varepsilon < 1$ there is no $\varepsilon \cdot \ln(|U|)$-approximation algorithm for MIN SET COVER (with universe U) unless P = NP. Since the reduction in the proof of Theorem 4 from SET COVER to SDES is cost preserving, the statement follows directly from the inapproximability result for MIN SET COVER. ■

3.4 Conclusion

This work rectifies the lack of formal results in the computational complexity analysis of the synthesis problem of decentralized energy systems. We present reductions from known (strongly) NP-hard problems to prove that the considered synthesis problem is difficult to solve from a theoretical point of view as there exists no polynomial time solution algorithm unless P = NP.

We specify the considered problem setting and formalize the synthesis problem of DES in form of a mathematical model with an objective, constraints, variables, and required input data. After that, we present three complexity results: As part of the synthesis problem, we prove that (i) already the operation problem of one load case is weakly NP-hard. Furthermore, we strengthen this complexity statement and prove that (ii) the synthesis problem of DES is NP-hard in the strong sense. Since our conducted reduction is cost preserving, it turns out that it is even (iii) NP-hard to approximate an optimal solution with a constant approximation factor.

Previous publications proposing solution approaches for synthesis of DES explain the difficulty of the problem by means of experience and insufficient arguments. In contrast, this work provides well-founded proofs on the computational complexity. Our results justify the use and development of heuristics and algorithms with potentially exponential runtime to compute feasible solutions or even to solve the synthesis problem of DES optimally or approximately.

3.5 Appendix: Auxiliary Lemma and Alternative Proof

The following lemma is used in the proof of Theorem 4 in order to strengthen the estimation in Equation (3.14).

Lemma 9 *For $a_1, \ldots, a_n \in \mathbb{N} \setminus \{0\},\ n \geq 2$ holds:*

$$\left(\sum_{i=1}^{n} a_i\right)^2 - \sum_{i=1}^{n} a_i^2 \geq 2.$$

Proof By the multinomial theorem, we have

$$\left(\sum_{i=1}^{n} a_i\right)^2 = \sum_{k_1+\ldots+k_n=2} \frac{2}{k_1! \cdot \ldots \cdot k_n!} \prod_{i=1}^{n} a_i^{k_i} = \sum_{i=1}^{n} a_i^2 + \sum_{1 \leq i < j \leq n} 2a_i a_j.$$

Thus,

$$\left(\sum_{i=1}^{n} a_i\right)^2 - \sum_{i=1}^{n} a_i^2 = \sum_{1 \le i < j \le n} 2a_i a_j \ge 2.$$

Note that the lower bound of 2 is attained for $n = 2$ and $a_1 = a_2 = 1$. ■

In the following, we provide an alternative proof of Theorem 4. Here, we conduct an reduction from SET COVER with an slightly adjusted instance. As pointed out in detail in the remark at the end of Section 3.3.2, the part-load performance functions of that problem instance fulfill the law of conservation of energy. This is not the case in the previously used instance. The following proof is conducted analogously to the one given on page 26 and uses the same argumentation, but contains some unpleasant calculations due to the done scaling.

Theorem 4 *SDES is strongly NP-hard.*

Proof (alternative to proof on page 26) Let $z \coloneqq (U, \mathcal{A}, k)$ with $U = \{1, \dots, n\}$, $n \in \mathbb{N}$, $\mathcal{A} = \{A_1, \dots, A_m\}$, and $k \le |\mathcal{A}|$ be an instance of SET COVER. Again, we stick to the exemplary DES setting given before to avoid too much abstraction. In the following, we construct an instance $z'(z)$ of SDES.

The set of considered energy forms is $F \coloneqq \{\text{heat}, \text{electricity (el)}, \text{gas}\}$ with $F^{\text{mkt}} \coloneqq \{\text{gas}, \text{el}\}$. Let $\varepsilon > 0$ with $|U| \cdot \varepsilon < 1$, e.g., $\varepsilon \coloneqq (|U|+1)^{-1}$. The set of load cases is $L \coloneqq U$ with demands

$$\dot{E}_\ell^{\text{heat}} \coloneqq \frac{\ell}{|U|}, \quad \dot{E}_\ell^{\text{el}} \coloneqq \left(\frac{\ell}{|U|}\right)^2 - \frac{\ell\varepsilon}{|U|^2}, \quad \dot{E}_\ell^{\text{gas}} \coloneqq 0,$$

and duration $\Delta_\ell \coloneqq 1$ for $\ell \in L$. The superstructure

$$S \coloneqq C \coloneqq \{c_A : A \in \mathcal{A}\}$$

consists of $|\mathcal{A}|$ CHP engines. Each CHP engine $c_A \in S$ corresponds to exactly one set $A \in \mathcal{A}$ and converts $F_{c_A}^{\text{in}} \coloneqq \{\text{gas}\}$ into $F_{c_A}^{\text{out}} \coloneqq \{\text{heat}, \text{el}\}$ with $f_{c_A}^{\text{main}} \coloneqq \text{heat}$. We define $\dot{\mathcal{V}}_s^{\text{N,set}} \coloneqq \{1\}$ for $s \in S$. The investment cost $I_s(\dot{V}_s^{\text{N}}) \coloneqq 1$ of $s \in S$ is independent of the selected capacity $\dot{V}_s^N$. Maintenance costs are neglected, i.e., $m_s \coloneqq 0$ for $s \in S$. For each CHP engine $c_A \in S$, $A \in \mathcal{A}$, we define

$$\dot{\mathcal{V}}_{c_A}^{\text{set}} \coloneqq \bigcup_{a \in A} \frac{a}{|U|}$$

as well as the part-load performance function

$$\dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}}) \coloneqq \dot{U}_{c_A}^{\text{gas}}(\dot{V}_{c_A\ell}) \coloneqq 2 \cdot \dot{V}_{c_A\ell},$$

and the electricity output

$$\dot{V}_{c_A}^{\text{el}}(\dot{V}_{c_A\ell}, \dot{V}_{c_A}^{\text{N}}) \coloneqq \dot{V}_{c_A}^{\text{el}}(\dot{V}_{c_A\ell}) \coloneqq \dot{V}_{c_A\ell}^2.$$

The remaining parameters are defined as APVF $\coloneqq 1$,

$$p^{\text{gas,buy}} \coloneqq \frac{\varepsilon}{2}, \quad p^{\text{gas,sell}} \coloneqq 0, \quad p^{\text{el,buy}} \coloneqq |\mathcal{A}| \cdot |U|^2, \text{ and } \quad p^{\text{el,sell}} \coloneqq |U|.$$

Clearly, this instance can be constructed in polynomial time and its encoding length is polynomially related to that of the input. Now we show that there is a cover $\mathcal{A}'$ of size $\beta \leq k$ for SET COVER instance z if and only if there is a feasible solution with objective value β for SDES instance $z'(z)$.

Let $\mathcal{A}'$ be a cover of size $\beta \leq k \leq |\mathcal{A}|$ for SET COVER instance z. Setting up CHP engines $c_A \in S$ corresponding to cover members $A \in \mathcal{A}'$ and choosing their respective capacities as $\dot{V}^{\text{N}}_{c_A} = 1$ leads to investment cost of β in the objective function of SDES. It remains to show that this energy system can satisfy all demands in all load cases with equality, without incurring extra cost. Consider an arbitrary load case $\ell^\star \in L$. Since $\mathcal{A}'$ is a cover of U, there exists $A^\star \in \mathcal{A}'$ with $\ell^\star \in A^\star$. Operating only CHP engine $c_{A^\star}$ in load case $\ell^\star$ with $\dot{V}_{c_{A^\star}\ell^\star} = \frac{\ell^\star}{|U|}$ satisfies the heat demand $\dot{E}^{\text{heat}}_{\ell^\star} = \frac{\ell^\star}{|U|}$. The operated CHP engine generates electricity $\dot{V}^{\text{el}}_{c_{A^\star}}(\frac{\ell^\star}{|U|}) = \left(\frac{\ell^\star}{|U|}\right)^2$. The demand $\dot{E}^{\text{el}}_{\ell^\star} = \left(\frac{\ell^\star}{|U|}\right)^2 - \frac{\ell^\star \varepsilon}{|U|^2}$ is fulfilled and surplus electricity $\dot{V}^{\text{el,sell}}_{\ell^\star} = \frac{\ell^\star \varepsilon}{|U^2|}$ is sold. The revenue $\dot{V}^{\text{el,sell}}_{\ell^\star} p^{\text{el,sell}} = \frac{\ell^\star \varepsilon}{|U|}$ equals the operation cost $\dot{U}^{\text{gas}}_{c_{A^\star}}(\frac{\ell^\star}{|U|}) \cdot p^{\text{gas,buy}} = \frac{\ell^\star \varepsilon}{|U|}$. Since $\ell^\star \in L$ was chosen arbitrarily, this holds for every load case $\ell \in L$. It follows: We found a feasible solution with objective value β for SDES instance $z'(z)$.

Now, let a feasible solution for SDES instance $z'(z)$ with objective value $\beta \leq k \leq |S|$ be given. We show that this solution consists of exactly β set up CHP engines $\{c_{A_{i_1}}, \ldots, c_{A_{i_\beta}}\} \subseteq S$ and that the corresponding set $\{A_{i_1}, \ldots, A_{i_\beta}\} \subseteq \mathcal{A}$ forms a cover for U of cardinality β.

Let $S_\ell \subseteq S$ be the set of operated CHP engines in load case $\ell \in L$ (and thus a subset of all set up ones). We start by showing that the total operating cost in each load case $\ell \in L$ is non-negative, i.e., no profit can be generated by operating units. The only possible way to gain profit in a load case is by selling surplus electricity. Since $\dot{V}^{\text{el}}_s : \dot{\mathcal{V}}^{\text{set}}_s \to \mathbb{Q}_{\geq 0}, \dot{V}_{s\ell} \mapsto \dot{V}^2_{s\ell}$ is (i) a superadditive function and (ii) $\dot{E}^{\text{heat}}_\ell = \frac{\ell}{|U|} = \sum_{s \in S_\ell} \dot{V}_{s\ell}$ holds, it follows that

$$\sum_{s \in S_\ell} \dot{V}^{\text{el}}_s(\dot{V}_{s\ell}) \overset{\text{(i)}}{\leq} \dot{V}^{\text{el}}_s\left(\sum_{s \in S_\ell} \dot{V}_{s\ell}\right) \overset{\text{(ii)}}{=} \dot{V}^{\text{el}}_s\left(\frac{\ell}{|U|}\right) = \left(\frac{\ell}{|U|}\right)^2. \tag{3.15}$$

Consequently, $\dot{V}^{\text{el,sell}}_\ell \leq \left(\frac{\ell}{|U|}\right)^2 - \dot{E}^{\text{el}}_\ell = \frac{\varepsilon \ell}{|U|^2}$ electrical energy can be sold with revenue $p^{\text{el,sell}} = |U|$ per unit. Since operating all CHP engines in S_ℓ leads to gas cost of $p^{\text{gas,buy}} \cdot 2\frac{\ell}{|U|} = \frac{\varepsilon \ell}{|U|}$, the total operating costs for all $\ell \in L$ are non-negative.

We now show that $|S_\ell| = 1$ holds for all $\ell \in L$. To that end, assume the contrapositive, i.e., that there exists $\ell^\star \in L$ in which (at least) two set up CHP engines are operated ($|S_{\ell^\star}| \geq 2$). It holds that $\sum_{s \in S_{\ell^\star}} \dot{V}_{s\ell^\star} = \dot{E}^{\text{heat}}_{\ell^\star} = \frac{\ell^\star}{|U|}$. In combination with $|S_{\ell^\star}| \geq 2$ this implies that

$\ell^\star \geq 2$ and with Lemma 10 in the Appendix we can strengthen our previous estimation in Equation (3.15) to

$$\sum_{s\in S_{\ell^\star}} \dot{V}_s^{\text{el}}(\dot{V}_{s\ell^\star}) \overset{\text{Lem. 10}}{\leq} \dot{V}_s^{\text{el}}\left(\sum_{s\in S_{\ell^\star}} \dot{V}_{s\ell^\star}\right) - \frac{2}{|U|^2} = \dot{V}_s^{\text{el}}\left(\frac{\ell^\star}{|U|}\right) - \frac{2}{|U|^2} = \frac{\ell^{\star 2}-2}{|U|^2}.$$

By construction, $|L|\varepsilon < 1$ and thus $\ell^\star\varepsilon < 1$, which implies $\sum_{s\in S_{\ell^\star}} \dot{V}_s^{\text{el}}(\dot{V}_{s\ell^\star}) \leq \frac{\ell^{\star 2}-2}{|U|^2} < \frac{\ell^{\star 2}-\ell^\star\varepsilon-1}{|U|^2} = \dot{E}_{\ell^\star}^{\text{el}} - \frac{1}{|U|^2}$. Consequently, $\dot{U}_{\ell^\star}^{\text{el,buy}} > \frac{1}{|U|^2}$ electricity has to be bought, implying cost $p^{\text{el,buy}} \cdot \dot{U}_{\ell^\star}^{\text{el,buy}} > |\mathcal{A}| = |S| \geq k$ in the objective of SDES. As we have previously shown that no profit can be generated that could reduce this cost, this yields a contradiction to the fact that the given solution for the SDES instance $z'(z)$ has an objective value $\beta \leq k$.

It follows that for each load case $\ell \in L$ we have $|S_\ell| = 1$, say $S_\ell = \{s_\ell\}$. CHP engine s_ℓ must fulfill the heat demand, i.e., $\dot{V}_{s_\ell\ell} = \frac{\ell}{|U|} = \dot{E}_\ell^{\text{heat}}$, and $\frac{\ell}{|U|} \in \dot{\mathcal{V}}_{s_\ell}^{\text{set}}$. Consequently, s_ℓ generates electricity $\dot{V}_{s_\ell}^{\text{el}}(\frac{\ell}{|U|}) = \left(\frac{\ell}{|U|}\right)^2$. The demand $\dot{E}_\ell^{\text{el}} = \frac{\ell^2-\ell\varepsilon}{|U|^2}$ is fulfilled and surplus electricity $\dot{V}_\ell^{\text{el,sell}} = \frac{\ell\varepsilon}{|U|^2}$ is sold. The revenue $\dot{V}_\ell^{\text{el,sell}} p^{\text{el,sell}} = \frac{\ell\varepsilon}{|U|}$ equals the operation cost $\dot{U}_{s_\ell}^{\text{gas}}(\frac{\ell}{|U|}) \cdot p^{\text{gas,buy}} = \frac{\ell\varepsilon}{|U|}$ and the total operation cost is 0.

Thus, we can conclude that the given solution for SDES instance $z'(z)$ with objective value $\beta \leq |S|$ must contain exactly β set up CHP engines $C^{z'(z)} \coloneqq \{c_{A_{i_1}}, \ldots, c_{A_{i_\beta}}\} \subseteq S$ causing investment costs β and operation cost 0. For all $\ell = 1, \ldots, |U|$ CHP engine $s_\ell = c_{A_{j_\ell}} \in C^{z'(z)}$ satisfies $\frac{\ell}{|U|} \in \dot{\mathcal{V}}_{c_{A_{j_\ell}}}^{\text{set}}$ with $\ell \in A_{j_\ell}$. Thus, $\{A_{j_\ell} : \ell \in L\} \subseteq \{A_{i_1}, \ldots, A_{i_\beta}\}$ is a set cover for U which implies that $\mathcal{A}' \coloneqq \{A_{i_1}, \ldots, A_{i_\beta}\}$ induced by $C^{z'(z)}$ is a set cover of size β for $z'(z)$.

In summary, a cover $\mathcal{A}'$ of size $\beta \leq |\mathcal{A}|$ for SET COVER instance z transforms into a feasible solution with objective value $\beta \leq |S|$ for SDES instance $z'(z)$, and vice versa. This completes the proof. ■

The following Lemma 10, used in the proof previously given, is a slight modification of Lemma 9 given before.

Lemma 10 *For $a_1, \ldots, a_n \in \mathbb{N} \setminus \{0\},\ n \geq 2$ and $\alpha \in \mathbb{N} \setminus \{0\}$ holds:*

$$\left(\sum_{i=1}^n \frac{a_i}{\alpha}\right)^2 - \sum_{i=1}^n \left(\frac{a_i}{\alpha}\right)^2 \geq \frac{2}{\alpha^2}.$$

Proof By Lemma 9 holds $\left(\sum_{i=1}^n a_i\right)^2 - \sum_{i=1}^n a_i^2 = \sum_{1\leq i<j\leq n} 2a_ia_j \geq 2$. By multiplying with $\frac{1}{\alpha^2} \geq 0$, this is equivalent to $\frac{1}{\alpha^2} \cdot \left(\sum_{i=1}^n a_i\right)^2 - \frac{1}{\alpha^2} \cdot \sum_{i=1}^n a_i^2 \geq \frac{2}{\alpha^2}$. ■

4 An Adaptive Discretization MINLP Algorithm for Optimal Synthesis of Decentralized Energy Supply Systems

Abstract Decentralized energy supply systems (DESS) are highly integrated and complex systems designed to meet time-varying energy demands, e.g., heating, cooling, and electricity. The synthesis problem of DESS addresses combining various types of energy conversion units, choosing their sizing and operations to maximize an objective function, e.g., the net present value. In practice, investment costs and part-load performances are nonlinear. Thus, this optimization problem can be modeled as a nonconvex mixed-integer nonlinear programming (MINLP) problem. We present an adaptive discretization algorithm to solve such synthesis problems containing an iterative interaction between mixed-integer linear programs (MIPs) and nonlinear programs (NLPs). The proposed algorithm outperformes state-of-the-art MINLP solvers as well as linearization approaches with regard to solution quality and computation times on a test set obtained from real industrial data, which we made available online.

4.1 Introduction

We propose an adaptive discretization algorithm for the superstructure-based synthesis of decentralized energy supply systems (DESS). The proposed optimization-based algorithm employs discretization of the continuous decision variables. The discretization is iteratively adapted and used to obtain valid nonconvex mixed-integer nonlinear program (MINLP) solutions within short solution time.

DESS can consist of several energy conversion components (e.g., boilers and chillers) providing different utilities (e.g., heating, cooling, electricity). DESS are highly integrated and complex systems due to the integration of different forms of energy and their connection to the gas and electricity market as well as to the energy consumers. The application of DESS encompasses, e.g., chemical parks (Maréchal and Kalitventzeff, 2003), urban districts (Jennings et al., 2014; Maréchal et al., 2008) and building complexes (Arcuri et al., 2007; Lozano et al., 2009). Energy costs usually match the companies' profits in magnitude (Drumm et al., 2013). Thus, optimally designed decentralized energy supply systems can lead to a considerable increase of profits.

The target of optimal synthesis of DESS is the identification of an (economically) optimal structure (which types of equipment and how many units?) and optimal sizing (how big?), while simultaneously considering the optimal operation of the selected components (which components are operated at which level at what time?) (Frangopoulos et al., 2002). These three decision levels could be considered sequentially. However, the levels influence each other, thus only a simultaneous optimization will find a global optimal solution. In this paper, we consider the simultaneous optimization using superstructure-based synthesis. A superstructure needs to be predefined and consists of a superset of possible components, which can be selected within the synthesis of the DESS. If the superstructure is chosen too small, optimal solutions could be excluded, if the superstructure is chosen too large, the computational effort becomes prohibitive. Therefore some of the authors proposed a successive superstructure expansion algorithm (Voll et al., 2013b).

The synthesis of DESS contains binary decisions for the selection of energy conversion components as well as the on/off status in the operation of each component. Combined with nonlinear part-load performance of the energy conversion components, nonlinear economy-of-scale effects in the investment cost curves and strict energy balances, the synthesis of DESS leads in general to a nonconvex MINLP (Bruno et al., 1998). Typically, an economic objective function is considered, e.g., the net present value is maximized or the total annualized costs are minimized, furthermore also ecologic objective functions can be considered (Østergaard, 2009).

Metaheuristic optimization approaches have been proposed for the synthesis of DESS: Evolutionary algorithms were proposed for superstructure-free linearized synthesis as well as superstructure-based MINLP synthesis (Dimopoulos and Frangopoulos, 2008; Voll et al., 2012). Stojiljkovic et al. (2014) proposed a heuristic for structural decisions and solved a mixed-integer linear program (MILP) for operation decision. These heuristic approaches do not provide any measure of optimality.

To allow rigorous optimization, mostly linearized approaches are considered for synthesis of practically relevant problems. In the resulting MILPs, the nonlinearities are approximated by piecewise-linearized functions. First, Papoulias and Grossmann (1983) linearized the investment cost functions, the nonlinear operation conditions are modeled as discrete, but fixed operation conditions. Continuous operation decision with constant efficiency is addressed by Lozano et al. (2009) for MILP synthesis of energy supply systems in the building sector using fixed capacities. Voll et al. (2013b) proposed an MILP model accounting for piecewise-linearized part-load dependent operation conditions and piecewise-linearized investment costs for continuous component sizing. Recently, Yokoyama et al. (2015) modeled the structure decision with integer variables for the type and discrete sizes of components, thus, modeling the nonlinear investment cost curve is not required. The operation power is modeled as linear function within allowed operation ranges.

The solution of the linarization approaches only results in approximated solutions. However solving the MINLP of superstructure-based synthesis is computationally demanding. First, an MINLP model for the operation of DESS was considered by Prokopakis and Maroulis (1996). The model takes into account the nonlinear size- and load-dependent components performance. Papalexandri et al. (1998) and Bruno et al. (1998) generalized the MINLP

formulation to the optimal synthesis of DESS. Due to the complexity of the problem, only one component of each type is considered in the superstructure and the demand is considered by a single load case. An MINLP model considering multiple, detailed components as well as multiple load cases for the demand profile has been proposed by Varbanov et al. (2004) and Varbanov et al. (2005). To solve the resulting large MINLP, nonlinearities of part-load performance are predefined in an iterative loop and internally MILPs are solved. Chen and Lin (2011) solved an MINLP for a steam-generation plant, the nonlinearities of part-load performance are optimized, nevertheless the model considers steam as a single demand type. The problem of integrated optimization of DESS and process system commonly results in large-scale MINLPs. Recently, Zhao et al. (2015) decomposed the integrated MINLP of optimal operation of DESS and process system into an MILP and NLP problem and the variables are exchanged between both problems. Moreover, Tong et al. (2015) proposed a discretization approach for the MINLP of optimal operation of DESS and process system. Further discretization approaches for solving nonconvex MINLP problems with different practical applications are discussed in Section 4.3.

Contribution In this paper, MINLP solutions are obtained by an adaptive discretization algorithm for the nonlinear synthesis problem of DESS. (Commercial) MINLP solvers such as BARON (Tawarmalani and Sahinidis, 2005) reach computational limits for relative small test cases of the considered MINLP, accounting for nonlinear investment cost and multivariate nonlinear part-load dependent operation performance. We developed a problem-tailored adaptive discretization algorithm to obtain valid solutions of the MINLP within short solution time. The algorithm discretizes the continuous component size within bounds given by practically available component size limits. The whole range of size can be selected for each type of component, since the discretization is iteratively adapted. Thus, the algorithm does not require predefining discrete sizes of the components in the superstructure. Moreover, the operation of each component for each load case is discretized with finer steps depending on the part-load performence of each type of energy conversion component. Thus, various energy conversion components with different capacities and with corresponding investment and maintenance costs can be selected and adjusted to meet the energy demands in each load case.

Outline We state our MINLP model of the DESS in Section 4.2. In Section 4.3, we describe the proposed adaptive discretization algorithm. In Section 4.4, we apply the algorithm to a test set of a real-world example. Solutions and performance are compared to a standard MINLP solver as well as state-of-the-art linearization approaches with MILP models.

4.2 Optimization Models for Decentralized Energy Supply Systems

In this section, we present an MINLP model for optimal synthesis of DESS (Section 4.2.2) as well as a piecewise-linearized model (Section 4.2.3), which we use as benchmark for our adaptive discretization algorithm. First of all, in Section 4.2.1, notations of parameters, decisions, and the optimization problem as a whole are given.

4.2.1 Equipment, Parameters, and Decisions

The set of energy conversion units, which can be set up to meet the demands, is denoted by superstructure

$$S = B \dot{\cup} C \dot{\cup} T \dot{\cup} A$$

and encompasses a set of boilers B, a set of combined heat and power engines C, a set of turbo-driven compressor chillers T and a set of absorption chillers A (Figure 4.1). Further equipment could be included, but we focus here on the problem introduced in our earlier work (Voll et al., 2013b). All units $s \in S$ in the superstructure are not further specified than their type of equipment. Note, that an optimal DESS is likely to contain multiple units of one type which is in strong contrast to classical process synthesis problems (Farkas et al., 2005).

The set of load cases considered for the operation of the DESS is denoted by L. The length of load case $\ell \in L$ is denoted by $\Delta_\ell \geq 0$. Furthermore,

$$\dot{E}_\ell^{\text{heat}} \geq 0, \quad \dot{E}_\ell^{\text{cool}} \geq 0, \quad \text{and} \quad \dot{E}_\ell^{\text{el}} \geq 0$$

denote the demands of heating, cooling, and electricity, which have to be satisfied with equality by the DESS in every load case $\ell \in L$.

For each unit $s \in S$, its continuous size $\dot{V}_s^{\text{N}}$ has to be determined. The size $\dot{V}_s^{\text{N}}$ specifies the maximum (nominal) output energy and has to be between a minimum size $\dot{V}_s^{\text{N,min}}$ and a maximum size $\dot{V}_s^{\text{N,max}}$. For combined heat and power (CHP) engines, the output is not unique (heat and electricity). In this case, the size refers to the maximum heat output. The investment cost of unit $s \in S$ depends on its size $\dot{V}_s^{\text{N}}$ and is given by the nonlinear function $I_s(\dot{V}_s^{\text{N}})$. Further, maintenance costs are considered as constant factors m_s in terms of investment costs.

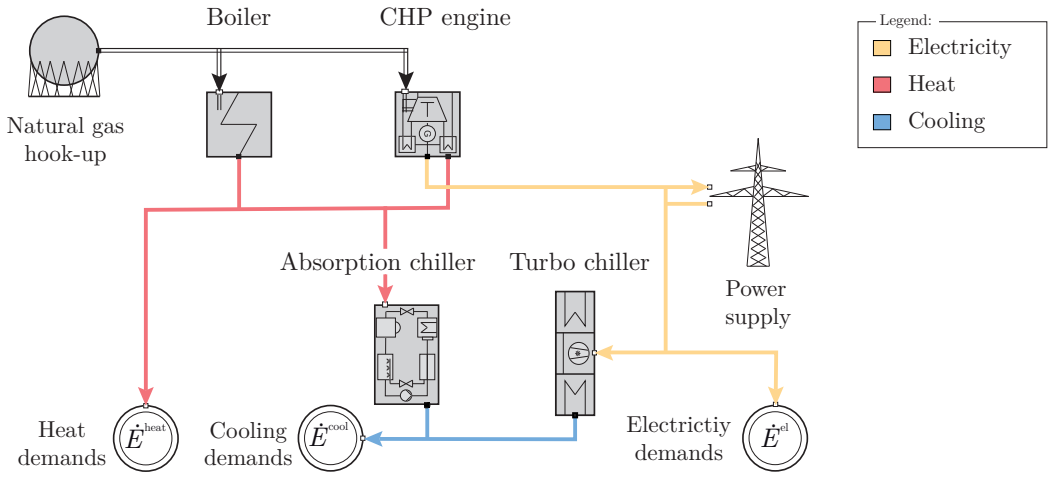


Fig. 4.1: Example of a decentralized energy supply system with exactly one unit of each considered type of equipment.

The output power of unit $s \in S$ at load case $\ell \in L$ is to be determined and is denoted by $\dot{V}_{s\ell}$. Again, for CHP, the output power refers to the heat output. The nonlinear function $\dot{V}^{\text{el}}_{s\ell}(\dot{V}_{s\ell}, \dot{V}^{\text{N}}_s)$ describes the electricity output of a CHP $s \in C \subseteq S$. For each unit $s \in S$ operated in load case $\ell \in L$, a minimum part-load operation is required. Thus, the condition $\alpha^{\text{min}}_s \dot{V}^{\text{N}}_s \leq \dot{V}_{s\ell} \leq \dot{V}^{\text{N}}_s$ with minimum part-load factor $0 \leq \alpha^{\text{min}}_s \leq 1$ has to hold. If $s \in S$ is not operated in load case $\ell \in L$, we set $\dot{V}_{s\ell} = 0$. The input needed to generate the output $\dot{V}_{s\ell}$ is described by the nonlinear part-load performance function $\dot{U}_s(\dot{V}_{s\ell}, \dot{V}^{\text{N}}_s)$.

Parameters $p^{\text{gas,buy}}$, $p^{\text{el,buy}}$, and $p^{\text{el,sell}}$ denote the purchase price of gas and electricity, and the selling price of electricity from and to the grid. To compute the objective value of a feasible DESS, i.e., the net present value, the parameter

$$\text{APVF}(i, \gamma^{\text{CF}}) := \frac{(i+1)^{\gamma^{\text{CF}}} - 1}{i \cdot (i+1)^{\gamma^{\text{CF}}}}$$

denotes the present value factor and depends on discount rate i and cash flow time γ^{CF}.

The equipment models including the analytical equations of the unit's input-output relations and all parameters can be found in the Appendix in Section 4.7.

4.2.2 MINLP Formulation

Variables For every unit $s \in S$, the variable $y_s \in \{0, 1\}$ denotes whether the unit is chosen and the continuous variable $\dot{V}^{\text{N}}_s \geq 0$ denotes the (nominal) size of unit s. The variable $\delta_{s\ell} \in \{0, 1\}$ denotes the on/off-status and the continuous variable $\dot{V}_{s\ell} \geq 0$ denotes the output power of unit $s \in S$ in load case $\ell \in L$. Furthermore, the continuous variables $\dot{U}^{\text{el,buy}}_\ell \geq 0$ and $\dot{V}^{\text{el,sell}}_\ell \geq 0$ denote the bought and sold electricity power from and to the grid in load case $\ell \in L$.

Formulation A mixed-integer nonlinear programming formulation for the considered problem for optimal synthesis of DESS is given by (4.1) – (4.12).

Objective In Objective (4.1), the net present value $\text{NPV} := \text{APVF}(i, \gamma^{\text{CF}}) \cdot R_{\text{CF}} - I$ is maximized. The NPV is calculated from the present value factor $\text{APVF}(i, \gamma^{\text{CF}})$, the net cash flow R_{CF} and the total investments I. The net cash flow R_{CF} are the annual revenues from sold electricity $\dot{V}^{\text{el,sell}}_\ell$ minus the cost for electricity $\dot{U}^{\text{el,buy}}_\ell$ bought from the grid and secondary energy $\dot{U}_s(\dot{V}_{s\ell}, \dot{V}^{\text{N}}_s)$ consumed by the boilers and CHP engines as well as maintenance costs.

Constraints Constraints (4.2) – (4.4) ensure that the demands for heating E^{heat}_ℓ, cooling E^{cool}_ℓ and electricity E^{el}_ℓ are fulfilled with equality in every load case $\ell \in L$ by the DESS. Constraints (4.5) restrict the size V^{N}_s to be in the technically allowed range $[V^{\text{N,min}}_s; V^{\text{N,max}}_s]$. Constraints (4.6) – (4.8) force $V_{s\ell} = 0$, if $\delta_{s\ell} = 0$ and, otherwise, limit $V_{s\ell}$ to the operation interval $[\alpha^{\text{min}}_s \cdot V^{\text{N}}_s; V^{\text{N}}_s]$. Constraints (4.9) ensure that a unit is chosen, if it is used in at least one load case.

$$\max \quad \text{APVF}(i,\gamma^{\text{CF}}) \cdot \Bigg[\sum_{\ell \in L} \Delta_\ell \cdot \Big(p^{\text{el,sell}} \cdot \dot{V}_\ell^{\text{el,sell}} - p^{\text{el,buy}} \cdot \dot{U}_\ell^{\text{el,buy}} - p^{\text{gas,buy}} \cdot \sum_{s \in B \cup C} \delta_{s\ell} \cdot \dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) \Big) - \sum_{s \in S} m_s \cdot I_s(\dot{V}_s^{\text{N}}) \cdot y_s \Bigg] - \sum_{s \in S} I_s(\dot{V}_s^{\text{N}}) \cdot y_s \tag{4.1}$$

$$\text{s.t.} \quad \sum_{s \in B \cup C} \dot{V}_{s\ell} = \dot{E}_\ell^{\text{heat}} + \sum_{s \in A} \delta_{s\ell} \cdot \dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) \qquad \forall\, \ell \in L \tag{4.2}$$

$$\sum_{s \in A \cup T} \dot{V}_{s\ell} = \dot{E}_\ell^{\text{cool}} \qquad \forall\, \ell \in L \tag{4.3}$$

$$\dot{U}_\ell^{\text{el,buy}} + \sum_{s \in C} \delta_{s\ell} \cdot \dot{V}_s^{\text{el}}(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) = \dot{E}_\ell^{\text{el}} + \sum_{s \in T} \delta_{s\ell} \cdot \dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) + \dot{V}_\ell^{\text{el,sell}} \qquad \forall\, \ell \in L \tag{4.4}$$

$$\dot{V}_s^{\text{N,min}} \le \dot{V}_s^{\text{N}} \le \dot{V}_s^{\text{N,max}} \qquad \forall\, s \in S \tag{4.5}$$

$$\dot{V}_{s\ell} \le \delta_{s\ell} \cdot \dot{V}_s^{\text{N,max}} \qquad \forall\, s \in S, \ell \in L \tag{4.6}$$

$$\dot{V}_{s\ell} \le \dot{V}_s^{\text{N}} \qquad \forall\, s \in S, \ell \in L \tag{4.7}$$

$$\dot{V}_{s\ell} \ge \alpha_s^{\text{min}} \cdot \dot{V}_s^{\text{N}} - (1 - \delta_{s\ell}) \cdot \alpha_s^{\text{min}} \cdot \dot{V}_s^{\text{N,max}} \qquad \forall\, s \in S, \ell \in L \tag{4.8}$$

$$y_s \ge \delta_{s\ell} \qquad \forall\, s \in S, \ell \in L \tag{4.9}$$

$$y_s \in \{0,1\},\ \dot{V}_s^{\text{N}} \ge 0 \qquad \forall\, s \in S \tag{4.10}$$

$$\delta_{s\ell} \in \{0,1\},\ \dot{V}_{s\ell} \ge 0 \qquad \forall\, s \in S, \ell \in L \tag{4.11}$$

$$\dot{U}_\ell^{\text{el,buy}}, \dot{V}_\ell^{\text{el,sell}} \ge 0 \qquad \forall\, \ell \in L \tag{4.12}$$

We note that the formulation is nonlinear due to the equipment models of the units (cf. Appendix, Section 4.7) and bilinear terms in Equations (4.1), (4.2), and (4.4) as well as nonconvex due to the investment cost function $I_s(\dot{V}_s^{\text{N}})$ (cf. Appendix, Section 4.7) and nonlinear equality Constraints (4.2) and (4.4).

4.2.3 Benchmarking to Piecewise-linearized Approach

The MINLP synthesis model (4.1) – (4.12) is commonly linearized for practical applications (Section 4.1). The solution obtained by the approximated MILP is in general not feasible for the nonlinear model (Bruno et al., 1998) (Section 4.4.1). In this section, we present an approach to obtain feasible solutions of the MINLP based on a solution of the MILP. The feasible MINLP solution based on the MILP result is considered as benchmark for our adaptive discretization algorithm (Section 4.3). Since, as explained above, a one-to-one comparison between MINLP and MILP solutions is not possible, we think that the presented analysis provides an insightful comparison between previous work and the algorithm proposed in this work.

The MILP stated by Voll et al. (2013b) with piecewise-linearized functions for the nonlinear investment cost curves and piecewise-linearized part-load operation curves are employed to compute the MILP solution. To obtain a feasible MINLP solution based on the solution $\delta^*_{s\ell}, \dot{V}^*_{s\ell}, y^*_s, \dot{V}^{\mathrm{N}*}_s$ of the MILP, we solve MINLP$^{\text{lin,feas}}$ (4.13) – (4.16).

$$\min \ |L| \cdot \sum_{s \in S} \left(\frac{\left| \dot{V}^{\mathrm{N}*}_s - \dot{V}^{\mathrm{N}}_s \right|}{\dot{V}^{\mathrm{N}*}_s} \right) + \sum_{\substack{s \in S, \ell \in L: \\ \delta^*_{s\ell}=1}} \left(\frac{\left| \dot{V}^*_{s\ell} - \dot{V}_{s\ell} \right|}{\dot{V}^*_{s\ell}} \right) \tag{4.13}$$

$$\text{s.t.} \ \ (4.2) - (4.12) \tag{4.14}$$

$$y_s = y^*_s \qquad \forall s \in S \tag{4.15}$$

$$\delta_{s\ell} = \delta^*_{s\ell} \qquad \forall s \in S, \ell \in L \tag{4.16}$$

The selected structure of the DESS y^*_s and the on/off status of the equipment $\delta^*_{s\ell}$ defined by the MILP is kept fixed. The objective function reflects minimizing the difference between the solution values of the MILP and the MINLP, in the solution space of the MINLP. Thus, feasible solutions for the MINLP are obtained which are 'near' the given solution of the MILP. The difference measure is defined by the sum of the normalized differences in optimal design $\dot{V}^{\mathrm{N}}_s$ and operation $\dot{V}_{s\ell}$.

4.3 Adaptive Discretization Algorithm

Solving the nonconvex MINLP (4.1) – (4.12) with state-of-the-art solvers like BARON (Tawarmalani and Sahinidis, 2005) leads to unsatisfying results. For several nontrivial test instances, it is even hard for solvers to compute a feasible solution (Section 4.4). Thus, the need of a problem-specific solution method providing primal MINLP solutions is evident.

It is a common approach to discretize (continuous) variables in a nonconvex nonlinear program to approximate it with an easier to solve mixed-integer linear one (Geißler et al., 2011; Gupte et al., 2013; Kolodziej et al., 2013; Leyffer et al., 2008; Pham et al., 2009; Yue and You, 2014). As an obtained solution might not be feasible for the original MINLP, we extend the discretization approach. Given an approximate solution, we fix selected solution-specific decisions (i.e., unit sizes and on/off statuses in the load cases), and solve the remaining NLP using a decomposition to arrive at a primal MINLP solution. To have a computational tractable approximation, only a few discretization points for the unit size and operation are used. However, to ensure a certain accuracy in our discretization algorithm, this two step algorithm is embedded in a loop of refinements of the discretization. At every iteration, the discretization grid is contracted and shifted in the direction of the discrete unit size chosen in the previous iteration, keeping the size of the discretized MILP.

The discretized problem formulation of the nonconvex MINLP (4.1) – (4.12) is described in Section 4.3.1, followed by the procedure to form a feasible MINLP solution using the approximate solution in Section 4.3.2. The adaptive part of the discretization algorithm is specified in Section 4.3.3. In the end and putting everything together, Section 4.3.4

provides a description of the adaptive discretization algorithm as a whole and some further comments.

4.3.1 Discretized Problem

To develop an approximation via discretization, we discretize all continuous variables with nonlinear dependencies. In MINLP (4.1) – (4.12) this involves the unit's size $\dot{V}_s^{\mathrm{N}} \geq 0$ and operation $\dot{V}_{s\ell} \geq 0$.

Unit size If unit $s \in S$ is chosen, i.e., $y_s = 1$ holds, we have to choose a size $\dot{V}_s^{\mathrm{N}}$ in the interval $[\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}]$. The investment cost function $I_s(\dot{V}_s^{\mathrm{N}})$ depends on the unit's size and is nonlinear (cf. Appendix, Section 4.7). We discretize the range of the continuous variable $\dot{V}_s^{\mathrm{N}} \in [\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}]$ by dividing the interval into $k_s^{\max}$ (equidistant) discrete sizes

$$\dot{V}_{s1}^{\mathrm{N,val}} < \dot{V}_{s2}^{\mathrm{N,val}} < \ldots < \dot{V}_{sk_s^{\max}}^{\mathrm{N,val}}$$

with $\dot{V}_s^{\mathrm{N,min}} \leq \dot{V}_{s1}^{\mathrm{N,val}}$, $\dot{V}_{sk_s^{\max}}^{\mathrm{N,val}} \leq \dot{V}_s^{\mathrm{N,max}}$ and $k_s^{\max} \in \mathbb{N}$ an odd number. These $\dot{V}_{sk}^{\mathrm{N,val}}$ are parameters and the related variables $\dot{V}_{sk}^{\mathrm{N}} \in \{0,1\}$ denote whether unit $s \in S$ is set up with the k-th discrete size $\dot{V}_{sk}^{\mathrm{N,val}}$. Thus, we transform every continuous variable $\dot{V}_s^{\mathrm{N}}$ in several binary variables $\dot{V}_{sk}^{\mathrm{N}}$. This implies that we do not need the nonlinear investment cost function in the discretized problem anymore, because for each discrete size $\dot{V}_{sk}^{\mathrm{N,val}}$ we can compute its investment costs $I_{sk}^{\mathrm{val}} := I_s(\dot{V}_{sk}^{\mathrm{N,val}})$ in advance.

Unit operation Together with the unit's size, one can compute the input energy needed to get a desired operation output $\dot{V}_{s\ell}$ using the nonlinear part-load performance functions $\dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\mathrm{N}})$ (cf. Appendix, Section 4.7). If $\dot{V}_{sk}^{\mathrm{N,val}}$ is chosen out of the discrete unit sizes and the unit is switched on, the possible output $\dot{V}_{s\ell}$ of this unit is bound by the size $\dot{V}_{sk}^{\mathrm{N,val}}$ and a minimal possible part-load $\alpha_s^{\min}\dot{V}_{sk}^{\mathrm{N,val}}$ with $0 \leq \alpha_s^{\min} \leq 1$. Again, we discretize the range of the continuous variable $\dot{V}_{s\ell} \in [\alpha_s^{\min}\dot{V}_{sk}^{\mathrm{N,val}}, \dot{V}_{sk}^{\mathrm{N,val}}]$ by dividing the interval into $j_{sk\ell}^{\max}$ (equidistant) discrete operations

$$\alpha_s \cdot \dot{V}_{sk}^{\mathrm{N,val}} =: \dot{V}_{sk\ell 1}^{\mathrm{val}} < \dot{V}_{sk\ell 2}^{\mathrm{val}} < \ldots < \dot{V}_{sk\ell j_{sk\ell}^{\max}}^{\mathrm{val}} := \dot{V}_{sk}^{\mathrm{N,val}}$$

with $j_{sk\ell}^{\max} \in \mathbb{N}$ and $j_{sk\ell}^{\max} \geq 2$. The variable $\dot{V}_{sk\ell j} \in \{0,1\}$ denotes whether unit $s \in S$ with size $\dot{V}_{sk}^{\mathrm{N,val}}$ has the j-th discrete operational output $\dot{V}_{sk\ell j}^{\mathrm{val}}$ in load case $\ell \in L$. We name

$$\dot{U}_{sk\ell j}^{\mathrm{val}} := \dot{U}_s(\dot{V}_{sk\ell j}^{\mathrm{val}}, \dot{V}_{sk}^{\mathrm{N,val}}) \text{ and } \dot{V}_{sk\ell j}^{\mathrm{el,val}} := V_s^{\mathrm{el}}(\dot{V}_{sk\ell j}^{\mathrm{val}}, \dot{V}_{sk}^{\mathrm{N,val}})$$

the values of the employed part-load performance function at the corresponding discrete size and discrete operation.

The discretization grid of size and operation and its notation is summarized in Figure 4.2.

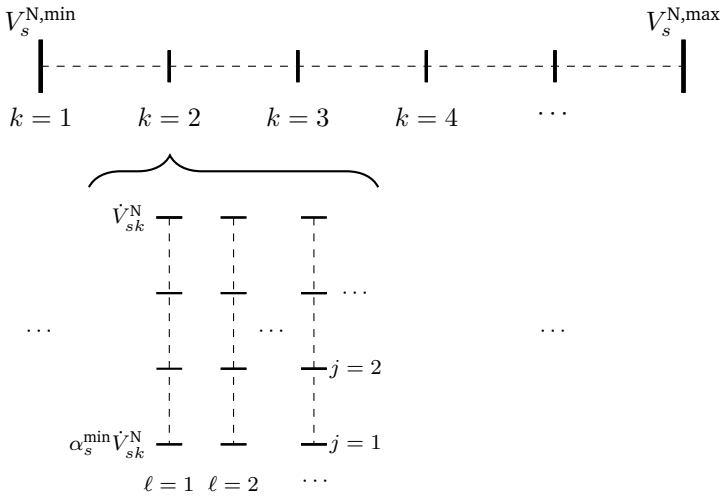


Fig. 4.2: Discretization and notation of unit size decisions (top) and operation decisions (bottom).

Since fulfilling the energy demands in heating, cooling, and electricity with equality is a requirement of our problem (constraints (4.2) – (4.4)), we want to enable equality in the energy balances of our discretized approximation as well (cf. Remark 11 in Section 4.3.4). A pure discretization with binary variables $\dot{V}_{sk\ell j}$ does not allow this in general. Therefore, we piecewise linearize the part-load performance functions $\dot{U}_s$ and $\dot{V}_s^{\mathrm{el}}$ using $\dot{V}_{sk\ell j}^{\mathrm{val}}$ as supporting points. We introduce a continuous variable

$$\dot{V}_{sk\ell j}^{\mathrm{cont}} \geq 0 \quad \text{with} \quad \dot{V}_{sk\ell j}^{\mathrm{cont}} \leq \dot{V}_{sk\ell j+1}^{\mathrm{val}} - \dot{V}_{sk\ell j}^{\mathrm{val}} =: \dot{V}_{sk\ell j}^{\mathrm{val,diff}}$$

and parameters

$$\dot{U}_{sk\ell j}^{\mathrm{lin}} := \frac{\dot{U}_{sk\ell j+1}^{\mathrm{val}} - \dot{U}_{sk\ell j}^{\mathrm{val}}}{\dot{V}_{sk\ell j}^{\mathrm{val,diff}}} \quad , \quad \dot{V}_{sk\ell j}^{\mathrm{el,lin}} := \frac{\dot{V}_{sk\ell j+1}^{\mathrm{el,val}} - \dot{V}_{sk\ell j}^{\mathrm{el,val}}}{\dot{V}_{sk\ell j}^{\mathrm{val,diff}}}$$

for each simplex, i.e., line segment between $\dot{V}_{sk\ell j}^{\mathrm{val}}$ and $\dot{V}_{sk\ell j+1}^{\mathrm{val}}$. Note that in the proposed approach the discretization of the unit *size* remains a pure one, where we do not add further continuous variables or piecewise linearize anything there.

Using the specified discretization and linearization, we are able to approximate the original MINLP (4.1) – (4.12) with the following mixed-integer linear program (4.17) – (4.27) (discretized MIP). For better readability, the limits of the indices $k = 1, 2, \ldots, k_s^{\max}$ and $j = 1, 2, \ldots, j_{sk\ell}^{\max}$ are not mentioned explicitly in the following formulation and sections. Indices s and ℓ without any set information mean $s \in S$ and $\ell \in L$.

The binary variables y_s and $\delta_{s\ell}$ in MINLP formulation (4.1) – (4.12) are not needed anymore in the discretized MIP (4.17) – (4.27), since the new binary variables $\dot{V}_{sk}^{\mathrm{N}}$ and $\dot{V}_{sk\ell j}$ together with constraints (4.22) and (4.23) include their role. Of course, the discretized problem (4.17) – (4.27) contains a lot more binary decisions, but the nonlinearities and actually the nonconvex nonlinearities are eliminated in that model. Moreover, some binary variables $\dot{V}_{sk}^{\mathrm{N}}$ and $\dot{V}_{sk\ell j}$ can be eliminated by preprocessing (Section 4.4.1) depending on the demands.

$$\max\ \text{APVF}(i,\gamma^{\text{CF}})\cdot\Bigg[\sum_{\ell\in L}\Delta_\ell\cdot\Big(p^{\text{el,sell}}\cdot\dot V_\ell^{\text{el,sell}}-p^{\text{el,buy}}\cdot\dot U_\ell^{\text{el,buy}} - p^{\text{gas,buy}}\cdot\sum_{s\in B\cup C}\sum_{k,j}\big(\dot U_{sk\ell j}^{\text{val}}\cdot\dot V_{sk\ell j}+\dot U_{sk\ell j}^{\text{lin}}\cdot\dot V_{sk\ell j}^{\text{cont}}\big)\Big) - \sum_{s,k} m_s\cdot I_{sk}^{\text{val}}\cdot\dot V_{sk}^{\text{N}}\Bigg]-\sum_{s,k} I_{sk}^{\text{val}}\cdot\dot V_{sk}^{\text{N}} \tag{4.17}$$

$$\text{s.t.}\ \sum_{s\in B\cup C}\sum_{k,j}\big(\dot V_{sk\ell j}^{\text{val}}\cdot\dot V_{sk\ell j}+\dot V_{sk\ell j}^{\text{cont}}\big) = \dot E_\ell^{\text{heat}}+\sum_{s\in A}\sum_{k,j}\big(\dot U_{sk\ell j}^{\text{val}}\cdot\dot V_{sk\ell j}+\dot U_{sk\ell l}^{\text{lin}}\cdot\dot V_{sk\ell j}^{\text{cont}}\big) \qquad \forall\,\ell\in L \tag{4.18}$$

$$\sum_{s\in A\cup T}\sum_{k,l}\big(\dot V_{sk\ell j}^{\text{val}}\cdot\dot V_{sk\ell j}+\dot V_{sk\ell j}^{\text{cont}}\big)=\dot E_\ell^{\text{cool}} \qquad \forall\,\ell\in L \tag{4.19}$$

$$\dot U_\ell^{\text{el,buy}}+\sum_{s\in C}\sum_{k,j}\big(\dot V_{sk\ell j}^{\text{el,val}}\cdot\dot V_{sk\ell j}+\dot V_{sk\ell j}^{\text{el,lin}}\cdot\dot V_{sk\ell j}^{\text{cont}}\big) = \dot E_\ell^{\text{el}}+\dot V_\ell^{\text{el,sell}}+\sum_{s\in T}\sum_{k,j}\big(\dot U_{sk\ell j}^{\text{val}}\cdot\dot V_{sk\ell j}+\dot U_{sk\ell j}^{\text{lin}}\cdot\dot V_{sk\ell j}^{\text{cont}}\big) \qquad \forall\,\ell\in L \tag{4.20}$$

$$\dot V_{sk\ell j}^{\text{cont}}\le\dot V_{sk\ell j}^{\text{val,diff}}\cdot\dot V_{sk\ell j} \qquad \forall\,s,k,\ell,j \tag{4.21}$$

$$\sum_k\dot V_{sk}^{\text{N}}\le 1 \qquad \forall\,s\in S \tag{4.22}$$

$$\sum_j\dot V_{sk\ell j}\le\dot V_{sk}^{\text{N}} \qquad \forall\,s,k,\ell \tag{4.23}$$

$$\dot V_{sk}^{\text{N}}\in\{0,1\} \qquad \forall\,s,k \tag{4.24}$$

$$\dot V_{sk\ell j}\in\{0,1\} \qquad \forall\,s,k,\ell,j \tag{4.25}$$

$$\dot V_{sk\ell j}^{\text{cont}}\ge 0 \qquad \forall\,s,k,\ell,j \tag{4.26}$$

$$\dot U_\ell^{\text{el,buy}},\dot V_\ell^{\text{el,sell}}\ge 0 \qquad \forall\,\ell\in L \tag{4.27}$$

4.3.2 Nonlinear Feasibility

After computing a solution of (4.17) – (4.27), post processing is needed to compute a primal feasible solution of the original MINLP (4.1) – (4.12). For this post processing, we fix the unit sizes and load case specific on/off statuses given by the approximate solution. Therefore, let $\dot V_{sk}^{\text{N}*}\in\{0,1\}$ and $\dot V_{sk\ell j}^{*}\in\{0,1\}$ be the values of the related variables of a given discretized problem solution. For each unit $s\in S$ and load case $\ell\in L$ parameters

$$y_s^{\text{par}}:=\sum_k\dot V_{sk}^{\text{N}*} \tag{4.28}$$

$$\dot V_s^{\text{N,par}}:=\sum_k\dot V_{sk}^{\text{N,val}}\cdot\dot V_{sk}^{\text{N}*} \tag{4.29}$$

$$\delta_{s\ell}^{\text{par}}:=\sum_{k,j}\dot V_{sk\ell j}^{*} \tag{4.30}$$

are defined. Fixing the variables $y_s \in \{0,1\}$, $\dot{V}_s^{\mathrm{N}} \geq 0$ and $\delta_{s\ell} \in \{0,1\}$ with these values in MINLP (4.1) – (4.12) implies that all binary variables and all constraints (4.5) – (4.9) linking load case are not needed anymore or become variable bounds. As a consequence, the problem is decomposable in independent nonlinear programs, one for every load case $\ell \in L$, named NLP_ℓ. Since the equality constraints (4.2) and (4.4) are still present, every NLP_ℓ remains nonconvex. However, as the computational results show in Section 4.4, the independent problems are solved quite fast for the considered test instances. It is not guaranteed that NLP_ℓ provides a feasible solution, since parts of an approximate solution are fixed. Whether NLP_ℓ provides a feasible solution depends on the form of the piecewise linearized functions and on the fineness of the discretization. It turns out that more discretization points, on the one hand, enlarge the probability to determine a feasible solution in NLP_l but, on the other hand, enlarge the computation times of solving NLP_l. However, the computational results (Section 4.4.1) show that for all test instances considered in this paper every single NLP_ℓ was feasible.

4.3.3 Adapting Discretization

Solving the discretized problem (4.17) – (4.27) followed by suited NLPs for nonlinear feasibility, a primal solution of the MINLP (4.1) – (4.12) is probably computed. This interaction of MIP and NLPs is incorporated into an iteration loop, as it is described as a whole in Section 4.3.4. At the end of every iteration, the discretization grid is adapted based on the just computed solution of the discretized problem in that step. Thereby, nearly the entire spectrum of possible unit sizes is enabled and a greater accuracy in the whole algorithm and therefore better primal solutions are achieved.

In the rest of this section, the procedure of adapting the discretization is described in detail. Proceed to Section 4.3.4 for an overview of the whole adaptive discretization algorithm.

Let $\dot{V}_{s1}^{\mathrm{N,val}} < \dot{V}_{s2}^{\mathrm{N,val}} < \ldots < \dot{V}_{sk_s^{\max}}^{\mathrm{N,val}}$ be the discretization of the size of unit $s \in S$ in a certain iteration and let $1 \leq k_s^* \leq k_s^{\max}$ be the index of the chosen discrete size of unit $s \in S$, i.e., $\dot{V}_s^{\mathrm{N,par}} = \dot{V}_{sk_s^*}^{\mathrm{N,val}}$ holds (cf. Equation (4.29)). We are faced with three different cases depending on k_s^* and $\dot{V}_s^{\mathrm{N,par}}$:

Case 1 (interior point):	$k_s^* \notin \{1, k_s^{\max}\}$
Case 2 (interval limit):	$k_s^* \in \{1, k_s^{\max}\}$ and $\dot{V}_{sk_s^*}^{\mathrm{N,val}} \notin \{\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}\}$
Case 3 (bound):	$k_s^* \in \{1, k_s^{\max}\}$ and $\dot{V}_{sk_s^*}^{\mathrm{N,val}} \in \{\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}\}$

Case 1 (interior point) For the case $k_s^* \notin \{1, k_s^{\max}\}$ the chosen discrete point lies not at the end of the discretization interval. We then contract the discrete grid points in the direction of the chosen size $\dot{V}_{sk_s^*}^{\mathrm{N,val}}$. More precisely, the equidistant division of the interval $[V_{sk_s^*-1}^{\mathrm{N,val}}, V_{sk_s^*+1}^{\mathrm{N,val}}]$ gets the new and adapted discretization. Notice, since $k_s^{\max}$ is odd, $\dot{V}_s^{\mathrm{N,par}}$ stays to be a grid point after the adaption.

Example (interior point) For $k_s^{\max} = 5$, $k_s^* \notin \{1, 5\}$ the adaption effects (Figure 4.3):

$$
\begin{aligned}
\dot{V}_{s1}^{\mathrm{N,val}} &\leftarrow V_{sk_s^*-1}^{\mathrm{N,val}} \\
\dot{V}_{s2}^{\mathrm{N,val}} &\leftarrow \frac{1}{2}\left(V_{sk_s^*}^{\mathrm{N,val}} + V_{sk_s^*-1}^{\mathrm{N,val}}\right) \\
\dot{V}_{s3}^{\mathrm{N,val}} &\leftarrow V_{sk_s^*}^{\mathrm{N,val}} \\
\dot{V}_{s4}^{\mathrm{N,val}} &\leftarrow \frac{1}{2}\left(V_{sk_s^*+1}^{\mathrm{N,val}} + V_{sk_s^*}^{\mathrm{N,val}}\right) \\
\dot{V}_{s5}^{\mathrm{N,val}} &\leftarrow V_{sk_s^*+1}^{\mathrm{N,val}}.
\end{aligned}
$$

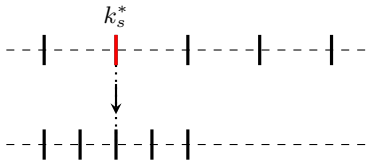


Fig. 4.3: Adaptive Discretization (interior point)

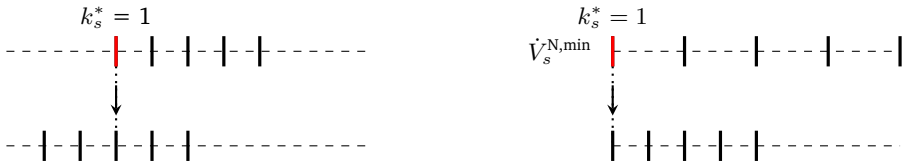
Case 2 (interval limit) If $k_s^* \in \{1, k_s^{\max}\}$ is the index of one of the end points of the discretization and $\dot{V}_{sk_s^*}^{\mathrm{N,val}} \notin \{\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}\}$ holds, we shift the grid in the direction of the chosen size (and do not contract it). Thus, for $k_s^* = 1$ (case $k_s^* = k_n^{\max}$ analog) the equidistant division of the interval

$$\left[2 \cdot \dot{V}_{sk_s^*}^{\mathrm{N,val}} - \dot{V}_{s\left\lceil \frac{k_s^{\max}}{2} \right\rceil}^{\mathrm{N,val}}, \dot{V}_{s\left\lceil \frac{k_s^{\max}}{2} \right\rceil}^{\mathrm{N,val}}\right]$$

results in the adapted discretization (Figure 4.4a). It is guaranteed that this discretization respects the initial size bounds $\dot{V}_s^{\mathrm{N,min}}$ and $\dot{V}_s^{\mathrm{N,max}}$.

Case 3 (bound) In the remaining case of $k_s^* \in \{1, k_s^{\max}\}$ and $\dot{V}_{sk_s^*}^{\mathrm{N,val}} \in \{\dot{V}_s^{\mathrm{N,min}}, \dot{V}_s^{\mathrm{N,max}}\}$ the chosen discrete point lies at a bound. Here, we assume $k_s^* = 1$ and $\dot{V}_{sk_s^*}^{\mathrm{N,val}} = \dot{V}_s^{\mathrm{N,min}}$ (other case analog). We contract the discretization, respecting the bounds $\dot{V}_s^{\mathrm{N,min}}$ and $\dot{V}_s^{\mathrm{N,max}}$. The equidistant division of the interval $[\dot{V}_s^{\mathrm{N,min}}, \dot{V}_{s\left\lceil \frac{k_s^{\max}}{2} \right\rceil}^{\mathrm{N,val}}]$ is the adapted discretization (Figure 4.4b).

Example (interval limit, bound) Figure 4.4 shows examples for the adaption of the discretization in case 2 and 3.



(a) case 2: chosen (interval limit) **(b)** case 3 (bound)

Fig. 4.4: Adaptive Discretization: (a) case 2 and (b) case 3

4.3.4 Adaptive Discretization Algorithm

The adaptive discretization algorithm is shown in Figure 4.5 as a whole. The algorithm consists of an iteration loop with a certain stop criterion, for example concerning an iteration or convergence limit. If the criterion is fulfilled, the algorithm terminates and the best MINLP solution found is output by the algorithm, otherwise, the algorithm continues with the next iteration step. Each step consists of (i) solving the discretized problem (Section 4.3.1) and (ii) solving NLP$_\ell$ for all $\ell \in L$ with parameters and bounds computed by (4.28) – (4.30) to

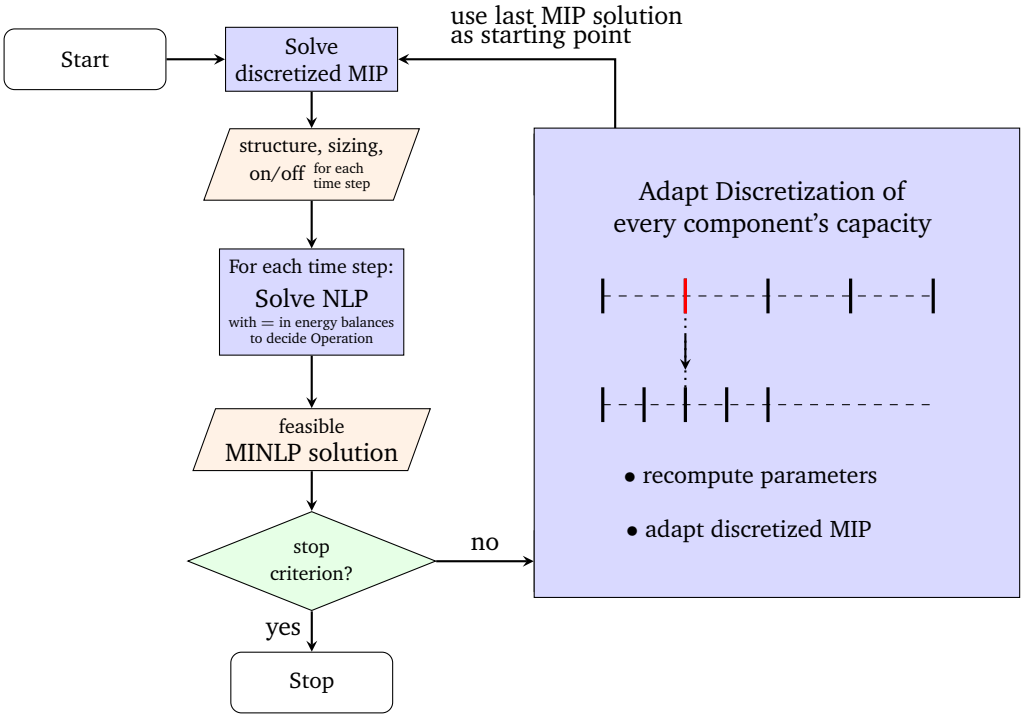


Fig. 4.5: Adaptive Discretization Algorithm

obtain a primal MINLP solution for the original problem (Section 4.3.2). After that and in the case of nontermination, (iii) the discretization is adapted as it is described in Section 4.3.3. All parameters concerning the discretization grid, including the operation discretizations $\dot{V}^{\text{val}}_{sk\ell 1} < \dot{V}^{\text{val}}_{sk\ell 2} < \ldots < \dot{V}^{\text{val}}_{sk\ell j^{\max}_{sk\ell}}$, which are based on the discrete sizes, and the formulation of the discretized problem (4.17) – (4.27) are updated. The next iteration step of the algorithm starts with solving the adapted discretized problem. Notice that the last iteration's solution of the discretized problem can be used to warm-start the discretized MIP, since the discrete decisions are still feasible in the adapted grid. This improves the performance of solving the MIP.

Remark 11 *(Alternative Approximations for the Discretized Problem)* To enable equality in the energy balances in the discretized problem, we expand the pure discretization of the operation to a piecewise linearization (Section 4.3.1). However, this is not necessary for the functionality of the proposed algorithm, since the discretized MIP is only used as an approximation of the original problem. We developed and tested other approaches for approximating the problem via discretization in addition to the discretized MIP (4.17) – (4.27). In a pure discretization, without the piecewise linearization, we can only request for at least fulfilling the energy demands. Consequently, energy excesses are possible. These excesses can occur since it is more favorable to produce electricity using CHP engines than to purchase it from the power grid. Thus, additional heat production by CHP engines can decrease operational costs of DESS. For that reason, there is more energy excess in solutions of a pure discretization than might be expected. Consequently, the approximation quality gets worse since overproduction is not allowed in the original problem. We develop two approaches to restrict the amount of energy excess in the pure discretization and to improve the approximation quality: First, by adding new and nontrivial constraints to the discretized

problem, secondly, by penalizing energy excess in the objective function. More details about these approaches are given in the Appendix in Section 4.6. It turns out that our adaptive discretization algorithm using the discretized problem with piecewise linearization of Section 4.3.1 outperforms these more sophisticated alternatives on the set of test instances (Section 4.4.1).

4.4 Computational Study and Results

In the computational study, we analyze the solution quality of our adaptive discretization algorithm (short AdaptDiscAlgo, Section 4.3) in comparison to (i) primal solutions of MINLP (Section 4.2.2) computed with BARON and to (ii) approximate solutions of piecewise linearized models following the explanations in Section 4.2.3. Furthermore, we examine the running times of all solving approaches.

Section 4.4.1 gives an overview and references of the online available considered test instances. In addition, details on the implementation of all approaches for computing MINLP solutions to synthesis of DESS are given. The computational results are presented in Section 4.4.2.

4.4.1 Problem Instances and Implementation

For the computational study on the performance of our algorithm, we derived a test-set: DESSLib (`www.math2.rwth-aachen.de/DESSLib`, Bahl et al., 2016a,b). The DESSLib contains categorized problem instances based on the original real-world example stated by Voll et al. (2013b). The categories are characterized by two dimensions, the number of considered units in the superstructure and the number of considered load cases. The category for the number of considered units is denoted by $S4, S8, S12, S16$, e.g., $S4$ corresponds to one unit for each type of equipment. The number of considered load cases is denoted by $L1, L2, L4, L6, L8, L12, L16, L24$. Each category (e.g., $S8L4$) consists of 10 instances with stochastic variations around the original demand time-series. We assign stochastic variations with latin hypercube sampling (Iman et al., 1981) and a variation of $\pm 5\%$ of the original demand. Thus, the resulting DESSLib consists of 320 problem instances. We use the DESSLib to evaluate the performance of the proposed adaptive discretization algorithm. The short notation, e.g., $S4L\{1,2\}$ denotes the set of all test instances of categories $S4L1$ and $S4L2$.

Software and Machine Our adaptive discretization algorithm (Section 4.3) was implemented in GAMS 24.4.3 (GAMS Development Corporation, 2015) using its Python-API. Computations are performed on one core of a Linux machine with 3.40GHz Intel Core i7-3770 processor and 32 GB RAM. To solve mixed-integer linear programs, i.e., discretized MIP (4.17) – (4.27) and MILP by Voll et al. (2013b) (Section 4.2.3), we use the default setting of CPLEX 12.6.1.0 (IBM, 2015). To solve (mixed-integer) nonlinear programs, i.e., MINLP (4.1) – (4.12), feasibility NLP (Section 4.3.2) and MINLP$^{\text{lin,feas}}$ (4.13) – (4.16), we use the default setting of BARON 14.4.0 (Tawarmalani and Sahinidis, 2005). BARON was selected as MINLP solver due its robustness in a preliminary study.

Discretization Grid The number of discrete sizes $k_s^{\max}$ and the number of discrete operations $j_{sk\ell}^{\max}$ in the discretized problem (Section 4.3.1) are $k_s^{\max} = 5$ and, with some exceptions, $j_{sk\ell}^{\max} = 10$. However, if the interval of possible operations $[\alpha_s^{\min}\dot{V}_{sk}^{\mathrm{N,val}}, \dot{V}_{sk}^{\mathrm{N,val}}]$ is smaller than 1800 kW, we reduce $j_{sk\ell}^{\max} \leq 10$ as much as necessary so that $\dot{V}_{sk\ell j}^{\mathrm{val,diff}} \geq 200$ kW or $j_{sk\ell}^{\max} = 2$ holds. These parameters have been determined in preliminary studies.

Limits and Stop Criterion For solving the discretized MIP (Section 4.3.1), a time limit of 300 seconds is implemented in the very first iteration of an algorithm run. For any further step, this time limit is set to 100 seconds and the last iteration's solution is used as a starting point. The time limit for solving the feasibility NLP (Section 4.3.2) is set to 100 seconds. Limits for the optimality gap are 0.1% (discretized MIP) and 0.001% (feasibility NLP). The adaptive discretization algorithm terminates, if the running time reaches the limit of one hour or the improvement of the best MINLP solution is less than 0.1% over the last two iterations.
For the benchmark MINLP (4.1) – (4.12), the same limit of one hour running time is implemented in each case. To obtain a feasible MINLP solution based on an approximate MILP solution, we solve MILP by Voll et al. (2013b) (Section 4.2.3) with a time limit of one hour and thereafter we solve MINLP$^{\mathrm{lin,feas}}$ (4.13) – (4.16) with a time limit of one hour as well.

Preprocessing on Discretization Grid Depending on the input data, particularly the demands of the load cases, some binary variables $\dot{V}_{sk}^{\mathrm{N}}$, $\dot{V}_{sk\ell j}$ can be eliminated by preprocessing. For chiller units $s \in A \cup T$, the operation variables $\dot{V}_{sk\ell j} \in \{0,1\}$ with $\dot{V}_{sk\ell j}^{\mathrm{val}} > \dot{E}_{\ell}^{\mathrm{cool}}$, i.e., supply greater than demand, will not be part of any feasible solution of the discretized problem. In analogy, for heat-producing units $s \in B \cup C$, an upper bound for $\dot{V}_{sk\ell j}^{\mathrm{val}}$ is given by the heat demand $\dot{E}_{\ell}^{\mathrm{heat}}$ plus the maximal possible heat demand of absorption chillers $s \in A$. If for indices s, k these constraints remove all discrete operation variables $\dot{V}_{sk\ell j}$, the corresponding discrete size variable $\dot{V}_{sk}^{\mathrm{N}}$ can be eliminated as well. This preprocessing on the discretization grid is quite natural, however, its effect may not be underestimated, because of the large number of binary variables in the discretized problem.

4.4.2 Computational Results

Before we analyze the robustness of our proposed algorithm compared to the two benchmarking approaches on basis of the entire set of 320 instances, we focus on one randomly chosen instance and compare the numerical solution results, i.e., DESS structure and equipment sizes, of all three considered approaches.

Table 4.1 shows the DESS structure and equipment sizes (numbers rounded) for DESSLib's instance $S8L4_8$ obtained by the solution approaches MINLP (Section 4.2.2), MINLP$^{\mathrm{lin,feas}}$ (Section 4.2.3), and AdaptDiscAlgo (Section 4.3). Table 4.1 does not contain the DESS resulting from the MILP of Voll et al. (2013b), which was the basis for the MINLP$^{\mathrm{lin,feas}}$ solution (cf. Section 4.2.3). The MILP solution differs from the MINLP$^{\mathrm{lin,feas}}$ solution just in a small increase of the boiler's sizing: from 11.45 MW to 12.02 MW. By this change, the solution becomes feasible. The three approaches mentioned in Table 4.1 lead to three different DESS structures, whereby the solution of AdaptDiscAlgo has the best objective value,

	MINLP	MINLP$^{\text{lin,feas}}$	AdaptDiscAlgo
Boiler #1	12.02 MW	11.45 MW	10.53 MW
Boiler #2	-	-	0.10 MW
CHP engine #1	3.20 MW	2.50 MW	3.20 MW
CHP engine #2	2.35 MW	2.30 MW	2.15 MW
Turbo chiller #1	7.88 MW	3.17 MW	3.48 MW
Turbo chiller #2	-	1.88 MW	1.90 MW
Absorption chiller #1	6.05 MW	6.43 MW	6.50 MW
Absorption chiller #2	-	2.43 MW	2.07 MW
Net present value	$-6.81 \cdot 10^7$	$-5.00 \cdot 10^7$	$-4.85 \cdot 10^7$

Tab. 4.1: DESS structure and equipment sizes computed by solution approaches MINLP, MINLP$^{\text{lin,feas}}$, and AdaptDiscAlgo for DESSLib's instance $S8L4_8$.

i.e., net present value. In fact, AdaptDiscAlgo's solution has, compared to the computed result of MINLP, a 28% higher net present value. With regard to MINLP$^{\text{lin,feas}}$, the presented AdaptDiscAlgo leads to a slightly, i.e., 3%, better solution. Looking at the DESS structures it turns out that using a second compressor chiller and a second absorption chiller is profitable in this problem instance. Furthermore, the total size of the boilers decrease, while the net present value of the three DESS systems increases.

In the further course of the computational results we evaluate the performance of AdaptDiscAlgo regarding objective value and computation times on the basis of the entire set of 320 problem instances. Among other things, we will see that the instance chosen for Table 4.1 is a good representative, in the sense that the solutions of AdaptDiscAlgo outperform the two benchmarking approaches.

For evaluating the quality of a feasible solution of a problem, we consider the *primal gap* to the objective value of a given reference solution, i.e., an optimal or other known solution.

Definition 12 *The primal gap of a feasible solution x with objective value $f(x)$ and a reference solution $x^\star$ with objective value $f(x^\star)$ is, except for trivial cases, defined by*

$$gap_p(x, x^\star) := \frac{f(x) - f(x^\star)}{|f(x^\star)|}.$$

We compute averages over parts of the test instances using the *shifted geometric mean*, which is customary in computational optimization, see (Achterberg, 2007).

Definition 13 *The shifted geometric mean of numbers $a_1, \ldots, a_k \in \mathbb{R}$ and a shift $\zeta \in \mathbb{R}_+$ with $(a_i + \zeta) > 0$, $i = 1, \ldots, k$ is defined by*

$$\gamma_\zeta(a_1, \ldots, a_k) := \left(\prod_{i=1}^{k} (a_i + \zeta) \right)^{\frac{1}{k}} - \zeta. \tag{4.31}$$

We use a shift of $\zeta = 100$ for time in seconds and values in percent, e.g., primal-dual bound, and a shift of $\zeta = 10$ for number of iterations.

The computational results of the solution quality of the benchmark MINLP and AdaptDiscAlgo is represented by a heatmap in Figure 4.6. For every test instance category, the average of relative improvement of the best solution of AdaptDiscAlgo in comparison to the best solution of MINLP (4.1) – (4.12) is indicated by the percentage and coloring of the heatmap square. To put it briefly, the greener, the better the solution quality of AdaptDiscAlgo compared to MINLP. The averages are calculated with the best MINLP solution as reference solution (Definition 12) and only instances are considered where both approaches provide an MINLP solution. Additionally and enclosed in brackets, the number of test instances (max. ten per category) is given, for which AdaptDiscAlgo (right number) respectively MINLP (left) computes an MINLP solution within the time limit.

For the smallest test instances, MINLP was able to solve every test instance of categories $S4L\{1, 2, 4, 6\}$ optimally within the time limit. For 63% (202 out of 320) of all considered test instances, at least a feasible solution was computed by MINLP, in all other cases the time limit was reached without any primal solution. In contrast, AdaptDiscAlgo was able to

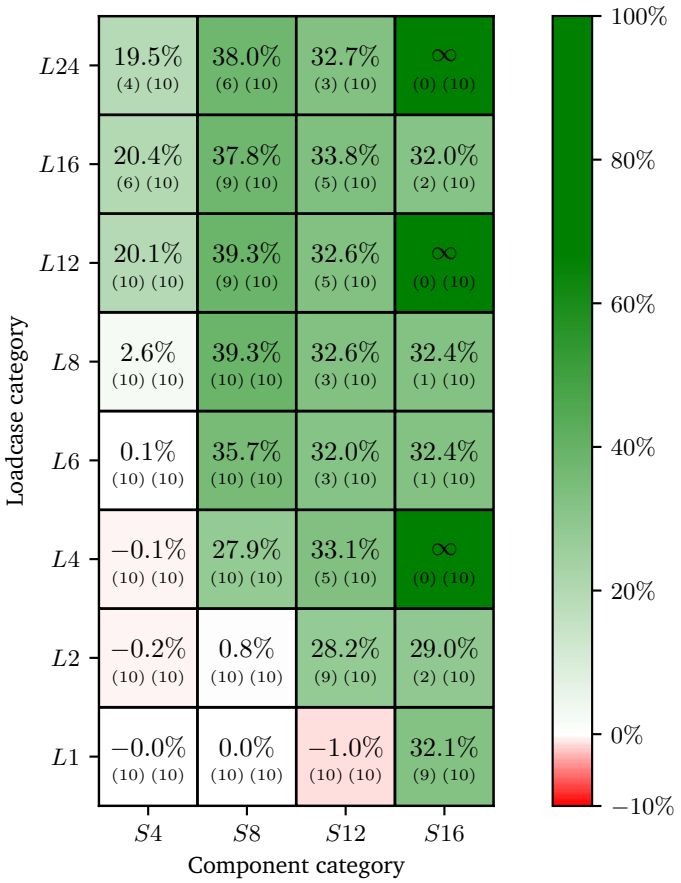


Fig. 4.6: Heatmap on the improvement of solution quality of AdaptDiscAlgo in relation to MINLP (4.1) – (4.12); averaged for each test instance category. In brackets: number of test instances (max. 10 per category), for which MINLP (left) respectively AdaptDiscAlgo (right) computes at least one MINLP solution in the time limit.

compute an MINLP feasible solution for every single test instance. Of course, the proposed algorithm can not ensure optimality of its solutions. However, AdaptDiscAlgo provides near-optimal solutions for test instances solved optimally by MINLP. Irritatingly, in category $S4L6$, AdaptDiscAlgo computes on an average a 0.1%-better solution than a (according to BARON) globally *optimal* solution of MINLP. This is due to the fact that BARON cuts off optimal solutions during the solution process for some of these instances. Unfortunately, this is not unusual in computational (nonlinear) optimization due to limited machine accuracy. All in all, except for the smallest instance categories, AdaptDiscAlgo is able to compute up to 40% better MINLP solutions than MINLP.

All primal bounds, dual bounds and computation times of the MINLP and AdaptDiscAlgo of the computations executed for this work are online available at www.math2.rwth-aachen.de/DESSLib (Bahl et al., 2016b).

Since common DESS-solving approaches consist of piecewise linearized models (Section 4.1), we compare approximate solutions of such a model with MINLP solutions of the proposed AdaptDiscAlgo following the explanations in Section 4.2.3. The structure y_s^* and sizing decisions $V_s^{\mathrm{N}*}$ of MILP solutions are in 85%, i.e., 273 out of 320 test instances, not feasible in



Fig. 4.7: Heatmap on the improvement of solution quality of AdaptDiscAlgo in relation to $\mathrm{MINLP}^{\mathrm{lin,feas}}$; averaged for each test instance category. Note, the color legend in this figure has a different scale than in Figure 4.6.

the original MINLP problem. If it was feasible, it was a test instance of small-sized category $S4$. For this reason, we consult MINLP$^{\text{lin,feas}}$ (4.13) – (4.16) to compute a MINLP-feasible solution *close to* the approximate MILP solution and evaluate it with the original objective (4.1). The comparison of the solution quality of MINLP$^{\text{lin,feas}}$ and AdaptDiscAlgo is shown by a heatmap in Figure 4.7. The averages are calculated with MINLP$^{\text{lin,feas}}$ solutions as reference solutions (Definition 12). In all categories, AdaptDiscAlgo provides comparably good or slightly better solutions as post-processed solutions of the piecewise-linearized approach.

The running times of all approaches are shown in Figure 4.8. Since only instances of categories $S4L\{1,2,4,6\}$ are solved optimally by MINLP, for all other test instances, the running time reaches the limit of one hour. The piecewise linearized model (MILP) runs for most instances less than one hour. However, to obtain an MINLP-feasible solution through MINLP$^{\text{lin,feas}}$, this whole approach runs up to two hours. In comparison, the proposed AdaptDiscAlgo terminates generally after a fraction of an hour and thus outperforms the compared approaches in terms of solution quality as well as running time, except for the very smallest test instances.

The running time of AdaptDiscAlgo is split up over the parts of the algorithm as follows: On average 93% of the running time is used for solving the discretized MIP (Section 4.3.1) and 5 iterations are passed on an average until the stop criterion of convergence is satisfied. For all considered test instances, the feasibility NLP (Section 4.3.2) was feasible in every single iteration. This was not the case for the alternative approaches of the discretized problem which are briefly mentioned in Section 4.3.4.

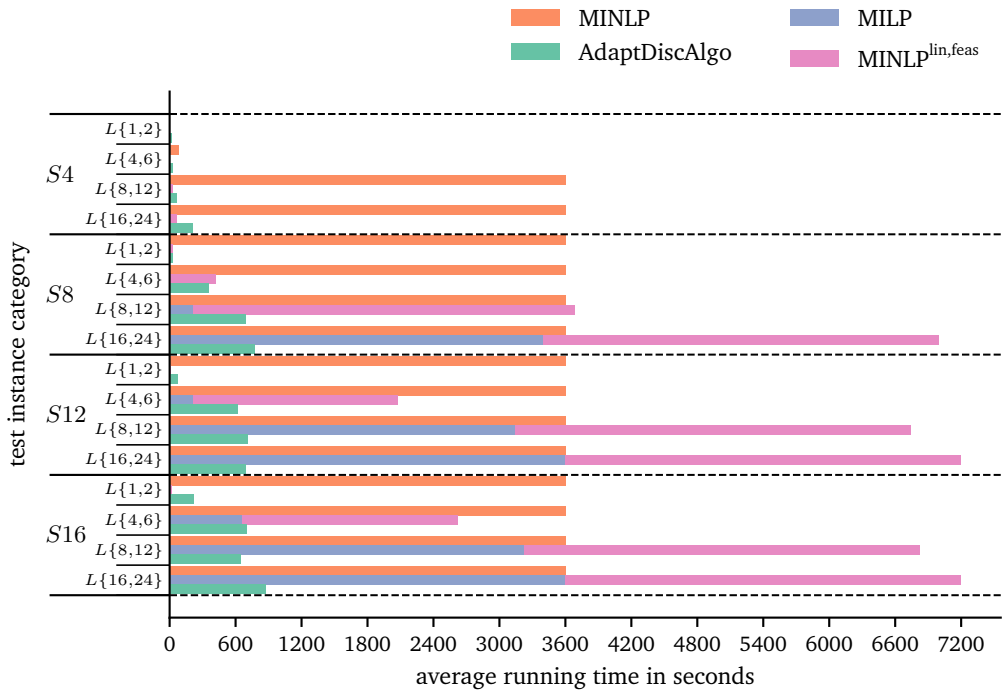


Fig. 4.8: Average running times of MINLP, MILP, MINLP$^{\text{lin,feas}}$, and AdaptDiscAlgo.

4.5 Summary and Outlook

The superstructure-based synthesis of decentralized energy supply systems can be formulated as a mixed-integer nonlinear program. By including, e.g., nonlinear part-load performances, investment costs, and strict energy balances, this optimization problem is unavoidably nonconvex. In this paper, we do not circumvent this issue via approximating the problem by linearizing the performance and investment cost models of all considered types of equipment. Such approximate solutions from linearized problems are not necessarily feasible for the original nonlinear problem. In this paper, we set the focus on computing solutions which are feasible for the nonlinear synthesis problem. Since global MINLP solvers, e.g., BARON, have difficulties to provide primal solutions for real-world-based test instances, we propose a problem-specific solution approach for the nonlinear synthesis of DESS. This optimization-based algorithm consists of a discretized and linearly formulated version of the synthesis problem, whose underlying discretization grid is iteratively adapted. The resulting approximate problem is of such a nature that solution-specific decisions are also feasible in the original nonlinear problem and by solving a decomposable NLP, this leads to MINLP solutions. A computational study based on a set of test instances obtained from real industrial data shows that the proposed adaptive discretization algorithm computes better MINLP solutions in less computation times than state-of-the-art solvers. Thus, the proposed algorithm provides an efficient solution method to the synthesis of decentralized energy supply systems.

In future work, one should expand the adaptive discretization algorithm concerning methods to compute dual bounds for the MINLP to estimate the optimality gap of the algorithm's primal solutions. The (mostly very weak) dual bounds provided by BARON do not contribute meaningful information.

A mathematically feasible or even optimal solution is usually only an approximation of a real-world implementation, since a model never represents the real problem perfectly. Real world decisions might be influenced by constraints not represented in the model, e.g., (missing) maintenance knowledge in the company for specific technologies. In (Voll et al., 2013a) and (Hennen et al., 2016) we show that several near-optimal solution alternatives exist. Analyzing these near-optimal solutions allows to derive real-world decision options. Since the proposed AdaptDiscAlgo efficiently provides feasible solutions of the nonlinear synthesis problem, in future work the algorithm could be expanded to efficiently generate many near-optimal solution alternatives.

To identify the suitable superstructure, one could complement the proposed algorithm with the successive superstructure expansion method of Voll et al. (2013b).

The application of the proposed discretization algorithm to other hard to solve synthesis problems seems quite promising.

4.6 Appendix: Variants of the Discretized Problem

We pick up Remark 11 stated in Section 4.3.4 and elaborate on variants of the discretized problem.

Recall Section 4.3.1: The discretization of all continuous variables with nonlinear dependencies of the original MINLP (4.1) – (4.12) involves the unit's size and operation. In the case of unit operation, a pure discretization with binary variables $\dot{V}_{sk\ell j}$ and corresponding values $\dot{V}^{\text{val}}_{sk\ell j}$ is extended by continuous variables $\dot{V}^{\text{cont}}_{sk\ell j} \geq 0$ with $\dot{V}^{\text{cont}}_{sk\ell j} \leq \dot{V}^{\text{val}}_{sk\ell j+1} - \dot{V}^{\text{val}}_{sk\ell j} =: \dot{V}^{\text{val,diff}}_{sk\ell j}$. These additional continuous variables, introduced for each line segment between $\dot{V}^{\text{val}}_{sk\ell j}$ and $\dot{V}^{\text{val}}_{sk\ell j+1}$, enables us to call for *equality* in the energy balances (4.18) – (4.20) in the discretized approximation.

However, expanding the pure discretization of the operation to a piecewise linearization is not necessary for the functionality of the proposed adaptive discretization algorithm. Other approaches for approximating the original problem via discretization are possible.

Pure Discretization of Operation

In anology to the discretized MIP (4.17) – (4.27) stated in Section 4.3.1 the MIP based on pure discretization of the operation reads as follows.

$$\begin{aligned}\max\ \text{APVF}(i,\gamma^{\text{CF}}) \cdot \Bigg[\sum_{\ell \in L} \Delta_\ell \cdot \Big(& p^{\text{el,sell}} \cdot \dot{V}^{\text{el,sell}}_\ell - p^{\text{el,buy}} \cdot \dot{U}^{\text{el,buy}}_\ell \\ & - p^{\text{gas,buy}} \cdot \sum_{s \in B \cup C} \sum_{k,j} \dot{U}^{\text{val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} \Big) \\ & - \sum_{s,k} m_s \cdot I^{\text{val}}_{sk} \cdot \dot{V}^{\text{N}}_{sk} \Bigg] - \sum_{s,k} I^{\text{val}}_{sk} \cdot \dot{V}^{\text{N}}_{sk} \end{aligned} \tag{4.32}$$

$$\text{s.t.} \sum_{s \in B \cup C} \sum_{k,j} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} \geq \dot{E}^{\text{heat}}_\ell + \sum_{s \in A} \sum_{k,j} \dot{U}^{\text{val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} \qquad \forall\, \ell \in L \tag{4.33}$$

$$\sum_{s \in A \cup T} \sum_{k,l} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} \geq \dot{E}^{\text{cool}}_\ell \qquad \forall\, \ell \in L \tag{4.34}$$

$$\dot{U}^{\text{el,buy}}_\ell + \sum_{s \in C} \sum_{k,j} \dot{V}^{\text{el,val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} = \dot{E}^{\text{el}}_\ell + \dot{V}^{\text{el,sell}}_\ell + \sum_{s \in T} \sum_{k,j} \dot{U}^{\text{val}}_{sk\ell j} \cdot \dot{V}_{sk\ell j} \qquad \forall\, \ell \in L \tag{4.35}$$

$$\sum_k \dot{V}^{\text{N}}_{sk} \leq 1 \qquad \forall\, s \in S \tag{4.36}$$

$$\sum_j \dot{V}_{sk\ell j} \leq \dot{V}^{\text{N}}_{sk} \qquad \forall\, s,k,\ell \tag{4.37}$$

$$\dot{V}^{\text{N}}_{sk} \in \{0,1\} \qquad \forall\, s,k \tag{4.38}$$

$$\dot{V}_{sk\ell j} \in \{0,1\} \qquad \forall\, s,k,\ell,j \tag{4.39}$$

$$\dot{U}^{\text{el,buy}}_\ell, \dot{V}^{\text{el,sell}}_\ell \geq 0 \qquad \forall\, \ell \in L \tag{4.40}$$

Due to the pure discretization, we can only request for at least fulfilling the energy demand of heat and cool, cf. $\geq$-sign in Equations (4.33) and (4.34). Consequently, energy excesses in a solution are very likely. Equality in the energy balance of electricity (4.35) is still possible due to the market access through continuous variables $\dot{U}_\ell^{\text{el,buy}}, \dot{V}_\ell^{\text{el,sell}} \geq 0$. The idea is that in spite of (hopefully small) energy excesses, the subsequent post processing via NLP (Section 4.3.2) computes an MINLP feasible solution. Thus, the adaptive discretization algorithm (Figure 4.5) can also be applied with discretized MIP (4.32) – (4.40) presented here instead of (4.17) – (4.27).

Excess in Energy Generation

It turns out that there are realistic parameter configurations for which the excess of energy in an optimal solution of the pure discretization (4.32) – (4.40) is greater than can be justified by the density of the discretization. That is, the excess may be greater than the discretization steps. The reason for this is that it can be more favorable to produce electricity using CHP engines than to purchase it from the power grid. Thus, additional heat production by CHP engines can decrease operational costs of DESS (Example 14).

Example 14 Consider an existing energy system with an absorption chiller AC_1, a turbo-driven compressor chiller TC_1, and two CHP engines CHP_1, CHP_2 of fixed size each and a load case with demand parameters

$$\dot{E}^{\text{heat}} = 2400, \quad \dot{E}^{\text{cool}} = 1170, \quad \dot{E}^{\text{el}} = 2320.$$

Assume, all conversion units are operating in this load case. Considering the original MINLP with one load case and fixed $y, \dot{V}^{\text{N}}, \delta$ as given leads to an NLP and following optimal solution:

- objective value: -5154119
- $\dot{V}_{AC_1} = 50$, $\dot{V}_{TC_1} = 1120$, $\dot{V}_{CHP_1} = 2000$, $\dot{V}_{CHP_2} = 474.626$, $\dot{U}^{\text{el,buy}} = 75.271$

Now we change $=$ into $\geq$ in the energy balances of heat (4.2) and cold (4.3), i.e., we only request for at least fulfilling the demands. This leads to following optimal solution (changed values are underlined):

- objective value: $\underline{-5116246}$ (i.e., an improvement of 37873)
- $\dot{V}_{AC_1} = 50$, $\dot{V}_{TC_1} = 1120$, $\dot{V}_{CHP_1} = 2000$, $\dot{V}_{CHP_2} = \underline{543.413}$, $\dot{U}^{\text{el,buy}} = \underline{0}$

Here, electricity is completely generated by the system itself, as this is cheaper than buying it. The electricity-covering operation point of the CHP engines generate more heat than required.

As a consequence, there can be more energy excess in solutions on the basis of a pure discretization than expected. This can lead to the fact that the approximation quality gets worse since overproduction is not allowed in the original problem. We developed two approaches to restrict the amount of energy excess in the pure discretization and therefore to improve the approximation quality. First, it is an option to penalize energy excess in the

objective function of the discretized problem. On the basis of the parameters, an upper bound for the profit of one heat unit can be estimated. It is important to penalize also cold overproduction in a comparable way, because otherwise heat excess is converted into cold. Our second approach restricts energy excess by adding new and nontrivial constraints to the discretized problem based on the applied discretization. We want to discuss this aspect in detail.

Restricting Energy Excess via additional Constraints

The following explanations and proofs are carried out exemplarily for the cooling demand. However, they can be easily adopted for other types of demand.

Example 15 To illustrate our results, consider the operation example depicted in Figure 4.9. Two chillers with capacity 2500 and 4000, respectively, are available to meet a cooling requirement of 2200. The orange area correspond to all feasible operation configuration. Note, also parts of the axes are orange since off-status of each chiller is also possible. The red parts as subset of the orange ones describe the feasible operation points meeting the given demand with equality. Furthermore, a chosen discretization of the component's operation is given by the black, blue, and green dots. For example, chiller 1 has discrete operations for the off-status, 800 output, 2400 output, and 4000 output. All dots above the demand line (green and blue dots) are feasible for the demand considering the pure discretization and $\geq$-energy balances. The three green dots correspond to the feasible operation configurations that lead to minimal energy excess – we name these solutions as *desired* ones.

We now develop constraints that, added to the discretized MIP, cut off blue dots but none of the green ones.

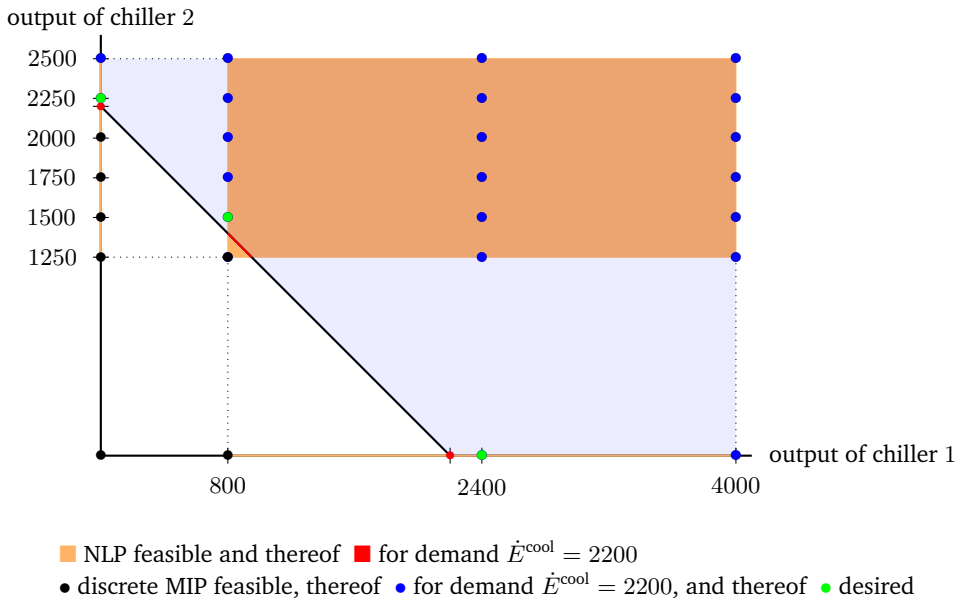


Fig. 4.9: Operation of two chillers to convert a cold demand: Feasible region/points for original problem and purely discretized problem.

Definition 16 *Let $\dot{V}^\star = (\dot{V}^\star_{sk\ell j})$ with $V^\star_{sk\ell j} \in \{0,1\}$ for indices $s \in S$, $k = 1,\dots,k_n^{\max}$, $\ell \in L$, $j = 1,\dots,j_{sk\ell}^{\max}$ be a* discretized solution *if $\dot{V}^\star$ can be expanded to a feasible solution for the discretized problem* (4.32) – (4.40).

By means of a discrete solution (if feasible) all other decisions of the discretized MIP can be derived to get a feasible solution for the discretized problem.

Definition 17 *Given a discretized solution $\dot{V}^\star$ and an index $s \in S$. The value $k_s^\star \in \{0,1,\dots,k_s^{\max}\}$ defined as*

$$k_s^\star := \max\left\{\sum_{k=1}^{k_s^{\max}}\sum_{j=1}^{j_{sk\ell}^{\max}} k\cdot\dot{V}^\star_{sk\ell j} : \ell \in L\right\}$$

denotes the index of discrete size selected. *Additionally, given a load case $\ell \in L$. The value $j^\star_{s\ell} \in \{0,1,\dots,\max\{j_{sk\ell}^{\max} : k = 1,\dots,k_s^{\max}\}\}$ defined as*

$$j^\star_{s\ell} := \sum_{k=1}^{k_s^{\max}}\sum_{l=1}^{l_{sk\ell}^{\max}} l\cdot\dot{V}^\star_{sk\ell j}$$

denotes the index of the discrete operation selected in load case ℓ.

We now characterize what desired discrete solutions are (cf. green dots in Figure 4.9). In order to be precise with this, for $j = 0$ we define $\dot{V}^{\text{val}}_{sk\ell j} := 0$.

Definition 18 *A discretized solution $\dot{V}^\star = (\dot{V}^\star_{sk\ell j})$ is called a* desired discretized solution w.r.t the cooling demand $\dot{E}^{cool} = (\dot{E}^{cool}_\ell)$, $\dot{E}^{cool}_\ell > 0\ \forall \ell \in L$ *if (∗), (∗∗), and (∗∗∗) hold for every $\ell \in L$:*

$$\sum_{\substack{s\in A\dot{\cup}T\\k,j}} \dot{V}^{val}_{sk\ell j}\cdot\dot{V}^\star_{sk\ell j} \geq \dot{E}^{cool}_\ell \tag{$*$}$$

$$\sum_{\substack{s\in A\dot{\cup}T\\k,j}} \dot{V}^{val}_{sk\ell j}\cdot\dot{V}^\star_{sk\ell j} > \dot{E}^{cool}_\ell \implies \exists s \in A\dot{\cup}T \text{ such that } j^\star_{s\ell} > 1 \tag{$**$}$$

$$\forall\ \hat{s} \in A\dot{\cup}T \text{ with } j^\star_{\hat{s}\ell} \neq 0 \text{ holds } \Big(\sum_{\substack{s\in A\dot{\cup}T\\s\neq\hat{s}\\k,j}} \dot{V}^{val}_{sk\ell j}\cdot\dot{V}^\star_{sk\ell j}\Big) + \dot{V}^{val}_{\hat{s}k^\star_{\hat{s}}\ell j^\star_{\hat{s}\ell}-1}\cdot\dot{V}^\star_{\hat{s}k^\star_{\hat{s}}\ell j^\star_{\hat{s}\ell}} < \dot{E}^{cool}_\ell \tag{$***$}$$

The conditions stated in Definition 18 ensure that $(*)$ the discrete solution fulfills the demand, $(**)$ the nonlinear δ_{nt}-decisions, which are implied by a discretized solution $V^\star$, can be expanded to a feasible solution for the nonlinear problem, and $(***)$ the discrete solution fulfills the demand with minimal excess. In Figure 4.9 the desired solutions are represented by green dots.

The constraints to restrict the energy excess are proposed in Theorems 19 and 20. Figure 4.10 shows their application in the example introduced in Figure 4.9.

Theorem 19 *Let $\dot{V}^\star$ be a desired discretized solution w.r.t the cooling demand then the following holds for every $\ell \in L$:*

$$\sum_{\substack{s \in A\dot{\cup}T \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} \leq E^{\text{cool}}_\ell + M^{\text{cool}}_\ell$$

with $M^{\text{cool}}_\ell := \max\{\dot{V}^{\text{val}}_{sk\ell j} - \dot{V}^{\text{val}}_{sk\ell j-1} \mid s \in A\dot{\cup}T, k = 1, \ldots, k^{\max}_s, j = 2, 3, \ldots, j^{\max}_{sk\ell}\}$ (Note, index $j = 1$ is not considered.).

Proof We distinguish two cases: (1) $\exists\, \tilde{s} \in A\dot{\cup}T : j^\star_{\tilde{s}\ell} > 1$ and (2) $\forall s \in A\dot{\cup}T : j^\star_{s\ell} \in \{0, 1\}$.
Case (1): It exists $\tilde{s} \in A\dot{\cup}T$ with $l^\star_{\tilde{s}\ell} > 1$. Then $(***)$ implies

$$\sum_{\substack{s \in A\dot{\cup}T \\ s \neq \tilde{s} \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} < \dot{E}^{\text{cool}}_\ell - \dot{V}^{\text{val}}_{\tilde{s}k^\star_{\tilde{s}}\ell j^\star_{\tilde{s}\ell}-1}$$

and after adding $\dot{V}^{\text{val}}_{\tilde{s}k^\star_{\tilde{s}}\ell j^\star_{s\ell}}$ on both sides it follows:

$$\sum_{\substack{s \in A\dot{\cup}T \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} < \dot{E}^{\text{cool}}_\ell + \left(\dot{V}^{\text{val}}_{\tilde{s}k^\star_{\tilde{s}}\ell j^\star_{\tilde{s}\ell}} - \dot{V}^{\text{val}}_{\tilde{s}k^\star_{\tilde{s}}\ell j^\star_{\tilde{s}\ell}-1}\right) \overset{\text{Def.}}{\underset{M^{\text{cool}}_\ell}{\leq}} \dot{E}^{\text{cool}}_\ell + M^{\text{cool}}_\ell$$

Case (2): For every $s \in A\dot{\cup}T$ it holds $j^\star_{s\ell} \in \{0, 1\}$. Then $(*)$ and $(**)$ imply

$$\sum_{\substack{s \in A\dot{\cup}T \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} \underset{(**)}{\overset{(*)}{=}} \dot{E}^{\text{cool}}_\ell \overset{M^{\text{cool}}_\ell \geq 0}{\leq} \dot{E}^{\text{cool}}_\ell + M^{\text{cool}}_\ell.$$

■

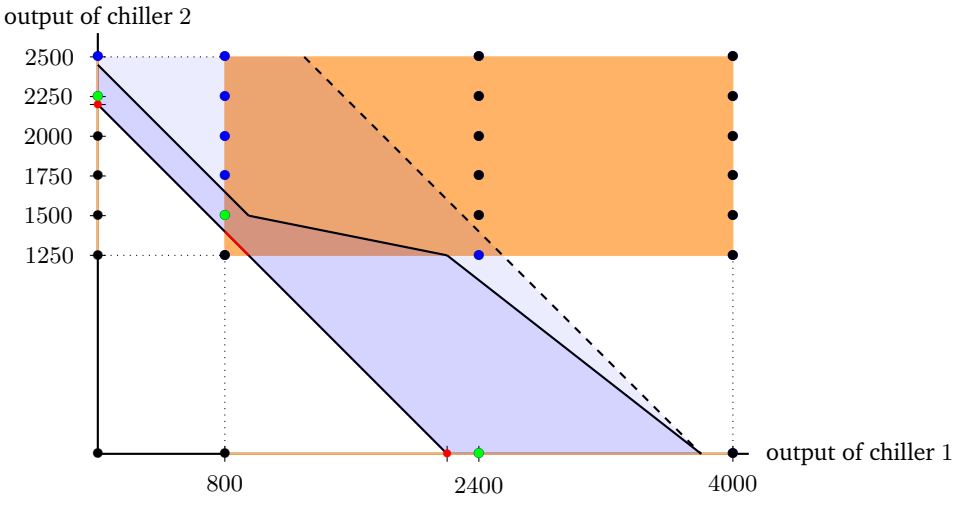


Fig. 4.10: Additional constraints to restrict energy excess: Constraint of Theorem 19 (dashed) and improved constraint of Theorem 20 (Please note that the space of the variables of the constraints does not correspond to the two-dimensional space shown here. The figure shown here is intended to visualize the effect of the developed constraints.). See Figure 4.9 for a legend.

The constraints given in Theorem 19 cut off discrete solutions but none of the desired ones. However, this set of constraints can be tightened and thus the excess further restricted.

Theorem 20 *Let $\dot{V}^\star$ be a desired discretized solution w.r.t the cooling demand then the following holds for every $\ell \in L$ and every $\hat{s} \in A\dot{\cup}T$:*

$$\sum_{\substack{s \in A\dot{\cup}T \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} \leq \dot{E}^{\text{cool}}_\ell + \sum_{k,j} \left(\dot{V}^{\text{val}}_{\hat{s}k\ell j} - \dot{V}^{\text{val}}_{\hat{s}k\ell j-1} \right) \cdot \dot{V}^\star_{\hat{s}k\ell j} + M^{\text{cool}}_\ell \cdot (1 - \sum_{k,j} V^\star_{\hat{s}k\ell j})$$

with (again) $M^{\text{cool}}_\ell := \max\{\dot{V}^{\text{val}}_{sk\ell j} - \dot{V}^{\text{val}}_{sk\ell j-1} \mid s \in A\dot{\cup}T, k = 1, \ldots, k^{\max}_s, j = 2, 3, \ldots, j^{\max}_{sk\ell}\}$.

Proof The inequality to be proven is equivalent to

$$\sum_{\substack{s \in A\dot{\cup}T \\ s \neq \hat{s} \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} + \sum_{k,j} \left(\dot{V}^{\text{val}}_{\hat{s}k\ell j-1} + M^{\text{cool}}_\ell \right) \cdot \dot{V}^\star_{\hat{s}k\ell j} \leq \dot{E}^{\text{cool}}_\ell + M^{\text{cool}}_\ell. \tag{4.41}$$

We consider three cases: (a) $j^\star_{\hat{s}\ell} = 0$, (b) $j^\star_{\hat{s}\ell} = 1$, and (c) $j^\star_{\hat{s}\ell} > 1$.
Case (a): Let $\hat{s} \in A\dot{\cup}T$ be such that $j^\star_{\hat{s}\ell} = 0$ holds. In this case Inequality (4.41), which has to be shown, states

$$\sum_{\substack{n \in A\dot{\cup}T \\ k,l}} V^{\text{val}}_{nktl} \cdot V^\star_{nktl} \overset{l^\star_{\hat{n}t}=0}{=} \sum_{\substack{n \in A\dot{\cup}T \\ n \neq \hat{n} \\ k,l}} V^{\text{val}}_{nktl} \cdot V^\star_{nktl} \leq E^{\text{cool}}_t + M^{\text{cool}}_t. \tag{4.42}$$

This holds as proven in Theorem 19.
Case (b): Let $\hat{s} \in A\dot{\cup}T$ be such that $j^\star_{\hat{s}\ell} = 1$ holds. In this case Inequality (4.41), which has to be shown, states

$$\sum_{\substack{s \in A\dot{\cup}T \\ s \neq \hat{s} \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} + M^{\text{cool}}_\ell \leq \dot{E}^{\text{cool}}_\ell + M^{\text{cool}}_\ell. \tag{4.43}$$

Condition $(***)$ implies this Inequality (4.43) after adding M^{cool}_t on both sides.
Case (c): Let $\hat{s} \in A\dot{\cup}T$ be such that $j^\star_{\hat{s}\ell} > 1$ holds. In this case Inequality (4.41), which has to be shown, states

$$\sum_{\substack{s \in A\dot{\cup}T \\ s \neq \hat{s} \\ k,j}} \dot{V}^{\text{val}}_{sk\ell j} \cdot \dot{V}^\star_{sk\ell j} + \dot{V}^{\text{val}}_{\hat{s}k^\star_{\hat{s}}\ell j^\star_{\hat{s}\ell}-1} \leq \dot{E}^{\text{cool}}_\ell \tag{4.44}$$

and this follows directly from condition $(***)$. ■

Applying additional constraints of Theorem 20 in the Example 15 leads to the fact that only desired solution remain feasible in the discretized MIP.

However, it turns out that our adaptive discretization algorithm using the discretized problem with piecewise linearization of Section 4.3.1 outperforms these more sophisticated alternatives on the considered set of test instances (Section 4.4.1).

4.7 Appendix: Economic Parameters and Equipment Models

The economic parameters for the objective function, i.e., net present value, are taken from Voll et al., 2013b and listed in Table 4.2. We list parameters of the considered types of equipment in Table 4.3.

$p^{\text{el,buy}}$	$p^{\text{el,sell}}$	$p^{\text{gas,buy}}$	i	γ^{CF}
0.16 ct/kWh	0.10 ct/kWh	0.06 ct/kWh	0.08	10 a

Tab. 4.2: Economic parameters of DESS synthesis problem

	$\dot{V}_s^{\text{N,min}}$	$\dot{V}_s^{\text{N,max}}$	m_s	α_s^{min}
Boiler $s \in B$	0.1 MW	14 MW	1.5	0.2
CHP engine $s \in C$	0.5 MW	3.2 MW	10	0.5
Absorption chiller $s \in A$	0.05 MW	6.5 MW	1	0.2
Turbo chiller $s \in T$	0.4 MW	10 MW	4	0.2

Tab. 4.3: Size ranges, maintenance cost factors, and minimum part-load factors of considered types of equipment.

We state the nonlinear models for part-load operation and investment cost curves used in this paper below. The part-load performance of CHP units is based on measured data-points for several existing units. Moreover we assume that the part-load operation is not depending on the size of equipment, thus scaling to a normalized output power is possible. The part-load efficiency for boilers and absorption chillers is modeled in analogy to Fabrizio (2008). The part-load performance behavior is modeled in analogy to Fabrizio (2008) and additional correspondence with turbo compression manufacturers. The nominal efficiency of the CHP engines was taken from (ASUE, 2011). Maintenance-cost is based on IUTA, 2002, the investment cost curves consider are composed on information from (IUTA, 2002) and databases of industrial partners.

Part-load performance: (4.45) – (4.49)

$s \in B$ (Boiler)

$$\dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) = \frac{1}{\eta^{\text{N,B}}} \left(C_1^{\text{B}} \cdot \frac{\dot{V}_{s\ell}^2}{\dot{V}_s^{\text{N}}} + C_2^{\text{B}} \cdot \dot{V}_{s\ell} + C_3^{\text{B}} \cdot \dot{V}_s^{\text{N}} \right) \tag{4.45}$$
$$\eta^{\text{N,B}} = 0.9,\ C_1^{\text{B}} = 0.1021,\ C_2^{\text{B}} = 0.8355,\ C_3^{\text{B}} = 0.0666$$

$s \in A$ (Absorption chiller)

$$\dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\text{N}}) = \frac{1}{\text{COP}^{\text{N,A}}} \left(C_1^{\text{A}} \cdot \frac{\dot{V}_{s\ell}^2}{\dot{V}_s^{\text{N}}} + C_2^{\text{A}} \cdot \dot{V}_{s\ell} + C_3^{\text{A}} \cdot \dot{V}_s^{\text{N}} \right) \tag{4.46}$$
$$\text{COP}^{\text{N,A}} = 0.67,\ C_1^{\text{A}} = 0.8333,\ C_2^{\text{A}} = -0.0833,\ C_3^{\text{A}} = 0.25$$

$s \in T$ (Turbo chiller)

$$\dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\mathrm{N}}) = \frac{1}{\mathrm{COP}^{\mathrm{N,T}}} \left(C_1^{\mathrm{T}} \cdot \frac{\dot{V}_{s\ell}^2}{\dot{V}_s^{\mathrm{N}}} + C_2^{\mathrm{T}} \cdot \dot{V}_{s\ell} + C_3^{\mathrm{T}} \cdot \dot{V}_s^{\mathrm{N}} \right) \tag{4.47}$$

$$\mathrm{COP}^{\mathrm{N,T}} = 5.54,\ C_1^{\mathrm{T}} = 0.8119,\ C_2^{\mathrm{T}} = -0.1688,\ C_3^{\mathrm{T}} = 0.3392$$

$s \in C$ (CHP engine)

$$\dot{U}_s(\dot{V}_{s\ell}, \dot{V}_s^{\mathrm{N}}) = C_1^{\mathrm{C}} + C_2^{\mathrm{C}} \cdot \frac{\dot{V}_{s\ell}}{\dot{V}_s^{\mathrm{N}}} + C_3^{\mathrm{C}} \cdot \dot{V}_s^{\mathrm{N}} + C_4^{\mathrm{C}} \cdot \left(\frac{\dot{V}_{s\ell}}{\dot{V}_s^{\mathrm{N}}} \right)^2 + C_5^{\mathrm{C}} \cdot \dot{V}_{s\ell} + C_6^{\mathrm{C}} \cdot \left(\dot{V}_s^{\mathrm{N}} \right)^2 \tag{4.48}$$

$$C_1^{\mathrm{C}} = 550.3,\ C_2^{\mathrm{C}} = -1328,\ C_3^{\mathrm{C}} = -0.4537,$$
$$C_4^{\mathrm{C}} = 668.3,\ C_5^{\mathrm{C}} = 2.649,\ C_6^{\mathrm{C}} = 9.571e-05$$

$$\dot{V}_s^{\mathrm{el}}(\dot{V}_{s\ell}, \dot{V}_s^{\mathrm{N}}) = C_7^{\mathrm{C}} + C_8^{\mathrm{C}} \cdot \frac{\dot{V}_{s\ell}}{\dot{V}_s^{\mathrm{N}}} + C_9^{\mathrm{C}} \cdot \dot{V}_s^{\mathrm{N}} + C_{10}^{\mathrm{C}} \cdot \left(\frac{\dot{V}_{s\ell}}{\dot{V}_s^{\mathrm{N}}} \right)^2 + C_{11}^{\mathrm{C}} \cdot \dot{V}_{s\ell} + C_{12}^{\mathrm{C}} \cdot \left(\dot{V}_s^{\mathrm{N}} \right)^2 \tag{4.49}$$

$$C_7^{\mathrm{C}} = 518.8,\ C_8^{\mathrm{C}} = -1203,\ C_9^{\mathrm{C}} = -0.5361,$$
$$C_{10}^{\mathrm{C}} = 579.3,\ C_{11}^{\mathrm{C}} = 1.464,\ C_{12}^{\mathrm{C}} = 7.728e-05$$

Investment cost: (4.50) – (4.53)

$s \in B$ (Boiler)

$$I(\dot{V}_s^{\mathrm{N}}) = 1.85484 \cdot \left[\left(11418.6 + 64.115 \cdot (\dot{V}_s^{\mathrm{N}})^{0.7978} \right) \cdot 1.046 \cdot \left(1.0917 - 1.1921 \cdot 10^{-6} \cdot \dot{V}_s^{\mathrm{N}} \right) \right] \tag{4.50}$$

$s \in A$ (Absorption chiller)

$$I(\dot{V}_s^{\mathrm{N}}) = 0.50401 \cdot 17554,18 \cdot \dot{V}_s^{\mathrm{N}\ 0.4345} \tag{4.51}$$

$s \in T$ (Turbo chiller)

$$I(\dot{V}_s^{\mathrm{N}}) = 0.8102 \cdot \dot{V}_s^{\mathrm{N}} \cdot \left(179.63 + 4991.3436 \cdot \dot{V}_s^{\mathrm{N}\ -0.6794} \right) \tag{4.52}$$

$s \in C$ (CHP engine)

$$I(\dot{V}_s^{\mathrm{N}}) = 9332.6 \cdot \left(\dot{V}_s^{\mathrm{N}} \cdot \frac{\eta_s^{\mathrm{N,el}}(\dot{V}_s^{\mathrm{N}})}{\eta_s^{\mathrm{N,th}}(\dot{V}_s^{\mathrm{N}})} \right)^{0.539} \tag{4.53}$$

$$\eta_s^{\mathrm{N,th}}(\dot{V}_s^{\mathrm{N}}) = 0.498 - 3.55 \cdot 10^{-5} \cdot \dot{V}_s^{\mathrm{N}}, \quad \eta_s^{\mathrm{N,el}}(\dot{V}_s^{\mathrm{N}}) = \eta_s^{\mathrm{N}} - \eta_s^{\mathrm{N,th}}(\dot{V}_s^{\mathrm{N}}), \quad \eta_s^{\mathrm{N}} = 0.87$$

5 Concluding Remarks

The conceptual synthesis of energy systems, especially those installed on site, is a significant task in the present and near future. More and more decision-makers from producing or researching institutions or housing complexes decide to cover their wide range of energy needs themselves. Decisions on the design and operation of energy generation facilities has a major impact on cost effectiveness, energy efficiency, and sustainability. Thus, research on optimal decision-making in energy systems goes along with one major challenge of the today's world: Supplying an ever-increasing number of people and more and more energy-driven technologies with the required energy in the age of the necessary energy transition, i.e. the structural change from the use of fossil fuels to a sustainable energy supply.

The contribution of this thesis to the optimization-based synthesis of decentralized energy systems is summarized in the following. Additionally, future research perspectives are discussed and follow-up work already done based on the documented research is outlined.

Computational complexity

In this thesis, the very first results on the computational complexity of the synthesis problem of decentralized energy systems are provided. Complexity statements are formally proven which have to date only been conjectured or concluded on the basis of insufficient arguments (cf. literature review in Section 3.1). A conducted polynomial reduction from SUBSET SUM implies that even the operation problem for one scenario (also time-step or load case) as a subproblem of the conceptual synthesis is at least weakly NP-hard (Section 3.3.1). Considering multiple scenarios a stronger complexity result for the synthesis problem is proven via a reduction from SET COVER: NP-hardness in the strong sense (Sections 3.3.2 and 3.5). It is shown that it is even NP-hard to approximate an optimal solution with a constant approximation factor or even with a factor of $\varepsilon \cdot \ln(|L|)$ (Section 3.3.3).

To summarize briefly Finally, there are well-founded justifications for developing and applying solution methods with potentially exponential runtime to compute feasible, approximate, or even optimal solutions for the synthesis problem of decentralized energy supply systems.

Further research perspectives

In order to refine the complexity analysis of the considered synthesis problem, the following aspects may be subject of further research. As an orientation the works of Furman and Sahinidis (2004), Letsios et al. (2018), Dey and Gupte (2015) and Haugland (2016) can

be considered as they are follow-up papers of comparable first complexity studies for other major problems in the field of process engineering (Alfaki and Haugland, 2013; Furman and Sahinidis, 2001).

In Section 3.3.1 it is shown that the operation problem is at least weakly NP-hard. It should be investigated whether this subproblem is also NP-hard in the strong sense. And if that is not the case: Is it possible to state a pseudo-polynomial algorithm or even an FPTAS for the operation problem? Due to the similarity of the (at least discrete) operation problem to SUBSET SUM or KNAPSACK, the development and analysis of approximation algorithms seems promising. In any case, developed problem-specific algorithms for the operation problem should be employed in integrated solution methods for the synthesis problem.

In Section 3.3.2 it is shown that the synthesis problem is strongly NP-hard even for settings restricted to one type of conversion technology with two forms of output energy. Complexity analyses of further special cases of the synthesis problem may be interesting.

Although in Section 3.3.3 it is shown that no $\varepsilon \cdot \ln(|L|)$-approximation algorithm for the synthesis problem exists unless P $=$ NP, approximation algorithms with a different performance guarantee should be elaborated.

Adaptive discretization algorithm

In this thesis, a novel solution approach is proposed to solve the superstructure-based synthesis problem of decentralized energy systems under consideration of non-linear technology models. The synthesis problem is commonly formulated as a two-stage stochastic program which leads to a non-convex MINLP (Section 4.2.2). Whereas in the literature the nonlinearities are usually (piece-wise) linearized (Section 4.2.3) and thus relevant physical and technical relations are simplified, the method proposed identifies good solutions for the non-convex MINLP within short computation time.

The solution approach consists of a coordinated interplay of MILPs and NLPs (Section 4.3.4). By discretization, the original non-convex problem can be approximated by a MILP (Section 4.3.1). Solving this MILP provides a suitable system structure. By fixing this structure, the original MINLP turn into a decomposable NLP which yields a feasible solution for the original synthesis problem (Section 4.3.2). Iteratively, the underlying discretization of the MILP is purposefully adapted based on the previous MILP solution (Section 4.3.3). The performed adaptation strategy improves the accuracy of the first-stage solution without enlarging the discretized problem in terms of, e.g., the number of variables.

On a freely available collection of 320 problem instances derived from real industrial data, the proposed adaptive discretization algorithm outperforms state-of-the-art solvers and common approaches based on piece-wise linearization (Section 4.4).

To summarize briefly A solution method for the synthesis problem of decentralized energy systems incorporating problem-related non-linearities is proposed, successfully applied, and evaluated. The designed approach overcomes non-convexity by adaptive concentrated discretization and provides iteratively improved solutions that are non-linear feasible due to short-duration post processing.

Further research perspectives

Based on the developed method and due to its successful application, aspects arise which may be subject of further research. We comment on some in the following.

One advantage of the adaptive discretization is that the discretized problem does not become larger with each iteration. The accuracy around the most profitable discretization grid point so far increases by concentrating the grid and not by increasing the number of discrete points (Section 4.3.3). However, the presented adaptive discretization algorithm remains a heuristic. It would be interesting to characterize problem instances where the approach is exact and where the output is an arbitrarily bad local optimum or even no non-linearly feasible solution is found at all. It may be possible to characterize non-linear functions for which a certain accuracy of the approach can be ensured.

Generally, one should work on the extension of the adaptive discretization algorithm concerning methods to compute dual bounds for the original MINLP (cf. next paragraph on follow-up work). Such bounds enable the estimation of the optimality gap of the algorithm's primal solutions.

In Section 4.6 we report in more detail on other possible discretized problems and thus alternatives to the one presented in Section 4.3.1. These alternatives are based on penalties in the objective function or additional constraints to restrict the energy excess. However, the more sophisticated discretized problems are defeated in a preliminary computational study and thus the approximate MIP based on discretization and linearization gets part of the adaptive discretization algorithm. Nevertheless, it would be interesting to investigate the other alternatives further. Can it be advantageous to choose a pure discretization (4.32)–(4.40) without continuous variables in between? Can the constraints of Theorem 20 be further tightened? Are there problem instances for which only the desired discrete solutions (Definition 18) are left under consideration of the constraints from Theorem 20?

To remedy the shortcoming of non-existing benchmark test sets (cf. Section 2.1), DESSLib should be expanded and further collections should be offered. In addition, a solution checker could be provided for the instances.

The application of the proposed adaptive discretization algorithm to other (non-convex) MINLP problems seems quite promising (cf. next paragraph on follow-up work). Perhaps the approach can even be generalized to more generic two-stage non-linear problems. In all cases, the structure of the discretized problem should be exploited to enable a speed up.

Follow-up work based on this thesis' research

Since our research documented in Chapter 4 has already been published (Goderbauer et al., 2016), there are subsequent papers citing our work. Two of these papers are addressed in the following.

In the field of mathematical optimization, a currently active field of research is the *exact* solution of (non-convex) MINLPs, e.g., based on discretizations. Citing our work, Nowak et al. (2018) recently proposed an decomposition-based inner- and outer-refinement procedure to solve non-convex MINLPs. Being part of a comprehensive solution framework, the concept of adaptive discretization is combined with other algorithmic approaches, e.g., by Duran and Grossmann (1986), to receive a dual bound for the original problem. Currently, the methods documented by Nowak et al. (2018) are being implemented as part of a new (non-convex) MINLP solver called Decogo (Muts et al., 2018). One motivation mentioned is the solution of large-scale energy system planning models under uncertainty.

Considering the design of water usage and treatment networks, Koster and Kuhnke (2018) recently successfully transferred our adaptive discretization approach to another two-stage synthesis problem. An integrated optimization of the network structure and its operation in consecutive load cases leads to a non-convex MINLP formulation. The operation subproblem encompasses a pooling problem and second-stage scenarios are linked since special units are able to store water. Besides the transferred adaptive discretization algorithm, Koster and Kuhnke (2018) developed a heuristic to speed up the solution process of the discretized problem. The authors conducted a computational study based on problem instances given by an industrial challenge. The proposed algorithm outperformed state-of-the-art MINLP solvers and improved the best known solution of almost all challenge instances.

Part II

POLITICAL DISTRICTING

Optimal (Re-)Districting and Decision Support
according to Legal and Judicial Requirements

6 Introducing Remarks and Contribution of this Thesis

> *Redistricting is among the least transparent processes in democratic governance.*
>
> **— M. Altman and M. P. McDonald (2011b)**

6.1 Optimal Design of Electoral Districts according to Law and Jurisprudence

In a democracy, transparency, objectivity, and the correct and meticulous handling of data are crucial. This applies in particular to elections, the heart of each democratic system. Every citizen eligible to vote must be able to understand how their will contributes to the overall decision (although this may require a detailed study of the electoral system). Votes must be duly received, possibly collected in electoral districts, and finally converted into a result for the whole electoral territory. All this must be done according to a transparent procedure and requires proper data handling.

The demand for transparency and correct data handling equally applies to the administrative work preceding an election. In most case, election preparation includes delimiting electoral districts (Handley, 2017). An *electoral district* or *constituency* is a territorial subdivision in which voters elect one (*single-member district*) or more members (*multi-member district*) to a legislative body. This is based on the idea that every part of the electoral territory is represented in parliament. As an example, Figure 6.1 shows the map of the 299 electoral districts for the German federal elections held in 2017.

In most democracies with an electoral district system, independent commissions are entrusted with the task of reviewing the latest districting plan and, if necessary, of developing options for adjustments. However, their elaborations are often not mandatory for the final decision-maker. The authority of the districting plan is often the legislature itself, i.e., the politicians in form of the parliament or the governing parties (Handley, 2017).

The boundaries of electoral districts can have a significant influence on an election's outcome, the composition of a parliament, and even the balance of power for the next legislative period. Consequently, the decision maker of the districting plan can have a major influence (cf. Fig. 6.2). This makes it all the more important that the decision-making process of electoral districts, called *(re)districting*, is conducted objectively and in accordance with clearly defined principles. Laws and jurisprudence provide principles that electoral districts

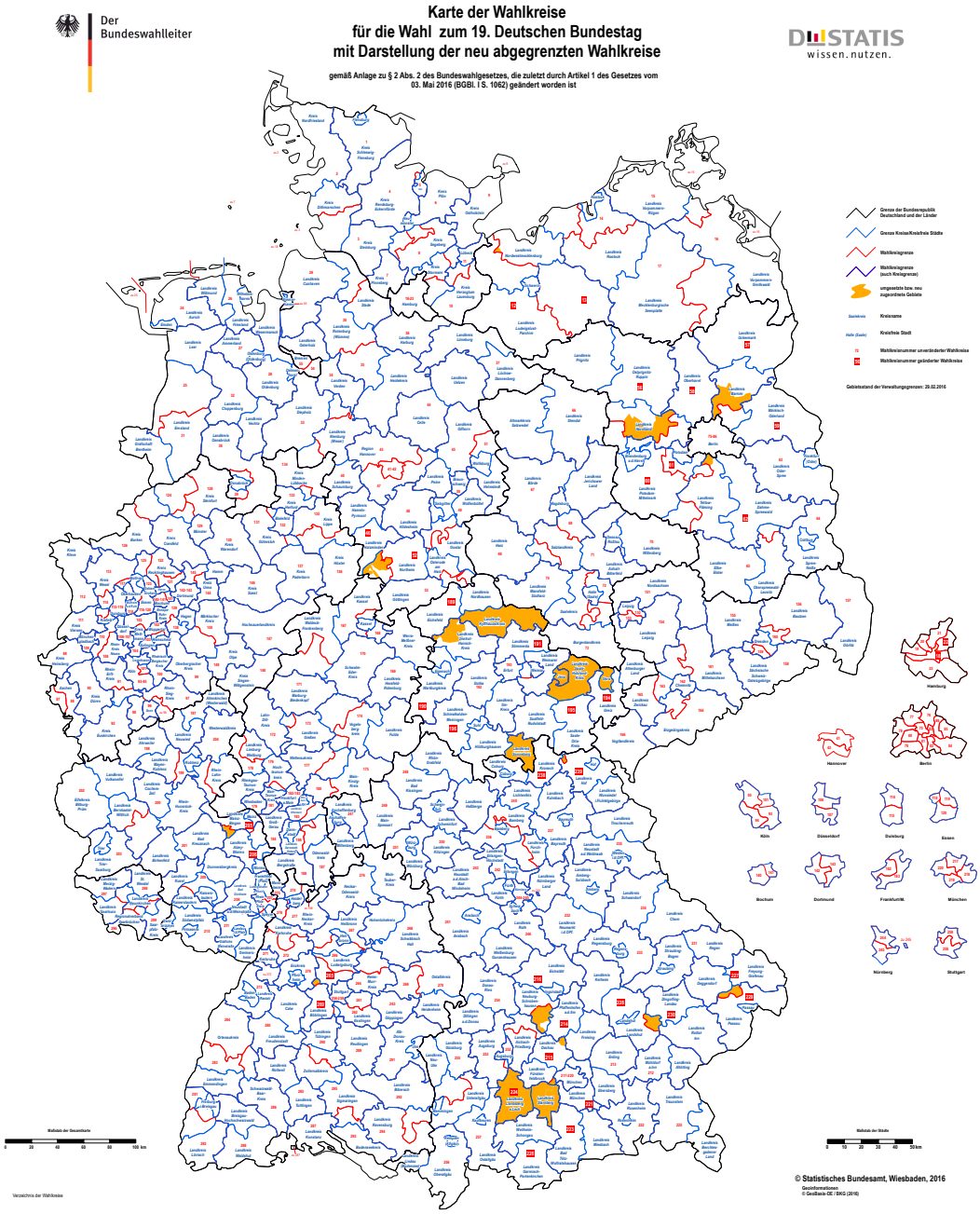


Fig. 6.1: Map of electoral districts for German federal elections 2017, published by the German Federal Returning Officer. Orange-colored areas were assigned to a different constituency compared to the previous delimitation of the elections 2013.

Source: `www.bundeswahlleiter.de`
© Der Bundeswahlleiter, Statistisches Bundesamt, Wiesbaden 2016,
Wahlkreiskarte für die Wahl zum 19. Deutschen Bundestag,
Basis of the geological information © Geobasis-DE / BKG (2016)

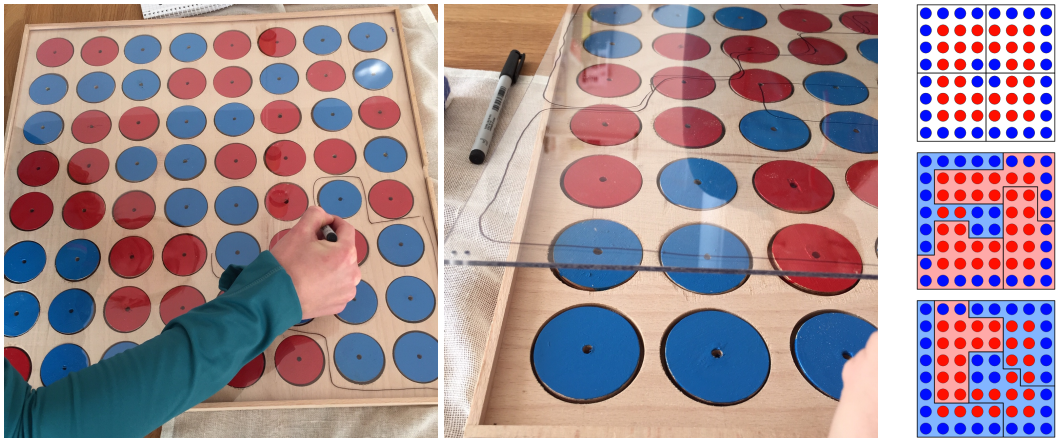


Fig. 6.2: Self-made board game: Discover the power of the one who decides the districting plan. There are as many voters of the blue party as of the red one. The voting intention may be derived from polls, previous elections, and other data. The game's question: Is it possible to partition the game board into four equally sized and contiguous districts so that the red party wins more of them? Is this also possible from the blue party's point of view? (The game has been part of the annual science night at RWTH Aachen University since 2015.)

must and/or should adhere to (Grofman and Handley, 2008; Handley, 2017). However, it is usually not clear how the decision-makers determine a districting plan based on the given requirements.

The questions that arise are as follows: Do further criteria influence the decision-making process? Are there districting plans that better comply with the legal requirements? Are high-quality or even law-optimal plans achievable with the tools currently used?

The lack of transparency and objectivity in districting processes is regularly criticized. There is even a specific term for it: *Gerrymandering*. It originated in the USA in the early 1800s: The acting governor of Massachusetts, Elbridge Gerry, initiated a redistricting in favor of his party. One of the new districts resembled the shape of a salamander. As a blend of the word "salamander" and governor Gerry's last name, the term "Gerry-Mander" was born (Griffith, 1907). Until today Gerrymandering is used to describe the malpractice of drawing district boundaries to gain advantage or disadvantage for certain persons (Cox and Katz, 2002; Grofman and Handley, 2008).
Besides the aspect of objectivity and transparency, a carelessly conducted districting process can lead to mistakes with serious consequences, as we will report in this introduction using the example of a German federal state.

> *Unbiased mathematics should be used to redesign electoral districts; only it can prevent the parties from tugging at the shape of each electoral district.*
>
> **— Christian Hesse (2019)**
> (translation from German)

The work presented in this thesis is mainly motivated by political districting issues in Germany. In the following, three regular and highly topical German (re)districting issues are highlighted. The thesis' work has already made important contributions on two of these issues. However, research and software presented in this work can be adapted to other districting applications – and not only in the context of electoral districts.

German Federal Elections: Redistricting ahead of each Election

For federal elections, Germany is (currently) partitioned into 299 electoral districts (cf. Fig. 6.1). Each electoral district sends one representative to parliament based on a first-past-the-post system. Thus half of the seats in parliament are determined via the electoral districts and the so-called *first votes*. The other seats are allocated proportionally using a *second vote* of the voters (Schreiber et al., 2017; Zittel, 2018). Every electoral district must preferably comprise the same number of people in order to comply with the principle of electoral equality. This principle is anchored in the German constitution. Population movements and demographic influences therefore require the redrawing of some electoral districts in preparation for each election (Schreiber et al., 2017). Figure 6.3 gives an outline of the process in which the districting plan of a last election is adjusted to the plan of an upcoming election.

A commission under the chairmanship of the Federal Returning Officer develops recommendations. Their report is published, e.g., BT-Drs. 19/7500 (2019). The commission's proposal is completely hand-made, based on experience and the guideline to receive legal districts with only minor changes (cf. Ch. 7 and Sec. 9.2.3). The commission works closely with the governments of the federal states. However, their reported adjustments are not

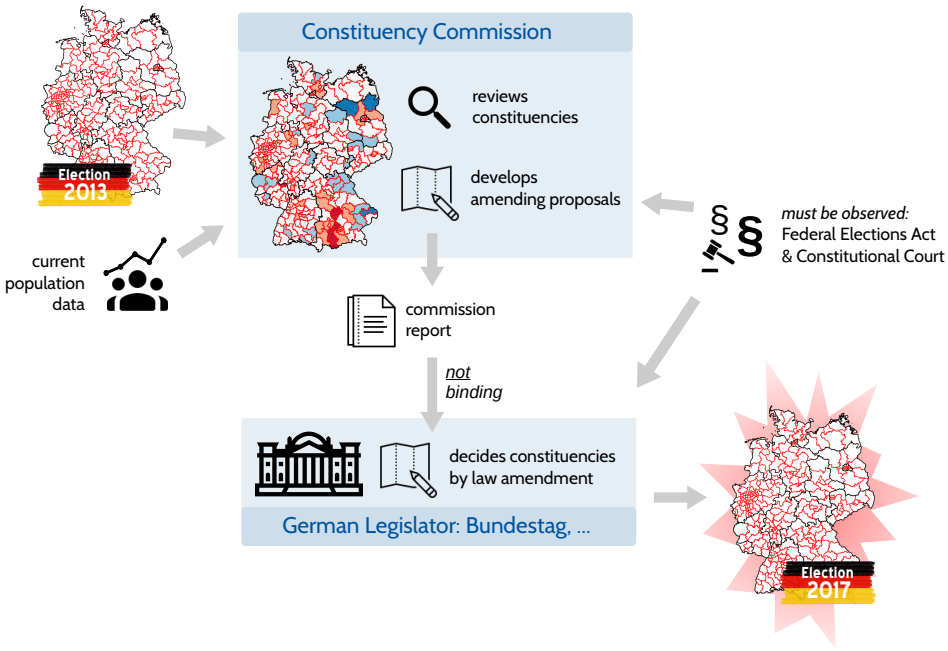


Fig. 6.3: The regular decision process in advance of every German federal election.
(Most icons by icons8.com. For note on geographical data cf. caption of Fig. 6.1.)

binding for the legislator who is the final decision-maker. Evaluations have shown that the legislator deviates from the proposals of the independent commission (Chapter 7). The result, i.e., the final districting plan, is published as a law amendment (Bundesgesetzblatt, 2016; BT-Drs. 18/7873, 2016). However, it is not known or documented how the final decision is reached.

The German electoral system is a mixed-member proportional representation. The composition of the parliament is determined not only by the electoral districts but also by elements of proportional representation (Zittel, 2018). As a result, the possible effects of gerrymandering are comparatively small. This is completely contrary to pure first-past-the-post systems as in the USA. In Germany, the electoral districts have an influence on the allocation of individual seats but generally not on the balance of power in parliament.

Nevertheless, the documentation of the decision-making process reveals a lack of objectivity and a tool to automatically provide high-quality districting amendments, based only on the legal requirements, for well-founded redistricting discussion in Germany.

German Federal Elections: Need for a Reform of the Electoral Law

Germany's electoral system has a weakness that is becoming a major problem: Before an election it is not known how many members the German parliament will comprise. A nominal size of 598 members is defined, but the actual number depends on the distribution of votes. As described, the voters of each electoral district send one member to parliament via their so-called first vote. In addition, every voter has a second vote which is given to a party. The distribution of second votes determines the relative strengths of the parties represented in parliament assuming a total size of 598 members. Along with the condition that each district winner has a guaranteed seat, this may result in won seats not being covered by the second vote result. In this case, coverage is artificially created by increasing the parliament's initial size (Behnke et al., 2017; Schreiber et al., 2017).

This weakness did not lead to any serious issues until the last election held in 2017. Today the German parliament has 709 members instead of 598 as planned (Federal Returning Officer, n.d., online). It has a size of historic dimensions and is effectively the largest democratically elected national parliament in the world. Election polls predict that the parliamentary expansion could be even larger after the next election scheduled to be held in 2021. A reform of the election law to handle this issue seems unavoidable. Under the chairmanship of the president of the German parliament a working group is currently discussing on a purposeful adjustment of the law (Baethge, 2018; Roßmann, 2019).

The reform debate includes the possibility to decrease the number of electoral districts (Behnke et al., 2017; Grotz and Vehrkamp, 2017; Hesse, 2019; Oppermann and Klecha, 2018; Pukelsheim, 2018). In order to evaluate and discuss various reform scenarios, practice-relevant districting plans for different numbers of electoral districts must be provided. The (political) redistricting process, as described in the previous section, takes several years. Thus, this manual approach is not appropriate for an urgent reform.

In fact, the work presented in this thesis enabled us to support the Federal Returning Officer in the context of the ongoing reform debate. Using our developed software (cf. Chapter 9), we contributed optimization-based districting plans for scenarios of 250, 200 and 125 electoral districts (Chapter 11; Goderbauer et al. (2018a,b); Goderbauer and Lübbecke (2019b)).

Hessian State Election 2018: Defective Electoral Districts

In addition to the German federal elections, there are regularly held elections in each of the 16 federal states. These are conducted through the use of electoral districts, too. In general, electoral districts of a state election do not coincide with those of a federal election.

In autumn 2018, state elections were held in Hesse which is the fifth-largest German federal state in terms of population. In preparation for this election, the districting plan with 55 electoral districts was established by law in December 2017.[1] But as it turned out in the first half of 2018, this law allowed for an inadmissible districting plan.

> *The error was detected by a scientist at RWTH Aachen University.*
>
> **— Spokesman of the Hessian Ministry of the Interior**
> on who uncovered the defective electoral districts.
> (translation from German; Frankfurter Allgemeine, 2018; Offenbach-Post, 2018)

Within this thesis' research and using the decision support software presented in Chapter 9, we analyzed the approved districting plan of Hesse in January 2018. We found out that the population data used by officials was incorrect. More precisely, when determining the population of the state's largest city Frankfurt, adults and children were incorrectly swapped. Using the wrong data, it was deduced that Frankfurt's electoral districts could be adopted unchanged from the last state election held in 2013. Taking into account the correct data, this was not the case. One electoral district had a much smaller population than what was legally permitted. The legal requirements would have forced adjustments to ensure admissibility, but none were made due to the incorrect data.
On February 15, 2018, we communicated our findings to the Hessian state election administration via email. On March 8, 2018, we received an email reply from the Ministry of the Interior. Simultaneously, the Ministry informed the political groups in the state parliament. The mistake we discovered became public for the first time (Frankfurter Allgemeine, 2018; Offenbach-Post, 2018).
On May 9, 2018 and based on a call of an opposition fraction, the issue was adjudicated by the state court of Hesse (2018). In an unprecedented trial, the judges confirmed the error we had discovered and ordered the legislator to perform corrections to the district plan before the election.

[1] A documentation of the parliamentary procedure as well as the publication of the law can be found in the database of the Hessian Parliament: `http://starweb.hessen.de` (last access March 29, 2019). The case is also documented in (Hessian State Court, 2018).

By the end of June, i.e., roughly four months before the Hessian election, a law was passed that regulates a minor change in the electoral districts of Frankfurt to obtain admissibility. The unanimous opinion was that a major districting reform should be carried out in the next legislative period.

Of course, any adjustment made to the electoral districts in Hesse led to controversial discussions. Also, in this decision-making process, one can identify a lack of transparency and objectively determined districting plans. Nevertheless, the case documented here shows a further dimension: possible consequences of improper data handling. It is not appropriate for such important decisions to produce serious errors. At least a plausibility check could have identified the unusually high change in the population of Frankfurt from the 2013 state elections. This kind of population development was reported for each electoral district in the appendix of the original law draft. If the error had not been noticed in time before the election, the election held in October 2018 could have been declared invalid afterward. The loss of confidence in the political authorities could haven been be immense.

The lack of **transparency**, the deficit of **well-founded bases for discussion**, and the practical need for **objectively determined districting plans** clearly call for research on **mathematical methods for optimal political (re)districting** according to legal and judicial requirements. In addition, practice shows the need for **problem-specific software** that combines **objective methods** with **adequate data handling**.

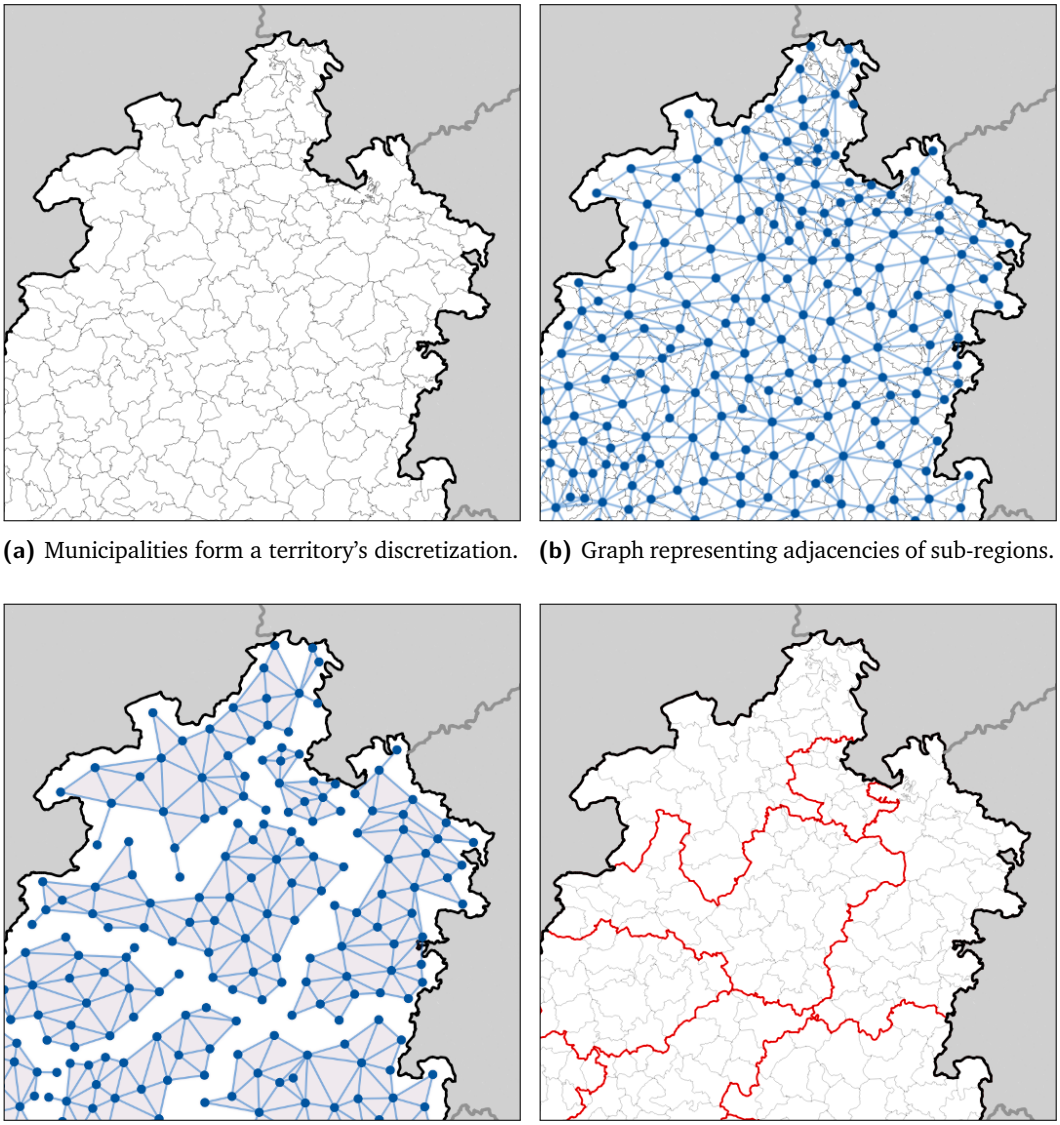
Optimal Political Districting and Decision Support

A territory has to be partitioned into a given number of electoral districts. Electoral laws and jurisprudence of the courts provide rules and guidelines for the delimitation of electoral districts.

Besides the natural requirement that each electoral district has to form a connected area, there are usually restrictions regarding the district's population. Most countries with single-member districts require that districts be as equal in population as possible. Since absolute equality is not realistic, specific limits for the permitted deviation from the population quota are usually set. Several other districting guidelines are applied (Grofman and Handley, 2008; Handley, 2017) – turning the problem mathematically into a multi-criteria task.

In practice, electoral districts are delimited based on the areas of cities, municipalities or, in the most detailed case, census tracts. Considering the enormous administrative effort that goes into an election, it makes sense to rely on existing administrative structures. For the mathematical modeling of the districting problem, a discretization of the territory into many sub-areas can be assumed (Ricca et al., 2011).

Using a given discretization of the territory (Fig. 6.4a), a graph can be prepared that represents adjacencies between the sub-areas (Fig. 6.4b; Ricca et al., 2011). On this basis,



(a) Municipalities form a territory's discretization.

(b) Graph representing adjacencies of sub-regions.

(c) Partition in connected subgraphs.

(d) Resulting districting plan.

Fig. 6.4: Defining electoral districts based on graph partitioning.
(Basis of the geological information © Geobasis-DE / BKG (2016))

the *political districting problem* can be modeled as a graph partitioning problem: Partition the graph's set of nodes in a pre-given number of subsets. Each node subset has to induce a connected subgraphs and has to fulfill further conditions (Fig. 6.4c). A multi-criteria objective function evaluates feasible node subsets and partitions. An (optimal) solution can then easily be translated into an optimal districting plan (Fig. 6.4d).

In order to define a certain political districting problem completely, to develop effective solution methods, and to enable practice-relevant solutions, the following aspects are necessary: adequate mathematical formalization of the legal requirements, detailed knowledge from practical experience, and detailed and current data of geography and population. Moreover, to link mathematical solution methods with a decision support system relevant for the practice, additional knowledge about the decision-making process and tools used are required.

Identified open research challenges and issues

In summary, the following open research topics have been determined. These have been identified during the work on this thesis, based on the literature on solution methods for optimal political districting, the literature on the practice of (re)districting, and the German issues presented above.

Missing evaluation of the German electoral districts in view of legal requirements Handley (2008) and Handley (2017) provide latest comparative studies on redistricting practice in the world. Most *numerical evaluations of districting plans* are conducted using US data with a focus on measuring gerrymandering (cf., e.g., Rossiter and Wong (2019), Stephanopoulos and McGhee (2015), and Warrington (2018)). The only study known to us that evaluates *German electoral districts* (in parts numerically) from the legal point of view is provided by Schrott (2006) on data up to the 2003 elections.
To be able to delimit practically relevant electoral districts, it is necessary to have information about the legal requirements as well as detailed insights into the interpretation and application of these in practice. Based on a comprehensive understanding, a *translation of legal requirements into formal mathematics* can be achievable.
There is no up-to-date and detailed numerical evaluation of German districting plans with regard to the observation of the legally prescribed principles. Until today, it has not been analyzed in detail to what extent the German requirements are observed in practice and whether there are criteria that are considered more important than others.

Proposed districting methods do not incorporate all German criteria A comprehensive literature survey on solution methods for the political districting problem (cf. Chapter 8, latest surveys of Ricca et al. (2011) and di Cortona et al. (1999)) reveals open research questions regarding German districting criteria. Almost all studied research papers were carried out for a specific application, each with its own criteria. As a result, numerous proposals for the numerical measurement of several criteria are proposed in the literature. However, the German requirements are not fully covered. Especially a suitable consideration of the *German version of administrative conformity* has not been developed yet. The legal guideline states that boundaries of electoral districts must comply with known administrative boundaries as far as possible. This includes several administrative levels, each consisting of differently populated areas; exactly this distinguishes the German version from others already considered (e.g., Bozkaya et al. (2003) and George et al. (1997)). Additionally, it turns out (cf. Chapter 7) that administrative conformity is one of the most important criteria in German practice. Consequently, this criterion must be appropriately considered in models and solution methods if electoral districts relevant to Germany are to be computed.

Demand from practice: objectively determined districting plans In the debate on a reform of the German electoral law, a change in the number of electoral districts is being discussed (Behnke et al., 2017; Oppermann and Klecha, 2018; Pukelsheim, 2018; Schäuble, 2019). The spectrum of proposals from scientists and politicians ranges from a moderate reduction in the number of electoral districts from 299 to 270 to halving the number and introduction of two-member-districts. Each discussed scenario implies the need for completely new districting of Germany. To discuss different numbers of electoral districts, it is not possible to

rely on the time-consuming and political decision-making process preceding every election. Thus, there is a need for *automatically and objectively determined districting plans tailored to the German case*. In order to guarantee transparency and impartiality, calculated electoral districts should only be evaluated on the basis of legal requirements. The goal is to determine practice-relevant districting plans that meet the legal requirements in a best possible way.

Spreadsheets, graphics software, paper maps, pencils – popular districting tools in Germany A survey among the election administrations of the German federal states (cf. Section 9.2.3 of Chapter 9) showed that the widespread state of the art of districting tools does not reflect the relevance of the task. This fact is also illustrated by the issue of the last state elections in Hesse described above. There is obviously a *lack of an integrated software solution* that is tailored to the German needs and offers optimal decision support for the (re)districting process.

6.2 Contribution of this Thesis

The major contribution of the thesis in the field of political districting encompasses five aspects. One of this is the expansion of the literature by a model and solution methods considering the German specifications. Therefore, among other things, a generalization of apportionment methods is proposed. Based on our research, a geovisual decision support system is developed. The software is used to support a commission of experts in preparing a reform of the German electoral law.

① **Numerical evaluation of recent electoral districts in Germany** Considering the electoral districts of the latest German federal elections, we analyze the *practice of German (re)districting* in detail to conclude the *practical interpretation of the given legal principles*. We analyze to what extent the requirements are met by the applied electoral districts. It turns out that *some criteria are preferred* over others in the German practice. Electoral equality, i.e., a homogenous distribution of the population among the electoral districts, appears to be less important. On the other hand, continuity and administrative conformity are of higher priority in practice. In the course of this analysis we formulate *numerical measures to quantify the observance of criteria*. These constitute an important component for the development of a practically relevant optimization model for the German political districting problem. In addition, we evaluate the suggestions made by an independent commission headed by the Federal Returning Officer. We analyze to what extent the German legislator, i.e., the decision-making authority, stuck to these proposals. It turns out that the legislator deviates from the commission's suggestions.

② **Detailed literature review of solution methods and districting software** Numerous optimization models and method for the political districting problem are proposed in the literature. To assess these regarding their application to the German case, we contribute a *comprehensive literature survey*. *Heuristic and exact solution methods* as well as *considered criteria* are presented. The review also illustrates how legal guidelines and criteria are transferred from the written law into mathematics. This is a crucial point since it determines whether the mathematical model is close to reality or not. In addition to mathematical models and

methods, we review the offered *software systems for districting*. These can be distinguished into those which provide (geovisual) assistance for manually districting and those which also provide decision support in the form of optimization-based automated districting.

③ **Optimization model and solution approaches tailored for German criteria** The problem of designing optimal electoral districts can be modeled as a *partitioning task on a graph*. This modeling approach is quite intuitive and widely used in the literature. The German variant of the problem is characterized by the fact that administrative conformity and continuity the most important criteria. Since the literature does not provide suitable consideration, especially for administrative conformity, we develop *functions that measure the level of adherence to the respective requirement*.
Based on that, we propose a *mixed-integer linear programming formulation* with a multi-criteria objective for the German political districting problem. The underlying *connectivity model* is well known for connected graph partitioning, but has not been applied before in the literature of political districting. To support the solution process of state-of-the-art MILP solvers, we develop an *exact preprocessing technique* and *primal heuristics*.
Beside a *MILP-based local search approach*, we propose a primal heuristic tailored to the criteria of administrative conformity as it is present in the German case. The heuristic is based on a novel *generalization of apportionment methods*. The classic version of these procedures are well studied in the literature and are widely applied in electoral practice. Apportionment methods are used to translate large vote counts of those to be represented into small numbers of parliamentary seats. We propose a generalized apportionment problem, analyze its computational complexity, provide a MILP formulation, and point out its application to support political districting.

④ **Geovisual and optimization-based decision support software** Our developed optimization approaches, the derived numerical measurements of legal requirements, and a comprehensive collection of data are packed into a *ready-to-use decision support system*. The presented software is based on a geographic information system, thus providing a *precise visualization* of districting plans. *Descriptive analytics* as well as the *application of optimization methods* are offered. The weighting of the objective criteria, i.e., priorities of continuity or electoral equality, can be specified by the user. Districting plans derived by optimization-based methods or provided as a user input can be *modified manually any time*. In this way, the user still holds the decision-making authority. Each change is evaluated according to the legal requirements. Districting plans and individual *electoral districts can be compared* with each other, both visually and numerically regarding the criteria.

⑤ **Supporting a commission working on a reform of German electoral law** Since spring 2018, experts and politicians have been advocating in a commission of the president of the German parliament, Wolfgang Schäuble, to elaborate a reform of the German electoral law. Developed reform proposals also include the *necessary redesign of electoral districts* in Germany. On behalf of the German Federal Returning Officer, we apply our developed optimization methods and decision support software to compute *districting plans considered by the commission*. To this end, we create a *data set of geoinformation and population numbers* of the German territory that was not previously available in such detail.

Mentioned contributions are documented in the following Chapters 7, 8, 9, 10, and 11.

7 Constituencies for German Federal Elections: Legal Requirements and Their Observance

Abstract About half of the seats in German Parliament (Bundestag) are assigned through relative majority vote in each of the 299 constituencies in German Federal Elections. Legal requirements and jurisprudence of courts regulate the characteristics and principles that have to or rather should be satisfied by constituencies in Germany. We investigate how well these requirements are met and whether some legal guidelines are given preferential treatment. We further analyze if, and to what extent, the decision-maker of the constituencies, i.e., the legislator, adopts proposals made by an independent Constituency Commission. No systematic and numerical study of constituency delimitation laws and practices in Germany has been conducted to date. This paper rectifies that shortcoming and provides the basis to prepare substantive arguments for upcoming delimitation debates in Germany. Our work is based on an extensive set of geographical and population data of the last five German Federal Elections, including the last one in September 2017.

7.1 Introduction

The delimitation of constituencies for the German Federal Election in autumn 2017 passed German legislation in spring 2016 (Bundesgesetzblatt, 2016; BT-Drs. 18/7873, 2016). Adaptations to the 299 constituencies compared to the German Federal Election of 2013 were necessary due to changes in population and local administrative reforms. Modifications to constituencies are common before each German Federal Election as is public dialogue about those rearrangements. Before a final decision is reached, an independent commission has to validate the current constituencies, report on changes in population figures, and make suggestions on how to modify the constituency boundaries (cf., e.g., BT-Drs. 18/3980 (2015) and BT-Drs. 18/7350 (2016)). This Constituency Commission is nominated by the German Federal President and consists of the Federal Returning Officer, a judge of the Federal Constitutional Court, and five other members. However, the commission's recommendations by the commission are not binding on the German legislator.

The Federal Election Act (German: Bundeswahlgesetz, abbreviated BWG) constitutes in section 3, subsection 1 the essential legal basis for the delimitation of constituencies for German Federal Elections. It lists details regarding the distribution of the 299 constituencies among the German Federal States as well as other principles that must be followed when

drawing constituency boundaries. For the sake of electoral equality required by the German constitution (German: Grundgesetz, abbreviated GG), all constituencies should ideally reflect the same share of the population. For this, the law defines population limits that each constituency should or must adhere to. Furthermore, established and historically evolved administrative borders should preferably be respected. In recent years, the legal requirements and guidelines for the delimitation of constituencies have been extended by decisions of the Federal Constitutional Court (German: Bundesverfassungsgericht, abbreviated BVerfG). For example, the court ruled that legislature has to strive for a certain degree of continuity in the spatial shape of the constituencies.

Contribution In practice, it is impossible to fulfill these competing and conflicting requirements entirely and simultaneously. The fact that the law does not clearly rank the principles complicates the matter further. In this context, we answer the following questions:

- To what extent are the legal principles for the delimitation of the German constituencies adhered to?
- Does the legislator take advantage of the liberty allowed by the vague phrasing of the legal requirements?
- Do the actual constituencies show that the legislator values certain principles more than others?
- To what extent is the German Federal Parliament following the suggestions of the Constituency Commission when deciding on a new delimitation of constituencies?

For all legal requirements and the mentioned questions above, we compile and visualize key figures in this article. Our work is based on an extensive data set, including population data, and detailed geographical information about the constituencies and administrative levels. We consider delimitation of constituencies for the German Federal Elections of the years 2009, 2013, and 2017 as well as the suggestions of the Constituency Commission regarding those elections. To the best of our knowledge, we created the most comprehensive, accurate, and current data set of this kind.

Related work A comparative survey of constituency delimitation laws and practices of 87 countries is provided by Handley (2008). The work includes a study on the practice of employing nonpartisan constituency commissions in the process of delimiting constituencies. Balinski et al. (2010) focus on the design of constituencies in the United Kingdom. The authors inform the public and analyze the consequences of a bill of 2010, changing the rules for defining constituencies in the UK. Schrott (2006) provides information about the history of redistricting in Germany between 1958 and 2003. The author concludes that the German legislator often accepts only constituency changes that are enforced by law, retaining the status quo as much as possible.

Overview The article is structured as follows: In Section 7.2, we present in detail the legal requirements and principles of the German Federal Election Act and Federal Constitutional Court concerning the German constituencies. In Section 7.3, we analyze the delimitations of constituencies in past German Federal Elections with respect to the observance of the requirements. In Section 7.4, we consider the Constituency Commission's proposed changes

and analyze to what extent the legislator accepts them. We close with a discussion and a summary in Section 7.5.

7.2 Legal Requirements for Delimitation of Constituencies

The principles that have to be considered during the delimitation of constituencies for German Federal Elections are stated in the Federal Election Act, section 3, subsection 1. In the last few years, those legal requirements have been complemented by the Federal Constitutional Court (BVerfGE 121, 226 (2008), BVerfGE 130, 212 (2012), and BVerfGE 95, 335 (1997)). In no particular order, the legal requirements are as follows.

Distribution of constituencies among Federal States (cf. sec. 3 subsec. 1 nos. 1 and 2 BWG). Since the German Federal Election in 2002, the territory of the German Federal Republic has been subdivided into 299 constituencies. By virtue of the constitutionally established federalism, the boundaries of the 16 German Federal States (German: Bundesländer) must be observed. Based on a state's population and a procedure described in the electoral law (cf. sec. 6 subsec. 2 sentences 2 to 7 BWG), the 299 constituencies are distributed among the states. This apportionment method is known as Webster/Sainte-Laguë procedure or divisor method with standard rounding. It is the subject of numerous mathematical publications (cf., e.g., Balinski and Young (1982) and Pukelsheim (2017)). The method ensures, in a certain sense, the best possible proportionality between the share of population and number of constituencies of the states.

Population numbers (cf. sec. 3 subsec. 1 sentence 2 BWG). The Federal Election Act states that *non-Germans* are not considered in the calculated population numbers for the constituencies. Therefore, the *German* population is the basis of assessment. The Federal Constitutional Court has extended the aspect to the effect that, additionally, the percentage of minors, thus, the proportion of non-eligible voters of the German population, has to be considered (BVerfGE 130, 212 (2012)). After examining the numbers, the Constituency Commission ascertained most recently that the percentage of minors in the German population varied insignificantly in most cases (cf. in particular section 2 in BT-Drs. 18/3980 (2015)). According to the commission, the German population figures can still be used as a reliable measurement. In addition, the Federal Constitutional Court instructs the legislator to take the trends of the long-term demographic development into account (BVerfGE 130, 212 (2012)).

Two-stage deviation limit of constituency's population (cf. sec. 3 subsec. 1 no. 3 BWG). According to the principle of electoral equality, each constituency must preferably comprise the same number of people. The law provides a two-staged scope for the deviation of the constituency's population from the average. Dividing the German population by the number of constituencies yields the expected average population per constituency. This currently is about $246\,000$. According to the Federal Election Act, the population of a constituency *should* not deviate more than 15% upward or downward from the average (15% tolerance limit).

The absolute maximum limit of the population deviation that *has* to be adhered to is 25%. This two-stage deviation limit with a should-regulation and a must-regulation is interpreted by the Constituency Commission as follows (cf. section 4.2.1, penultimate paragraph in BT-Drs. 17/4642 (2011)): "The absolute maximum limit of 25% may not be maxed out ad libitum. Exceeding the 15%-tolerance limit can only be justified on a case-by-case basis and by factually founded reasons."[1]

Conformity of constituency boundaries with administrative boundaries (cf. sec. 3 subsec. 1 no. 5 BWG). As far as possible, the delimitation of constituencies should be oriented toward (administrative) boundaries of the districts, urban districts, and municipalities. Even though it is not mentioned in the legal principles, the observance of the boundaries of municipal associations, possible existing governmental districts, and constituencies for the Federal State's election is supported. The conformity with known boundaries helps the territorial roots of a constituency from the voters' perspective as well as the electoral candidate. Thereby, the constituency can be easier to identify. Furthermore, and this aspect can not be neglected, it simplifies the administrative and organizational work around an election.

Connectedness of constituency (cf. sec. 3 subsec. 1 no. 4 BWG). Every constituency is supposed to form a connected, i.e., a coherent area. With respect to this and the aforementioned principle about the observance of historically rooted or administrative boundaries, the Federal Constitutional Court notes that a constituency should be a cohesive and rounded entity (BVerfGE 95, 335 (1997)). This serves as an additional visual aspect of a constituency. Its territory should resemble a circle than a lengthened and frayed entity. The concept of compactness of a constituency does not play a relevant role in public debates and legal requirements in Germany, in marked contrast to the electoral discussions in the United States of America (cf. public and political discussion as well as American legislation on the subject of Gerrymandering).

Continuity of delimitation of constituencies (BVerfGE 130, 212 (2012) and BVerfGE 95, 335 (1997)). The Federal Constitutional Court argues that it would be contrary to the principles of democratic representation, if constantly large and numerous changes were made to the constituencies. A certain degree of continuity is needed in the geographic layout of the constituencies to enable the establishment of adequate relationship between the representative and the constituency's population. While the continuity of constituencies is not mentioned in the Federal Election Act, it can justify exceeding the 15%-tolerance deviation limit from the viewpoint of the Federal Constitutional Court. The Constituency Commission notes that the reasons have to be more and more solid the closer the deviation of population moves toward the maximum limit of 25% (cf. section 4.2.1, penultimate paragraph in BT-Drs. 17/4642 (2011)).

[1] Original German quote: "Hierbei darf die 25 Prozent-Grenze nicht nach Belieben ausgeschöpft werden, sondern es müssen im Einzelfall besondere, sachlich fundierte Gründe vorliegen, um ein Abgehen von der 15 Prozent-Toleranzgrenze rechtfertigen zu können." (BT-Drs. 17/4642 (2011))

7.3 Observance of the Legal Requirements and Principles

We analyze in the following sections the extent to which the legal requirements and principles of the constituencies for German Federal Elections are observed. Sections 7.3.1 – 7.3.5 deal with one regulation as introduced in Section 7.2. In Section 7.4, we analyze the extent to which the suggestions of the Constituency Commission were considered by the German Federal Parliament. The key figures and outcomes rely on population and territory data from the Federal Statistical Office and the Federal Agency for Cartography and Geodesy, respectively.[2] Key figures are available on request from the corresponding author.

7.3.1 Distribution of Constituencies among Federal States

As the constituencies are distributed among the Federal States through a predetermined and unambiguous algorithm there is no leeway. Nevertheless, we want to evaluate how well the principle of electoral equality is being respected. The distribution of the constituencies yields for each state a different average population number compared to the national average. The state-specific deviations measure how a state's number of constituencies relates to the state's share of the German population.

For most Federal States, it is possible to be within a 5% range of the national population average. It is, however, different for states with comparably few constituencies. For the 2013 and 2017 elections, the states Thuringia (9 and 8 constituencies, respectively), Mecklenburg-Vorpommern (6), and Saarland (4) amounts to between 5% and 10%. In all the analyzed elections, the least populous German state, Bremen, has a state-specific deviation that exceeds even 15%. Thus, it is not possible to delimit constituencies in Bremen, all of which observe the 15%-tolerance limit. Calculations of Goderbauer (2016a,b) reveal that increasing the number of German constituencies – staying, however, close to 299 – can lead to deviation values above the admissible 25% in Bremen.

7.3.2 Deviation of Constituency Population from Average

Even though the constituencies are defined up to 18 months before a German Federal Election, their delimitation must take place in such a way that the constituencies meet the legal requirements at the time of the election. Owing to permanent population changes, foresight is necessary with regard to the population deviation limits.

The cartogram[3] in Figure 7.1 shows for each constituency of the 2017 German Federal Election the individual deviation of the constituency population from the national average.

[2] Sec. 7.3.1: German population with key dates: 2002/12/31 (Election 2002), 2005/12/31 (Election 2005), 2009/09/30 (Election 2009), 2013/09/30 (Election 2013), 2015/12/31 (Election 2017). Sec. 7.3.2 – 7.3.5: German population and geodata with key dates: 2009/12/31 (Election 2009), 2013/12/31 (Election 2013), 2015/06/30 (Election 2017, German population), 2016/02/29 (Election 2017, geodata).

[3] Hexagonally tiled cartogram with one hexagon per constituency. Tile map generated with own implementation, based on work of McNeill and Hale (2017).

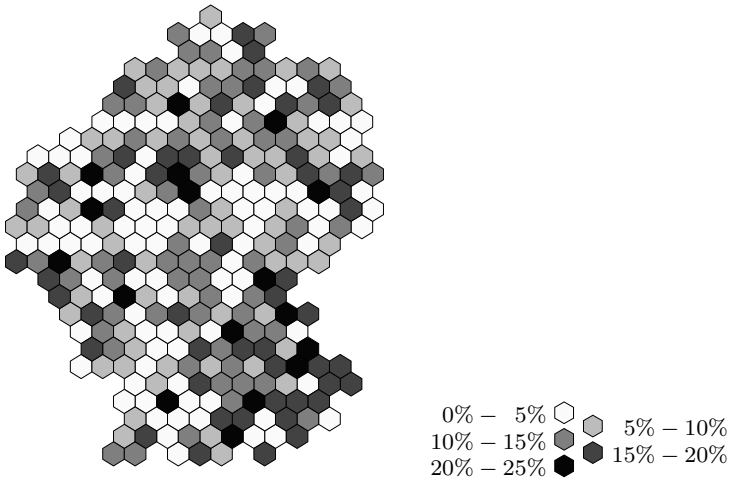


Fig. 7.1: One-hexagon-per-constituency cartogram showing population deviations.

The darker the coloring of a constituency's hexagon, the greater is its deviation. The most populous constituency has 303,880 Germans (constituency 243 Fürth, Bavaria, $+23.1\%$ deviation). The other extreme can also be found in Bavaria: Just 189,238 Germans live in the least populous constituency (constituency 238 Coburg, Bavaria, -23.1% deviation).

Figure 7.2 shows the distribution of the deviation values of the constituency populations over the course of time. It becomes clear that the modifications to the delimitation of constituencies for the 2017 Federal Election led to improvements in terms of population deviations: The histogram classes $(-25\%, -20\%)$ and $(20\%, 25\%)$ of the 2013 election are losing in favour of more inward classes. The two constituencies of 2013 with deviations above 25% and below -25% also left their histogram class for the 2017 election. Slightly

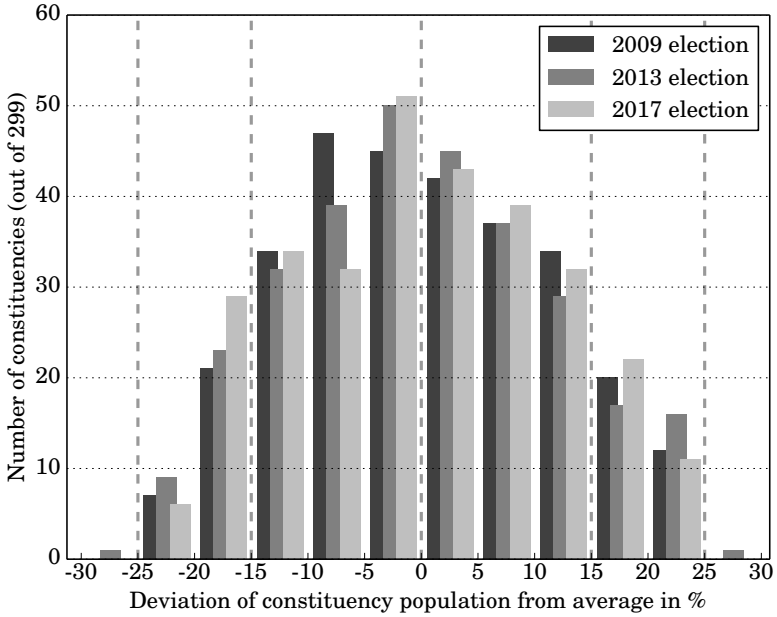
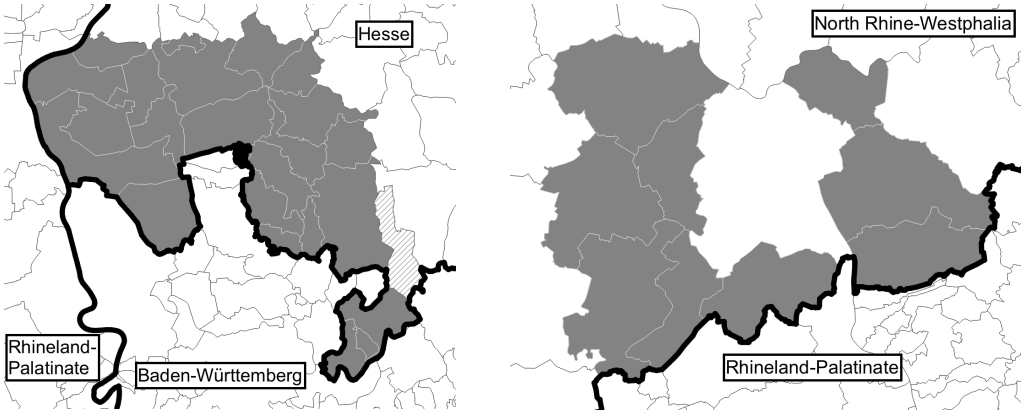


Fig. 7.2: Distribution of the population deviations of constituencies for the 2009, 2013, and 2017 elections.

more than every second constituency remains below the deviation value of 10%. About four out of five German constituencies comply with the legal tolerance limit of 15%. Since we calculated the deviation values of the constituencies for the 2017 election on the basis of population data as of 06/30/2015, it remains to be seen whether the delimitation for 2017 was robust enough and chosen with sufficient farsightedness.

7.3.3 Connectedness of Constituency

According to the Federal Election Act, the area of each constituency should form a coherent area. For the 2013 and 2017 elections, we found that this legal principle was adhered to in general. However, there are exceptions. Apart from some negligible cases, we would like to emphasize two non-connected constituencies. Negligible cases are, for example, non-connected constituencies, where islands, exclaves or non-connected municipalities cause the non-connectivity.



(a) Constituency 188 Bergstraße. **(b)** Constituency 98 Rhein-Sieg-Kreis II.

Fig. 7.3: Two non-connected constituencies of the elections in 2013 and 2017. Boundary lines: ©GeoBasis-DE / BKG 2011 (data changed).

The Hessian constituency Bergstraße (see Figure 7.3a) was created for the first election in West Germany after World War II in 1949 and has since been a part of the delimitation of constituencies. It consists entirely of the non-connected district of Bergstraße. Interestingly, for the three elections in the years 1965 – 1972, a municipality from a neighbouring district was assigned to the constituency so that it was connected during this time (see the highlighted municipality in Figure 7.3a).

The North Rhine-Westphalian constituency Rhein-Sieg-Kreis II (see Figure 7.3b) consists of two separate parts of the Rhine-Sieg district. The western part of this constituency consists entirely of the left-Rhine municipalities of the Rhine-Sieg district and, thus, is delineated by the district boundaries as well as the natural border of the Rhine River. This non-connected constituency around the city of Bonn has existed in this form since the 1980 election.

7.3.4 Conformity with Administrative Borders

The Federal Election Act requires that the boundaries of municipalities, districts and urban districts should be respected as much as possible. It is apparent that other administrative and/or historical boundaries are also included in the planning. In a hierarchical order, this includes boroughs, city districts, municipal associations, and potential governmental districts. Seen on the basis of their population strengths, the districts and urban districts are most comparable in size to a constituency. There are, on the one hand, constituencies which contain several (urban) districts completely. On the other hand, there are (urban) districts that are divided into multiple constituencies. Municipalities (apart from large cities, which are mostly administered as urban districts) and also municipal associations are usually too small to form a constituency by themselves. Governmental districts, however, are too large and comprise several constituencies.

Governmental districts (German: Regierungsbezirke). Four German Federal States are subdivided into governmental districts and the following applies to the constituencies in those states at the 2013 and 2017 elections. In Bavaria (7 governmental districts) and North Rhine-Westphalia (5), all governmental districts are respected by the delimitation of constituencies. In Baden-Wurttemberg (4) and Hesse (3) only a few constituencies cover areas from more than one governmental district.

Districts and urban districts (German: Kreise und kreisfreie Städte). An interpretation of the legal requirement for conforming to administrative boundaries is that the delimitation of constituencies should have as few differences as possible with the boundaries of the (urban) districts. In other words: The share of the constituency boundaries, which at the same time are also boundaries on the district level, should be as large as possible. We chose the length of the constituency borders as a basis for assessment. This so-called border classification number can be expressed for each constituency, and also for a region or for Germany as a whole. Examples of the 2017 election: (i) Constituency 248 matches exactly with the union of three districts in northern Bavaria. All boundaries of this constituency are also the boundaries of the district level, that is, a border classification number of 100%; (ii) Constituency 283 consists of the district Emmendingen and the southern part of the district Ortenaukreis. The northern and the north-western borders of the constituency are not district boundaries. The border classification number of this constituency amounts to 64%.

Figure 7.4 shows the distribution of the border classification number of the constituencies for the 2017 election in a class histogram. It shows that the majority of constituencies tend to comply with boundaries of districts and urban districts. 90 of the 299 constituencies are in the last histogram class. In 88 of these constituencies, the boundaries even correspond to 100% with boundaries at the district level. Five constituencies have a border classification number of 0%. These are the two constituencies of Hanover (which is officially not an urban district, but a municipality in the district of Hanover) and three constituencies of Berlin, which lie completely within the city/Federal State area. Seen across the whole of Germany, 86.6% of the constituency boundaries in the Federal Elections in 2017 coincide

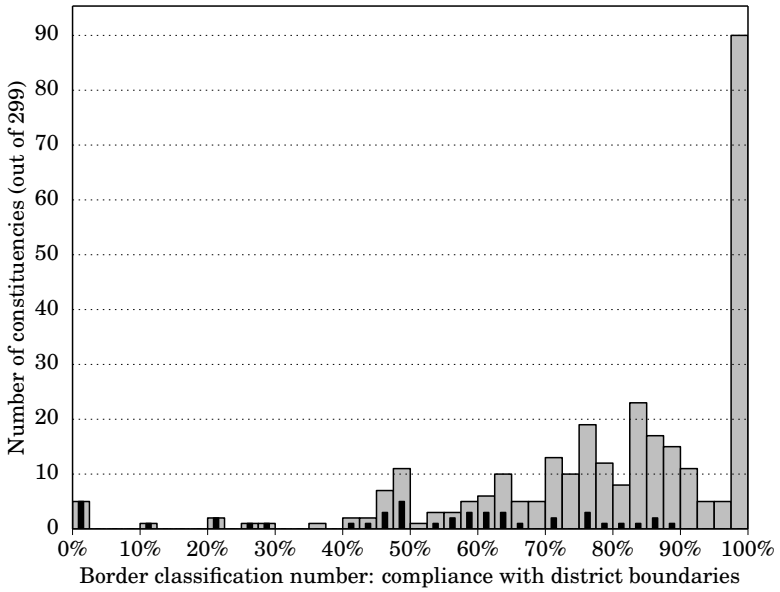


Fig. 7.4: In gray: Distribution of the border classification number (compliance with the boundaries of (urban) districts) of the constituencies for the election in 2017. In black: Constituencies whose border classification number is not very meaningful, since they are part of a set of constituencies that exactly partition a (urban) district.

with boundaries at the district level. This value is similar for the 2013 election (86.7%) and the 2009 election (88.0%).

For certain constituencies, the border classification numbers is a questionable key figure. For example, the urban district of Munich is made up of exactly four constituencies. None of these constituencies contains areas outside the urban area. Thus, the entire border of Munich is a constituency border. Within Munich, the four constituencies are forced to create borders that deviate from Munich's city borders. Thus, the border classification numbers of these constituencies are less than 100%, namely around 50%. But constituencies that match the exact area of a (highly populated) district or urban district fulfill, in our view, the principle of observance of district boundaries completely. Obviously, the border classification numbers do not take this into account. According to this interpretation, an additional 44 constituencies (including the mentioned four in Munich) for the 2017 election were fully in line with the boundaries of the districts and urban districts. In Figure 7.4, these constituencies are represented in the form of the black class fractions.

Municipal associations (German: Gemeindeverbände). A municipal association is the association of at least two municipalities. In Germany, there are almost $1\,300$ municipal associations. At the delimitation of constituencies for the 2013 election, four municipal associations were not fully in one constituency. For the 2017 election, this number increases by one.

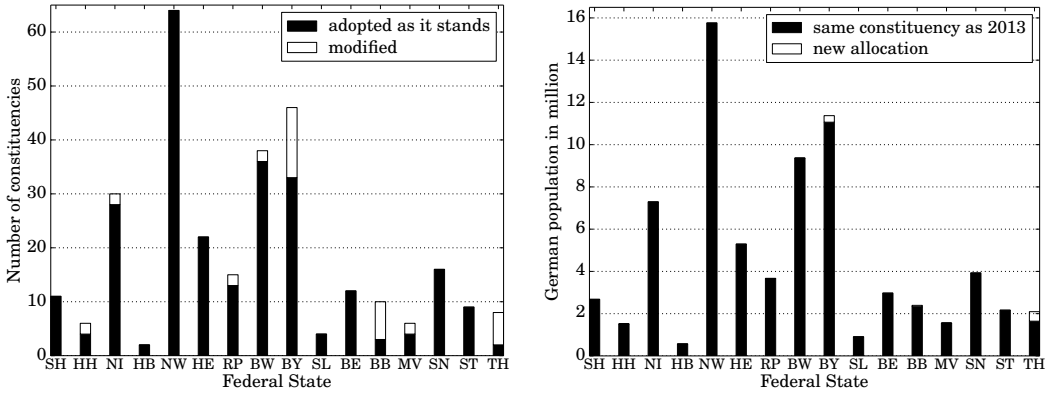
Municipalities (German: Gemeinden). In general, the boundaries of the municipalities are respected when defining constituencies. In fact, mathematically, there is only one understandable reason why a municipality is not completely in one constituency or not

partitioned into a certain number of constituencies: The restriction of the constituency population in the form of the deviation limit of 25%. The deviation limit can imply the existence of a constituency containing parts of a city and of the city's surrounding area.

7.3.5 Continuity of Delimitation of Constituencies

The requirement that as few modifications to the constituencies as possible should be made between one election and the next is not formulated in the Federal Election Act. This was imposed by the Federal Constitutional Court. We measure the continuity by the number of modified constituencies and the population that has changed its constituency.

In all, 267 of the 299 constituencies were adopted unchanged from the 2009 to the 2013 elections. This corresponds to about 89%. In the transition to the 2017 election, 263 of the 299 constituencies of the 2013 election, i.e., 88%, remain intact. Figure 7.5 illustrates the extent of the continuity of constituencies for the 2017 election, based on the number of (un)altered constituencies and the newly allocated population per Federal State. The Federal States where the numbers of constituencies were changed (Bavaria $+1$, Thuringia -1) recorded the most significant adjustments. With the exception of these states, the newly assigned population is so small that their share in the diagram is hard to recognize. Nationwide, almost 1.2% of the population has changed its constituency from the 2013 to the 2017 elections.



(a) Proportion of unchanged constituencies (black) per Federal State.

(b) Proportion of newly allocated population (white) per Federal State.

Fig. 7.5: The extent of continuity from 2013 to 2017 elections as measured by the share of (a) adopted constituencies and (b) newly allocated population (Federal States are abbreviated with their ISO 3166-2:DE code).

7.4 Adoption of Proposed Amendments suggested by Constituency Commission

The proposals developed by the Constituency Commission about amendments to the delimitation of constituencies are not binding on the legislator's decision. This section states whether, and to what extent, the constituencies decided by the legislator deviate from the commission's recommendations.

For the 2017 election, the Constituency Commission proposed changes to a total of 62 constituencies[4] due to excessive deviations in the constituency population (BT-Drs. 18/3980 (2015) and BT-Drs. 18/7350 (2016)).[5] In the final delimitation for the 2017 election, only 34% (21 out of 62) of these suggested amendments were adopted. In addition, 11 other constituencies underwent changes, which were not proposed by the commission, through the legislator. Thus, about one in three constituencies changed for the election in 2017 were drafted not by the commission, but by parliamentary parties of the Bundestag (BT-Drs. 18/7873, 2016).[6]

7.5 Summary and Discussion

Our analysis shows that the observance of legal principles varies in the delimitation of constituencies for German Federal Elections varies. The requirements and legal principles are incorporated differently into the decision-making process. Some legal guidelines are given preference. Differences in the interpretation of the regulations between the legislator and the Constituency Commission are identified.

Regarding the constituency population, about one in every five constituencies exceeds the 15%-tolerance deviation limit. Approximately one in every ten constituencies has a deviation of 20% and more. Overall, the legally permissible deviation interval up to the maximum limit of 25% has been exhausted. The population deviation distribution (cf. Figures 7.2 and 7.6) shows that the 15%-tolerance limit is not a limit that is actively targeted.

Much more attention is paid to the principle of compliance with administrative boundaries. Boundaries of governmental districts are almost fully respected, municipal associations are, almost without exception, enclosed in a constituency, and municipalities are, generally, only divided into several constituencies in the form of some large cities. In addition, constituency boundaries are clearly aligned with the boundaries of districts and urban districts. It is also shown in Figure 7.6 that the principle of administrative conformity is much more respected than the one concerning population deviations.

[4] The dissolved constituency in Thuringia and the newly founded one in Bavaria are counted only once.

[5] On occasion, the commission has prepared more than one proposal for certain issues. In these cases, the suggestion which is named first by the commission is used as their unique proposal in our analysis.

[6] For completeness it should be stated that further proposals for amendments were suggested and partly accepted: (i) In order to have a unique assignment of certain unincorporated and uninhabited areas (in contrast to past delimitations of constituencies) two further minor changes were proposed by the commission and adopted by the legislator. (ii) On the basis of official regional changes, the commission proposed amendments to four constituencies. The legislator approved two of them.

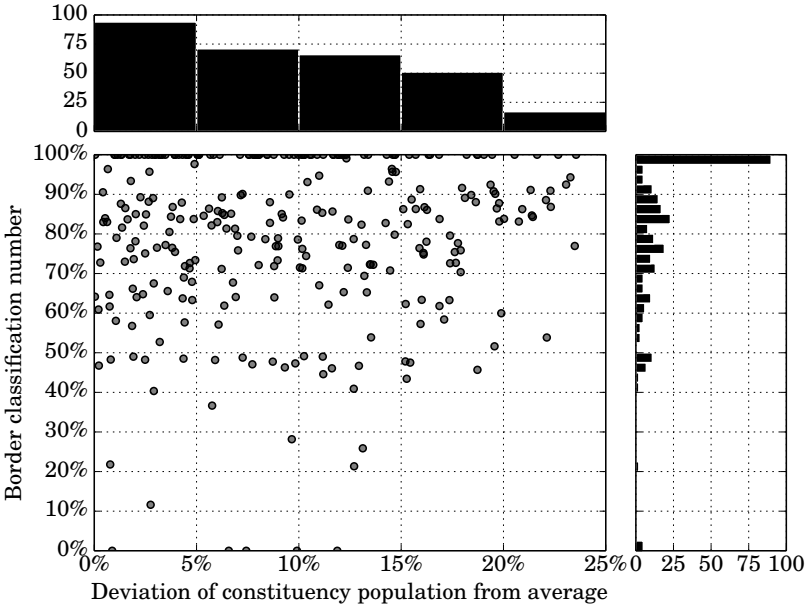


Fig. 7.6: Scatterplot and histograms of the population deviations as well as border classification numbers for the delimitation of constituencies for the 2017 election.

Furthermore, the analysis shows that continuity of the constituencies is preferred. Before an election, as few constituencies as possible are modified as little as possible. Here, the views of the legislator and the commission differ as follows. The legislator only modifies constituencies that are currently infeasible due to their population deviations or are in danger of becoming so until the day of the election. That is, in practice, only the absolute maximum limit of 25% is used for the revision of constituencies. In contrast, the commission presents a large number of amendments justified by the exceeding of the 15%-tolerance limit. These are generally not considered by the legislator. The official justification of the law, which defines the delimitation of constituencies for the 2017 election, states unequivocally (BT-Drs. 18/7873, 2016): 'If a constituency is beyond the tolerance limit of $\pm 15\%$, an amendment to the constituency boundaries is generally avoided under the aspect of continuity.'[7]

The coherence, i.e., connectivity of the constituencies, is usually present just as the legal requirements stipulate. However, two constituencies contain municipalities that are separated from the rest of the constituency. Since these two constituencies have existed in the current form for several decades, we assumed that this non-connectivity would be permitted for reasons of continuity. In the course of this analysis, we have not received any comment on the disregarding of the coherence principle either by the Bundestag or the commission.

In summary, the analysis of the delimitation of constituencies shows that the legislator values the requirements differently. The population deviation limit of 25% is regarded as a condition for the feasibility of a constituency. The same applies (with a few historical exceptions) to the connectivity of a constituency's area. The continuity of constituencies is absolutely the ultimate goal. If something has to be modified in the run-up to an election in order to maintain legal admissibility, the legislator values the objectives in the following

[7] Original German quote: 'Soweit Wahlkreise jenseits der Toleranzgrenze von $\pm 15\%$ [...] liegen, sieht der [Gesetz-] Entwurf von einer Neueinteilung unter dem anerkannten Aspekt der Wahlkreiskontinuität [...] grundsätzlich ab.' (BT-Drs. 18/7873, 2016)

order: (i) maximize continuity, (ii) maximize observance of administrative boundaries, and (iii) minimize the deviation of constituency population.

The analysis also shows that the legislator uses the right to treat the report of the Constituency Commission only as a proposal. The fact that so many suggestions for amendments are not accepted by the legislator, and that numerous amendments are decided that are not part of the commission's work is surprising. In their reports, the commission stated that they had been in regular contact with the governments of all Federal States and parties represented in the German Bundestag (BT-Drs. 17/4642 (2011), BT-Drs. 18/3980 (2015), and BT-Drs. 18/7350 (2016)). Many of the commission's suggestions for amendments contain the note that it would be supported by the government of the respective Federal State. It is evident that in the commission's proposals the tolerance limit of 15% for population deviation is considered. The commission is willing to abandon continuity in order to prevent the crossing of the 15% limit. In this respect, the approach of the Constituency Commission differs completely from that of the legislator.

There are a variety of arguments and justifications favoring the continuity and observance of administrative or known borders as important objectives. It may, however, be surprising that the deviation of constituency population plays a subordinate role in the German practice. The difference in population between the least and most populated constituency could, theoretically, constitute almost half a constituency. Regardless of the actual extent, the German legal deviation limits are very generous compared to European norms. The Council of Europe, whose decisions are represented by Germany as a member, recommends in a Code of Good Practice in Electoral Matters (Venice Commission, 2002) that countries comply with a population deviation tolerance limit of 10% and a maximum limit of 15%. Germany is far away from that — in practice as well as legal principles. Nearly every second German constituency exceeds the recommended tolerance limit of 10%. After the last two German Federal Elections in 2009 and 2013, election observers from the OSCE (Organization for Security and Co-operation in Europe) indicated that Germany should reduce the population deviations as recommended by the decision of the Council of Europe (OSCE, 2009, 2013).

8 Political Districting Problem: Literature Review and Discussion with regard to Federal Elections in Germany

Abstract Electoral districts have great significance for many democratic parliamentary elections. Voters of each district elect a number of representatives into parliament. The districts form a partition of the electoral territory, meaning each part of the territory and population is represented. The problem of partitioning a territory into a given number of electoral districts, meeting various criteria specified by laws, is known as the Political Districting Problem. In this paper, we review solution approaches proposed in the literature and survey districting software, which provides assistance with interactive districting by hand or even decision support in the form of optimization-based automated districting. As a specific application, we consider the Political Districting Problem for the federal elections in Germany. Regarding the present requirements and objectives, we discuss and examine the applicability of the approaches mentioned in the literature to this specific German Political Districting Problem.

8.1 Introduction

In preparation for an upcoming parliamentary election, a country is generally subdivided into *electoral districts*. These districts are of fundamental importance in democratic elections, because the voters of each district elect a number of representatives into parliament. In general, the number of seats staffed by an electoral district is determined a priori in line with the district's population. In many cases, exactly one seat is assigned to each electoral district. This calls for a balance in population distribution among the districts. Owing to population changes, the partition into electoral districts, i.e., the *districting plan*, needs regular adjustments.

The *Political Districting Problem* (PDP) denotes the task of partitioning a geographical territory, such as a country, into a given number of electoral districts while considering different constraints and (optimization) criteria. Every country has its own electoral system and laws. Therefore, the legal requirements and their particular importance for a districting plan differ across application cases.

Models and solution approaches proposed in the literature are primarily addressed to the PDP in the United States of America. The particular motivation is mostly to tackle the suspicion

of applying *gerrymandering*. Gerrymandering is the practice of creating (dis)advantages from the territorial subdivision for a certain political party, a candidate, or a social class in order to gain or lose seats. The term "gerrymandering" dates back to the early 1800s when Elbridge Gerry, the acting governor of Massachusetts, signed a bill that redistricted the state to benefit his Democratic-Republican Party. A cartoonist[1] realized that one of the new districts resembles the shape of a salamander. As a blend of the word salamander and Governor Gerry's last name, the "Gerry-Mander" was coined (Griffith, 1907). Basically, gerrymandering can be utilized in pure majority voting systems (first-past-the-post systems). By contrast, pure proportional representation precludes gerrymandering. The symptoms of manipulating geographic political boundaries are usually odd-shaped districts, such as the original gerrymander from 1812. For deeper insights into the topic of gerrymandering, see (Cox and Katz, 2002; McGann et al., 2016).

Today, we have to deal with "the *digital gerrymander*," as Berghel (2016) recently stated. Nowadays, computers and mathematics are exploited in an arms race between subtly performing and objectively identifying gerrymandering. Mathematical models and algorithms are transparent as they are defined in a precise way. However, they are only unbiased as long as they are not fed with political or social data.[2]

One answer to the highly discussed malpractice of gerrymandering is the *compactness* of electoral districts. Odd-shaped districts are undesirable, because this might be an indication for gerrymandering. The more circle-like or square-like an area is shaped, and the less elongated and frayed it is, the more compact it is. However, there is no uniform definition of compactness and its measurement, neither in the literature nor in court decisions. Horn et al. (1993) lists over 30 compactness indicators. For detailed discussions about compactness, see (Chambers and Miller, 2010; Fryer and Holden, 2011; Niemi et al., 1990; Young, 1988).

Of late, another proposed measure of gerrymandering has gained (public) attention. The Supreme Court of the United States of America considers the *efficiency gap* in a partisan gerrymandering case in Wisconsin.[3] The efficiency gap captures the difference in "wasted votes" between two parties engaged in an election. See (McGhee, 2014; Stephanopoulos and McGhee, 2015) for more details and the calculation of the efficiency gap in a hypothetical election scenario.

Besides compactness, the following two criteria are mostly considered in the literature of PDP: *Contiguity*: Each electoral district has to be geographically contiguous. *Population balance*: In order to comply with the principle of electoral equality, i.e., one person-one vote, the differences in population among the electoral districts have to be preferably small. In practice, the law defines a limit on the deviation.

One specific application, which is only partly addressed in the literature is the PDP for the German parliamentary elections: the *German Political Districting Problem* (GPDP). Since

[1] The first known use of the word "gerrymandering" appeared in "The Gerry-Mander: A new species of Monster which appeared in Essex South District in Jan. 1812", *Boston Gazette*, March 26, 1812. The article is available at `http://www.masshist.org/database/1765` (visited on Oct 1, 2018).

[2] Former US president Ronald Reagan is cited in (Altman, 1997): "There is only one way to do reapportionment – feed into the computer all the factors except political registration."

[3] *Gill v. Whitford*, United States Supreme Court case, No. 15-cv-421-bbc, 2016 WL 6837229 (E.D. Wis. Nov. 21, 2016), docket no. 16-1161.

Germany's electoral system is a mixture of proportional representation and uninominal voting in the electoral districts, the effect of applying gerrymandering is comparatively small. However, the design of the electoral districts is frequently called into question by the German public, too. Additionally, the European organization OSCE (2009, 2013) officially criticized the German districting plan regarding its large population imbalance. Referring to the Code of Good Practice in Electoral Matters of the Venice Commission (2002), it is pointed out that the deviations of district population are way too large in Germany.

The PDP is a special *districting problem*, *territory design problem*, or *zone design problem*. This kind of problem has been applied to an extensive number of fields. Within this survey, we disregard all works not specifically addressing the PDP. A broad review of different districting applications is given by Kalcsics et al. (2005). Moreover, Kalcsics et al. (2005) provides one of few papers that consider the districting problem independently from a concrete practical background.

Contribution In this article, we review solution approaches, models, and algorithms proposed in the literature for the PDP. The considered constraints and optimization criteria differ across applications. Besides a general literature survey, we specifically consider the legal requirements and principles given for the delimitation of electoral districts for federal elections in Germany. In addition to the review of solution approaches and a suitability evaluation for the German case, we survey districting software that offers either assistance with manually districting or decision support in the form of optimization-based automated districting. Unfortunately, most software is only commercially available and promising open source projects are outdated.

If a reader is not interested in the specific German application but in the general literature review of the solution approaches for the PDP and districting software, one can skip Sections 8.3 and 8.5.

Outline In Section 8.2, we present a definition of the PDP and provide a unified mathematical model. We discuss extensions and comment on the problem's computational complexity. In Section 8.3, we introduce the basics of the German electoral system, comment on specifics, and define the GPDP on the basis of presented legal requirements. In Section 8.4, we review the literature's solution approaches as well as available (re)districting software for PDP. We discuss the approaches' applicability to the considered German problem in Section 8.5. The paper closes with a conclusion in Section 8.6.

8.2 Political Districting Problem

A territory, e.g., a country or federal state, has to be partitioned into $k \in \mathbb{N}$ electoral districts meeting certain (legal) criteria. For this purpose, a discretization of the territory is given in the form of a partition into $n \in \mathbb{N}$, $n \gg k$ geographical units. These units can be, e.g., municipal associations, municipalities, city districts, or census tracts. Most PDP models assume that each unit has to be assigned to exactly one electoral district, i.e., a unit can not be split. This assumption is not a relevant restriction for applications in practice, as a main

requirement is not to split up existing administrative units like municipalities or city districts. We follow this assumption in our modeling.

After the introduction of a population graph in Section 8.2.1, a basic definition of the PDP is given in Section 8.2.2. In Section 8.2.3, the computational complexity of the PDP is analyzed.

8.2.1 Population Graph

To model PDP, it is a widely spread and quite natural idea to use a connected graph $G = (V, E)$ representing adjacencies. In the so-called *population graph* (or *contiguity graph*) G, a *node* $i \in V$ represents a geographical unit. Each node $i \in V$ is weighted with its population $p_i \in \mathbb{N}$. It is common to call V the set of *population units*. An undirected *edge* $(i, j) \in E$ with nodes $i, j \in V$ exists if and only if the corresponding areas share a common border. Depending on the given criteria, further parameters for the nodes and edges may be given. See Figure 8.1 for an exemplar population graph and its construction based on a given discretization of the territory.



Fig. 8.1: Constructing a population graph: population units as nodes, edges represent adjacent units (administrative boundaries: © GeoBasis-DE / BKG 2016).

8.2.2 Mathematical Model

Based on a given population graph $G = (V, E)$ and a number of electoral districts $k \in \mathbb{N}$, we give a basic definition of the PDP. It can be extended with further criteria and requirements.

The task is to find a districting plan $\mathcal{D}$, i.e., a partition of the set of population units V in electoral districts

$$\mathcal{D} = \{D_1, D_2, \ldots, D_k\} \text{ with disjoint } D_\ell \subseteq V \ \forall \ell \text{ and } \bigcup\nolimits_\ell D_\ell = V. \tag{8.1}$$

The basic PDP calls for electoral districts D_ℓ with contiguity and population balance. Continuity leads to the constraint

$$G[D_\ell] \text{ connected} \qquad \forall \ell \in \{1, \ldots, k\}, \tag{8.2}$$

where graph $G[D_\ell] := (D_\ell, E(D_\ell))$ with set of edges $E(D_\ell) := \{(i, j) \in E : i, j \in D_\ell\}$ is the subgraph of $G = (V, E)$ induced by node set $D_\ell \subseteq V$.

Population balance can be aimed for in the objective function or, as stated in the following, implemented as a range constraint limiting the amount of legal imbalance. Let $\bar{p}$ be the *average population of an electoral district*. As per definition, a district D_ℓ with $\sum_{i \in D_\ell} p_i = \bar{p}$ has perfect population balance. In most applications $\bar{p} = \frac{\sum_{i \in V} p_i}{k}$ holds.[4] For given bounds $\check{p}$, $\hat{p}$ with $\check{p} \leq \bar{p} \leq \hat{p}$ the districting plan $\mathcal{D}$ has to fulfill the range constraint of population balance

$$\check{p} \leq \sum_{i \in D_\ell} p_i \leq \hat{p} \qquad \forall \ell \in \{1, \ldots, k\}. \tag{8.3}$$

The basic PDP (8.1)–(8.3) can be extended by further criteria that are implemented in the form of an objective function or (range) constraints. The multiplicity of relevant criteria is extensively discussed in (Kalcsics et al., 2005; Webster, 2013; Williams, 1995), and (di Cortona et al., 1999, Chapter 10). Let c be a criterion, e.g. compactness. Let $c(\mathcal{D})$ and $c(D_\ell)$ be indicators that measure the criterion for a districting plan $\mathcal{D}$ and an electoral district D_ℓ, respectively. Note that the measurement of most criteria, e.g., compactness, is not clearly given by the legal requirements and is subject to discussion. The basic PDP is extended with criterion c by adding objective

$$\text{maximize / minimize} \qquad c(\mathcal{D}) \tag{8.4}$$

or adding district sharp range constraints with given bounds $\check{c}, \hat{c}$

$$\check{c} \leq c(D_\ell) \leq \hat{c} \qquad \forall \ell \in \{1, \ldots, k\}. \tag{8.5}$$

Range constraints $\check{c} \leq c(\mathcal{D}) \leq \hat{c}$ regarding the entire districting plan $\mathcal{D}$ are possible as well. Implementing more than one criterion as objective leads to a multi-criteria optimization problem.

8.2.3 Complexity

PDP (8.1)–(8.3) with its two basic criteria, contiguity and population balance, is equivalent to the following combinatorial task: Partition a node-weighted graph into a given number of connected and weight-restricted subgraphs. On paths and trees this problem can be solved in linear time (Lucertini et al., 1993) and polynomial time (Ito et al., 2012), respectively. For series-parallel graphs this problem gets NP-hard (Ito et al., 2006). Thus, the PDP is NP-hard in general.

Minimizing population imbalance $\sum_{\ell=1}^{k} |\bar{p} - \sum_{i \in D_\ell} p_i|$ in the objective of the PDP instead of limiting it with constraints (8.3) leads to an NP-hard optimization problem even on trees (De Simone et al., 1990).

The most frequently cited work in the context of the PDP's complexity is (Altman, 1997). Among other things, the author shows that computing a districting plan with maximally

[4] This equation does not hold for the German case in general (cf. Section 8.3): The GPDP decomposes into 16 independently solvable PDPs, each with the same $\bar{p}$ specified by the entire GPDP instance and not by the individual subproblem.

compact electoral districts is NP-hard. Thereby, population units are given as points in the plane and the considered decision problem asks if these points can be covered by k discs of a certain diameter (Johnson, 1982). Connectivity conditions are neglected.

8.3 German Political Districting Problem

In Germany, the effect of applying gerrymandering is comparatively small, because an electoral system with mixed-member proportional representation is applied. Nevertheless, German electoral districts are regularly revised and discussed.[5] Continually and even from an official authority, the very liberal and practically exploited deviation limits for a district's population are criticized (OSCE, 2009, 2013).

In Section 8.3.1, the basic elements of the German electoral system including the role of electoral districts is introduced. More details are given in the Federal Election Act (German: Bundeswahlgesetz, abbreviated to BWG, cf. Schreiber et al. (2017)) and on the website of the German Federal Returning Officer (n.d., online). In Section 8.3.2, the German legal requirements for electoral districts are presented in detail. Based on that and the basic PDP (cf. Section 8.2.2), the German Political Districting Problem (GPDP) is defined in Section 8.3.3. Its problem size is analyzed in Section 8.3.4.

8.3.1 Electoral System of Germany and the Role of Electoral Districts

In German federal elections, voters elect the members of the national parliament, which is called *Bundestag* (cf. Fig. 8.2). The Bundestag can be compared to the lower house of parliament, such as the House of Commons of the United Kingdom or the United States House of Representatives. The German election system is that of a so-called *personalized proportional representation*, i.e., proportional representation in combination with a candidate-centered first-past-the-post system in the electoral districts.

Every German voter has two votes. With the first one, voters select their favorite candidate to represent their electoral district in the parliament. Parties may nominate electoral district candidates, but independent candidates are also possible. Every candidate who wins one of the 299 electoral districts is guaranteed a seat. Approximately half the seats in the Bundestag are assigned by these *direct mandates*. The second vote is given to a party. The result of these votes determines the relative strengths of the parties represented in the Bundestag. This, together with the fact that every district winner has a seat for sure, forms the root of a major weakness in the German electoral system — the inability to determine the size of the parliament in advance. This is explained in the following.

[5] (i) 2002 German federal election: *Bundestagswahl 2002 - Die umstrittenen Wahlkreise*, S. Eisel and J. Graf, Konrad-Adenauer-Stiftung e.V., Jan. 2002.
(ii) 2017 North Rhine-Westphalia state election: *Im Essener Süden ist die SPD jetzt klar im Vorteil*, WAZ, online, 06/11/2015.
(iii) 2018 Hessian state election: *Beuthe-Wahlkreise*, Frankfurter Rundschau, online, 12/11/2017.



(a) Reichstag building in Berlin.



(b) Plenary chamber of the Reichstag building.

Fig. 8.2: The meeting place of the German parliament, the German Bundestag (`pixabay.com`).

From the legally prescribed total of 598 ($= 2 \cdot 299$) seats, the number of seats each party is entitled to is determined on the basis of the result of the second votes. Whenever a party won more direct mandates than it was entitled to by its share of second votes, the so-called *overhang mandates* arose. In other words, overhang mandates are direct mandates not covered by second votes. To maintain proportionality, which is given by the distribution of second votes, additional *balance mandates* for otherwise underrepresented parties are created. This leads to new seats exceeding the initially targeted total of 598. Thus, the size of the Bundestag depends on the outcome of the elections and is theoretically unbounded.

In the 2017 election, the described weakness led to a parliamentary size of historic dimension. The election yielded the largest Bundestag ever and, simultaneously, the largest democratically elected national parliament in the world. A total of 46 overhang mandates led to 65 additional balance mandates – the resulting Bundestag had 709 members instead of 598 as planned. This fact highlights the need for a reform. In order to limit growth in the number of seats, (political) scientists discuss whether to change the number of electoral districts in Germany (Behnke et al., 2017; Grotz and Vehrkamp, 2017; Pukelsheim, 2018). This implies numerous carefully considered adjustments to the districting plan. Hence, in Germany the PDP is more relevant than ever before, and suitable solution methods have to be part of current discussions.

8.3.2 Legal Requirements and Criteria for German Electoral Districts

The essential legal basis of electoral districts and their delimitation for German federal elections is documented in the Federal Election Act (BWG).[6] Those legal requirements have been complemented by the German Constitutional Court (German: Bundesverfassungsgericht, abbreviated to BVerfGE).[7] In Germany, the *number of electoral districts* $k \in \mathbb{N}$ stands at 299. In no particular order, the following principles shall be observed when partitioning Germany into electoral districts.

[6] Cf. section 3, subsection 1 BWG.
[7] Cf. BVerfGE 95, 335 in 1997, BVerfGE 121, 226 in 2008, BVerfGE 130, 212 in 2012.

(a) Decomposability into 16 subproblems Germany comprises 16 federal states (German: Bundesländer, cf. Table 8.1), denoted by the set S. The constitutional principle of federalism implies that electoral districts have to respect the federal states' boundaries. The number of electoral districts is apportioned among the states $s \in S$ by means of the *divisor method with standard rounding*. For more insights into apportionment methods, see (Balinski and Young, 1982; Pukelsheim, 2017). We denote the *number of electoral districts of state* $s \in S$ with $k(s) \in \mathbb{N}$, $k(s) \geq 1$. Of course, $\sum_{s \in S} k(s) = k$ holds. Overall, the GPDP can be subdivided into 16 independently solvable PDPs – one for each federal state.

(b) Population balance In order to comply with the principle of electoral equality, which is anchored in the German constitution, every electoral district must preferably comprise the same number of people. The law defines a two-staged deviation scope: A *tolerance limit*, stating that a deviation from the average district population should not exceed 15%. If the deviation is greater than 25% (*maximum limit*), the appropriate district's boundaries shall be redrawn. In determining population figures, only German people are considered.

(c) Contiguity Each electoral district should form a continuous area.

(d) Conformity to administrative boundaries Where possible, the boundaries of administrative subdivisions should be respected. This criterion supports conformity between the boundaries of electoral districts and already existing official and rooted regions, i.e., municipalities, and rural and urban districts.

(e) Continuity Between two consecutive elections, the adjustments of the electoral districts should be as small as possible. The aim is to achieve the greatest possible continuity in the districting plan.

8.3.3 Definition of German Political Districting Problem (GPDP)

Based on the legal requirements presented in Section 8.3.2, we distinguish between *hard* and *soft requirements* corresponding to the GPDP's constraints and objectives, respectively.

Decomposability into 16 subproblems (a), maximum population deviation limit in (b), and contiguity (c) are *hard constraints*. All remaining requirements are *soft constraints*: tolerance population limit in (b), administrative conformity (d), and continuity (e). We model the GPDP as 16 independently solvable multi-objective PDPs. Every individual soft constraint, i.e., objective criterion, influences others. For example, improving the conformity to administrative boundaries may need adjustments to the districts which is in contrast to the criterion of continuity. Officially, there is no explicit order or trade-off between the objective criteria in law nor court resolutions. Goderbauer and Wicke (2017) analyzed the districting plans of the 2013 and 2017 German elections in detail, and deduced the following descending order of importance for the objective criteria in practice: (e) continuity, (d) administrative conformity, and (b) tolerance population limit.

Given a suitable population graph $G = (V, E)$ of Germany, number of electoral districts $k(s) \in \mathbb{N}, k(s) \geq 1$ for each state $s \in S$ with $k := 299 = \sum_{s \in S} k(s)$, and average district population $\bar{p} := \frac{\sum_{i \in V} p_i}{k}$. The 16 German federal states $s \in S$ partition the set of population units $V = \bigcup_{s \in S} V_s$. For each state $s \in S$ a population graph $G_s := (V_s, E_s) := G[V_s]$ arises. Solving the GPDP is equivalent to solving the following PDP (cf. Section 8.2.2) for each $s \in S$.

Find

$$\mathcal{D}_s = \{D_1, \ldots, D_{k(s)}\} \text{ with disjoint } D_\ell \subseteq V_s \; \forall \ell \text{ and } \bigcup\nolimits_\ell D_\ell = V_s \tag{8.6}$$

so that

$$G_s[D_\ell] \text{ connected} \qquad \forall \ell \in \{1, \ldots, k(s)\} \tag{8.7}$$

$$0.75\,\bar{p} \leq \sum_{i \in D_\ell} p_i \leq 1.25\,\bar{p} \qquad \forall \ell \in \{1, \ldots, k(s)\} \tag{8.8}$$

while

max continuity to the previous election's districts (8.9)

max conformity between elect. districts and adm. boundaries (8.10)

max number of districts complying with 15% tolerance limit (8.11)

min amount of deviations between district population and $\bar{p}$ (8.12)

The union $\mathcal{D} := \bigcup_{s \in S} \mathcal{D}_s$ describes a *districting plan* for the GPDP. Objective criteria (8.9) and (8.10) refer to the most important soft constraints (e) and (d), respectively. The tolerance limit of population balance and the population balance (b) itself are implemented by objective criteria (8.11) and (8.12), respectively.

German law provides no measurement of these criteria. We deliberately omit to cast (8.9)–(8.12) in mathematical terms. Determining suitable measurement functions for especially the two most important objectives in German practice, continuity and administrative conformity, does not seem to be a straight-forward task. We additionally elaborate the literature review in this work to record suitable measurements for the GPDP's objectives.

With regard to administrative conformity, Goderbauer and Wicke (2017) point out that, in the German case, this objective deals with at least the following hierarchical divisions (cf. Figure 8.3): municipalities, municipal associations, rural and urban districts, and governmental regions. The rural and urban districts are most comparable in population numbers to an electoral district. On the one hand, there are electoral districts that contain several urban/rural districts completely. On the other hand, some urban/rural districts are divided into multiple electoral districts. Apart from large cities, municipalities and municipal associations are usually too small to form an electoral district. Governmental districts comprise several electoral districts. A measurement for administrative conformity has to consider these characteristics.

8.3.4 Size of German Political Districting Problem

As mentioned, the GPDP decomposes into 16 independently solvable PDPs. Table 8.1 gives an overview of the sizes of the PDPs.

The column entitled Gem (=Gemeinden in German) indicates the number of municipalities, giving an impression of the order of magnitude of population units in the population graphs. Since there are German cities (being in particular municipalities) with a population greater than the maximum population limit $1.25\,\bar{p}$, these cities have to be divided at least on the level of their boroughs to facilitate a feasible districting plan. Since the GPDP is defined on the basis of indivisible population units (cf. Eq. (8.6)), this leads to more population units than municipalities. As has been pointed out already, the conformity between electoral districts and administrative boundaries is an important objective and involves several levels of administrative units, e.g., rural and urban districts, municipal associations. For orientation purposes, Table 8.1 provides the numbers of units at different administrative levels. The administrative divisions, along with their acronyms used in Table 8.1, are given in Figure 8.3. See (Goderbauer et al., 2016) for illustrations of a municipality-level population graph for each German federal state and information about the number of edges in these graphs.

	federal state	German population	$k(s)$	number of units at administrative level			
				RB	Kr	VB	Gem
01	Schleswig-Holstein	2 680 368	11	1	15	173	1 112
02	Hamburg	1 521 536	6	1	1	1	1
03	Niedersachsen	7 292 572	30	1	46	434	998
04	Bremen	569 478	2	1	2	2	2
05	Nordhein-Westfalen	15 758 084	64	5	53	396	396
06	Hessen	5 293 234	22	3	26	430	430
07	Rheinland-Pfalz	3 671 099	15	1	36	192	2 306
08	Baden-Württemberg	9 372 306	38	4	44	462	1 103
09	Bayern	11 372 546	46	7	96	1 426	2 099
10	Saarland	905 965	4	1	6	52	52
11	Berlin	2 972 331	12	1	1	1	1
12	Brandenburg	2 395 418	10	1	18	200	417
13	Mecklenburg-Vorpommern	1 553 846	6	1	8	116	754
14	Sachsen	3 926 810	16	1	13	312	426
15	Sachsen-Anhalt	2 160 479	9	1	14	122	218
16	Thüringen	2 090 264	8	1	23	219	849
	Germany	73 536 336	299	31	402	4 538	11 164

Tab. 8.1: German population, number of electoral districts $k(s)$ of federal state $s \in S$ at federal elections in 2017, number of units at different administrative levels. German population as of 2015/09/30, based on Census 2011 and number of units at different administrative levels as of 2016/09/30 (© Statistisches Bundesamt, Wiesbaden, 2016). See Fig. 8.3 for used acronyms in last four columns.

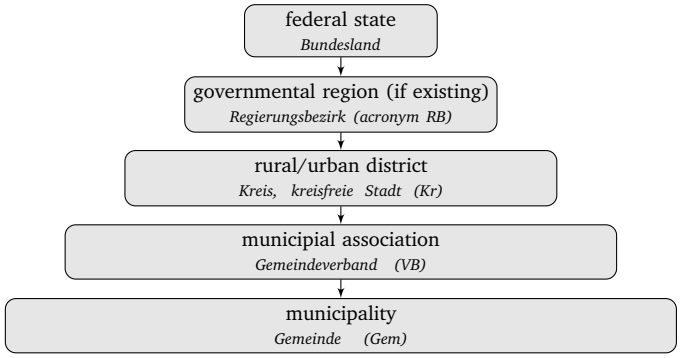


Fig. 8.3: Hierarchical administrative divisions in Germany.

8.4 Literature Review: Solution Approaches and Software

In this survey, we focus on work proposing solution approaches with explicit reference to the PDP by mentioning keywords such as *political (re)districting*, *non-partisan districting*, or *electoral district design*. This leads us to a set of 49 publications. Each of these publications is represented by a point in Figure 8.4, indicating its year of publication and the number of citations. Do note that some points overlap each other. In the next sections, we restrict our attention to the 28 black, labeled publications. These curated papers provide pioneering or ground-breaking results; mainly recent ones offer promising new approaches. The 21 remaining publications (grey dots) are not discussed further in this overview, as they tend

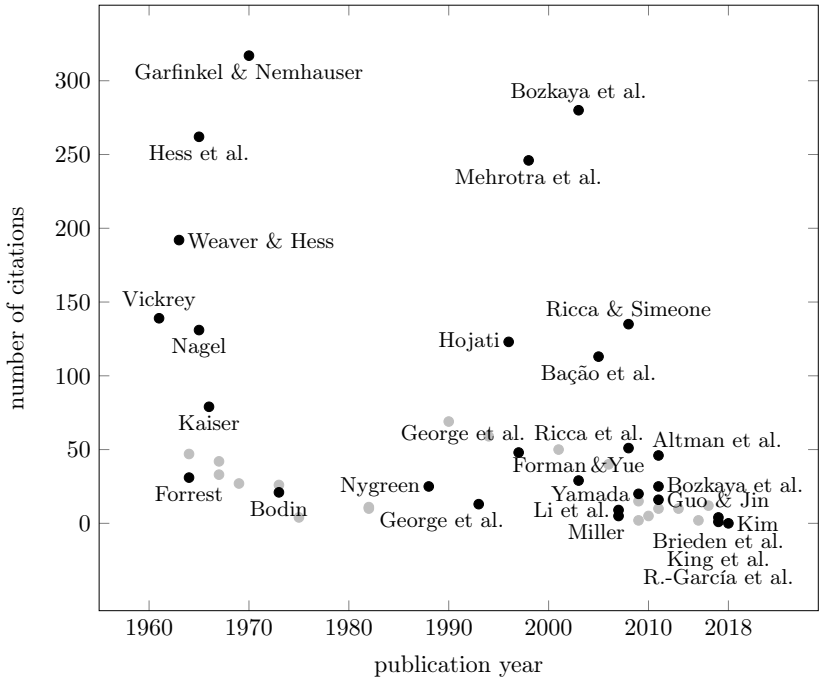


Fig. 8.4: Publications on PDP, its year of publication, and number of citations (source of number of citations: Google Scholar as of Oct. 6, 2018).

to contribute to applications rather than methodology. They mostly take up the work of the discussed PDP papers or propose methods and models with only little modifications to previous (PDP) results.[8] When separating the grey papers, we ensure that they do not contain any contributions to the measurement of the GPDP criteria. The gray publications are not cited in the next sections but listed in the "Further Reading" bibliography in the appendix in Section 8.7.

Other literature reviews on the PDP are (Papayanopoulos, 1973; Ricca et al., 2011; Williams, 1995) and (di Cortona et al., 1999, Chapter 12).

In the following Section 8.4.1, the PDP literature and its solution approaches are discussed. In Section 8.4.2 software tools for redistricting are presented.

8.4.1 Solution Approaches for PDP in Literature

Exact Methods

Since the PDP is NP-hard (cf. Section 8.2.3), most approaches are heuristics and assure appropriate computational effort. Nevertheless, there are some *exact methods* for solving the PDP. Garfinkel and Nemhauser (1970) presented a two-phase algorithm and solved instances of up to 40 population units and 7 districts in a reasonable amount of time. After generating *all* feasible electoral districts, a set partitioning model was used to provide a districting plan. This implicit enumeration approach was not sufficient for solving large-scale instances. (Garfinkel and Nemhauser, 1970) is the most cited publication in the surveyed literature of the PDP (cf. Figure 8.4).

An algorithm comparable with the work of Garfinkel and Nemhauser was presented by Nygreen (1988). Using implicit enumeration and a set partitioning problem, the author grouped 38 parliamentary districts of Wales together into 4 European electoral districts. In the conclusions of the paper, the author noted that the equivalent PDP for England (with $\geq$ 500 parliamentary districts, $\geq$ 60 European electoral districts) would be too large for the approach to terminate in reasonable computation time.

Li et al. (2007) used a quadratic programming model to redistrict New York. The model's decision variables are continuous, denoting the percentage of assigning a population unit to an electoral district. The authors thus assumed to be able to split population units at any position. This is contrary to our definition of the PDP given in Section 8.2.2.

Kim (2018) applied a contiguity model proposed by Williams (2002a,b) to solve PDPs on artificial grid instances. Assuming planarity of the used graph, Williams (2002b) developed a remarkably small and strong mixed-integer programming model that ensures connectivity of node-induced subgraphs. However, Validi and Buchanan (2018) have shown, that the

[8] An exception to this is the work of Chou and Li (2006a) (grey dot, 40 citations). The authors carry out a simulation using a q-state Potts model that has been in use in statistical physics since the 1950s but has not yet been mentioned in connection with the PDP.

formulation of Williams is incorrect. Fortunately, the same authors provide a simple fix. Based on this, the work of Kim (2018) needs to be revised.

Exact/Heuristic: Column Generation

Since the already mentioned enumeration approach of Garfinkel and Nemhauser (1970) is not suitable to deal with larger instances, Mehrotra et al. (1998) evolved the idea into a *column generation/branch and price* procedure. They considered more criteria and got faster results, without reducing the quality of the obtained solutions in any significant way. The procedure generated suitable electoral districts iteratively in the subproblem of a column generation approach. In fact, districts are required to be subtrees of shortest path trees (Zoltners and Sinha, 1983) which induces connectedness and compactness. The master problem of the column generation approach is a set partitioning problem. In this problem, k districts are selected out of the set of already generated feasible districts. In general, the technique of column generation and of branch and price can be used to solve optimization problems exactly (Lübbecke and Desrosiers, 2005). Even so, the algorithm of Mehrotra et al. (1998) remains a heuristic, since some contiguous but most likely irrelevant districts are excluded due to the contiguity model used.

Heuristic: Greedy

Probably the first *heuristic approach* for the PDP was a *multi-kernel growth method* introduced by Vickrey (1961). Vickrey's publication in a political journal contained a quite rudimentary description of a *greedy algorithm*. Bodin (1973), who presented another multi-kernel procedure, was one of the first to mathematically introduce the concept of a population graph.

The main steps of multi-kernel growth methods are illustrated in Figure 8.5. First, the centers of the districts must either be given or found by a preprocessing step (Fig. 8.5, left). Next, the districts grow from their respective centers by adding neighboring units according to a chosen algorithm (Fig. 8.5, middle). The procedure stops when every unit

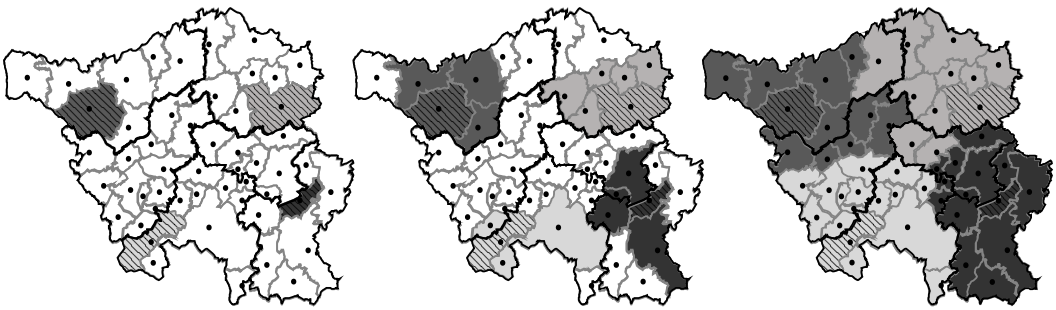


Fig. 8.5: Greedy heuristic (boundaries: © GeoBasis-DE / BKG 2016):
Left: Every district has a given starting point (crosshatched areas).
Middle: Add neighbouring population units to the districts.
Right: Stop when every unit is assigned to one district.

is assigned to one district, hopefully producing a feasible districting plan (Fig. 8.5, right). Although, multi-kernel growth methods are fast, they usually generate districting plans with a low population balance as well as a low compactness factor due to left-over population units during the growth process. Therefore, a postprocessing step is necessary to produce satisfying results.

Heuristic: Location-Allocation

Weaver and Hess (1963) pioneered in applying a *location-allocation* approach to solve the PDP. In a second paper, they formalized their work (Hess et al., 1965). In several publications, other authors used their model as a basis.

This kind of method consists of repeating location and allocation steps until the assignment of units to districts does not change anymore. As shown in Figure 8.6, a location-allocation step takes an assignment of units to districts as input (Fig. 8.6, left). Thereafter, the centers of the current districts are located according to some measurements (Fig. 8.6, middle). The output is a new mapping from each unit to its nearest new center (Fig. 8.6, right). Afterward, this new assignment is used as an input for the next iteration. To ensure population balance, some models allow assigning population units to more than one district, e.g., with a certain percentage. To resolve those splits, a second algorithm is implemented. All in all, these location-allocation methods can not ensure producing connected districts.

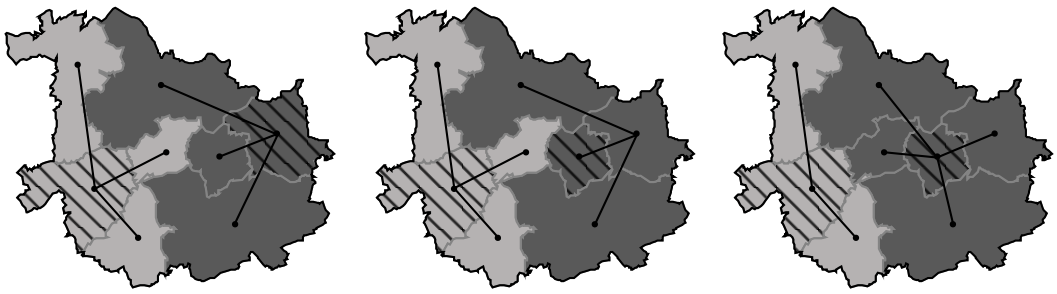


Fig. 8.6: Location-allocation step/heuristic (boundaries: © GeoBasis-DE / BKG 2016):
Left: Allocate points to nearest (given) center.
Middle: Locate new centers of the districts.
Right: Allocate points to nearest new center.

George et al. (1993, 1997) expanded the location-allocation approach of Hess et al. (1965) by solving a minimum cost network flow problem. In their network, population units are assigned to new district centers in the following manner. Each population unit i is represented as a node with supply p_i, its population. Each electoral district is represented as a node with no demand or supply, and all electoral district nodes are connected to a super sink node with demand $\sum_i p_i$. Flow from every population unit to the super sink is possible through each electoral district. With respect to flow balance equation and nonnegativity constraints, a minimum cost flow is computed and determines how population units are allocated to electoral districts. The authors point out several options to choose the arc costs in that network and to consider various types of criteria. Population units that are allocated

to more than one electoral district, i.e., splits, are reassigned solely to the district with the highest proportion of population for that unit.

Hojati (1996) used a Lagrangian relaxation method from the general location-allocation literature to find the district centers and resolved the occurring splits using a sequence of capacitated transportation problems.

Heuristic: Local Search

Nagel (1965) and Kaiser (1966) solved the PDP by transferring and swapping population units between neighboring electoral districts, as described in Figures 8.7 and 8.8. The candidate districts involved in a swap/transfer are chosen according to some criteria such as size and compactness (Fig. 8.7 and 8.8, left). Units to swap/transfer are determined using an objective function calculating the benefits of the resulting solution (Fig. 8.7 and 8.8, middle). Population units with a best score are swapped/transferred (Fig. 8.7 and 8.8, right). Once again, the algorithm stops when no improving candidates can be found or a stop criterion is reached. The swap/transfer method can be seen as an early approach to the modern *local search heuristics*.

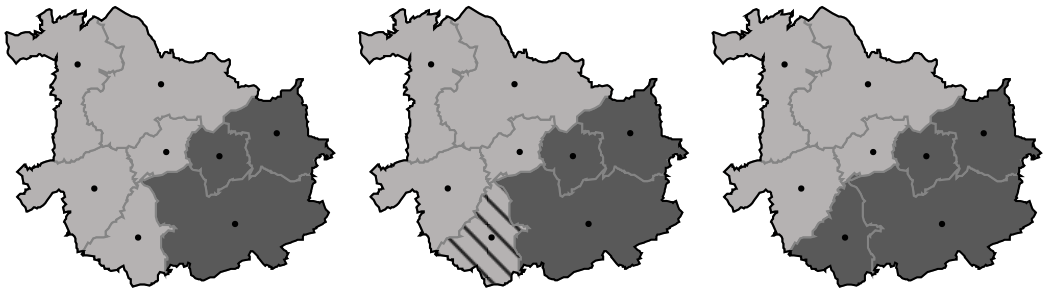


Fig. 8.7: Transfer step, local search heuristic (boundaries: © GeoBasis-DE / BKG 2016):
Left: Choose a "donor" (light gray) and "receiver" district (dark gray).
Middle: Find best unit to transfer.
Right: The chosen unit is now assigned to the receiver district.

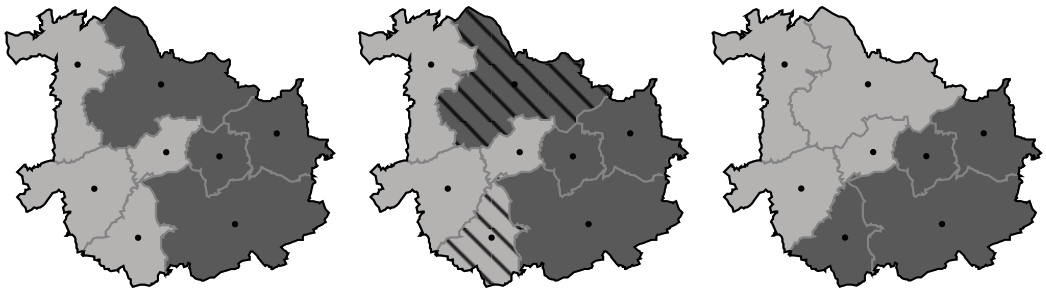


Fig. 8.8: Swap step, local search heuristic (boundaries: © GeoBasis-DE / BKG 2016):
Left: Choose two districts that will swap a population unit.
Middle: Find best units to swap.
Right: Swap the chosen units between the two districts.

Bozkaya et al. (2003) proposed a tabu search algorithm considering a group of criteria in the objective function. The algorithm is enhanced with an adaptive memory procedure (Rochat and Taillard, 1995) that constantly combines districts of good solutions to construct other high quality districting plans. This concept is also known in the field of genetic algorithms. In (Bozkaya et al., 2011), the same authors report on their successful implementation of new electoral districts for the city council elections in Edmonton, Canada.

Yamada (2009) formulated the PDP as a minimax spanning forest problem and presented two local search algorithms operating on trees on the population graph. Owing to the tree model, the algorithms guarantee contiguity of the obtained districts.

Ricca and Simeone (2008) applied several local search variations to the PDP and compared their respective performance in a case study. They determined advantages and disadvantages of these methods.

King et al. (2017) improved local search approaches for the PDP by proposing a procedure which substantially reduces computations needed for the connectivity check. They use a framework called geo-graph (King et al., 2015, 2012). Applying this concept decreases the contiguity-related computations by at least three orders of magnitude compared to simple graph search algorithms like breadth-first search and depth-first search as used by, e.g., Ricca and Simeone (2008). To apply the geo-graph model, assumptions are made concerning the population units, especially the geometry of the units' boundaries. Forbidden are: (i) units whose area is fully nested inside the area of another unit and (ii) units with several non-contiguous areas. King et al. (2017) proposed preprocessing methods to eliminate violations of these assumptions. To evaluate the performance of the geo-graph model, a simple steepest descent local search algorithm is implemented. The authors were able to handle instances with up to $340\,000$ population units and 29 electoral districts.

Heuristic: Nature-inspired and Probabilistic Algorithms

Forman and Yue (2003) proposed a *genetic algorithm* to solve the PDP. Their work is based on existing genetic algorithms for the traveling salesman problem (Larranaga et al., 1999). Bação et al. (2005) picked up on the same idea, although they decided to use a clustering heuristic as a basis for their procedure. In a comparative study, Rincón-García et al. (2017) analyzed the performance of four different *nature-inspired and probabilistic metaheuristics* for PDP: simulated annealing, particle swarm optimization, artificial bee colony, and a method of musical composition.

Heuristic: Geometric

As the PDP asks for a partition of the plane into districts, it seems reasonable to apply methods from the field of *computational geometry*. Forrest (1964) was the first to work on this for the PDP. Unfortunately, no explicit algorithm or computational results are given for the proposed method of diminishing halves. Other authors took up the idea and developed

methods based on the concept of *Voronoi diagrams* (Aurenhammer and Klein, 2000; Okabe et al., 2009). Voronoi regions are inherently compact and contiguous, which is why they are often named in the context of striving against gerrymandering.

Miller (2007) applied an algorithm for (centroidal) Voronoi diagrams on data of the US state Washington. As the author puts no population constraints on the Voronoi diagram, the method creates districts with bad population balance.

In contrast to Miller, who considered the territory as a continuous area, Ricca et al. (2008) proposed a Voronoi heuristic for the PDP on the basis of the population graph. They define a graph-theoretic counterpart of the ordinary Voronoi diagram, denoted as discrete weighted Voronoi regions. After applying a heuristic location procedure to define k district centers, the Voronoi regions are determined. The distance between a pair of population units is defined as the length of a shortest path with respect to road distances. Thereafter, an iterative procedure starts incorporating population balance. Distances are updated based on the population of computed regions. This adjustment supports pushing units of (population-wise) heavy districts in directions of light ones. Several variants of the algorithm are executed on randomly generated rectangular grids and instances of Italian regions. The presented computational results are note worthy, especially due to the bad population balance.

Brieden et al. (2017), who presented a paper on constrained clustering, applied their presented approaches on data of parts of German federal states (leaving out larger cities) to achieve districting plans. Their work is based on the close connection between geometric diagrams and clustering. In fact, using the duality of linear programming, the authors work out a relationship between constrained fractional clusterings and additively weighted generalized Voronoi diagrams. First, district centers are heuristically defined, e.g., using the centroids of the current districts in order to obtain similar new districts. A linear program with a population equality constraint is solved with a state-of-the-art solver to achieve fractional assignments of population units to district centers. To come up with integral assignments and to ensure connected districts, some post processing is needed. The centerpiece of this generally described approach is mainly the choice of metrics or more general distance measures. It is worth highlighting that for each cluster, for example, an individual *ellipsoidal* norm can be used. Thus, information regarding current electoral districts can be integrated to achieve a low ratio of voter pairs that used to share a common district but are now assigned to different ones. Depending on the applied metric and post processing, the presented computations need between seconds and several hours to finish.

Case studies and considered requirements of GPDP Every considered publication (except for (Forrest, 1964; Vickrey, 1961)) contains a case study with (real-world) data. Table 8.2 provides a summary of applications and problem sizes. Additionally, Table 8.3 offers an overview of the criteria considered. Beyond the criteria mentioned in Table 8.3, Nagel (1965) and King et al. (2017) also discussed political balance, and Bozkaya et al. (2011, 2003) considered socio-economic homogeneity. A detailed discussion of the implemented measurement functions concerning the requirements of GPDP (cf. Section 8.3) is provided in Section 8.5.

method	citation	application	number of population units	number of electoral districts
exact methods	Garfinkel et al. (1970)	Washington, USA	39	7
	Nygreen (1988)	Wales	38	4
	Li et al. (2007)	New York, USA	62	29
	Kim (2018)	artificial data, grid graph	25, 100	3
col. generation	Mehrotra et al. (1998)	South Carolina, USA	46	6
greedy	Vickrey (1961)	–	–	–
	Bodin (1973)	Arkansas, USA	75	3, 5, 9
location/ allocation	Hess et al. (1963, 1965)	a county in Delaware, USA	?	6
	Hojati (1996)	Saskatoon, Canada	42	11
	George et al. (1993, 1997)	New Zealand	35 000	100
local search	Nagel (1965)	Illinois, USA	90	18
	Kaiser (1966)	Illinois, USA	101	12
	Bozkaya et al. (2003, 2011)	Edmonton, Canada	400	12
	Ricca, Simeone (2008)	5 regions in Italy	246 – 1 208	8 – 28
	Yamada (2009)	Kanagawa Prefecture, Japan	49	17
	King et al. (2017)	4 states in USA	147 565 – 339 933	3 – 29
nature-insp./ probabilistic	Forman and Yue (2003)	3 states in USA	70 – 350	5 – 13
	Bação et al. (2005)	Lisbon, Portugal	52	7
	R. García et al. (2017)	8 states in Mexico	192 – 860	5 – 40
geometric	Forrest (1964)	–	–	–
	Miller (2007)	Washington, USA	1 318	9
	Ricca et al. (2008)	4 regions in Italy	305 – 1 208	8 – 28
	Brieden et al. (2017)	(parts of) 13 states of Germany	52 – 2 304	4 – 48

Tab. 8.2: PDP solution approaches in literature and their case study with problem size.

method	citation	criteria considered in objective and/or constraints					
		contiguity	population balance	compactness	adm. boundaries	continuity	other
exact	Garfinkel et al. (1970)	•	•	•			
	Nygreen (1988)	•	•	•	•		
	Li et al. (2007)	•	•	•			
	Kim (2018)	•	•	•			
column gen.	Mehrotra et al. (1998)	•	•	•	•		
greedy	Vickrey (1961)	•	•	•			
	Bodin (1973)	•	•				
location/ allocation	Hess et al. (1963, 1965)	•	•	•			
	Hojati (1996)	•	•	•			
	George et al. (1993, 1997)	•	•	•	•	•	
local search	Nagel (1965)	•	•	•			•
	Kaiser (1966)	•	•	•			
	Bozkaya et al. (2003, 2011)	•	•	•	•	•	•
	Ricca, Simeone (2008)	•	•	•	•		
	Yamada (2009)	•	•				
	King et al. (2017)	•	•	•			•
nature-insp./ probabilistic	Forman and Yue (2003)	•	•	•			
	Bação et al. (2005)	•	•	•			
	R.-García et al. (2017)	•	•	•			
geometric	Forrest (1964)	•	•	•			
	Miller (2007)	•		•			
	Ricca et al. (2008)	•	•	•			
	Brieden et al. (2017)	•	•			•	

Tab. 8.3: PDP solution approaches in literature and considered criteria. A • indicates that the criteria of the column is considered in the cited work, either in an objective or (also) as constraints.

8.4.2 Districting Software

Redistricting software became the predominant tool during the (re)districting process (Altman et al., 2005; Altman and McDonald, 2011b). On the one hand, software is used to analyze current districting plans, organize and evaluate population data, and modify plans manually. On the other hand, driven by the methods and algorithms for the PDP, more and more software provides automated and optimization-based redistricting. A downside is that these is professional software, which is designed to assist decision-makers to perform gerrymandering. In all conscience, we leave out software packages supporting the execution of the malpractice of gerrymandering.

Most of the redistricting software tools are based on a geographic information system (GIS). A GIS allows displaying, managing, analyzing, and capturing characteristics of spatial or geographic data. While editing, e.g., a districting plan, the user perceives the consequences of every change in real time. Altman et al., 2005 reported that in 2001 every US American state (except for Michigan) officially used some kind of redistricting software. Nevertheless, *automated* software was officially employed by very few states (Altman et al., 2005).

In Germany, the Electoral District Commission and its chairman, the Federal Returning Officer, use a software tool called WEGIS (acronym for the German word Wahlkreis-Einteilungs-GIS) (Heidrich-Riske, 2014). It was developed in-house as a plugin for ArcGIS, a commercial software distributed by the company Esri. WEGIS has been in use since the preparation for federal elections in 2002. In those days, the number of German electoral districts was reduced from 328 to 299. This decision triggered the need for a software tool for supporting redistricting. WEGIS does not provide automated redistricting. It is used for displaying and exporting information, and for facilitating manual redistricting. The software tool is not available to the public. Suggestions for delimiting electoral districts posed by, e.g., political parties, is performed in-house and evaluated by request (Heidrich-Riske and Krause, 2015). The ArcGIS plugin is specifically tailored to meet German legal requirements. For example, after importing a districting plan and population data, districts exceeding the 15% soft population deviation limit are highlighted in color. This enables the user to quickly spot all districts that should be examined and possibly redrawn.

In the remaining part of this section, we present available software, both commercial and open source, which can be used in the (re)districting process. We distinguish between software that provides an algorithm that can automatically form new districting plans and software enabling only manual modifications. Some of these redistricting tools come with an accompanying scientific publication. More and more tools have become available as web-based applications ensuring that redistricting software is available to millions of non-expert users. However, some software packages are not available to the public, but only to officials or decision-makers of state administrations.

Assisting redistricting by hand

Esri and Caliper are two commercial software vendors that provide licenses for standalone as well as online versions of their redistricting software (Caliper, n.d., online; Esri, n.d., online). Both systems assist in manual redistricting and are not able to form legal districting plans automatically (Altman and McDonald, 2011a, Sec. 6.1). Owing to their pricing, these programs are not practical for private individuals. Esri and Caliper rather address state and local governments, legislators, and advocacy groups. Several US states used their software in the 1990 and 2000 congressional redistricting (Altman et al., 2005).

Dave's Redistricting App (Bradlee, n.d., online), a free web-based tool, has been developed by an individual software engineer since 2009. Data of every US state (as of 2000 and 2010) is provided and embedded into a mapping service. Furthermore, the population units (voting districts and block groups) can be highlighted in color based on demographic aspects or recent election results. Besides ready-to-use data of US states, own data can be imported. Unfortunately, the tool does not support the common shapefile format. The user can draw electoral districts onto the map and receives population numbers and votes.

Another software package for manual redistricting is DistrictBuilder (not to be confused with the software tool of Bozkaya et al. (2011), which is named exactly the same in their publication). The tool is developed under supervision of authors Altman and McDonald, who have already been cited in the paper. The open-source project allows hosting of online public redistricting initiatives and competitions (Altman and McDonald, 2011b). A software partner builds custom applications as per request.

In order to analyze the 2015 Malaysian districting plan, a non-governmental organization developed a plugin for QGIS, an open-source GIS (Tindak Malaysia, n.d., online). The free tool comes with population and geographical data of Malaysian states and electoral districts, and enables redistricting by hand, providing several statistics.

Optimization-based redistricting software

AutoBound, distributed by Citygate GIS (formerly known as Digital Engineering Corporation), is a software tool that promises "intelligent automated redistricting" (Citygate GIS, n.d., online). The product website gives no information about underlying algorithms. According to Altman et al. (2005), a simple greedy multi-kernel growth algorithm as sketched in (Hejazi and Dombrowski, 1996) is used. The vendor states that AutoBound was used for 2000 congressional redistricting in over 30 US states (according to Altman et al. (2005) in only 19 US states) and in Canada for country wide redistricting most recently in 2011. Unfortunately, a demo version of this software is not available.

In a journal paper, Guo and Jin (2011) presented a software called iRedistrict. The system provides optimization-based automated redistricting. Its underlying heuristic is based on a tabu search algorithm, whose performance is evaluated in a study (Iowa, USA: 99 population units, 5 districts). The authors recognize the indispensability of human judgment in presence

of criteria that may be vaguely defined and therefore not uniquely quantifiable. The user of iRedistrict can define the weights of the multi-criteria objective, is authorized to select sets of population units to be handled as indivisible units, and can also manipulate computed plans manually. Furthermore, the tool provides useful and customized plots to analyze each objective. iRedistrict can be purchased via the company ZillionInfo as a commercial product (ZillionInfo, n.d., online). Unfortunately, neither a demo version nor pricing information is available on the website.

A tool called BARD (Altman and McDonald, 2011, online) was presented by Altman and McDonald (2011a) in a journal paper. The name is an acronym for "Better Automated Redistricting". BARD is an open-source software package and comes in the form of a module for the R programming language project for statistical computing. The software tool utilizes different procedures for automatically generating plans. The following four metaheuristics are available to refine them: simulated annealing, genetic algorithms, tabu search, and greedy randomized adaptive search (Altman and McDonald, 2011a, Section 6.3). Unfortunately, the software has not been updated since 2011 and is no longer available through the official R module repository.

In Section 8.4.1, we reviewed the work of Bozkaya et al. (2011, 2003). Their tabu search heuristic with an adaptive memory procedure was implemented as a plugin for ArcGIS. The authors described how it was used to assist the official designing process of new electoral districts for the city of Edmonton, Canada. One of the authors informed us that their software works fine with ArcGIS version 8 (Bozkaya, 2016). Unfortunately, this outdated version is not available anymore and the plugin's code has not been upgraded to work with the newest versions of ArcGIS, i.e., as of October 2018, ArcGIS 10.6.1.

The open-source software Auto-Redistrict (Baas, n.d., online) is developed by a private person and includes a genetic algorithm to form districting plans. Details about the genetic algorithm are available on the software's homepage (Baas, n.d., online). It is possible to load custom shapefiles, to adjust weights of the criteria and to enforce the latter via constraints. It is also possible to shift population units from one district to another by hand. The tool is regularly updated and allows oversight of improvements made by the genetic algorithm in real time as solutions are constantly displayed. Unfortunately, Auto-Redistrict does not support population deviation limits, neither as constraint nor as objective. Just the minimization of squared deviations is possible. Furthermore, one can request equal population as a constraint. Auto-Redistrict supports compactness and some "fairness criteria" concerning bias on the basis of election data (Baas, n.d., online).

In summary, it is unsatisfactory that the majority of presented software tools providing automated redistricting are not available to us for testing. Either, the plugins are outdated and not compatible with current versions of the underlying software, or the districting tools are distributed commercially having no demo version. As presented above, Auto-Redistrict (Baas, n.d., online) is an exception. Including the tools that assist manual redistricting, this software survey highlights that it is a good choice to develop districting software as a plugin of a GIS and to benefit from its features and already implemented functionality. Choosing an open-source GIS, e.g., QGIS, enables any interested person to utilize it.

8.5 Discussion and Suitability Evaluation for GPDP

To evaluate the suitability of the reviewed PDP solution approaches (cf. Section 8.4.1) for solving the GPDP, we bring together each publication's considered criteria and the GPDP's constraints as well as objectives. In contrast to Table 8.3, we will make a careful distinction between whether a criterion is implemented as a constraint or as an objective. Furthermore, we discuss if the concrete measurement of the criteria is rigorous enough for the GPDP. Table 8.4 contains a summary of the evaluation. The first two columns of Table 8.4 indicate the superordinate approach as well as the author(s), whereas the remaining columns represent the GPDP's essential criteria (8.7)–(8.8) and objectives (8.9)–(8.12) (cf. Section 8.3.3). For each criterion we analyze, if it is considered in the paper's algorithm or model. A "+" indicates that the criterion is implemented in such a way that it could be used without changes for the GPDP. An "o" means that the criterion is taken into account but in a way that is not applicable to the GPDP. No cell entry translates into an omission of the respective criterion. However, this does not imply that it is impossible to adapt the method in this regard.

In the following, we discuss our findings in detail. We take a closer look at literature's measurements of the GPDP's objectives (8.9) and (8.10), i.e., continuity and administrative conformity, since we did not cast them in mathematical terms in Section 8.3.3 and this does not seem to be trivial either.

The size of the GPDP instances are by far greater than the instances solved by exact methods in the literature (cf. Table 8.1 and 8.2). Since these results are up to almost 50 years old, one should investigate if and to what extent today's solvers and computer technologies can handle larger instances using these models. There is no doubt that the exact method of Garfinkel and Nemhauser (1970) becomes more promising through the reasonable embedding of Mehrotra et al. (1998) in a branch and price approach. Mehrotra et al. (1998) apply a postprocessing step in which population between districts is shifted in line with the objective of minimizing the number of split population units, in this case counties. Overall, this can be seen as an weak implementation of administrative conformity which is clearly not rigorous enough for the GPDP.

Nygreen (1988) considers conformity to administrative boundaries insofar as the author forces all population units of the same city to belong to the same electoral district. This implementation is insufficient for the GPDP since the criterion of administrative conformity is far more comprehensive in the German case. The model of Li et al. (2007) is not compatible with the definition of the GPDP either. For example, there is no guarantee that this formulation will produce contiguous districts, although this is favored in the objective function. From a practical perspective, their assumption to split population units at any position is debatable. This requires additional effort to transform a solution into a legal districting plan.

The contiguity model of Williams (2002a,b) used by Kim (2018) should be pursued further, of course following the note by Validi and Buchanan (2018). The formulation could also be implemented in a pricing problem as in (Mehrotra et al., 1998) to ensure contiguity

method	citation	constraints (8.7) and (8.8)		objectives (8.9)–(8.12)			
		contiguity	max pop. deviation	continuity	adm. boundaries	tol. pop. deviation	pop. balance
exact	Garfinkel et al. (1970)	+	+				+
	Nygreen (1988)	+	+		o		+
	Li et al. (2007)	o	+				o
	Kim (2018)	+					+
column gen.	Mehrotra et al. (1998)	+	+		o		o
greedy	Vickrey (1961)	o	+				o
	Bodin (1973)	+					+
location/ allocation	Hess et al. (1963, 1965)	o	+				
	Hojati (1996)	o	+				
	George et al. (1993,1997)	o	+	+	o	+	+
local search	Nagel (1965)	+	+				
	Kaiser (1966)	o	+				+
	Bozkaya et al. (2003,2011)	+	o	+	o	+	+
	Ricca, Simeone (2008)	+			o		+
	Yamada (2009)	+					+
	King et al. (2017)	+	+				+
nature-insp./ probabilistic	Forman and Yue (2003)	o	o			+	
	Bação et al. (2005)	o	o				+
	R.-García et al. (2017)	o	o				+
geometric	Forrest (1964)	o	o				o
	Miller (2007)	+					
	Ricca et al. (2008)	+					o
	Brieden et al. (2017)	+		o			+

Tab. 8.4: Overview of the criteria considered in the literature.
+: Criterion considered and implemented according to the formulation of the GPDP.
o: Criterion considered, but not rigorously enough for the GPDP.

of generated electoral districts. This would remove the disadvantage of the model of Mehrotra et al. (1998), since Williams' formulation encompasses all connected subgraphs while Mehrotra et al. (1998) ignores some. An exact solution method based on branch and price would be the outcome. As stated, Williams (2002b) utilizes planarity of the used graph. For the GPDP, the population graph is not always planar. There are municipal areas that do not themselves form a contiguous area, and this results in a population graph not being planar (Goderbauer et al., 2016, Example 8.3). However, one can imagine some preprocessing to obtain planarity in the GPDP instances.

All considered multi-kernel growth methods are not suitable for the German case due to the wide diversity of criteria and objectives considered in the GPDP. It seems to be inappropriate to incorporate more criteria than contiguity and population balance in such greedy algorithms. A greedy setting seems to be unqualified especially for considering conformity to hierarchically structured administrative boundaries. However, since such algorithms are very fast, they may be used to compute a starting solution. For example, this is the case in (Bozkaya et al., 2011, 2003).

Location-allocation approaches mentioned in the literature on the PDP have a simple but fundamental drawback: They do not ensure contiguity of resulting electoral districts. Nevertheless, the location-allocation method of George et al. (1993, 1997) managed to consider more or less all criteria and objectives of the GPDP. As mentioned before, George et al. solves a minimum-cost network flow problem in the allocation step. Using different arc costs in the underlying network, almost every imaginable objective can be modeled. To give an example, George et al. penalizes each crossing of natural barriers (e.g., mountain ranges, rivers) with a constant. However, this does not encompass the multilevel GPDP objective of conformity to administrative boundaries. To support continuity in the districting plan, it is penalized if a population unit is assigned to a district different from a previously given districting plan. This penalty is implemented as arc costs of the mentioned network and depends on the distance between population-wise centers of gravity of units and districts. It should be noted that George et al. provides different versions of their model, each incorporating a subset of all discussed objectives. On the one hand, this illustrates the flexibility of their approach. On the other hand, they bypass the difficulties of the multi objective nature of the problem and the trade-off between the different objectives.

Considering the local search algorithms in Table 8.4, the work of Bozkaya et al. (2011, 2003) stands out from others. Their tabu search algorithm considers most of the essential criteria and objectives of the GPDP. Contiguity is treated as the only hard constraint. All other criteria are implemented through measures combined into a weighted additive multicriteria function. According to the authors, they propose a new measure in order to compare similarity of a computed districting plan with an existing plan. Their continuity index endorses districts which have large overlapping areas with an existing district. This index can be used even if old and new plans do not contain the same number of districts. However, since it considers the overlapping area of regions, this measure serves more the visual continuity between districting plans – which certainly can be a legitimate objective. Owing to the vast differences in population density and the interpretation that the goal of continuity refers to population (as the most important component in an democratic election), this measure is potentially debatable at least for the GPDP. In contrast, measuring the district overlay by means of

involved population may be a small but suitable modification of the similarity index proposed by Bozkaya et al. (2011, 2003).

In addition, Bozkaya et al. (2011, 2003) implemented a criterion called *integrity of communities*, which requires that communities with common interests be kept within the same electoral district. In the context of electoral districts in the Canadian city of Edmonton, Bozkaya et al. (2011) give the example of French-speaking communities. From the point of view of administrative units as communities of interest, it would be interesting to rephrase this criterion as the GPDP's administrative conformity and analyze if it is appropriate. Bozkaya et al. (2011, 2003) defines $f_{\text{int}}(\mathcal{D})$ as the measurement of integrity of communities for a districting plan $\mathcal{D} = \{D_1, \ldots, D_k\}$. As an objective function which is to be *minimized* the measurement reads

$$f_{\text{int}}(\mathcal{D}) := 1 - \frac{\sum_{\ell=1}^{k} G(D_\ell)}{\sum_{i \in V} p_i}$$

where $G(D_\ell)$ represents the population of the most represented community in electoral district D_ℓ. As before, $\sum_{i \in V} p_i$ equals the total population of the PDP instance.

In terms of the GPDP, we consider every rural and urban district as a community of interest. As per the definition of f_{int}, electoral districts D_ℓ with $G(D_\ell) = \sum_{i \in D_\ell} p_i$ contribute in the best possible way to the objective function. These electoral districts contain only units of *one* community of interest, i.e., rural or urban district, regardless of whether the electoral district coincides exactly with the administrative unit or comprises only a part of it. That is suitable for the GPDP. For example, with regard to urban/rural districts, this is the case for (i) the electoral district which matches exactly with the rural district of Warendorf in North Rhine-Westphalia and (ii) each electoral district of the city and urban district of Munich in Bavaria (Federal Returning Officer, n.d., online). However, there are German electoral districts which are identical to up to four urban and rural districts. In German practice, this is as good to evaluate as an electoral district which is exactly identical to *one* administrative area. Unfortunately, this fact is not taken into account and actually penalized in the conformity index by Bozkaya et al. (2011, 2003).

Ricca and Simeone (2008) used an administrative conformity index which is not described in detail in their publication but in (di Cortona et al., 1999, Section 11.3). We review the proposed administrative conformity index in detail and explain why it is not suitable for the GPDP.

Let h be a type of administrative area, e.g., h indicates the level of rural/urban districts. Let A_h denote the number of administrative areas of type h. The conformity index $C(D_\ell, h)$ for electoral district D_ℓ and administrative area type h is based on the distribution of district's units $i \in D_\ell$ among the areas of type h: Let $\delta_{\ell,a}$ denote the number of units $i \in D_\ell$, which belong to area $a \in \{1, \ldots, A_h\}$ of administrative area type h. di Cortona et al. (1999) define the conformity index which has to be *maximized* as

$$C(D_\ell, h) := \frac{1}{|D_\ell|^2} \sum_{a=1}^{A_h} \delta_{\ell,a}^2.$$

The index $C(D_\ell, h) \in [\frac{1}{A_h}, 1]$ is maximal, i.e., $C(D_\ell, h) = 1$, if D_ℓ contains only units of *one* administrative area of type h. The proposed conformity index is minimal, i.e., $C(D_\ell, h) = \frac{1}{A_h}$, when units $i \in D_\ell$ are equally distributed among all A_h administrative areas of type h. A global conformity index is defined as average over all districts and all types of administrative areas.

In the German context, the weakness of the conformity index proposed by di Cortona et al. (1999) is the same as pointed out for the work of Bozkaya et al. (2011, 2003): The measurement penalizes if an electoral district exactly matches more than one administrative area of one type. Thus, the proposed measurement of di Cortona et al. (1999) is not suitable for an administrative level containing numerous areas which are too sparsely populated to define their own electoral district.

Using the framework of nature-inspired and probabilistic algorithms, Forman and Yue (2003), Bação et al. (2005), and Rincón-García et al. (2017) consider the districts' contiguity only in a single fitness function or in an additional contiguity check. Neither continuity nor administrative conformity is regarded. Of course, this fact does not exclude the concept of these metaheuristics for being adequate to solve the GPDP but rather leaves room for further research.

Algorithms using Voronoi regions by Miller (2007) and Ricca et al. (2008) focus mainly on maximizing the compactness of the electoral districts. In contrast to the PDP in the USA, for example, compactness is not a (primary) goal to achieve in the German case. It is widespread in the PDP literature and especially in Voronoi approaches to use squared Euclidean distances or road distances to achieve compactness. In this respect, the work of Brieden et al. (2017) is refreshing. The authors apply an individual ellipsoidal norm for each electoral district in their anisotropic power diagram approach. Since these norms are computed on the basis of pre-given electoral districts, it favors the computation of similar districts. Nevertheless, this approach strives for continuity only implicitly. Brieden et al. (2017) evaluate the extent of continuity after the solution computation, namely by the ratio of voter pairs that are used to share a common district but are assigned to different ones in the solution output.

Summary of suitability evaluation

By summing up the suitability evaluation of the solution approaches for GPDP, we propose the following three aspects.

Firstly, a column generation/branch and price approach as proposed by Mehrotra et al. (1998) seems promising. Besides the previous related work of Garfinkel and Nemhauser (1970), the implicit enumeration of Mehrotra et al. (1998) is one of the few that ensures the two essential criteria of the GPDP (see Table 8.4). Mehrotra et al. (1998) identifies the compactness of each generated district with its costs in the objective. The sum of costs is minimized in the set partitioning problem. It is possible to consider more diverse costs and thus to make the approach suitable for the GPDP. As mentioned, only subtrees of shortest

path trees are considered as possible electoral districts in the pricing problem. Therefore, Mehrotra et al. (1998) provide only an optimization-based heuristic. Using another model to ensure a connected subgraph in the pricing problem, e.g., (Williams, 2002b) with (Validi and Buchanan, 2018), can eliminate this drawback, since the technique of branch and price can solve problems exactly.

Second, the local search heuristic of Bozkaya et al. (2011, 2003) nearly fits each requirement of the GPDP. It is possible to consider more diverse and GPDP-tuned costs. Concerning the measurement of continuity, this can easily be done by using the population number as a basis for assessment rather than the surface area. The speed-up of continuity checks as provided by King et al. (2017) should be implemented in a local search.

Third, the PDP literature does not provide any measurement for conformity of administrative boundaries completely fulfilling all requirements of the objective of the GPDP. As described before, every suggestion has drawbacks regarding the hierarchical multi-level character of administrative divisions in Germany. Moreover, that electoral districts which are part of exactly one rural/urban district and electoral districts which exactly match a number of rural/urban districts should be rated well.

8.6 Summary and Outlook

In this work, we examine the optimization problem of partitioning a territory into electoral districts: the Political Districting Problem (PDP). We provide a unified and extendable formulation of the PDP, based on two basic criteria: contiguity and population balance. As has been pointed out, this leads to an NP-hard problem. As a specific application, we consider the German Political Districting Problem (GPDP). We introduce the German electoral system and point out the significance and topicality of the GPDP in ongoing (political) discussions. We present all legal requirements for German electoral districts and define the GPDP as a multi-objective partitioning problem. The PDP is widely discussed in the literature. We review solution approaches, models, and algorithms proposed for the PDP. Only a few published solution approaches solve the PDP exact, the focus is clearly on heuristics. Various software packages are offered which provide assistance for state administrations during the redistricting process, or enable interested citizens to analyze and compute districting plans. Unfortunately, most software is only commercially available and some open-source projects are outdated.

The review of the exact solution approaches illustrates that reported computational results are approximately as old as 50 years. One should investigate to what extent today's technologies can handle larger instances. Ensuring contiguity efficiently seems to be an issue in exact methods. Furthermore, in most cases, the solution methods provided in the literature are green-field approaches that do not utilize current districting plans. In practice, however, a districting plan is often given and has to be adjusted, preferably as little as possible. One can focus on combinatorial redistricting problems occurring in connection with the regular adjustment of districting plans, thereby combining complexity questions of the occurring (continuity) problems with application-oriented answers for decision-makers.

Our literature review reveals that the German case differs from the most widely discussed PDP variants in the following aspects. Continuity is rarely considered in the literature. In Germany, however, it is a very important objective and, in general, a quite natural one. The number of electoral districts *with respect to German federal states* changes sometimes. Consequently, attention should be paid to the objective of continuity also in case of increasing or decreasing the number of electoral districts. In most approaches in the literature, compactness is a fundamental objective. In Germany, neither legal requirements, nor court decisions nor exterior discussions call for (maximally) compact electoral districts. In Germany, it is important to favor conformity between electoral districts and administrative boundaries. This includes several levels of the hierarchical administrative structure. In a sense, pursuing this conformity implicitly leads to compact electoral districts. As we conclude from the literature review, no suitable measurement for this objective has been proposed to date. Having one population deviation limit as a constraint (maximum limit of 25%) and another within an objective (tolerance limit of 15%) makes the GPDP unique. The GPDP consists of subproblems, in which sizes (measured by the size of population graph on municipality level) surpass most test instances studied in the literature.

On the whole, the GPDP stands out from classical PDPs in various aspects. Therefore, we think that studying the GPDP with its associated constraints and objectives in detail would enrich the literature on the PDP.

8.7 Appendix: Additional Bibliography

In the following, the 21 publications are listed that are part of the literature on the political districting problem but are not cited in the survey (cf. Section 8.4). This section of "Further Reading" corresponds to the grey dots in Figure 8.4.

Further Reading

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9 A Geovisual Decision Support System for Optimal Political Districting

Abstract. The design of electoral districts is – on the one hand – a highly relevant process and – on the other – a highly sensitive and controversial one. The demand for transparency and objectivity in this process can be met by making an effort to apply unbiased mathematics. In this paper, methods of mathematical optimization are presented, which are integrated into a software tool to provide optimal decision support. Applied criteria and optimization goals are derived transparently from (and only) the legally prescribed requirements. Nevertheless, all decision-making power remains in the hands of the user of the geovisual software. High-quality electoral districts provides by optimization algorithms are displayed on an interactive map and the user can perform adjustments by hand and immediately notice the effects regarding the legal requirements.

9.1 Introduction

Most democratic political systems include the delimitation of electoral districts to conduct elections (Handley, 2008; Handley, 2017). Therefore, the territory is partitioned into electoral districts and the voters of each district elect members to a legislative body. Depending on the electoral system, additional mandates may be assigned via e.g. party-list proportional representation. For electoral districts, a distinction is made between single-member districts, where voters elect exactly one candidate to represent their district, and multi-member districts with two or more representatives. The number of seats staffed by an electoral district is in proportion to the population it encompasses. The principle of electoral equality ("one person, one vote") implies legal constraints on the population of the electoral districts. A single-member district system, for example, calls for a balance in population among the districts. Together with the quite natural requirement that each electoral district has to form a contiguous area of municipalities, census blocks or the like, the laws and jurisprudence turn the task of designing electoral districts (called *political districting problem*) into a complex and in fact a NP-complete problem (Altman, 1997; Goderbauer and Winandy, 2017). In practice, political districting is not a one-off task — *re*districting is regularly on the agenda: Owing to population changes, electoral districts require regular adjustments in order to remain legally permissible. In addition to contiguity and population balance, further common districting criteria are geographic compactness, preservation of political subdivisions or continuity (di Cortona et al., 1999; Webster, 2013).

(Re)districting is a very delicate process — not only politically. The shape of electoral districts may influence the outcome of the election. For a candidate, its (re)entry into parliament and therefore future employment may depend on it. From the voters' point of view, it is not desirable to belong to an electoral district other than the last election, due to (necessary) changes in the districting plan. The parties want as many candidates as possible as winners of electoral districts. Discussions about planned or implemented adjustments regularly include the accusation that changes to electoral districts are politically motivated. The practice of drawing electoral district boundaries to deliberately favor one political party, a special interest group, or a single candidate over others is known under the term *"Gerrymandering"*, especially in the USA.

In the majority of countries with an electoral district system, independent commissions have been set up and entrusted with the task to prepare or adapt electoral districts (Handley, 2008). However, their elaborations are not always mandatory for the decision-maker (Goderbauer and Wicke, 2017; Handley, 2008). The authority of the final districting plan is often the legislature itself, i.e., the parliament or the governing parties (Handley, 2008).

Our investigations on the example of Germany shows that particularly for elections at the level of the 16 German federal states, the tools used by parliamentary groups, committees and electoral administrations to (manually) create and discuss change proposals are limited and do not do justice to the matter. Moreover, it is rarely transparent how districting decisions are reached. This fact naturally fuels discussions in public and the media. Altman and McDonald (2011b) summarized that "redistricting is among the least transparent processes in democratic governance". Due to combinatorial explosion there are unmanageable many possibilities to delimit (feasible) electoral districts. Applying mathematics can satisfy the need for objectivity and impartiality: Mathematical models are able to incorporate all possible configurations, so that not a single one is excluded or favored in advance. Mathematical solution methods are transparent because they are defined in a precise way. Thus, there is no space for possible manipulation as long as objectives and criteria comply with legal requirements. In fact, the applied criteria has to be derived transparently from the legally prescribed requirements and principles – and only from these.

Contribution. In this paper, we present a software tool that provides optimization-based geovisual decision support for the crucial issue of (re)districting. The tool enables a transparent and objective (re)districting procedure with mathematical methods based on legal requirements. Decision-makers, involved parties, or interested persons are offered well-founded solutions to serve as a solid basis for upcoming districting discussions. Developed optimization methods can be applied to achieve electoral districts which are best possible according to laws and jurisdictions. We present underlying optimization models and methods as well as our numerical measurements of criteria specified by laws and jurisdictions. Despite the possibility of computational optimization, the user retains the authority in our geovisual tool. Imported districting plans as well as computed high-quality proposed amendments are displayed on an interactive map with all relevant data. The user can perform (additional) adjustments by hand and immediately notice the effects these have on the compliance with the legal requirements. Descriptive analytics is provided for each electoral district and districting plan as a whole.

Structure of the paper. In the subsequent Section 9.2, related work on the political districting problem is presented. This includes solution methods presented in literature as well as offered software. In addition, we collect information on which tools are used in practice to assign constituencies. In Section 9.3, the political districting problem considered in this work is defined. For this purpose, the legal requirements on German electoral districts are formalized in mathematics. The defined problem is modeled as a mixed-integer linear program in Section 9.4. Next to the model, a preprocessing technique and primal heuristics are presented. Section 9.5 focuses on the geovisual decision support software which incorporates the developed methods of mathematical optimization, descriptive analytics, and options for manually editing of electoral districts. In Section 9.6, a case study is presented that has been carried out using the software tool introduced before. The paper closes with an conclusion and outlook in Section 9.7.

9.2 Related Work

We review relevant literature on computational solution approaches for political districting and survey (re)districting software. In addition, we present details about redistricting in practice with a special focus on software used.

Political Districting Problem For the purpose of partitioning a territory into $k \in \mathbb{N}$ electoral districts, commonly a discretization of the territory is given in the form of a partition into $n \in \mathbb{N}$, $n \gg k$ *geographical units* (Goderbauer and Winandy, 2017). These units can be, e.g., municipalities, municipal associations, or census tracts. Given this discretization, the *political districting problem* (PDP) is modeled as a graph partitioning problem on the following graph (Goderbauer and Winandy, 2017). Based on the geographical units and its adjacencies, the so-called *population graph* $G = (V, E)$ is defined: Each *node* $i \in V$ represents a geographical unit and is weighted with the *unit's population* $p_i \in \mathbb{N}$. We define $p(D) := \sum_{i \in D} p_i$ for $D \subseteq V$. An undirected *edge* $(i, j) \in E$ with nodes $i, j \in V$ exists if and only of the corresponding areas share a common border.
We denote $\mathcal{P}(V) := \{\{D_1, \dots, D_n\} | \, V = \bigcup_{i=1}^{n} D_i$ with disjoint $D_i \subseteq V$ and $n \in \mathbb{N}\}$ as the *set of all partitions of set* V. Given $G = (V, E)$ and $k \in \mathbb{N}$, the PDP consists of finding a partition $\mathcal{D} = \{D_1, \dots, D_k\} \in \mathcal{P}(V)$ of the units V in k *electoral districts* $D_\ell \subseteq V$ observing application specific constraints and objectives. Such a partition $\mathcal{D} \in \mathcal{P}(V)$ is called feasible *districting plan*.

9.2.1 Solution Approaches in the Literature

The first algorithmic approach for political districting is said to be the work of Vickrey (1961). Published in a political journal, the author presents a rudimentary description of a greedy multi-kernel growth heuristic.

Hess et al. (1965) pioneered in applying a discrete location-allocation model. Their work is considered the earliest operations research paper in political districting. Many other authors

followed using their work as a basis. The presented integer programming model does not ensure contiguity of the districts since this is only targeted by the objective function.

Garfinkel and Nemhauser (1970) proposed a two-phase algorithm. After generating all feasible districts, a set partitioning model is used to compute a districting plan. The work of Garfinkel and Nemhauser (1970) is the most cited one in the mathematical optimization literature of political districting (Goderbauer and Winandy, 2017). Mehrotra et al. (1998) evolved this enumeration approach into a branch and price procedure. They generate suitable districts iteratively in the pricing problem. To ensure contiguity, districts are required to be subtrees of shortest path trees (Zoltners and Sinha, 1983). The master problem consists of a set partitioning formulation which forms a districting plan on basis of already generated feasible districts. In general, the technique of branch and price can be applied to solve optimization problems exactly (Lübbecke and Desrosiers, 2005). However, the algorithm of Mehrotra et al. (1998) remains a heuristic, since some contiguous but most likely irrelevant districts are excluded due to the used contiguity model.

Bozkaya et al. (2003) proposed a local search algorithm within an adaptive memory search framework. The enhanced procedure is based on tabu search and constantly combines districts of good solutions to construct other high-quality districting plans.

Kim (2018) applied a contiguity model by Williams (2002a,b) for political districting. Under the condition that the used graph is planar, Williams (2002a,b) ensures connectivity of node-induced subgraphs via a quite small and strong mixed-integer programming formulation. However, Validi and Buchanan (2018) demonstrate that the formulation of Williams (2002a,b) is incorrect. Fortunately, the same authors provide a simple repair.

Following publications propose solution approaches while concentrating on the PDP in Germany. Goderbauer (2016a,b) proposed a multi-stage heuristic which is specialized for the very important and multilayered German requirement of administrative conformity (cf. Section 9.3.1). Brieden et al. (2017) worked out a relation between constrained fractional clusterings and additively weighted generalized Voronoi diagrams. In a case study, their approaches were applied on data of parts of German federal states.

Broad literature reviews on solving methods as well as criteria for political districting and proposals to measure them are given by Williams (1995), di Cortona et al. (1999), Ricca et al. (2011), Goderbauer and Winandy (2017).

9.2.2 Software Tools

The aforementioned local search by Bozkaya et al. (2003) was the basis of a plugin for ArcGIS (a commercial geographic information system (GIS) of the vendor Esri). In (Bozkaya et al., 2011) the authors describe how it was used to assist the official designing process of new electoral districts for municipal elections in Edmonton, Canada in 2010. The software works fine with version 8 of ArcGIS. Unfortunately, this outdated version of ArcGIS is not available anymore and the plugin's code has not been upgraded (Bozkaya, 2016).

Guo and Jin (2011) present a software called iRedistrict. It provides heuristic solutions based on tabu search. The software can be purchased via the company ZillionInfo (n.d., online) as a commercial product.

A further software tool for political districting is BARD (Better Automated Re-Districting) by Altman and McDonald (2011, online). BARD is an open source software package and comes as a module for the R programming language project for statistical computing. The software tool utilizes different procedures for automatically generating districting plans (Altman and McDonald, 2011a, Section 6.3). The code was not updated since 2011 and is no longer available through the official R module repository.

Dave's Redistricting App (Bradlee, n.d., online) is a free web-based tool and has been developed by an individual software engineer since 2009. The user can draw electoral districts onto the map and receives population numbers and votes. The tool does not offer automated redistricting. Data of US states is provided and embedded into a mapping service. Recently, this application was used by Bycoffe et al. (2018) in a large online project about Gerrymandering in the USA.

Further (optimization-based) redistricting software tools proposed in literature are gathered in the survey of Goderbauer and Winandy (2017).

9.2.3 Tools used in Practice

United States of America. Redistricting software is the predominant tool during the (re)districting process in the USA (Altman et al., 2005). Some US states have developed their own software internally by legislative staff (Storey, 2011). Most US states are using commercial products, e.g., Esri Redistricting (n.d., online) or Maptitude for Redistricting (n.d., online). Some of the offered software packages provide the functionality to automatically compute districting plans using heuristics (Altman et al., 2005, Table 6). These programs cost between "$3,000" (Southwell, 2011), "$6,000 per work station" (Storey, 2011), and "tens of thousends of dollars" (Altman and McDonald, 2011b).

Germany. Elections in Germany include elections to Germany's federal parliament, i.e., the Bundestag, and state elections to parliaments of the 16 German states (Länder). In all these elections, electoral districts are of great importance. For German federal elections a software tool called WEGIS is used to evaluate and adjust electoral districts (Heidrich-Riske, 2014; Statistisches Bundesamt, 2003). It was developed internally by the Federal Returning Officer as a plugin for ArcGIS and has been in use since the preparation for German federal elections in 2002. WEGIS does not provide automated redistricting and is only available for employees of the Federal Returning Officer. Suggestions for delimiting electoral districts posed by, e.g., political parties, are performed and evaluated in-house by request (Heidrich-Riske and Krause, 2015).

German federal states. Each electoral administration of the 16 German states has its own process and tools to evaluate and possibly adjust the districting plan in preparation for state elections. We received details on this issue from 12 federal states via email (Bundeswahlleiter,

2018, contact details of Land returning officers) in the first half of 2018. It turned out that German federal states are lagging behind in terms of technology. The majority stated that the main work of redistricting is performed with Microsoft Excel. Coloured pencils, paper maps, graphics software (e.g. Microsoft Paint), and calculators are other mentioned tools. Only a few administrations use customized software. In Berlin an internally developed ArcGIS-based application is in use since 2016. The administration of Bavaria uses an ArcGIS-based application developed in-house in 2017. Auxiliary calculations are made in Excel. In Lower Saxony the development of an software tool was started in the beginning of 2018. Excel sheets were used up to now.

Further details and analyses on the practice of redistricting in various countries and states are given by Handley et al. (2006), Grofman and Handley (2008), Moncrief (2011), and Handley (2017).

9.3 Political Districting Problem

We use and adopt the modeling of the PDP in form of a graph partitioning problem as is common in literature (cf. beginning of Section 9.2). The (electoral) law of a country or state usually contains criteria which are obliged to consider when delimiting electoral districts. Sometimes court precedents complement these principles. These legal guidelines lead to the constraints and objectives of the PDP. At least contiguity and a kind of population balance are present in most districting requirements (Handley et al., 2006). When several conflicting objectives are mentioned, the law usually does not name a hierarchy or trade-off between them. From practical experience, however, preferences can be derived (Goderbauer and Wicke, 2017).

In the following, we focus on the design of electoral districts for *German federal elections*. The legal requirements to be observed are presented in following Section 9.3.1. Subsequently, in Section 9.3.2, the criteria are divided into strict constraints to be adhered and objectives to be aimed for. We develop numerical measurements in order to evaluate the characteristics of the legal requirements for a given electoral district or districting plan. Altogether, this forms the mathematical definition of the considered PDP. With regard to Germany, Goderbauer and Winandy (2017) analyzed the PDP literature and evaluated used measurements for legal requirements. Their findings and open questions are a basis of the following sections.

9.3.1 Legal Requirements for Electoral Districts in Germany

The German Federal Elections Act contains principles to be observed at the delimitation of electoral districts. In recent years, these guidelines have been complemented by jurisdictions of the Federal Constitutional Court. The legal requirements are as follows (Goderbauer and Wicke, 2017; Schreiber et al., 2017).

(i) Distribution among federal states. For federal elections the territory of Germany is subdivided into 299 single-member electoral districts. Due to the constitutionally established

federalism, the boundaries of the 16 federal states must be strictly observed. Based on the states' population numbers the 299 electoral districts are distributed among the states. As apportionment method the divisor method with standard rounding (Pukelsheim, 2017) is used.

(ii) Contiguity. Every electoral district should form a contiguous, i.e., coherent area.

(iii) Two-stage population deviation limit. The principle of electoral equality implies that each electoral district must preferably comprise the same number of people. The German law enables a two-staged scope for the deviation of the district's population from the average. The deviation *should* not be larger than 15% (tolerance limit). The absolute maximum limit of population deviation, which *has* to be adhered to, is expressed with 25%. The German population is the basis of assessment, i.e., German minors are included and all non-Germans are not taken into account.

(iv) Continuity. Between two consecutive elections the adjustments of the electoral districts should be as small as possible. It would be contrary to the principles of democratic representation if large and numerous changes were constantly made.

(v) Administrative conformity. Electoral districts should, as far as possible, follow (administrative) boundaries of rural districts, urban districts, and municipalities. In practice, this principle of conformity also encompasses the boundaries of municipal associations and possibly existing governmental districts.

9.3.2 Mathematical Formalization

The apportionment of electoral districts among the German federal states implies the decomposition of the PDP into 16 independent subproblems – one for each federal state. Based on the remaining legal requirements stated in Section 9.3.1, we distinguish between constraints (Sec. 9.3.2.1) and objectives (Sec. 9.3.2.2) for a districting plan.

9.3.2.1 Constraints

The law formulates contiguity of the electoral districts as a should-criterion (cf. (ii) in Sec. 9.3.1). However, exceptions of this principle are permitted only in duly justified cases like exclaves or islands (Schreiber et al., 2017). Goderbauer and Wicke (2017) pointed out that currently two (long-established) German electoral districts form a non-connected territory whose incoherence cannot be explained by islands or exclaves. We consider connectedness as a constraint and perform some data processing in order to achieve feasibility of the two mentioned electoral districts. In the course of the modeling as a graph partition problem this implies the requirement for connected subgraphs induced by each electoral district $D \subseteq V$. Next to connectedness, each electoral district has to fulfill the maximum population deviation limit of 25% (cf. (iii) in Sec. 9.3.1). We denote parameter $\bar{p}$ as the *average population of an electoral district*. In most applications $\bar{p} = \frac{p(V)}{k}$ holds. In the

German case, however, $\bar{p}$ is the same for each federal state instance, since the parameter is not determined for each state but for Germany as a whole.

Definition 21 (feasible electoral district) *A set $D \subseteq V$ is a* feasible electoral district *if and only if following holds*

(i) the induced subgraph $G[D]$ is connected and

(ii) $\left|\frac{p(D)}{\bar{p}} - 1\right| \leq 25\%$.

9.3.2.2 Objectives and their measurements

The objectives are the maximization of *continuity* (cf. (iv) in Sec. 9.3.1), of *administrative conformity* (cf. (v)), and the minimization of *population deviation* (cf. (iii)). Except perhaps for the latter, evaluation functions of the objectives are not given in the law. In order to get closer to numerical formulations of the objective functions, we phrase the situation which implies total fulfillment of each:

- *Continuity* (abbreviated with cont): Perfect continuity is given if an electoral district of a given districting plan is not adjusted, i.e., stays the same.
- *Administrative conformity* (adm): An electoral district has perfect administrative conformity if it exactly matches a (number of) rural/urban district(s). Perfect conformity is also present in the case where an electoral district is entirely within a rural/urban district which, due to population restrictions, must be divided into several electoral districts (e.g., a big city).
- *Population deviation* (pop): The best possible population deviation from average is obviously 0%.

For each objective we will assess to what extent the best possible situation is achieved. For this purpose we define a function E^σ for each objective $\sigma \in \{\text{cont, pop, adm}\}$. The value $E^\sigma(D) \in [0,1]$ rates an electoral district $D \subseteq V$ with regard to σ. Total compliance with an objective σ, i.e., perfect/total fulfillment, leads to $E^\sigma(D) = 1$. The multi-objective character is treated as the maximization of a weighted additive multicriteria function

$$\max \quad \sum_{\sigma} \omega^\sigma \sum_{\ell=1}^{k} E^\sigma(D_\ell) \tag{9.1}$$

where $\omega^\sigma \geq 0$ is the weight for criterion σ with $\sum_\sigma \omega^\sigma = 1$.

Instead of being part of the objective function, it can also be useful to consider a criterion like continuity or population deviation as a *budget constraint*. For continuity, such a budget constraint can specify the maximum amount of difference between a calculated districting plan and the previous one. For population deviation, the constraint given in Definition 21 (ii) can be strengthened by, e.g., the law's should-requirement of 15%. The use of a budget constraint for criterion σ instead of being part of the objective function (i.e., $w^\sigma = 0$) can make it easier to choose the weights $w^{\sigma'}$ of remaining objective criteria σ'.

In the following, we develop measurements E^σ for objectives $\sigma \in \{\text{cont, pop, adm}\}$. Thereby we incorporate the intended option to consider objectives cont and pop in form of budget constraints.

Continuity. The consideration of continuity is possible if an appropriate districting plan $\mathcal{D}^{\text{old}} \in \mathcal{P}(V)$ is given, from which a new plan $\mathcal{D}$ is to emerge. We assume that the number of electoral districts $k = |\mathcal{D}|$ of a PDP instance equals the number of a given districting plan $\mathcal{D}^{\text{old}} \in \mathcal{P}(V)$, i.e., $|\mathcal{D}^{\text{old}}| = |\mathcal{D}|$. For a districting plan $\mathcal{D}$ the notation of its initial plan $\mathcal{D}^{\text{old}}$ is unique. For a district $D \in \mathcal{D}$ we denote the unique district from which D has emerged with $D^{\text{old}} \subseteq V$.
In order to assess the similarity of an electoral district $D \subseteq V$ with an existing one $D^{\text{old}} \in \mathcal{D}^{\text{old}}$, we measure how much the electoral district has changed. The numerical quantification of a change is based on the population that has been taken out $p(D^{\text{old}} \setminus D)$ and that has been added $p(D \setminus D^{\text{old}})$, i.e., based on the symmetric difference of D^{old} and D. The literature of PDP measures continuity based on the *size* of reallocated area (Bozkaya et al., 2011, 2003) or the *number* of reallocated geographical units (George et al., 1993, 1997). We think that continuity should be measured by the population affected by the changes.

Definition 22 (continuity of a district: objective measurement) *Let $D \subseteq V$ be an electoral district that has emerged from electoral district $D^{old} \subseteq V$ of a given districting plan $\mathcal{D}^{old}$. The* measurement of continuity of D *is defined as*

$$E^{cont}(D) := \max\left\{0,\ 1 - \frac{p(D^{old} \setminus D) + p(D \setminus D^{old})}{\bar{p}}\right\}. \tag{9.2}$$

The case $E^{\text{cont}}(D) = 0$ in (9.2) occurs if electoral district D changes by more population than an average electoral district comprises. This limit seems reasonable to speak of non-existing continuity.

Example 23 *Compare Figure 9.1. Given a districting plan with $\bar{p} = 245\,958$, including an electoral district D_1^{old} (Fig. 9.1a). In the course of an adjustment, areas change between three districts (cf. orange colored areas in Fig. 9.1b): $p(D_3^{old} \cap D_1) = 9\,824$ and $p(D_1^{old} \cap D_2) = 6\,898$. Then, the measurement of continuity of D_1 is:*

$$E^{cont}(D_1) = 1 - \frac{p(D_1^{old} \setminus D_1) + p(D_1 \setminus D_1^{old})}{\bar{p}} = 1 - \frac{9\,824 + 6\,898}{245\,958} = 0.93$$

Based on this, we define also a measurement for an entire districting plan $\mathcal{D} \in \mathcal{P}(V)$. This will be use in the course of a budget constraint to ensure a minimum degree of continuity. Such a minimum of continuity describes how much population of the entire electoral territory at least should remain in their original electoral district and thus how much population at most can be transferred to a different district. For example: For a districting plan having an optimization-based revision, a maximum of 10% of the population should be assigned to another electoral district.

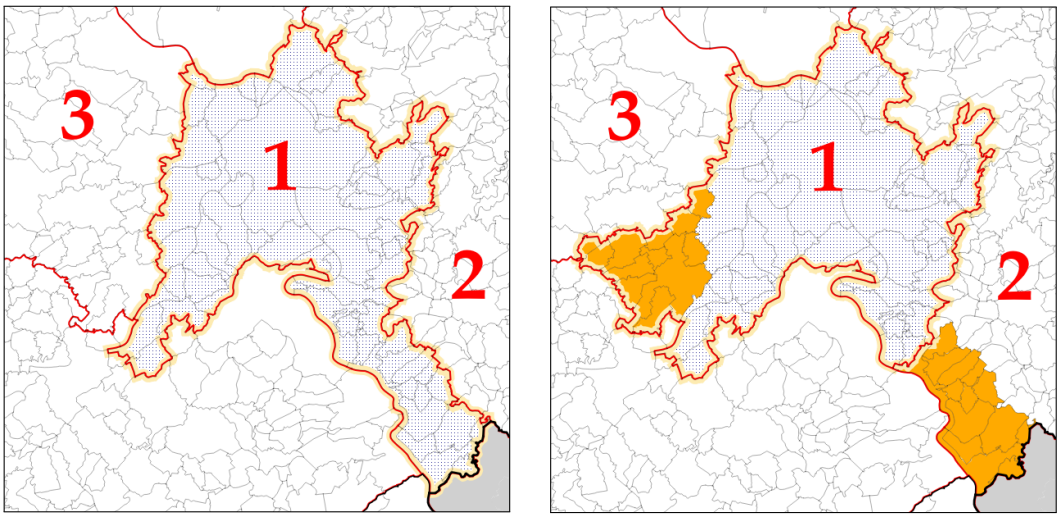
Definition 24 (continuity of a plan: budget measurement) *Let $\mathcal{D} \in \mathcal{P}(V)$ be a districting plan that has emerged from $\mathcal{D}^{old} \in \mathcal{P}(V)$ with $|\mathcal{D}| = |\mathcal{D}^{old}|$. The* measurement of continuity of *$\mathcal{D}$ is defined as*

$$E^{cont}(\mathcal{D}) := 1 - \frac{\sum_{D \in \mathcal{D}} p(D \setminus D^{old})}{p(V)}. \tag{9.3}$$

Under the assumption that $E^{\text{cont}}(D) \geq 0$ holds for each $D \in \mathcal{D}$, the continuity of a districting plan (Def. 24) and of its districts (Def. 22) have the following relationship:

$$\begin{aligned} E^{\text{cont}}(\mathcal{D}) &\overset{\text{Def. 24}}{:=} 1 - \frac{\sum_{D \in \mathcal{D}} p(D \setminus D^{\text{old}})}{p(V)} \\ &= 1 - \frac{\frac{1}{2} \sum_{D \in \mathcal{D}} p(D^{\text{old}} \setminus D) + p(D \setminus D^{\text{old}})}{|\mathcal{D}| \cdot \bar{p}} \\ &= 1 - \frac{\frac{1}{2} \sum_{D \in \mathcal{D}} \frac{p(D^{\text{old}} \setminus D) + p(D \setminus D^{\text{old}})}{\bar{p}}}{|\mathcal{D}|} \\ &\overset{\text{Def. 22}}{=} 1 - \frac{\frac{1}{2} \sum_{D \in \mathcal{D}} (1 - E^{\text{cont}}(D))}{|\mathcal{D}|} \end{aligned}$$

Administrative conformity. The territory of Germany is partitioned into administrative areas of different hierarchically arranged levels. We identify each *administrative level* with its partition $\mathcal{A} = \{A_1, A_2, \ldots\} \in \mathcal{P}(V)$ in *administrative subdivisions* $A_i \subseteq V$. The law requires that electoral districts should be oriented towards these levels and subdivisions (cf. (v) in Sec. 9.3.1). Goderbauer and Winandy (2017) pointed out that for the German PDP this criterion has to be assessed in the objective primary for the administrative level of *rural and urban districts* (in German: *Landkreise und kreisfreie Städte*). Germany is partitioned



(a) Initial districting plan $\mathcal{D}^{\text{old}}$.

(b) Electoral districts after adjustments.

Fig. 9.1: Electoral district D_1 (Fig. 9.1b) is derived from electoral district D_1^{old} (Fig. 9.1a) as follows. Parts of D_1^{old} are transposed to a neighbouring electoral district with index 2. In addition, D_1^{old} is extended by parts of another neighbouring district with index 3. Areas whose electoral district assignment has been changed are highlighted in orange.
(boundaries: © GeoBasis-DE / BKG 2016)

in roughly $400 = |\mathcal{A}|$ rural/urban districts (Goderbauer and Winandy, 2017) and each rural/urban district belongs to exactly one federal state. On the one hand, there are electoral districts that include up to four rural/urban districts. On the other hand, rural/urban districts exist which are forced to be divided into multiple electoral districts because of population strengths. Therefore, our interpretation of this legal requirement is twofold: (i) Consider a highly populated city in form of a urban district, which necessarily has to be divided into several electoral districts. In that case, the aim is to support electoral districts which contain only areas of that city and none outside of it. Such an approach is also appreciated in practice due to administrative matters. (ii) In all other cases, the share of electoral district boundaries, which are also boundaries of rural/urban districts, should be as large as possible. Electoral districts should define as few borders as possible that differ from those of rural and urban districts. As a basis of assessment, the length of boundaries was chosen. The purpose of this is to form electoral districts, in some sense, as compactly as possible on the basis of rural and urban districts.

As pointed out by Goderbauer and Winandy (2017), the PDP literature does not provide a usable measurement for administrative conformity in the German case. Thus, we contribute a suitable measurement.

We denote following parameters. For an electoral district $D \subseteq V$, let $\text{perim}(D) \in \mathbb{R}_+$ be the *length of the perimeter of the area of* D. For an administrative level $\mathcal{A}$, e.g., rural/urban districts, let $\text{perim}^{\mathcal{A}}(D) \in \mathbb{R}_+$ be the *perimeter's length of the area of electoral district* $D \subseteq V$ *which matches with boundaries of administrative level* $\mathcal{A}$. Thus, we consider the border of D which is simultaneously part of the boundaries of administrative level $\mathcal{A}$. It holds $\text{perim}(D) \geq \text{perim}^{\mathcal{A}}(D)$ for $D \subseteq V$ in general. For a union $\bigcup A_i$ of some administrative subdivisions $A_i \in \mathcal{A}$ holds equality $\text{perim}(\bigcup A_i) = \text{perim}^{\mathcal{A}}(\bigcup A_i)$.

Definition 25 (administrative conformity: objective measurement) *The* measurement of administrative conformity *of an electoral district* $D \subseteq V$ *is defined with following distinction of cases:*

- *If* $D \subseteq A$ *holds for a rural/urban district* $A \in \mathcal{A}$, $A \subseteq V$ *with* $p(A) > 1.25 \cdot \bar{p}$ *we define*

$$E^{adm}(D) := 1,$$

- *otherwise we define*

$$E^{adm}(D) := \frac{perim^{\mathcal{A}}(D)}{perim(D)} \in [0,1],$$

i.e., the share of the perimeter of electoral district D *which is also border of the administrative level of rural and urban districts.*

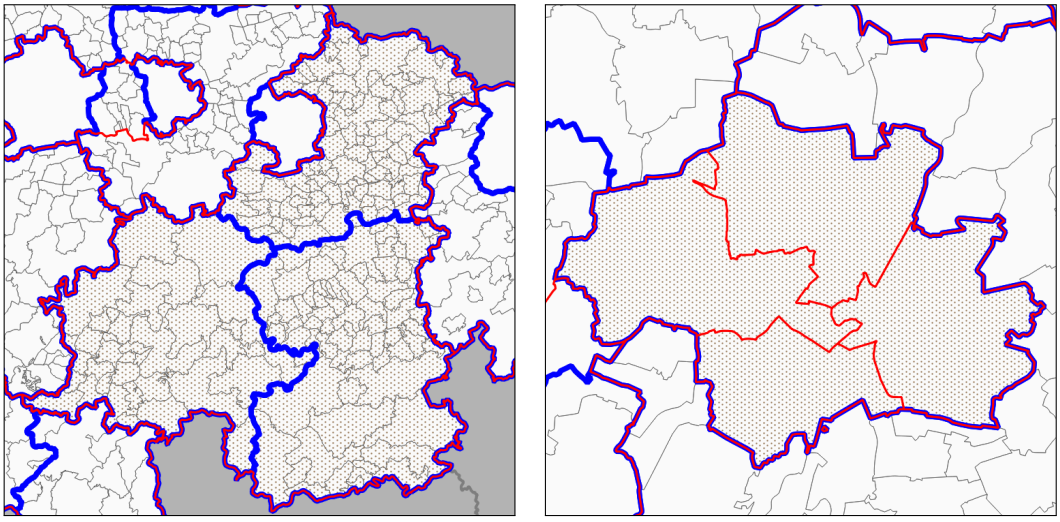
Example 26 *Compare Figures 9.2 and 9.3. The electoral districts highlighted in Fig. 9.2a and 9.2b fully comply with the objective of administrative conformity. The boundaries of the one in Fig. 9.3a match to* 90% *the boundaries of the considered administrative level. In Fig. 9.3b this is slightly lower with* 85%.

A budget constraint for administrative conformity is not practical from our point of view. We cannot imagine that a delimitation is requested where, for example, the boundary of each electoral district has to correspond to a certain percentage with given administrative boundaries. Also, the specification of a minimum number of electoral districts with full administrative conformity does not seem reasonable. For this reason, we do not develop budget constraints for the criterion of administrative conformity.

Population deviation. In practice, a deviation of a few percent from the average electoral district population $\bar{p}$ is as good as no deviation, i.e., 0%. In fact, the German law describes deviations of up to 15% as acceptable. The European Venice Commission (2002) favors a maximum deviation of 10% in its Code of Good Practice in Electoral Matters. To evaluate smaller deviations similarly well and to punish larger deviations disproportionately strongly, we utilize a flexibly selectable function to map the interval of permissible deviations $[0\%, 25\%]$ to the evaluation interval $[0, 1]$.

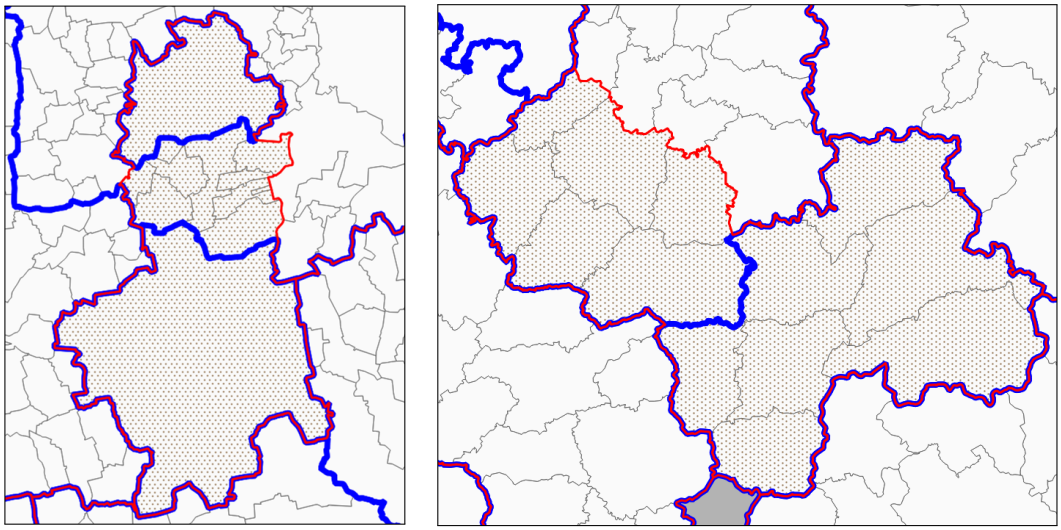
Definition 27 (population deviation: objective measurement) *Based on a piecewise linear, monotonically decreasing, concave function* $f : [0\%, 25\%] \to [0, 1]$ *with* $f(0\%) = 1$ *and* $f(25\%) = 0$*, the* measurement of population deviation *of an electoral district* $D \subseteq V$ *is defined as*

$$E^{pop}(D) := f\left(\left|\frac{p(D)}{\bar{p}} - 1\right|\right). \tag{9.4}$$



(a) $E^{\text{adm}}(D) = 1$ **(b)** For all highlighted applies: $E^{\text{adm}}(D) = 1$

Fig. 9.2: The boundaries of rural/urban districts are colored in blue, the one of electoral districts in red. If both match, the boundary appears to be purple. The measured electoral districts are filled with dot patterns. In Fig. 9.2b the partitioned rural district encompasses more than $1.25 \cdot \bar{p}$ population. (boundaries: © GeoBasis-DE / BKG 2016)



(a) $E^{\text{adm}}(D) = 0.9$ **(b)** $E^{\text{adm}}(D) = 0.85$

Fig. 9.3: Addition to Figure 9.2. The boundaries of rural/urban districts are colored in blue, the one of electoral districts in red. If both match, the boundary appears to be purple. The measured electoral districts are filled with dot patterns. (boundaries: © GeoBasis-DE / BKG 2016)

Concavity of f is essential for the following reason. Considering the population deviation objective of the whole districting plan $\sum_{\ell=1}^{k} E^{\text{pop}}(D_\ell)$ (cf. Eq. (9.1)), it should not be advantageous to get a small deviation improvement of an already quite well rated electoral district for an larger deviation of an already strongly deviating electoral district. We use linear function segments here to be able to apply linear programming techniques to model the objective function in Section 9.4.1. Figure 9.4 shows a possible function f which is used in this work.

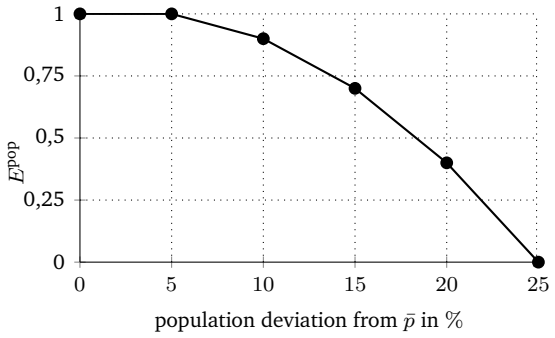


Fig. 9.4: Mapping a district's population deviation to its measurement (cf. Def. 27).

In the context of a budget constraint on population deviation, it is possible to restrict the deviation of each electoral districtg stronger by modifying constraint (ii) given in Definition 21.

9.3.3 Definition of Political Districting Problem in Germany

All in all, the considered political districting problem reads as follows.

POLITICAL DISTRICTING PROBLEM (PDP)

Given

- population graph $G = (V, E)$ with ...
  - population $p_i \in \mathbb{N}$ for $i \in V$
  - current districting plan $\mathcal{D}^{\text{old}} \in \mathcal{P}(V)$
  - rural/urban districts $\mathcal{A} \in \mathcal{P}(V)$
  - geographical data, e.g., border lengths for perim$(D), D \subseteq V$
- number of electoral districts: $k \in \mathbb{N}$ (with $k = |D^{\text{old}}|$)
- avergage population of electoral district: $\bar{p} \in \mathbb{R}_+$ (with possibly $\bar{p} = \frac{p(V)}{k}$)
- population bounds of electoral district: $\check{p}, \hat{p} \in \mathbb{N}$ with $\check{p} \leq \bar{p} \leq \hat{p}$
- objective weights $\omega^\sigma \geq 0$ with $\sum_\sigma \omega^\sigma = 1$.
- max. proportion of $p(V)$ allowed to change electoral district: $\text{bdg}^{\text{cont}} \in [0, 1]$

Find

$$\mathcal{D} = \{D_1, \ldots, D_k\} \text{ with disjoint } D_\ell \subseteq V \ \forall \ell \text{ and } \bigcup_\ell D_\ell = V \tag{9.5}$$

so that

$$G[D_\ell] \text{ connected} \qquad \forall \ell \in \{1, \ldots, k\} \tag{9.6}$$

$$\check{p} \leq \sum_{i \in D_\ell} p_i \leq \hat{p} \qquad \forall \ell \in \{1, \ldots, k\} \tag{9.7}$$

$$E^{\text{cont}}(\mathcal{D}) \geq 1 - \text{bdg}^{\text{cont}} \tag{9.8}$$

while

$$\text{maximizing} \quad \sum_{\ell=1}^{k} \left\{ \begin{array}{rl} & \omega^{\text{cont}} \cdot E^{\text{cont}}(D_\ell) \\ + & \omega^{\text{adm}} \cdot E^{\text{adm}}(D_\ell) \\ + & \omega^{\text{pop}} \cdot E^{\text{pop}}(D_\ell) \end{array} \right\} \tag{9.9}$$

9.4 Optimization Model and Methods for Political Districting

Based on the problem's definition developed in Section 9.3.2 the considered political districting problem is modeled as a mixed-integer linear program (MILP). This is done in Section 9.4.1. The modeling of connectivity and the objective functions takes the largest part in the formulation. In Section 9.4.2 a preprocessing technique is presented which reduces the size of the underlying graph without neglecting any feasible districting plan. In addition, start and improvement heuristics presented in Section 9.4.3 are employed to obtain good primal solutions in the solving process of the political districting problem MILP.

In order to clearly distinguish between decision variables and parameters in the following explanations, we denote variables consistently with capital letters. For a shorter notation, we define $[n] := \{1, \dots, n\}$ for $n \in \mathbb{N}$.

9.4.1 Mixed-Integer Linear Programming Formulation

We model the political districting problem as a mixed-integer linear program (MILP). Thereby, we utilize binary decision variables $X_{i\ell} \in \{0, 1\}$. An assignment variable $X_{i\ell}$ equals 1 if and only if unit $i \in V$ is part of electoral district D_ℓ, i.e., $i \in D_\ell$ holds.

$$X_{i\ell} \in \{0, 1\} \qquad \forall i \in V, \ell \in [k] \tag{9.10}$$

In order that a resulting districting plan $\mathcal{D} = \{D_1, \dots, D_k\}$ with electoral districts $D_\ell := \{i \in V : X_{i\ell} = 1\}$, $\ell \in [k]$ forms a partition of units V, we add set partitioning constraints (9.11). Following Definition 21 (ii), the population deviation of each electoral district is limited via constraints (9.12).

$$\sum_{\ell=1}^{k} X_{i\ell} = 1 \qquad \forall i \in V \tag{9.11}$$

$$0.75 \cdot \bar{p} \leq \sum_{i \in V} p_i X_{i\ell} \leq 1.25 \cdot \bar{p} \qquad \forall \ell \in [k] \tag{9.12}$$

It remains to ensure connectivity of $G[D_\ell]$ for each $\ell \in [k]$, to model the objective functions, i.e., E^{cont}, E^{adm}, E^{pop}, and the budget constraint for continuity. This is set out in the following Sections 9.4.1.1 and 9.4.1.2.

9.4.1.1 Connectivity

There are plenty of integer programming formulations for ensuring connectivity in (sub-) graphs. In the following we give a brief insight into the related literature. Then we point out and argue which approach we apply. Overall, we divide MILP connectivity models into three classes: (i) based on *trees*, (ii) based on *flows*, and (iii) based on *cuts*.

Following MILP models work with finding a spanning tree in the selected subgraph. Originally developed for the traveling salesman problem, the famous *Dantzig-Fulkerson-Johnson subtour elimination constraints* (Dantzig et al., 1954) as well as *Miller-Tucker-Zemlin (MTZ) formulation* (Miller et al., 1960) can be utilized to ensure subgraph connectivity. Sherali and Driscoll (2002) propose a linearization of a nonlinear MTZ formulation, thereby they tighten its relaxation. Williams (2002a,b) and Validi and Buchanan (2018) develop a connectivity model for *planar graphs* exploiting the behave of spanning trees in the primal planar graph and its corresponding dual graph. Zoltners and Sinha (1983) model that the spanning tree has to be a *shortest path subtree*. This model has the restriction that a known unit must already be assigned to the subgraph; this unit is used as the root of the shortest path tree. Cova and Church (2000) generalize this approach and allow k-shortest paths as connection between a node and the root.

Using *network flow* conditions, Shirabe (2005, 2009) impose connectivity of a selected subgraph. Shirabe was certainly not the first applying this approach. Commodity flow formulations were already used in the context of the traveling salesman problem (Langevin et al., 1990).

We employ a connectivity model based on *cuts*. The reason for this consists of the following three aspects. (i) All models mentioned so far induce connectivity relying on at least additional variables for the set of edges. In contrast, connectivity of a subgraph can be modeled in the original space of variables (i.e., $X_{i\ell} \in \{0,1\}$) using *separator inequalities*. Apart from the fact that these inequalities do not require any further variables, (ii) relevant computational successes (Álvarez-Miranda et al., 2013; Buchanan et al., 2015; Carvajal et al., 2013; Fischetti et al., 2016) and (iii) a facet defining property (Wang et al., 2017) has been achieved. To our knowledge, this connectivity model has not yet been applied to the PDP.

Separator inequalities are based on *node separators*, defined in the following.

Definition 28 (node separator) *Let $G = (V, E)$ be a graph. For two distinct nodes $a, b \in V$, a subset of nodes $S \subseteq V \setminus \{a, b\}$ is called* a,b-separator *if and only if there is no path from a to b in $G[V \setminus S]$. A separator S is* minimal *if $S \setminus \{i\}$ is not a a,b-separator for any $i \in S$. Let $\mathcal{S}(a, b)$ denote the* family of all a, b-separators.

We ensure connectivity of electoral districts $D_\ell = \{i \in V : X_{i\ell} = 1\}$, $\ell \in [k]$ by considering following *a, b-separator inequalities* (9.13) in our model.

$$X_{a\ell} + X_{b\ell} - \sum_{i \in S} X_{i\ell} \leq 1 \qquad \forall \ell \in [k],\ a \neq b \in V,\ S \in \mathcal{S}(a, b) \tag{9.13}$$

Given an integer solution X, these inequalities force connectivity of D_ℓ as follows: Whenever two distinct units $a, b \in V$ are in electoral district D_ℓ, i.e., $X_{a\ell} = X_{b\ell} = 1$, at least one unit $i \in S$ from any separator $S \in \mathcal{S}(a, b)$ has to be in that district as well. This ensures that there exists a path between a and b and therefore connectivity. Only minimal separators $S \in \mathcal{S}(a, b)$ have to be considered in (9.13) since they dominate the remaining ones.

Wang et al. (2017) showed that the minimal a, b-separator inequalities *induce facets* of the *connected subgraph polytope*

$$\mathcal{P}(G) := \text{conv}\{x^D \in \{0,1\}^{|V|} : D \subseteq V, G[D] \text{ connected}\},$$

where x^D denotes the characteristic vector of $D \subseteq V$ and $G = (V, E)$ a connected graph.

There can be exponentially many (minimal) separator inequalities (9.13). Therefore, we implement (9.13) as lazy constraints, separate them on the fly based on an integer point and using the linear time algorithm proposed by Fischetti et al. (2016, Algorithm 1). Thereby, we cut off infeasible integer points during the branch-and-bound procedure. Fischetti et al. (2016) comments on the possibility additionally separating (9.13) on the basis of fractional solutions. Referring to computational experience, however, the authors argue that this is too

ineffective to be worth the time consuming effort. We follow this statement and separate on integer points only.

9.4.1.2 Objective functions and budget constraints

We add decision variables (9.14) – (9.16) to our MILP. These represent the measurement of the three objectives for each electoral district $\ell \in [k]$. The objective is given by (9.17).

$$E_\ell^{\text{cont}} \in [0,1] \qquad \forall \ell \in [k] \tag{9.14}$$
$$E_\ell^{\text{adm}} \in [0,1] \qquad \forall \ell \in [k] \tag{9.15}$$
$$E_\ell^{\text{pop}} \in [0,1] \qquad \forall \ell \in [k] \tag{9.16}$$

$$\max \quad \omega^{\text{cont}} \sum_{\ell=1}^{k} E_\ell^{\text{cont}} + \omega^{\text{adm}} \sum_{\ell=1}^{k} E_\ell^{\text{adm}} + \omega^{\text{pop}} \sum_{\ell=1}^{k} E_\ell^{\text{pop}} \tag{9.17}$$

Continuity. For a pair of a current electoral district $D_\ell^{\text{old}} \in \mathcal{D}^{\text{old}}$ and an electoral district to be determined D_ℓ, the population that has been left $p(D_\ell^{\text{old}} \setminus D_\ell)$ and that has been added $p(D_\ell \setminus D_\ell^{\text{old}})$ can be modeled as $\sum_{i \in D_\ell^{\text{old}}} p_i \cdot (1 - X_{i\ell})$ and $\sum_{i \in V \setminus D_\ell^{\text{old}}} p_i \cdot X_{i\ell}$, respectively. We add (9.18) and (9.19) to our MILP; computing a temporary measurement of continuity.

$$E_\ell^{\text{cont,temp}} \in \mathbb{R} \qquad \forall \ell \in [k] \tag{9.18}$$
$$E_\ell^{\text{cont,temp}} = 1 - \frac{\sum_{i \in D_\ell^{\text{old}}} p_i \cdot (1 - X_{i\ell}) + \sum_{i \in V \setminus D_\ell^{\text{old}}} p_i \cdot X_{i\ell}}{\bar{p}} \qquad \forall \ell \in [k] \tag{9.19}$$

Because of population limits (9.12), it holds

$$-0.25 - \frac{p(D_\ell^{\text{old}})}{\bar{p}} = 1 - \frac{p(D_\ell^{\text{old}}) + 1.25\,\bar{p}}{\bar{p}} \leq E_\ell^{\text{cont,temp}} \leq 1.$$

To model $E_\ell^{\text{cont}} = \max\{0, E_\ell^{\text{cont,temp}}\}$, we use auxiliary variables $\text{AUX}_\ell^{\text{cont}} \in \{0,1\}$. We add (9.20) – (9.22) to our MILP formulation.

$$\text{AUX}_\ell^{\text{cont}} \in \{0,1\} \qquad \forall \ell \in [k] \tag{9.20}$$
$$E_\ell^{\text{cont}} \leq E_\ell^{\text{cont,temp}} + \left(0.25 + \tfrac{p(D_\ell^{\text{old}})}{\bar{p}}\right) \cdot \left(1 - \text{AUX}_\ell^{\text{cont}}\right) \qquad \forall \ell \in [k] \tag{9.21}$$
$$E_\ell^{\text{cont}} \leq \text{AUX}_\ell^{\text{cont}} \qquad \forall \ell \in [k] \tag{9.22}$$

The objective sense of the MILP (cf. (9.17)) ensures that such pairs $D_\ell^{\text{old}} \leftrightarrow D_\ell$ are obtained, so that $\sum_{\ell=1}^{k} E_\ell^{\text{cont}}$ is maximum.

The measurement of continuity can be used additionally or as a substitute for the continuity objective at $\omega^{\text{cont}} = 0$ to add a budget limit on the continuity for the whole districting plan $\mathcal{D}$.

$$\sum_{\ell=1}^{k} \sum_{i \in D_\ell^{\text{old}}} p_i \cdot (1 - X_{i\ell}) \leq \text{bdg}^{\text{cont}} \cdot p(V)$$

The budget parameter $\text{bdg}^{\text{cont}} \in [0, 1]$ states the maximum proportion of people allowed to change their electoral district.

Administrative conformity. We start modeling with the second case of administrative conformity's Definition 25. Using the geographical data and the partition in rural/urban districts $\mathcal{A}$, we denote the following parameters for $i \in V$ and $\{i, j\} \in E$:

$$\begin{aligned}
b_i &:= \text{perimeter's length of the area of unit } i \in V \\
b_i^{\mathcal{A}} &:= \begin{cases} \text{length of the perimeter of area of unit } i \in V \\ \text{which matches with boundaries of rural/urban districts } \mathcal{A} \end{cases} \\
b_{ij} &:= \text{length of the shared border between } i, j \in V \text{ with } \{i, j\} \in E \\
b_{ij}^{\mathcal{A}} &:= \begin{cases} \text{length of the shared border between } i, j \in V \text{ with } \{i, j\} \in E \\ \text{corresponding to boundaries of a rural/urban district } A \in \mathcal{A} \end{cases}
\end{aligned}$$

In general, $b_i \geq b_i^{\mathcal{A}}$ and $b_{ij} \geq b_{ij}^{\mathcal{A}}$ holds. For adjacent units $i, j \in V$ which are in the same rural/urban district $A \in \mathcal{A}$ holds: $b_{ij}^{\mathcal{A}} = 0$. For the case $i \in A_1 \in \mathcal{A}$ and $j \in A_2 \in \mathcal{A}$ with $A_1 \neq A_2$ holds: $b_{ij} = b_{ij}^{\mathcal{A}}$.

We add decision variables $Y_{ij\ell} \in \{0, 1\}$ for $\{i, j\} \in E$ to indicate if an edge $\{i, j\} \in E$ is part of the electoral district's subgraph $G[D_\ell]$. Using (9.23) – (9.26), variable $Y_{ij\ell}$ equals one if and only if $X_{i\ell} = 1$ and $X_{j\ell} = 1$ holds.

$$Y_{ij\ell} \in \{0, 1\} \qquad \forall \{i, j\} \in E, \ell \in [k] \tag{9.23}$$

$$X_{i\ell} \geq Y_{ij\ell} \qquad \forall \{i, j\} \in E, \ell \in [k] \tag{9.24}$$

$$X_{j\ell} \geq Y_{ij\ell} \qquad \forall \{i, j\} \in E, \ell \in [k] \tag{9.25}$$

$$X_{i\ell} + X_{j\ell} - 1 \leq Y_{ij\ell} \qquad \forall \{i, j\} \in E, \ell \in [k] \tag{9.26}$$

The perimeter $\text{perim}(D_\ell)$ of an electoral district $D_\ell \subseteq V$ as used in Definition 25 can be modeled linearly as follows. We sum up the length of the perimeter of each unit $i \in D_\ell$ with $X_{i\ell} = 1$ and subtract twice the length of the boundaries shared by adjacent units $i, j \in D_\ell$, $\{i, j\} \in E$ with $Y_{ij\ell} = 1$. Likewise, $\text{perim}^{\mathcal{A}}(D_\ell)$ can be modeled:

$$\text{perim}(D_\ell) = \sum_{i \in V} b_i \cdot X_{i\ell} - \sum_{\{i,j\} \in E} 2b_{ij} \cdot Y_{ij\ell}\,, \quad \text{perim}^{\mathcal{A}}(D_\ell) = \sum_{i \in V} b_i^{\mathcal{A}} \cdot X_{i\ell} - \sum_{\{i,j\} \in E} 2b_{ij}^{\mathcal{A}} \cdot Y_{ij\ell}.$$

We add variables (9.27) to our MILP, storing a temporary measurement of administrative conformity.

$$E_\ell^{\text{adm,temp}} \in [0, 1] \qquad \forall \ell \in [k] \tag{9.27}$$

We continue with the following steps.

$$E_\ell^{\text{adm,temp}} \overset{\text{Def. 25}}{=} \frac{\text{perim}^{\mathcal{A}}(D_\ell)}{\text{perim}(D_\ell)} = \frac{\sum_{i\in V} b_i^{\mathcal{A}} \cdot X_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij}^{\mathcal{A}} \cdot Y_{ij\ell}}{\sum_{i\in V} b_i \cdot X_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij} \cdot Y_{ij\ell}}$$

$$\iff \sum_{i\in V} b_i \cdot E_\ell^{\text{adm,temp}} \cdot X_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij} \cdot E_\ell^{\text{adm,temp}} \cdot Y_{ij\ell} = \sum_{i\in V} b_i^{\mathcal{A}} \cdot X_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij}^{\mathcal{A}} \cdot Y_{ij\ell}$$

The products $E_\ell^{\text{adm,temp}} \cdot X_{i\ell} =: \tilde{X}_{i\ell} \in [0,1]$ and $E_\ell^{\text{adm,temp}} \cdot Y_{ij\ell} =: \tilde{Y}_{ij\ell} \in [0,1]$ of bounded continuous and binary variables can be linearized (folklore). We add decision variables (9.28) and (9.29), and equations (9.30) – (9.36) to our MILP. We come up with a formulation for the objective of administrative conformity.

$$\tilde{X}_{i\ell} \in [0,1] \qquad \forall i \in V, \ell \in [k] \tag{9.28}$$

$$\tilde{Y}_{ij\ell} \in [0,1] \qquad \forall \{i,j\} \in E, \ell \in [k] \tag{9.29}$$

$$\tilde{X}_{i\ell} \leq X_{i\ell} \qquad \forall i \in V, \ell \in [k] \tag{9.30}$$

$$\tilde{X}_{i\ell} \leq E_\ell^{\text{adm,temp}} \qquad \forall i \in V, \ell \in [k] \tag{9.31}$$

$$\tilde{X}_{i\ell} \geq E_\ell^{\text{adm,temp}} + X_{i\ell} - 1 \qquad \forall i \in V, \ell \in [k] \tag{9.32}$$

$$\tilde{Y}_{ij\ell} \leq Y_{ij\ell} \qquad \forall \{i,j\} \in E, \ell \in [k] \tag{9.33}$$

$$\tilde{Y}_{ij\ell} \leq E_\ell^{\text{adm,temp}} \qquad \forall \{i,j\} \in E, \ell \in [k] \tag{9.34}$$

$$\tilde{Y}_{ij\ell} \geq E_\ell^{\text{adm,temp}} + Y_{ij\ell} - 1 \qquad \forall \{i,j\} \in E, \ell \in [k] \tag{9.35}$$

$$\sum_{i\in V} b_i \cdot \tilde{X}_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij} \cdot \tilde{Y}_{ij\ell} = \sum_{i\in V} b_i^{\mathcal{A}} \cdot X_{i\ell} - \sum_{\{i,j\}\in E} 2b_{ij}^{\mathcal{A}} \cdot Y_{ij\ell} \qquad \forall \ell \in [k] \tag{9.36}$$

Following Definition 25, the temporary measurement $E_\ell^{\text{adm,temp}}$ equals E_ℓ^{adm} in the definition's second case. In addition, we now model the first case in the following, i.e., the case where D_ℓ consists of units of a single rural/urban district $A \in \mathcal{A}$ with $p(A) > 1.25 \cdot \bar{p}$.

We define a subset of nodes $V^{\text{adm,aux}} \subseteq V$ and subset of edeges $E^{\text{adm,aux}} \subseteq E$:

$$V^{\text{adm,aux}} := \{i \in V \,:\, i \in A \text{ with } A \in \mathcal{A},\, p(A) \leq 1.25 \cdot \bar{p}\}$$
$$E^{\text{adm,aux}} := \{\{i,j\} \in E \,:\, i \in A_1,\, j \in A_2 \text{ with } A_1, A_2 \in \mathcal{A},\, A_1 \neq A_2\}$$

If $V^{\text{adm,aux}} = V$ holds, no rural/urban district exceeds the legal limit of electoral district population. For such an problem instance, we simply add $E_\ell^{\text{adm}} = E_\ell^{\text{adm,temp}}$ $\forall \ell \in [k]$ to our MILP and the following specifications have not to be taken into account. However, the following modeling is feasible for any kind of $V^{\text{adm,aux}}$.

We introduce an auxiliary binary variable $\text{AUX}_\ell^{\text{adm}}$ that is forced to be 1 by Constraints (9.38) – (9.39) if electoral district D_ℓ contains a unit from a rural/urban district A with $A \leq 1.25 \cdot \bar{p}$ or an edge that traverses a rural/urban district boundary.

$$\text{AUX}_\ell^{\text{adm}} \{0,1\} \qquad \forall \ell \in [k] \tag{9.37}$$

$$\text{AUX}_\ell^{\text{adm}} \geq \frac{1}{|V^{\text{adm,aux}}|} \sum_{i \in V^{\text{adm,aux}}} X_{i\ell} \qquad \forall \ell \in [k] \tag{9.38}$$

$$\text{AUX}_\ell^{\text{adm}} \geq Y_{ij\ell} \qquad \forall \{i,j\} \in E^{\text{aux,adm}}, \ell \in [k] \tag{9.39}$$

In the case of $V^{\text{adm,aux}} = \emptyset$, equations (9.38) are omitted. Finally, Definition 25 can be carried out with $E_\ell^{\text{adm}} = \max\left\{E_\ell^{\text{adm,temp}}, 1 - \text{AUX}_\ell^{\text{adm}}\right\}$. Due to the maximization of objective function (9.17), this can be expressed via following equations (9.40).

$$E_\ell^{\text{adm}} \leq E_\ell^{\text{adm,temp}} + (1 - \text{AUX}_\ell^{\text{adm}}) \qquad \forall \ell \in [k] \tag{9.40}$$

If electoral district D_ℓ is entirely contained within a rural/urban district A with $p(A) > 1.25 \cdot \bar{p}$, $E_\ell^{\text{adm}} = 1$ holds since $\text{AUX}_\ell^{\text{adm}}$ may assume the value 0. Otherwise, electoral district D_ℓ must contain a unit from a rural/urban district A with $p(A) \leq 1.25 \cdot \bar{p}$ or units from different rural/urban districts. In both cases, $\text{AUX}_\ell^{\text{adm}}$ is forced to 1 and it holds $E_\ell^{\text{adm}} = E_\ell^{\text{adm,temp}}$.

Population deviation. First, we add variables $\text{DEV}_\ell \geq 0$, ℓ to our MILP, cf. (9.41). To have in mind the objective sense and the fact that f is monotone decreasing, equations (9.42) and (9.43) model $\text{DEV}_\ell = \left| \frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \right|$.

$$\text{DEV}_\ell \in [0, 25\%] \qquad \forall \ell \in [k] \tag{9.41}$$

$$\text{DEV}_\ell \geq \frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \qquad \forall \ell \in [k] \tag{9.42}$$

$$\text{DEV}_\ell \geq -\left(\frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \right) \qquad \forall \ell \in [k] \tag{9.43}$$

There are several options to model $E_\ell^{\text{pop}} = f(\text{DEV}_\ell)$ with an piecewise linear function f. We do it as follows. Let $g_s \in [0, 25\%]$ for $s = 0, \ldots, n^{\text{pwl}}$, $n^{\text{pwl}} \in \mathbb{N}$ be the grid points of f with corresponding monotonically decreasing function values $f(g_s)$. In Figure 9.4 holds $g_0 = 0$, $g_1 = 10\%$, $g_2 = 15\%$, $g_3 = 25\%$ with $f(0) = 1$, $f(10\%) = 1$, $f(15\%) = 0.75$, $f(25\%) = 0$. Let $\text{grd}_h^{\text{pwn}}$ be the gradient of segment h, i.e.,

$$\text{grd}_h^{\text{pwn}} := \frac{f\left(g_h^{\text{pwl}}\right) - f\left(g_{h-1}^{\text{pwl}}\right)}{g_h^{\text{pwl}} - g_{h-1}^{\text{pwl}}}, \qquad h \in [n^{\text{pwl}}].$$

With the help of additional variables $S^{\text{pwl}}_{\ell h}$ and $T^{\text{pwl}}_{\ell h}$ we model $E^{\text{pop}}_{\ell} = f(\text{DEV}_\ell)$ in equations (9.44) – (9.49).

$$S^{\text{pwl}}_{\ell h} \in \{0,1\} \qquad \forall \ell \in [k], h \in [n^{\text{pwl}}] \tag{9.44}$$

$$\sum_{h=1}^{n^{\text{pwl}}} S^{\text{pwl}}_{\ell h} = 1 \qquad \forall \ell \in [k] \tag{9.45}$$

$$T^{\text{pwl}}_{\ell h} \in [0, g^{\text{pwl}}_h] \qquad \forall \ell \in [k], h \in [n^{\text{pwl}}] \tag{9.46}$$

$$g^{\text{pwl}}_{h-1} S^{\text{pwl}}_{\ell h} \leq T^{\text{pwl}}_{\ell h} \leq g^{\text{pwl}}_h S^{\text{pwl}}_{\ell h} \qquad \forall \ell \in [k], h \in [n^{\text{pwl}}] \tag{9.47}$$

$$\text{DEV}_\ell = \sum_{h=1}^{n^{\text{pwl}}} T^{\text{pwl}}_{\ell h} \qquad \forall \ell \in [k] \tag{9.48}$$

$$E^{\text{pop}}_{\ell} = \sum_{h=1}^{n^{\text{pwl}}} f(g^{\text{pwl}}_h) S^{\text{pwl}}_{\ell h} + \text{grd}_h \left(T^{\text{pwl}}_{\ell h} - g^{\text{pwl}}_h S^{\text{pwl}}_{\ell h} \right) \qquad \forall \ell \in [k] \tag{9.49}$$

The presented MILP formulation (9.10)–(9.49) is named

Political Districting Problem MILP (PDP-MILP).

Even if the formulation contains next to $X_{i\ell}$ numerous further decision variables through the modeling of the objective function, their unique values can be derived completely from given values of the $X_{i\ell}$ variables.

9.4.2 Preprocessing

Due to the connectivity requirement and population minimum of each electoral district (cf. Definition 21), an exact preprocessing procedure is possible. One can identify a set of nodes which are definitely in the same electoral district. Therefore, the subgraph induced by these nodes can be contracted to one single node. This preprocessing procedure is exact, i.e., no feasible solution gets lost, and is based on *articulation nodes*.

Definition 29 (articulation node) *Let $G = (V, E)$ be a graph. A node $i \in V$ is called* articulation node *if $G[V \setminus \{i\}]$ decomposes into at least two components.*

The set of all articulation nodes can be computed in $\mathcal{O}(|V| + |E|)$ time (Hopcroft and Tarjan, 1973). In our case, only articulation nodes are of interest that yield to (at least) one component with population less than the population minimum of a legal electoral district. The nodes of such a component are in the same electoral district for sure. For each articulation node and their resulting components we check the mentioned condition. If successful, we contract the articulation node and all components with population less than the minimum of a electoral district to a single node. If the node resulting from such a contraction covers more population than is legally allowed for one electoral district, it can be concluded that the instance is infeasible. In the course of a contraction, the population

and geographical data must be adjusted accordingly. When iterating through the set of articulation nodes, a articulation node may already have been part of a contraction. In that case, this node can be skipped.

9.4.3 Start- and Improvement Heuristics

Based on the PDP-MILP presented in Section 9.4.1, we develop heuristic approaches to compute primal solutions. The procedures either aim to improve a feasible solution (Sec. 9.4.3.1) or work towards the goal of converting an infeasible partition of the graph into a valid districting plan (Sec. 9.4.3.2).

On the one hand, these approaches are used to supply the PDP-MILP with a good start solution. In addition, the improvement heuristic is triggered by every new primal solution found by the MILP solver during the solving procedure.

Figure 9.5 provides an overview of the interaction between the PDP-MILP described in Section 9.4.1 and the methods and models presented in the following sections.

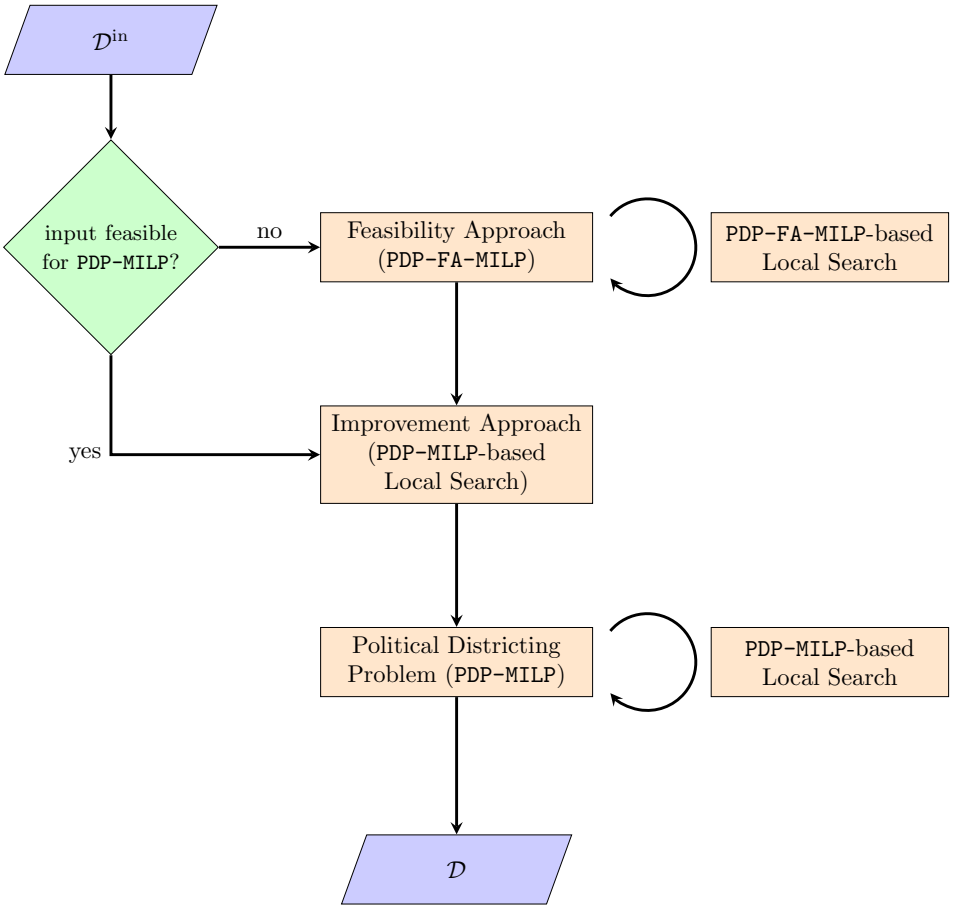


Fig. 9.5: Flowchart of the interaction of start/improvement heuristics and the PDP-MILP.

9.4.3.1 MILP-based Local Search

Local search algorithms are based on a solution and an iterative "movement" to another solution by applying local changes. Such a movement is called a step. The local search procedure stops if no improving solution can be found in a step's search space, a time bound elapsed, or another criterion applies. A local search step can be performed based on combinatorial algorithms. In our work, we take advantage of the performance of state-of-the-art MILP solvers and thereby use the opportunity to explore a larger search space in each step. The definition of search space exploited here uses the presented PDP-MILP formulation.

For now, a districting plan $\mathcal{D}^{\text{in}} = \{D_1^{\text{in}}, \dots, D_k^{\text{in}}\}$ is given which is feasible for PDP-MILP ($\mathcal{D} := \mathcal{D}^{\text{in}}$). In addition, we state in the upcoming Section 9.4.3.2 how a comparable local search procedure is used in a feasibility heuristic based on an infeasible districting plan.

The idea of the PDP-MILP-based local search is to modify PDP-MINLP by fixing all assignments $X_{i\ell}$ between units $i \in V$ and electoral districts ℓ given by $\mathcal{D}^{\text{in}}$, except for those units adjacent to units of another electoral district in $\mathcal{D}^{\text{in}}$. That is, we fix $X_{i\ell}$ for all $i \in V$ except for units i at the boundaries of the given electoral districts. For this, we define *boundary units*.

Definition 30 (boundary unit and edge) *Given a districting plan $\mathcal{D}^{in} = \{D_1, \dots, D_k\}$. A unit $i \in V$ is called* boundary unit*, if at least one other unit $j \in V$ exists with $\{i, j\} \in E$ and being in a different electoral district, i.e., $i \in D_{\ell_i}$ and $j \in D_{\ell_j}$ with $\ell_i \neq \ell_j$. The set of all boundary units is denoted with $B^V(\mathcal{D})$. An edge $\{i, j\} \in E$ is called* boundary edge*, if $i, j \in B^V(\mathcal{D})$ are boundary units. The set of all boundary edges is denoted with $B^E(\mathcal{D})$.*

Using this definition, following additions to PDP-MILP are performed. We fix the districting assignment given by $\mathcal{D}^{\text{in}}$ for all units except for boundary units.

$$X_{i\ell} = 1 \qquad \forall i \in V \setminus B^V(\mathcal{D}^{\text{in}}), \ell \in [k] : i \in D_\ell^{\text{in}} \tag{9.50}$$

For boundary units, we limit the assignment options to the assigned electoral district in $\mathcal{D}^{\text{in}}$ and neighboring ones. Note, a boundary unit can be adjacent to more than one electoral district.

$$X_{i\ell} + \sum_{\substack{\tilde{\ell} \in [k] : \\ \exists \{i,j\} \in B^E(\mathcal{D}^{\text{in}}) \\ \text{with } j \in D_{\tilde{\ell}}^{\text{in}}}} X_{i\tilde{\ell}} = 1 \qquad \forall i \in B^V(\mathcal{D}^{\text{in}}), \ell \in [k] : i \in D_\ell^{\text{in}} \tag{9.51}$$

The resulting MILP formulation depends on the input $\mathcal{D}^{\text{in}}$ and is named *PDP-MILP-based Local Search MILP for $\mathcal{D}^{in}$ (PDP-LS-MILP($\mathcal{D}^{in}$))*.

With regard to the set partitioning constraints (9.11), the fixations (9.50) and equations (9.51) imply fixations of several further variables and in particular $X_{i\ell}$ variables to the value 0. Thus, the performed fixations of $X_{i\ell}$ variables thins out the MILP a lot since all decision variables added to model the objective functions are easily computed when values of $X_{i\ell}$

variables are known. A lot of variables and constraints can be neglected in advance or are removed during the presolving performed by the MILP solver. Simultaneously, almost all symmetry, naturally given by assignment variables, is broken in the MILP. Furthermore, the solution given by $\mathcal{D}^{\text{in}}$ is still feasible for PDP-LS-MILP. We take advantage of this and provide a start solution to the solver. In order to ensure connectivity of the electoral districts, we also separate a,b-separator inequalities on the fly in the solution process as indicated in Section 9.4.1.1

PDP-LS-MILP is solved until optimality, a predefined number of solutions, or a time limit is reached. The best found solution $\mathcal{D}^{\text{impro}}$ is used as input for the next local search step, i.e. solving PDP-LS-MILP($\mathcal{D}^{\text{impro}}$). The procedure stops if no improving solution is found.

Algorithm 1 gives a gathered overview of the PDP-MILP-based local search procedure.

Algorithm 1: MILP-based local search to improve districting plan

Input: feasible districting plan $\mathcal{D}^{\text{in}}$
initialize $\mathcal{D}^{\text{impro}} \leftarrow$ `none`
do
  if $\mathcal{D}^{\text{impro}} \neq$ `none` **then**
    $\mathcal{D}^{\text{in}} \leftarrow \mathcal{D}^{\text{impro}}$
  end
  solve PDP-LS-MILP($\mathcal{D}^{\text{in}}$)
    · with possibly timelimit or solution limit
    · use $\mathcal{D}^{\text{in}}$ for warmstart
  $\mathcal{D}^{\text{impro}} \leftarrow$ best found solution
while $\mathcal{D}^{\text{impro}} \neq \mathcal{D}^{\text{in}}$
Output: feasible (improved) districting plan $\mathcal{D}^{\text{impro}}$

9.4.3.2 MILP-based Feasibility Approach

The procedure given in the following is based on a districting plan $\mathcal{D}^{\text{in}} \in \mathcal{P}(V)$ which is not feasible for PDP-MILP.

The PDP-MILP presented in Section 9.4.1 is relaxed by removing the population constraints (9.12). Furthermore, objective (9.17) is replaced. In the course of this, the variables and conditions for modeling the objective function (9.17) are also removed. In the new objective function, the number of electoral districts that meet the population limit of $\pm 25\%$ deviation is to be maximized. In addition, the sum of absolute deviation values of the electoral districts is minimized.

We introduce binary decision variables $\text{FEAS}_\ell^{\text{pop}} \in \{0, 1\}$ for each electoral district $\ell \in [k]$. Such a variable $\text{FEAS}_\ell^{\text{pop}}$ equals 1 if and only if the population deviation of electoral district ℓ is inside the legal interval $[-25\%, 25\%]$.

$$\text{FEAS}_\ell^{\text{pop}} \in \{0,1\} \qquad \forall \ell \in [k] \tag{9.52}$$

$$-0.25 - 0.75 \cdot (1 - \text{FEAS}_\ell^{\text{pop}}) \leq \frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \qquad \forall \ell \in [k] \tag{9.53}$$

$$0.25 + \text{bigM} \cdot (1 - \text{FEAS}_\ell^{\text{pop}}) \geq \frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \qquad \forall \ell \in [k] \tag{9.54}$$

As parameter bigM one can choose $\text{bigM} := \frac{\sum_{i \in V} p_i}{\bar{p}} - 1.25$.

To model the second part of the new objective function, we use a formulation known from the modeling of population deviation objective function in Section 9.4.1.2, cf. equations (9.41)–(9.43).

$$\text{DEV}_\ell \geq 0 \qquad \forall \ell \in [k] \tag{9.55}$$

$$\text{DEV}_\ell \geq \frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1 \qquad \forall \ell \in [k] \tag{9.56}$$

$$\text{DEV}_\ell \geq -\left(\frac{\sum_{i \in V} p_i X_{i\ell}}{\bar{p}} - 1\right) \qquad \forall \ell \in [k] \tag{9.57}$$

With this, we formulate the new objective function for the feasibility approach.

$$\max \sum_{\ell \in [k]} \text{FEAS}_\ell^{\text{pop}} - \text{DEV}_\ell \tag{9.58}$$

The resulting MILP formulation is named *PDP Feasibility Approach MILP (PDP-FA-MILP)*.

To ensure connectivity, lazy constraints in form of a,b-separator inequalities are separated on the fly (cf. Section 9.4.1.1). Although $\mathcal{D}^{\text{in}}$ may contain non-connected electoral districts, $\mathcal{D}^{\text{in}}$ is offered to the solver as a starting solution. Potentially, first violated a,b-separator inequalities are added to the MILP to reach connected electoral districts as quickly as possible.

The solving process of PDP-FA-MILP is supported by a MILP-based local search, analogous to the one in Section 9.4.3.1 for LS-MILP. The local search is implemented as a start heuristic and an improvement heuristic based on each found primal solution of PDP-FA-MILP. Adding fixations (9.50) and equations (9.51) to PDP-FA-MILP leads to *PDP-FA-MILP-based Local Search MILP for $\mathcal{D}^{in}$ (PDP-FA-LS-MILP($\mathcal{D}^{in}$))*. The local search procedure can repair connectivity if district's components are not scattered too much across the graph. In the best case, the local search procedure computes a feasible districting plan starting from $\mathcal{D}^{\text{in}}$.

9.5 Decision Support System for Optimal Political Districting

Based on an open-source geoinformation software system, we designed a decision support software for optimal political (re-)districting. A screenshot of the sofware is given in Figure 9.6. A user of WKOPT, as the software is called, is able to analyze a pregiven districting plan and modify some electoral districts by hand or define a complete new one. In addition, the developed methods of mathematical optimization can be applied to obtain optimal adjustments of the districting plan which can be used as a objective basis for decision-making.

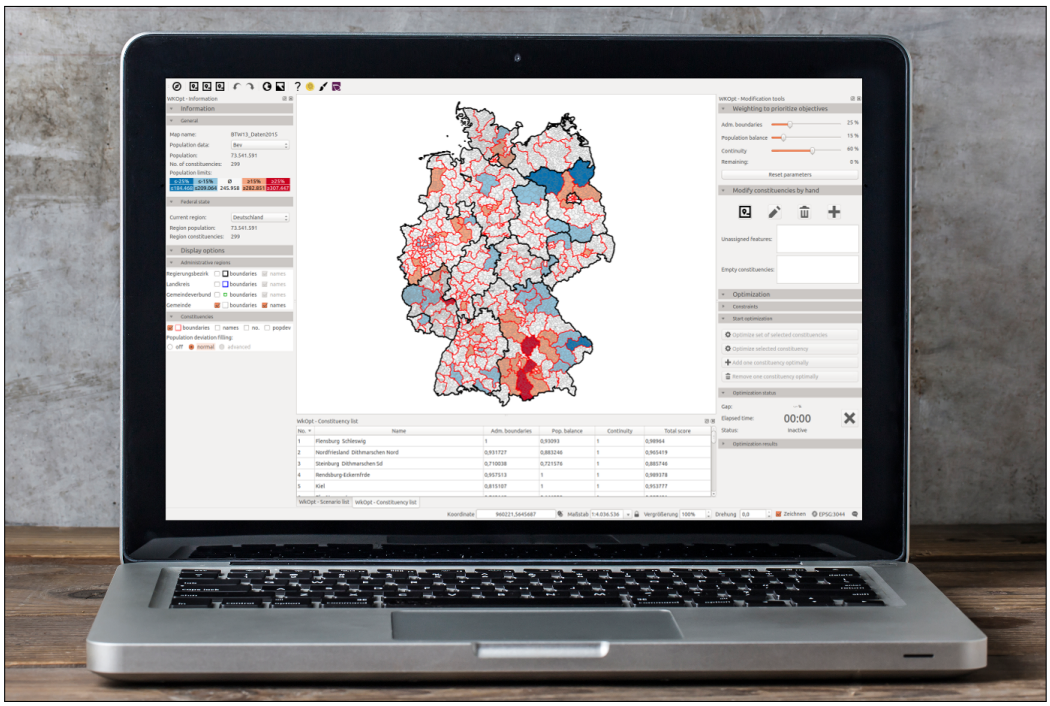


Fig. 9.6: Geovisual decision support system WKOPT with districting plan of German federal elections 2013 on population data as of June 30, 2015.

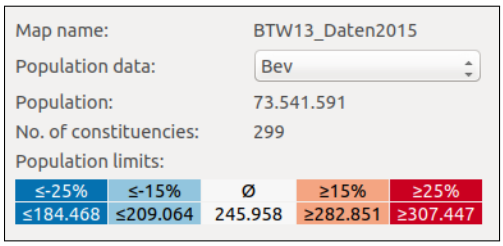
WKOPT combines the technology of a geoinformation system with descriptive analytics and specialized methods of mathematical optimization. The criteria used for the numerical evaluation and optimization of electoral districts are derived directly from the legal requirements (cf. Sec. 9.3.2). It is important to mention that the user still has all decision-making power, as manual changes to the districting plan can be made and evaluated at any time – this also holds for optimization-based computed electoral districts. The software thus offers optimal support in issues concerning political (re-)districting.

In the following Subsections 9.5.1 – 9.5.3, the functionality and features of WKOPT are presented in detail.

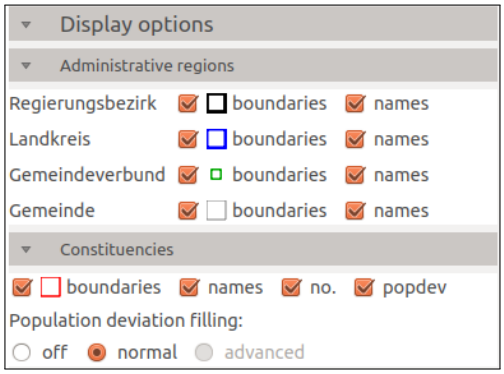
9.5.1 Appearance, Options, Descriptive Analytics

After starting the software, the user is able to load a map via the toolbar. The data format shapefile `shp`, which is known for geodata, is expected. In addition to geographical information, the number of German population, the official municipality key, and, if applicable, the electoral district is required for each (sub-)area. Figure 9.6 shows a screenshot of the software after loading the map of Germany with the districting plan of the Bundestag elections in 2013. In addition, it is also possible to load only individual regions or federal states to prepare e.g. state elections.

The interactive map shows all relevant administrative boundaries as well as the names of their areas (depending on zoom level). The user has the option to hide any type of boundary and label (cf. Fig. 9.7b). Boundaries of the current electoral districts are also displayed. According to a electoral district's population and the resulting deviation from an average one, the area of the electoral district is colored. The legend given in the tool is shown in Figure 9.7a. Dark red and dark blue colored electoral districts do not comply with the legal requirements and need appropriate revisions. White electoral districts have less than 15% population deviation.



(a) Color fillings of electoral districts.



(b) Display options for boundaries and labels.

Fig. 9.7: General information 9.7a and display options 9.7b of a loaded map in WKOPT.

The entire color scheme of the map has been adopted from the official districting maps published by the German federal election commissioner and the districting commission (BT-Drs. 19/7500, 2019). Since the visualization is based on a geoinformation system, one can study the map intuitively by zooming and moving with the mouse. Thus the exact location of a electoral district boundary can be obtained, matches with the boundaries of rural and urban districts can be checked, and names of smaller areas can be read.

Starting from the software screen showing the entire German territory, as in Figure 9.6, the user can select a single federal state. Then the map zooms to this state and grays out all other areas (cf. Fig. 9.8). Now one can concentrate on the state's electoral districts. One can see immediately that Brandenburg's districting plan from the 2013 election is no longer admissible. The population of two electoral districts deviates more than 25% from the average. Another four electoral districts show a deviation of more than 19%. The electoral districts of Brandenburg need definitely a revision for the Bundestag elections in 2017.

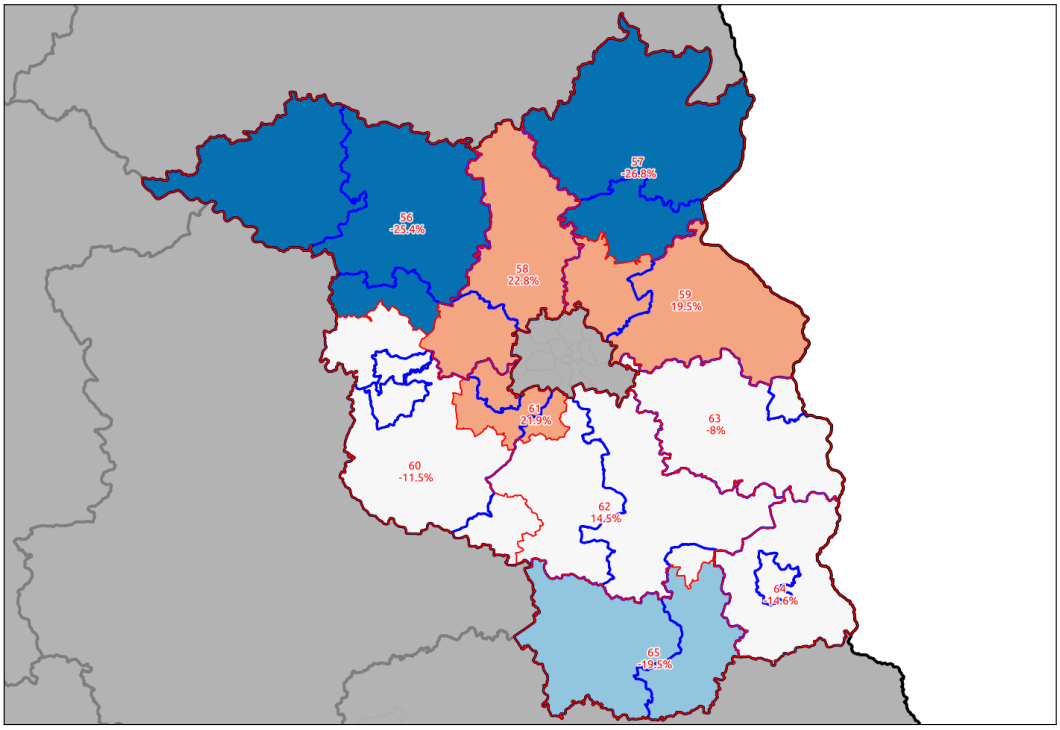


Fig. 9.8: Map after federal state of Brandenburg has been selected.

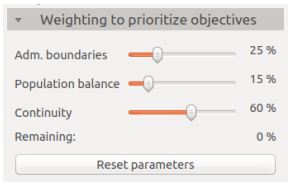
After selecting Brandenburg, the focus of descriptive analytics is now limited to the electoral districts of the federal state. For this, a list of electoral districts is displayed under the map (cf. Fig. 9.9a). Each electoral district is evaluated based on the three objectives defined in Section 9.3.2. The total score of each electoral district D_ℓ (last column in Fig. 9.9a) is calculated by

$$\text{total Score}(D_\ell) = \omega^{\text{adm}} E_\ell^{\text{adm}} + \omega^{\text{pop}} E_\ell^{\text{pop}} + \omega^{\text{cont}} E_\ell^{\text{cont}}$$

and depends on the choice of weights ω^σ of the objective functions (cf. equations (9.1)). The weighting can be chosen and adjusted by the user with sliders (cf. Fig. 9.9b), the overall rating of the electoral districts is updated immediately.

No.	Name	Adm. boundaries	Pop. balance	Continuity	Total score
56	Prignitz Ostprignitz-Ruppin Havelland I	0,859687	0	1	0,814922
57	Uckermark Barnim I	0,854964	0	1	0,813741
58	Oberhavel Havelland II	0,941323	0,177608	1	0,861972
59	Mrkisch-Oderland Barnim II	0,831307	0,432679	1	0,872729
60	Brandenburg an der Havel Potsdam-Mittelmark I Ha...	0,587645	0,841613	1	0,873153
61	Potsdam Potsdam-Mittelmark II Teltow-Flming II	0,457298	0,247213	1	0,751406
62	Dahme-Spreewald Teltow-Flming III Oberspreewald...	0,721429	0,720356	1	0,888411
63	Frankfurt (Oder) Oder-Spree	1	0,940404	1	0,991061
64	Cottbus Spree-Neie	1	0,716339	1	0,957451

(a) List of electoral districts and their evaluation.

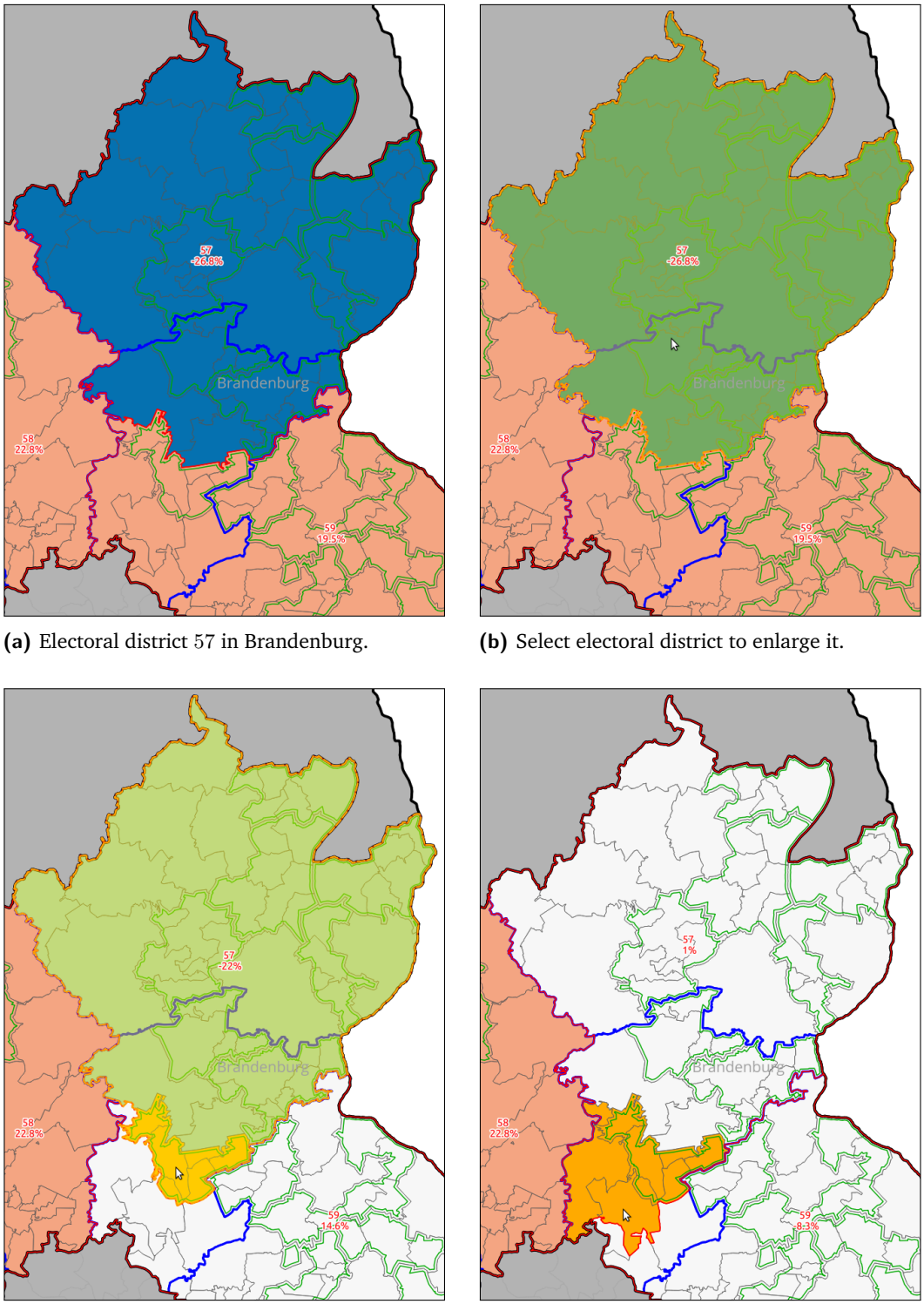


(b) Sliders for weights ω^σ.

Fig. 9.9: The electoral districts are evaluated according to the choice of relative weights of the three objectives E^{adm}, E^{pop}, E^{cont}.

9.5.2 Modify Electoral Districts by Hand

The user can change the districting plan manually using an easy-to-use select & click function. An example of this is given in Figure 9.10d. First, the user has to select the electoral district



(a) Electoral district 57 in Brandenburg.

(b) Select electoral district to enlarge it.

(c) Add territories to electoral district by hand.

(d) Deselected electoral district.

Fig. 9.10: Process of manually modifying the districting plan. Transposed areas (compared to the initial plan) are highlighted in orange. Colors of fillings, labels, boundaries, evaluation scores, etc. are updated live.

he wants to enlarge with additional areas (cf. Fig. 9.10b). Selecting an electoral district is possible directly on the map or via the list shown in Figure 9.9a. Next, by clicking on the areas to be added, the selected electoral district is enlarged (cf. Fig. 9.10c). Areas that are now assigned to a different electoral district compared to the initial plan are highlighted in orange. Immediately after each change, the visualization and information in the tool are updated. Of course, undo and redo buttons are available in the tool bar of the software.

A districting plan for a map is called *szenario* in WKOPT. To store performed changes a new szenario can be created. All szenarios of a map, including the initial one, are organized in the scenario manager list (cf. Fig. 9.11). In this list, the scenarios, i.e., different districting plans, can be compared with regard to the three objective functions and total score. In addition to create scenarios, it is also possible to change their names or delete them. In addition, the plans of two scenarios can be compared. Thereby areas where the electoral district differs are highlighted in orange.

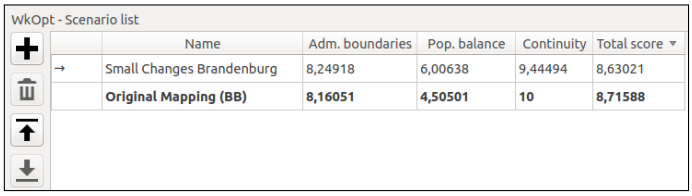


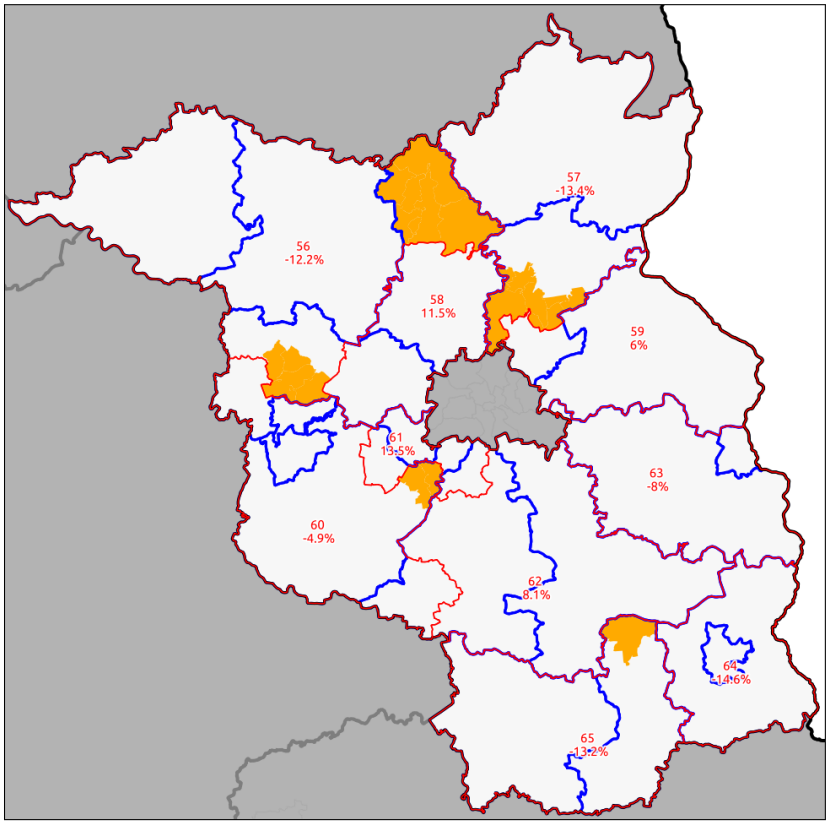
Fig. 9.11: Scenario manager list with the initial districting plan of Brandenburg (2nd row) and the one after adjustments done in Figure 9.10 (1st row).

The entries in the list of Figure 9.11 indicate that the changes performed in Figure 9.10 improve the administrative conformity and population deviation of Brandenburg's districting plan. This of course comes at the expense of continuity.

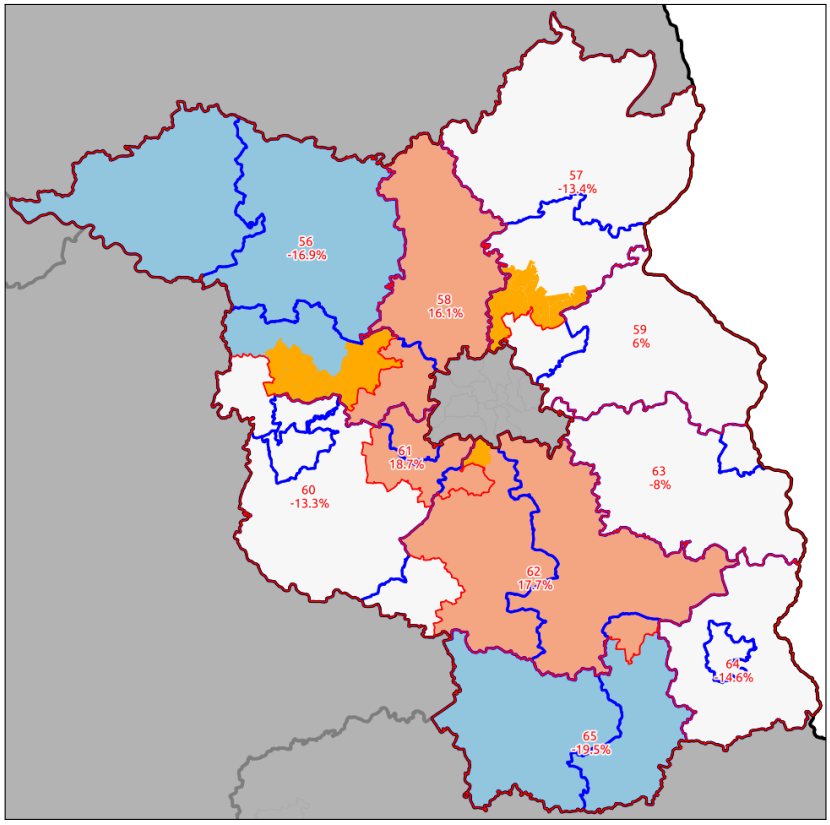
9.5.3 Apply Mathematical Optimization

As an example, the mathematical optimization methods developed in Section 9.4 are now applied on the federal state of Brandenburg. After selecting all 10 electoral districts of Brandenburg and selecting the objective weights as shown in Figure 9.9b (25% administrative conformity, 15% population balance, 60% continuity), the user can start the optimization by clicking on the corresponding button. During the optimization, all feasible solutions found are automatically transferred to WKOPT as scenarios and displayed in the list (cf. Fig. 9.13). The map always shows the best solution found so far.

10 seconds after Brandenburg's optimization was started, a feasible districting plan was found using the feasibility approach (cf. Sec. 9.4.3.2) starting from the invalid plan displayed in Fig. 9.8. After 15 iteratively improved solutions and a total of 2 minutes computing time, the improvement approach (cf. Sec. 9.4.3.1) handed over the best solution found to PDP-MILP. The MILP started with an optimization gap of 7.13%. By raising the dual bound, the gap was reduced to 4.56% in 1 minute and 30 seconds. At that time the calculation was terminated by the user. The primal bound was not improved by the MILP solver in this time. The best solution found after a total of 3 minutes and 30 seconds computation time is shown in Figure 9.12a.



(a) Best found districting plan after 3:30 minutes computation time.



(b) Official plan for German federal elections 2017

Fig. 9.12: Output of optimization procedure (a) and districting plan for elections 2017 (b). In both maps, transposed areas in comparison to elections 2013 (BT-Drs. 18/7873, 2016) are highlighted in orange.

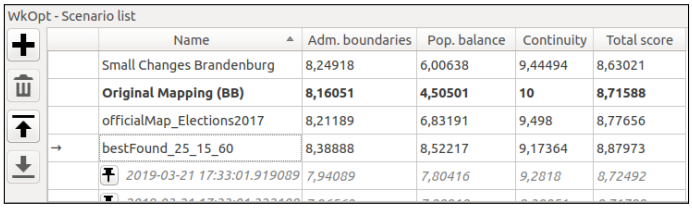


Fig. 9.13: Scenario list after optimization: scenario *Small Changes Brandenburg* was manually developed in Fig. 9.10, *bestFound_25_15_60* is depicted in Fig. 9.12a, *officialMap_Election2017* in Fig. 9.12b. All rows with grey font color contain temporary scenarios that were found during the optimization procedure. By clicking on the needle next to the temporary name, a temporary scenario can be made permanent, so that it is saved and will not be lost when closing the software.

After the optimization has been applied, the scenario list looks as shown in Figure 9.13. By hand, we have added the official changes made by the legislator to the 2017 election as a scenario called *officialMap_Election2017*. See Figure 9.12b for the map of this scenario.

In WKOPT it is also possible to select only certain electoral districts and optimize these. In Brandenburg, for example, this could be done for the two legally inadmissible electoral districts in the north and its neighbors. Each scenario can be manually modified and used as a starting point for optimization. In addition, the weighting of the objectives can be changed at any time. The numerical evaluation of the electoral districts and plans is immediately recalculated. The optimization methods always use the objective weights that were set at their start.

9.6 Case Study: German Federal Elections

On behalf of the German federal returning officer, we applied the presented software tool WKOPT to compute new districting plans for Germany. Optimization-based computations were requested in context of a debate on reducing the number of electoral districts in Germany from 299 to, e.g., 250, 200, or 125. The results are documented (in German) in the reports of Goderbauer et al. (2018a,b), the paper of Goderbauer and Lübbecke (2019b), and an online map (Goderbauer et al., 2019, online).

In this paper we present additional results: a new and optimization-based districting plan for Germany in 299 electoral districts. The result is numerically compared with the current 299 electoral districts applied in the federal elections 2017.

The case study is based on detailed geographical and population data as of September 30, 2017 (Goderbauer et al., 2018a). The weights of the objectives used are: 50% administrative conformity, 50% population balance, 0% continuity.

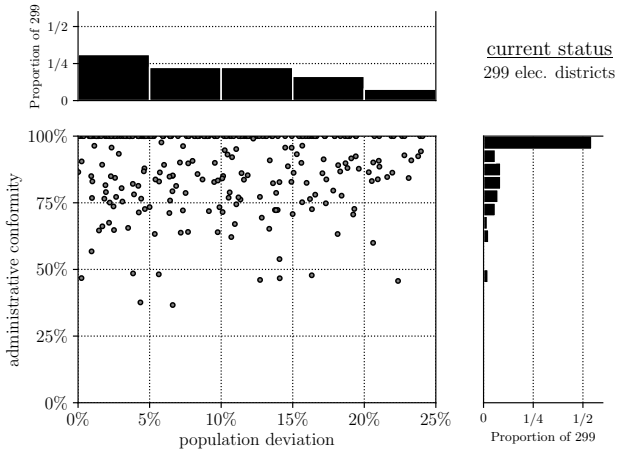
$$\omega^{\text{cont}} := 0, \qquad \omega^{\text{adm}} := 0.5, \qquad \omega^{\text{pop}} := 0.5$$

As required by law, the study is conducted for each federal state. Additionally, for federal states that are subdivided into governmental regions (German: Regierungsbezirke), the delimitation of electoral districts took place on this level. This was also performed in the

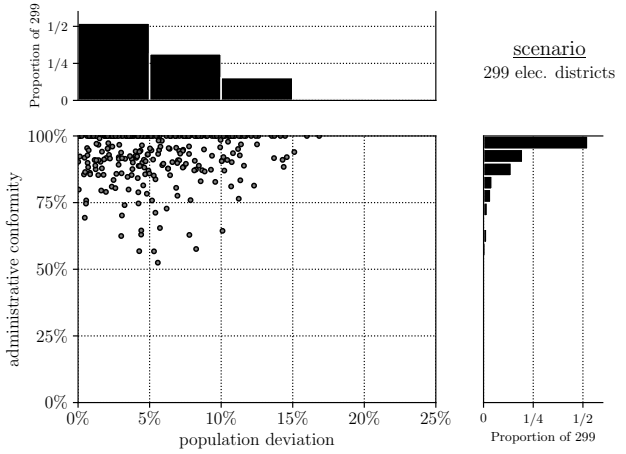
studies for the federal returning officer (Goderbauer et al., 2018a,b) and is preferred in practice.

The results reported in the flowing were obtained by using the optimization methods and the interactive possibility of the software to restart the optimization on a collection of electoral districts of the best solution found so far. Within short time, this leads to improved districting plans in most cases. Each optimization round lasted only for a few minutes and the selection of subproblems was performed manually by the user. As described in Section 9.5 it is one part of the concept of WKOPT to give the user the opportunity to actively participate in the optimization with problem knowledge. The used MILP solver was GUROBI 7.5.1 and the software ran on a single thread of a personal laptop with an Intel Core i7 1.80 GHz.

In this case study, each instance's best found solution is characterized by the fact that the local search on the entire instance did not find any further improvement within a timelimit of 30 seconds. In order to assess the quality of a found solution in form of a proven optimality gap, we used the found solution as a starting point in a final PDP-MILP run. Each run was



(a) Current districting plan.



(b) Optimized districting plan.

Fig. 9.14: Evaluation of the current districting plan and the optimized one on the basis of the two objective functions population deviation and administrative conformity.

performed with SCIP 6.0 (Gleixner et al., 2018) in default settings but deactivating all primal heuristics, a time limit of 12 hours, and on a single thread of a Xeon L5630 Quad Core 2.13 GHz with 16 GB DDR3 RAM. The dual bound was used to determine the optimality gap of the starting solution. Possibly better primal solutions have been neglected.

The objective value and gap of each instance's best found solution is presented in Table 9.1. In addition, we evaluate the computed districting plan regarding the objectives and compare it with the current districting plan. In Figure 9.14 each point represents an electoral district D and indicates its administrative conformity $E^{\text{adm}}(D)$ and population deviation $|\frac{p(D)}{\bar{p}} - 1|$. In addition, the distribution of both objectives is evaluated in histograms.

Tab. 9.1: Results of optimization-based districting.

Federal State / Governmental Region (GR)	k	obj.val.	dual	gap
Schleswig-Holstein	11	10.34	10.90	5.5%
Mecklenburg-Vorpommern	6	5.54	5.90	6.5%
Hamburg	6	5.68	5.86	3.3%
Lower Saxony	30	28.04	29.91	6.7%
Bremen	2	1.69	1.69	opt
Brandenburg	10	9.55	9.94	4.1%
Saxony-Anhalt	9	8.54	8.85	3.7%
Berlin	12	11.62	11.81	1.7%
North Rhine-Westphalia				
GR Düsseldorf	18	17.05	17.90	5.0%
GR Köln	16	15.31	15.85	3.5%
GR Münster	10	9.04	9.37	3.7%
GR Detmold	7	6.37	6.37	opt
GR Arnsberg	13	12.36	12.75	3.1%
Saxony	16	15.30	15.93	4.2%
Hesse				
GR Darmstadt	13	12.41	12.93	4.2%
GR Gießen	4	3.72	3.79	1.9%
GR Kassel	5	4.47	4.66	4.3%
Thuringia	8	7.83	7.88	0.7%
Rhineland-Palatinate	15	14.43	14.87	3.0%
Bavaria				
GR Upper Bavaria	16	15.00	15.93	6.2%
GR Lower Bavaria	4	3.34	3.47	3.9%
GR Upper Palatinate	4	3.83	3.95	3.3%
GR Upper Franconia	4	3.89	3.98	2.2%
GR Middle Franconia	6	5.78	5.88	1.8%
GR Lower Franconia	5	4.90	4.98	1.7%
GR Swabia	7	6.77	6.97	3.0%
Baden-Württemberg				
GR Stuttgart	14	13.16	13.90	5.6%
GR Karlsruhe	10	9.63	9.84	2.2%
GR Freiburg	8	7.60	7.94	4.4%
GR Tübingen	6	5.35	5.51	3.1%
Saarland	4	3.59	3.59	opt
Germany	299			

9.7 Conclusion and Outlook

In this paper a geovisual software system for optimal decision-making in political districting issues is proposed (cf. Fig. 9.15). The decision support system is designed for the collaborative work of human users and mathematical methods. The offered optimization algorithms and underlying MILP formulation is developed in detail within this paper. Applying these methods relieves the decision-maker from the manual and time-consuming process of adjusting electoral districts in order to be legally admissible. High-quality districting plans are achievable that fulfill all legal requirements and optimize the objective criteria according to user specified preferences. Optimization-based districting plans can be still adjusted by hand in the software, thus the decision-making authority remains in the hands of the user.

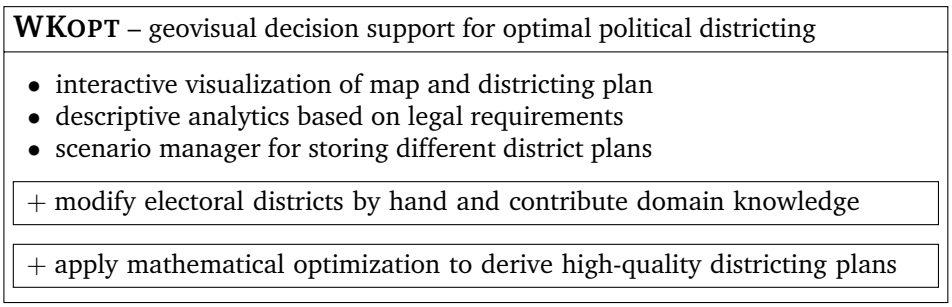


Fig. 9.15: Union of geoinformation system, manual operation, and mathematical methods.

The paper focuses on the application case in Germany and involved legal requirements and criteria. The conducted research is motivated by the fact that German (re)districting issues has so far been completely solved by hand and mostly under the use of tools or software that are not tailored to the task.

In addition to the fact that our work can simplify and improve the process of (re)districting in practice, there is another aspect to be mentioned. The reported research and methodology can lead to more transparency and objectivity in districting issues. The lack of this is regularly subject of discussion and critical reviews. Proposed solution methods are able to compute districting plans that meet all legal requirements and fulfill districting criteria best possible. Using the geovisual software system, a numerical and visual comparison of an optimization-based districting plan and the officially decided one is possible. The ability to generate districting plans objectively and transparently on the basis of legal guidelines enables new questions and discussion to be addressed. This covers further research in mathematics, political science and law. Any work on this issue can only benefit the two important aspects of a democracy: Transparency and objectivity in decision-making.

The presented model and solution approaches for political districting are flexible to be extended. It is possible to consider other legally given criteria; e.g., the criteria of compactness which holds a high regard in discussions on political districting issues in the USA. Thereby the research described can also be transferred to other applications. In addition, the developed decision support system can be extended towards, e.g., the consideration of presented budget constraints on continuity.

Methodically and algorithmically it is interesting from the perspective of the German problem, to further research on the criteria of administrative conformity. The conducted computational study shows that a consideration of this criteria as modeled in the paper leads to bad dual bounds. This is surely due to the fact that the modeling contains multiple linearizations of products of decision variables. Possibly this type of modelling can be reinforced with additional constraints or a better formulation can be found. Also the development of criterion specific heuristics can be a research direction. A first approach to this is offered by Goderbauer and Ermert (2019).

10 Proportional Apportionment for Connected Coalitions

Abstract In order to divide up resources that can only be distributed in integer units as fairly as possible, apportionment methods are used. A practical example in this respect is the allocation of seats of a fixed size parliament to parties after an election. In this case, a fair distribution means the best possible proportionality to the ratio of votes received. In this paper, we generalize extensively studied apportionment methods by allowing the formation of coalitions, i.e. the grouping of allocation recipients, in order to increase the resulting apportionment quality. In the classical setting, these coalitions are limited to singletons. For the generalized apportionment problem, we prove NP-hardness and develop a mixed-integer linear program. We point out the application of our findings to the political districting problem.

10.1 Introduction

In electoral systems, which are based on proportional representation, each political party is represented in parliament in proportion to the number of people who vote for it. To translate large vote counts of those to be represented into small numbers of parliamentary seats, procedures called *apportionment methods* are employed. Since a total number of seats is usually prespecified by law and must be dealt out precisely, simply rounding is not sufficient. Apportionment methods are able to meet this requirement and, more importantly, ensure proportionality.

In Germany, an apportionment method is not only used after a federal election, but also in its preparation: A prespecified number of electoral districts is apportioned among the 16 German federal states in proportion to their population figures. After that, electoral districts are designed in each state separately. The task of partitioning a geographical territory into a given number of electoral districts is called *political districting problem* and includes different constraints and (optimization) criteria. The fact that an apportionment method is part of the very first step in the design process of electoral districts in, e.g., Germany, leads to the basic motivation of our work: Development of generalized apportionment methods that are applicable in further steps of the (re)districting process.

Contribution Classical apportionment methods assign one integer to each *recipient*. We generalize a prime class of apportionment methods by allowing *coalitions* of recipients: The latter can be grouped in order to improve proportionality of the apportionment. We show that this additional combinatorics leads to an *NP-hard* problem. In contrast, the standard setting can be solved in linear time. We propose a *mixed-integer linear program* (MILP) for

the generalization, discuss extensions, and point out its application in the *political districting problem*.

Related work Apportionment methods were studied by Balinski and Young (1982), Kopfermann (1991), and Pukelsheim (2017). The political districting problem is discussed in surveys of Goderbauer and Winandy (2017) and Ricca et al. (2011). The idea to generalize apportionment methods was triggered by work of Goderbauer (2016a,b).

10.2 Apportionment Problem and Divisor Methods

The general setting of an apportionment problem reads as follows. For a vector $v \in \mathbb{R}^n$, $n \in \mathbb{N}$ we define the sum of its components as $v_+ := \sum_{i=1}^{n} v_i$.

Definition 31 (apportionment problem) *Given* target size $h \in \mathbb{N}_{\geq 1}$*, number of* recipients $\ell \in \mathbb{N}_{\geq 2}$*, and* weight vector $0^\ell \neq w = (w_1, .., w_\ell) \in \mathbb{Q}^\ell_{\geq 0}$*. An* apportionment problem *asks for an* apportionment vector $x = (x_1, .., x_\ell) \in \mathbb{N}^\ell_{\geq 0}$ *with* $x_+ = h$*, i.e., an allocation* x_i *for each recipient* i *so that target size is met.*

An apportionment problem does not contain any requirement on proportionality between w and x since there exists no unique measurement of disproportionality. Certainly, of interest are apportionment vectors x with

$$\frac{x_i}{h} \approx \frac{w_i}{w_+}$$

for all i. Equality in all equations is called *perfect proportionality*. Minimizing the deviation from perfect proportionality is the purpose of suitable solution methods.

To define solution methods for the apportionment problem, some notation is introduced. For target size $h \in \mathbb{N}_{\geq 1}$ and weight vector $w \in W := \bigcup_{\ell \geq 2} \mathbb{Q}^\ell_{\geq 0} \setminus \{0^\ell\}$, denote the dimension of w as $\ell(w)$ and define the set of all feasible apportionment vectors as

$$\mathbb{N}^{\ell(w)}(h) := \{x \in \mathbb{N}^{\ell(w)}_{\geq 0} : x_+ = h\} \in X := \bigcup_{h \geq 1} \bigcup_{\ell \geq 2} \mathbb{N}^\ell(h).$$

Definition 32 (apportionment method) *A mapping*

$$A : \mathbb{N}_{\geq 1} \times W \to X$$

with $\emptyset \neq A(h, w) \subseteq \mathbb{N}^{\ell(w)}(h)$*,* $h \in \mathbb{N}_{\geq 1}$*,* $w \in W$ *is an* apportionment method.

In the following, we consider the "most powerful apportionment methods" (Pukelsheim, 2017, p. 72): *divisor methods*. At its core, divisor methods use a flexible divisor to scale the weights to interim quotients of an appropriate order of magnitude and round these to integers using a specific rule. We focus on the *divisor method with standard rounding*, but our findings can be transfered to other divisor methods.

Definition 33 (rule of standard rounding) *The* rounding rule of standard rounding $[\![\cdot]\!]$ *is defined for* $t \in [0, \infty)$ *and* $n \in \mathbb{N}_{\geq 0}$ *with* $[\![t]\!] := \{0\}$ *if* $t = 0$ *and*

$$[\![t]\!] := \begin{cases} \{n\} & \text{if } t \in \left(n - \frac{1}{2}, n + \frac{1}{2}\right), \\ \{n-1, n\} & \text{if } t = n - \frac{1}{2} > 0. \end{cases}$$

Lemma 34 *For all* $t \in [0, \infty)$ *and* $n \in \mathbb{N}_{\geq 0}$ *holds:*

$$n \in [\![t]\!] \Leftrightarrow n - \frac{1}{2} \leq t \leq n + \frac{1}{2}.$$

Lemma 34 is a direct consequence of Definition 33. The divisor method induced by the rule of standard rounding is denoted with *DivStd* and defined as follows.

Definition 35 (DivStd) *The* divisor method with standard rounding *reads*

$$\text{DivStd}(h, w) := \left\{ x \in \mathbb{N}^{\ell}(h) : x_1 \in \left[\!\left[\frac{w_1}{D}\right]\!\right], \ldots, x_\ell \in \left[\!\left[\frac{w_\ell}{D}\right]\!\right] \text{ for some } D > 0 \right\}.$$

The solution set of divisor methods, including DivStd, is easily computable. In fact, after a sensible initialization of divisor D, it needs linear many iterations to meet the target size with the summed up rounded quotients (Pukelsheim, 2017).

Theorem 36 $\text{DivStd}(h, w)$ *is computable in* $\mathcal{O}(\ell(w))$ *for* $h \in \mathbb{N}_{\geq 1}$ *and* $w \in W$.

Sainte-Laguë (1910) proved the following optimality characteristic (Pukelsheim, 2017).

Theorem 37 *It holds:*

$$x \in \text{DivStd}(h, w) \Leftrightarrow x \in \underset{y \in \mathbb{N}^{\ell(w)}(h)}{\arg\min} \sum_{i=1}^{\ell(w)} w_i \cdot \left(\frac{y_i / h}{w_i / w_+} - 1 \right)^2.$$

10.3 Proportional Apportionment for Coalitions

A *coalition* is a non-empty set of recipients. In the literature, it is analyzed which apportionment method encourages coalitions or, quite the opposite, encourages schisms (Balinski and Young, 1979, 1982). Coalitions are encouraged, if the expected success rate, e.g., number of seats, is higher if recipients form a coalition before allocation instead of standing alone. An apportionment method is called *coalition-neutral* if coalitions are just as likely to gain as to lose one unit of the allocated resource.

So far, the concept of coalitions has not been part of an apportionment problem itself. In our generalization, forming coalitions gets part of the decision to be made in order to increase

the apportionment quality globally. In the classical apportionment setting, these coalitions are fixed to singletons. The following theorem guarantees that the formation of coalitions in our generalization of DivStd does not lead to (dis)advantages for recipients.

Theorem 38 (Balinski and Young, 1982) DivStd *is the unique divisor method that is coalition-neutral.*

In applications, not every coalition may be desired. Therefore, we consider a graph $G = (V, E)$ with set of recipients $V = \{1, \dots, \ell\}$ as input of the generalized problem and request that the *subgraph induced by* each coalition $C \subset V$, denoted with

$$G[C] := (C, \{(i_1, i_2) \in E : i_1, i_2 \in C\}),$$

has to be connected.

10.3.1 Generalized Apportionment Problem and Divisor Methods

Our generalized apportionment problem for connected coalitions reads as follows.

Definition 39 (apportionment prob. for connected coalitions (APCC)) *Given $h \in \mathbb{N}_{\geq 1}$, $w \in W$, an apportionment method A, and a graph $G = (V, E)$ with $V = \{1, .., \ell(w)\}$. An* apportionment problem for connected coalitions (APCC) *asks for a partition of V in $2 \leq p \leq \ell(w)$ coalitions $\mathcal{C} = \{C_1, .., C_p\}$ with $G[C_j]$ connected for all j, and an apportionment vector $x \in A(h, w^{\mathcal{C}})$ with coalition weight $w_j^{\mathcal{C}} := \sum_{i \in C_j} w_i$ for $j = 1, \dots, p$.*

We exclude $p = 1$ since the trivial partition $\mathcal{C} = \{V\}$ has always perfect proportionality. Let $\mathcal{P}_{\geq 2}(V)$ be the set of all non-trivial partitions of V. To evaluate a solution of APCC, i.e., coalitions $\mathcal{C}$ (with its apportionment $x \in A(h, w^{\mathcal{C}})$), a function $f : \mathcal{P}_{\geq 2}(V) \times X \to \mathbb{R}_{\geq 0}$ can be employed. Such an f is called *APCC objective* if a value of f equals zero if and only if the evaluated apportionment has perfect proportionality. DivStd's measurement of disproportionality (Theorem 37) fulfills this requirement. However, applications may require a different objective.

Definition 40 (DivCoalStd) *Given an APCC instance with apportionment method* DivStd *and an APCC objective f. We define* DivStd for connected coalitions under objective f (DivCoalStd^f) *with the following characterization:*
$(\mathcal{C}, x) \in \text{DivCoalStd}^f(h, w, G) :\Longleftrightarrow \mathcal{C} = \{C_1, \dots, C_p\}$, x optimal solution of

$$\begin{aligned} &\min\ f(\mathcal{C}, x) \\ &\text{s.t.}\ \ p \in \mathbb{N},\ 2 \leq p \leq \ell \\ &\qquad \mathcal{C} = \{C_1, .., C_p\} \text{ partition of } V \text{ with } C_j \neq \emptyset \quad \forall j = 1, \dots, p \\ &\qquad G[C_j] \text{ connected} \quad \forall j = 1, \dots, p \\ &\qquad x \in \text{DivStd}(h, w^{\mathcal{C}}) \end{aligned} \tag{10.1}$$

10.3.2 Complexity

Computing DivStd takes linear time (cf. Theorem 36). We show that DivCoalStd is more complex. This is not only due to the required connectedness of the coalitions, which itself is NP-hard. Let K_ℓ be the complete graph on ℓ nodes.

Theorem 41 ((Dyer and Frieze, 1985), problem no. 6 in (Johnson, 1982)) *Partitioning a graph into connected subgraphs of bounded size or weight is NP-hard.*

Theorem 42 *Computing* $(\mathcal{C}, x) \in \text{DivCoalStd}^f(h, w, G)$ *is NP-hard even if* G *is complete.*

Proof Reduction from PARTITION (Garey and Johnson, 1979). Let $U = \{1, \ldots, \ell\}$, $\ell \in \mathbb{N}_{\geq 2}$ with $s_i \in \mathbb{N}_{\geq 1}$, $i \in U$ be given. Prove: There is $U' \subseteq U$ with $\sum_{i \in U'} s_i = \sum_{i \in U \setminus U'} s_i$ iff $\text{DivCoalStd}^f(h, w, K_\ell)$ with $h := 2$, $w_i := 2 \cdot \frac{s_i}{s_+}$ $\forall i = 1, .., \ell$ (note, $w_+ = h$) has a solution with perfect proportionality, i.e., objective value 0 in (10.1) for all f.
$\Rightarrow$: $C_1 := U'$, $C_2 := U \setminus U'$ fulfills $\sum_{i \in C_1} w_i = \sum_{i \in C_2} w_i = 1$. Choose $x := (1, 1)$.
$\Leftarrow$: Since $w_+ = h$, perfect proportionality is equivalent to $x_j = \sum_{i \in C_j} w_i$ $\forall j$ and therefore to $\sum_{i \in C_j} w_i \in \mathbb{N}$ $\forall i$. Since $\mathbb{N}$ is closed under addition, coalitions can be merged: W.l.o.g. assume $p = 2$. Since $w_i > 0$ $\forall i$, we get $x_1 = \sum_{i \in C_1} w_i = 1 = \sum_{i \in C_2} w_i = x_2$, implying $\sum_{i \in C_1} s_i = \sum_{i \in C_2} s_i$. Choose $U' := C_1$. ■

If additional conditions are specified on a solution $(\mathcal{C}, x)$ (cf. application in Section 10.4), the complexity statement can be strengthened. In the following case, strong NP-hardness is proven.

Theorem 43 *Computing* $(\mathcal{C}, x) \in \text{DivCoalStd}^f(h, w, G)$ *with* $x^{\min} \leq x_j \leq x^{\max}$ $\forall j$ *for given bounds* $x^{\min}, x^{\max} \in \mathbb{N}_{\geq 0}$ *is NP-hard in the strong sense even if* G *is complete.*

Proof Reduction from 3-PARTITION which is NP-hard in the strong sense (Garey and Johnson, 1979): Finite set $A = \{1, \ldots, 3m\}$, $m \in \mathbb{N}$, bound $B \in \mathbb{N}$, size $s_a \in \mathbb{N}$ for each $a \in A$ such that $\frac{B}{4} < s_a < \frac{B}{2}$ and such that $\sum_{a \in A} s_a = mB$. 3-PARTITION asks for a partition into m disjoint sets $A_1, \ldots, A_m \subseteq A$ such that $\sum_{a \in A_j} s_a = B$ $\forall j$. Construct an instance of apportionment problem for coalitions as follows: target size $h := mB$, set of nodes $\{1, \ldots, \ell\}$ with $\ell := n$, weight vector $w \in \mathbb{Q}^\ell_{>0}$ with entries $w_i := s_i$ $\forall 1 \leq i \leq n$, and $x^{\min} := x^{\max} := B$.
Claim: A partition $\mathcal{C} = \{C_1, \ldots, C_p\}$, $p > 1$, of the nodes and an apportionment vector $x \in \mathbb{N}^p$, $x_+ = h$, $x^{\min} \leq x_j \leq x^{\max}$ $\forall j$, with perfect proportionality exist if and only if there is a solution for the 3-PARTITION instance.
$\Rightarrow$: Here, perfect proportionality is equivalent to $\sum_{i \in C_j} w_i = B$ $\forall j$. Thus $p = m$ holds and sets $A_j := C_j$, $1 \leq j \leq p$ form a solution for the 3-PARTITION instance.
$\Leftarrow$: Coalitions $C_j := A_j$, $1 \leq j \leq p$ form a partition of the nodes. Apportionment vector x with $x_j = B$ $\forall j$ completes the solution with perfect proportionality. ■

10.3.3 Mixed-Integer Linear Programming (MILP) Formulation

DivStd can be formulated as integer points of a linearly described region.

Lemma 44 *It holds:*

$$\text{DivStd}(h,w) = \left\{ (x_1,\dots,x_{\ell(w)}) : \begin{array}{l} \sum_i x_i = h,\ x_i \in \mathbb{N}_{\geq 0}\ \forall i, \\ -\frac{1}{2} \leq w_i\mu - x_i \leq \frac{1}{2}\ \forall i,\ \mu \geq 0 \end{array} \right\}.$$

Proof With $D := 1/\mu$, Lemma 34 reads $x_i \in [\![w_i\mu]\!] \Leftrightarrow -\frac{1}{2} \leq w_i\mu - x_i \leq \frac{1}{2}$. Note, $\mu = 0$ is only feasible on the right side of the equation for $h = 0$ and this is not allowed as input. ■

In the following, we propose a formulation for problem (10.1). Let $B = \{1,\dots,\ell\}$ be coalitions' indices. Consider variables: Binary $\delta_{i,b}$ equals 1 iff coalition $b \in B$ contains recipient $i \in V$. Binary γ_b equals 1 iff coalition $b \in B$ is non-empty. Integer x_b denotes allocation for $b \in B$. A formulation of all feasible points reads:

$$\begin{array}{rlrl} \sum_{b\in B} x_b = h, \quad \sum_{b\in B} \gamma_b \geq 2 & & & \\ \sum_{b\in B} \delta_{i,b} = 1 & \forall i \in V & \mu \geq 0 & \\ -\frac{1}{2} \leq \left(\sum_{i\in V} w_i\delta_{i,b}\right)\cdot\mu - x_b \leq \frac{1}{2} & \forall b \in B & x_b \in \mathbb{N}_{\geq 0} & \forall b \in B \\ G[\{i \in V : \delta_{i,b} = 1\}] \text{ connected} & \forall b \in B & \gamma_b \in \{0,1\} & \forall b \in B \\ \delta_{i,b} \leq \gamma_b \leq \sum_{i\in V} \delta_{i,b} & \forall i \in V, b \in B & \delta_{i,b} \in \{0,1\} & \forall i \in V, b \in B \end{array} \tag{10.2}$$

Theorem 45 *If APCC objective f can be modeled linearly, problem* (10.1) *and therefore* DivCoalStd^f *can be formulated as an MILP.*

Proof Consider formulation (10.2). Products $\delta_{i,b} \cdot \mu$ can be linearized by introducing a new variable and additional constraints (folklore) since $\mu \leq \frac{h+\frac{1}{2}}{\max_i w_i}$ holds. Connectedness of subgraphs can be ensured by, e.g., *separator inequalities* (Wang et al., 2017). ■

10.4 Application: Political Districting Problem

For the design of electoral districts, German law stipulates that boundaries of rural and urban districts (a level of administrative subdivisions) should be respected where possible (Goderbauer and Winandy, 2017). It is preferred that a boundary of an electoral district matches a boundary of a rural/urban district. This guideline, called *administrative (adm.) conformity*, is an important objective in German political districting (PD) practice (Goderbauer and Wicke, 2017). Another legal aim requests for preferably equal population in each electoral district, i.e., small electoral district's *population deviation*.

We utilize our results to allocate a federal state's number of electoral districts among connected coalitions of rural and urban districts. This APCC results in a number of smaller

PD instances, one from each non-empty connected coalition C_b. Each resulting instance has (i) a modest number of electoral districts, (ii) adm. conformity for at least the instance's external borders, and (iii) small population deviation. Coalitions C_b with $x_b = 1$ lead to already solved PD instances with perfect adm. conformity. Remaining instances can be solved with PD algorithms (Goderbauer and Winandy, 2017; Ricca et al., 2011). As an example, we examine the federal state of Hesse.

APCC instance for DivCoalStd. Hesse has $h = 22$ electoral districts and $\ell = 26$ rural and urban districts, each with a given population of $w_i \in \mathbb{Z}_{\geq 1}$, $1 \leq i \leq \ell$. Let $G = (V, E)$ be the *contiguity graph* on rural/urban districts V, i.e., $\{i, j\} \in E$ iff areas of $i, j \in V, i \neq j$ have a common border (which is not negligibly short).

APCC objective. In order to minimize population deviations accompaning with apportionment $x \in \text{DivStd}(h, w^{\mathcal{C}})$, define $f(\mathcal{C}, x) := \sum_{1 \leq b \leq p} x_b \cdot \left| \frac{\sum_{i \in C_b} w_i}{x_b} - \frac{w_+}{h} \right|$. Objective f can be formulated linearly with variables of (10.2): $\min f(\mathcal{C}, x) \iff \min \sum_b z_b$ s.t. $\sum_{i \in V} w_i \delta_{i,b} - \frac{w_+}{h} x_b \leq z_b$, $\frac{w_+}{h} x_b - \sum_{i \in V} w_i \delta_{i,b} \leq z_b$, $z_b \geq 0 \; \forall b$.

Additional constraints. To get feasible PD instances, each coalition needs at least one electoral district, i.e., $x_b \geq \gamma_b \; \forall b$. In order not to dilute administrative conformity too much, add an upper bound $x_b \leq x^{\max} \; \forall b$. We choose $x^{\max} := 4$.

In our implementation, we utilize separator inequalities as lazy constraints to ensure connectedness (Fischetti et al., 2016; Wang et al., 2017), we add $\gamma_b \geq \gamma_{b+1} \; \forall b \in B \setminus \{\ell\}$ and fix $\gamma_b = 1$ for $b = 1, \ldots, \lceil \frac{h}{x^{\max}} \rceil$ in purpose of symmetry breaking.

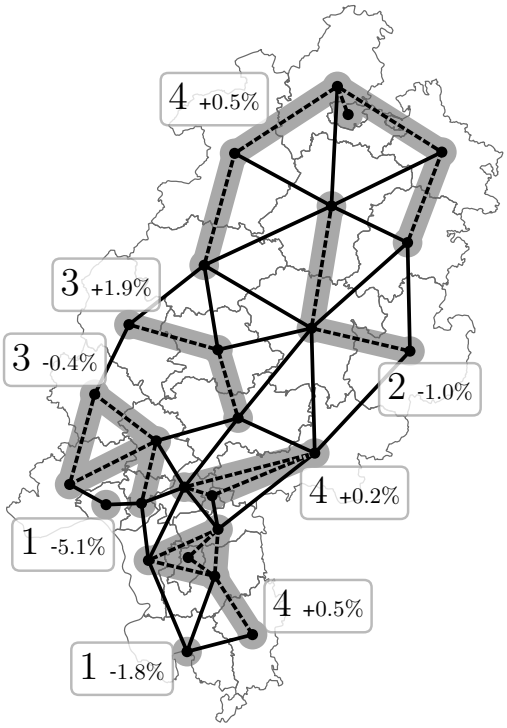


Fig. 10.1: Contiguity graph of the 26 rural and urban districts of the German federal state of Hesse, and the best found solution of DivCoalStd^f: The solution consists of eight connected coalitions (grey, dashed edges). Next to each coalition, a two-number box (such as 4, $+0.5\%$) indicates the electoral district apportionment of that coalition ($4 = x_b$), and resulting (average) population deviation ($+0.5\%$). Population figures used are of June 2015.

Using GUROBI as MILP solver, we perform 5 independent runs with a timelimit of 10 minutes each. The best solution found is shown in Figure 10.1. Unfortunately, its quality in terms of an optimality gap can not be assessed, since the solver was not able to compute a dual bound better than the trivial one, i.e., 0.

The latter fact leaves room for further research. In addition, a link to a suitable PD algorithm for designing electoral districts in coalitions with $x_b > 1$ should be implemented – perhaps even with a response to DivCoalStd in order to be able to evaluate coalitions there on the basis of designed electoral districts.

11

Reform der Bundestagswahlkreise: Unterstützung durch mathematische Optimierung

Abstract. *Reform of constituencies for Bundestag elections: Support provided by mathematical optimization*. The current debate on an amendment to the electoral law for the German Bundestag also includes a possible reduction of the number of constituencies. On behalf of the Federal Election Commissioner, we have computed possible delimitations of constituencies for the scenarios of 250, 200 and 125 constituencies. The application of mathematical optimization guarantees objectivity and transparency: All legal criteria are strictly adhered to and delimitation principles from law and regulations are fulfilled in the best possible way. No other conditions or restrictions were included, not a single legally possible delimitation of constituencies was excluded in advance. In addition to the results of our studies, the article shows that carelessly deciding on the number of constituencies can have considerable consequences and can even lead to numerical inadmissibility. Following the federal structure of Germany, the article emphasizes that the most suitable numbers of constituencies are 248 and 145, for one- and two-person constituencies, respectively. Our studies as well as all optimization-based computed constituencies can be studied in an interactive map on the internet.

Zusammenfassung. Die gegenwärtig geführte Debatte um eine Novellierung des Wahlrechts für den Deutschen Bundestag beinhaltet auch eine mögliche Reduktion der Wahlkreisanzahl. Im Auftrag des Bundeswahlleiters haben wir mögliche Wahlkreiseinteilungen Deutschlands für die Szenarien 250, 200 sowie 125 Bundestagswahlkreise berechnet. Der Einsatz mathematischer Optimierung sichert dabei Objektivität und Transparenz: Alle gesetzlichen Kriterien werden strikt eingehalten und Einteilungsgrundsätze aus Recht und Gesetz bestmöglich erfüllt. Keine anderen Vorgaben oder Einschränkungen flossen ein, keine einzige, gesetzlich mögliche Einteilung wurde im Vorfeld ausgeschlossen. Neben den Ergebnisse unserer Studien zeigt der Artikel auf, dass eine achtlose Festlegung der Wahlkreisanzahl erhebliche Folgen haben, sogar zu numerischer Unzulässigkeit führen kann. Der bundesstaatlichen Struktur der Bundesrepublik folgend, wird im Artikel herausgestellt, dass Wahlkreisanzahlen 248 bzw. 145 für Ein- bzw. Zweipersonenwahlkreise am geeignetsten sind. Unsere Studien sowie sämtliche optimierungsbasiert berechnete Einteilungen können in interaktiven Wahlkreiskarten im Internet studiert werden.

11.1 Einleitung

Nicht zuletzt ausgelöst durch den nach der Wahl 2017 abgeordnetenstärksten Deutschen Bundestag aller Zeiten wird über eine Reform des Bundeswahlrechts diskutiert. Inhalt der Debatte ist auch die Möglichkeit einer *Abänderung der Anzahl der Bundestagswahlkreise* von gegenwärtig 299 (Behnke et al., 2017; Hesse, 2019; Pukelsheim, 2018). Im Rahmen dessen wird ebenso eine Abkehr von *Einerwahlkreisen* hin zu der Einführung von *Zweierwahlkreisen* erörtert (Behnke et al., 2017; Behnke, 2010b; Oppermann und Klecha, 2018; Weinmann, 2014).

Als damaliger Bundestagspräsident beklagte Norbert Lammert noch kurz vor der Bundestagswahl im September 2017 bezüglich der und insbesondere seiner Bemühungen um eine Wahlrechtsreform fehlende „öffentliche Unterstützung“ und „in allen Fraktionen keine genügende Bereitschaft“ (Lammert, 2017). Es sei eine „Abwehrfront im Bundestag“ vorhanden, so Lammert (2017).
Nach Ablösung Lammerts als Bundestagspräsident übernahm Nachfolger Wolfgang Schäuble neben dem Amt auch den Eifer Lammerts, sich für eine Novellierung des Wahlrechts einzusetzen. Schäuble kündigte nach Amtsübernahme bezüglich einer Wahlrechtsreform an, der Bundestag habe jetzt „einen neuen Präsidenten, der ein Scheitern nicht zulassen will“ (Roßmann, 2018). Unter seinem Vorsitz berät seit Frühjahr 2018 nicht-öffentlich eine fraktionsübergreifende Arbeitsgruppe zum Themenkomplex Wahlrechtsreform (Baethge, 2018; Roßmann, 2019). Diese sei bestrebt „bis zur Osterpause eine gemeinsame Position“ vorweisen zu können, so Schäuble (2019). Mit Blick auf eine mögliche Reduktion der Wahlkreisanzahl fügte Schäuble (2019) hinzu, es sei „schwierig, es so zu machen, dass die Wahlkreise nicht betroffen sind“.

In der Praxis ist es üblich, dass bei der im Vorfeld jeder Bundestagswahl stattfindenden Revision der Wahlkreiseinteilung durch die Wahlkreiskommission und den Gesetzgeber auf die Einteilung der letzten Wahl zurückgegriffen wird (BT-Drs. 17/4642, 2011; BT-Drs. 18/3980, 2015). Falls unter Verwendung neuster Bevölkerungszahlen Wahlkreise nicht mehr gesetzeskonform sind, werden manuell und – begründet mit der vom Bundesverfassungsgericht angewiesenen Wahlkreiskontinuität (BVerfGE 130, 212, 2012) – möglichst minimalinvasiv Änderungen vorgenommen (Goderbauer und Wicke, 2017).
Dieses Vorgehen ist bei einer Änderung der Wahlkreisanzahl nicht mehr möglich, da eine vollständige Neueinteilung vorzunehmen ist. Aufgrund kombinatorischer Explosion gibt es unüberschaubar viele Möglichkeiten, Wahlkreise abzugrenzen. Sich davon nur eine geringe Auswahl händisch herauszugreifen ist kaum begründbar und schwerlich objektiv. Im Gegenteil sollten die angewendeten Kriterien transparent aus den rechtlich vorgegebenen Einteilungsgrundsätzen – und nur diesen – folgen. Genau diese Meinung vertritt in der aktuellen Wahlrechtsdebatte auch Hesse (2019): „Die Reduzierung der Wahlkreise muss nach einem objektiven und damit für alle Parteien fairen Verfahren erfolgen. Für den Neuzuschnitt der Wahlkreise sollte die unparteiische Mathematik bemüht werden“. Ähnlich formuliert es Behnke (2017, S. 176): „Sollte tatsächlich eine neue Wahlkreiseinteilung vorgenommen werden, sollte dies auch möglichst unter objektiven Kriterien geschehen“.

In diesem Artikel stellen wir Wahlkreisneueinteilungen Deutschlands vor, die wir mithilfe eigens entwickelter *Modelle und Methode der mathematischen Optimierung* berechnet haben. So geben wir Antworten auf die Notwendigkeit und die Forderungen nach Objektivität und Unparteilichkeit bei einer möglichen Wahlkreisreform. Gesetzliche Muss-Vorgaben werden eingehalten und die größtmögliche Erfüllung weiterer rechtlicher Einteilungsgrundsätze angestrebt. Die Überführung der aus Gesetz und Rechtsprechungen gegebenen Vorgaben an eine Wahlkreiseinteilung in mathematische Nebenbedingungen und numerisch bemessene Zielkriterien wird dargelegt. Unsere Arbeit und sämtliche Berechnungen sind frei von politischen, soziokulturellen, -ökonomischen o.ä. Daten und berücksichtigen ausschließlich die angegebenen Vorgaben und Kriterien. Durch Anwendung der objektiven Verfahren können Einteilungen in Bundestagswahlkreise gefunden werden, die *robuster gegenüber zukünftigen Bevölkerungsbewegungen* sind und zugleich bestmöglich Verwaltungsgrenzen beachten um u.a. den *administrativen Aufwand gering zu halten*, der bei Wahldurchführung und Arbeit in den Wahlkreisen besteht.

Grundlage dieses Artikels sind u.a. von uns im Auftrag des Bundeswahlleiters in der zweiten Jahreshälfte 2018 durchgeführte Studien. In diesen wurden mithilfe der von uns entwickelten optimierungsbasierten Software Neueinteilungen für die Szenarien 250, 200 sowie 125 Bundestagswahlkreise berechnet. Die Studien sowie berechnete Wahlkreiskarten sind auf der Internetseite des Lehrstuhls für Operations Research der RWTH Aachen University verfügbar (Goderbauer et al., 2019, online; Goderbauer et al., 2018a,b). Neben diesen drei Szenarien stellen wir in dem vorliegenden Artikel zusätzlich berechnete Einteilungen zum Vergleichsszenario 299 (Goderbauer und Lübbecke, 2019a) sowie 248 und 145 Wahlkreise vor. Eine ausführliche numerische Begründung der beiden letztgenannten Anzahlen erfolgt im Verlaufe des Artikels.

Warum mathematische Optimierung? Um eine enorme Zahl voneinander abhängiger Entscheidungen zu modellieren, bedienen wir uns der diskreten und ganzzahligen Optimierung. Diese ermöglicht uns, *sämtliche* Konfigurationen gesetzeskonformer Wahlkreiseinteilungen kompakt zu beschreiben, Ziele wie möglichst geringe Abweichung zur durchschnittlichen Bevölkerungszahl zu definieren und bezüglich dieser Ziele *beweisbar* bestmögliche Einteilungen zu berechnen. Alle dabei formulierten Bedingungen werden eingehalten, keine anderen Vorgaben oder Einschränkungen berücksichtigt. Diese Methodik grenzt sich scharf von heuristischen und manuellen Vorgehen ab, bei denen nur einige wenige plausible Alternativen bestimmt und bewertet werden. In der mathematischen Optimierung wird von vornherein keine einzige denkbare Konfiguration ausgeschlossen. Sie bietet daher eine nur auf nachprüfbaren Fakten beruhende (bestmögliche) Entscheidungsgrundlage.

11.2 Rechtsgrundlagen und mathematische Formalisierung

Basierend auf den rechtlichen Vorgaben (Abschnitt 11.2.1) wird die Aufgabe der Wahlkreiseinteilung in Abschnitt 11.2.2 in ein mathematisches Modell überführt. Nach begründeter Trennung zwischen strikten Bedingungen und angestrebten Einteilungszielen, beinhaltet

die Modellierung auch numerische Bewertungsfunktionen der Ziele. Schließlich wird in Abschnitt 11.2.3 ein interaktives Software-Tool vorgestellt, welches den Nutzern optimierungsbasierte Entscheidungsunterstützung bei der Einteilung von Wahlkreisen bietet und auch für die vorliegende Arbeit verwendet wurde.

11.2.1 Rechtliche Vorgaben

Das Bundeswahlgesetz (BWG) sowie Entscheidungen des Bundesverfassungsgerichts (BVerfG) bilden die Rechtsgrundlage für Bundestagswahlkreise und deren Einteilung. Folgende Vorgaben und Grundsätze sind zu beachten (die Reihenfolge stellt keine Gewichtung dar):

(1) *Grenzen der Bundesländer sind einzuhalten* (§3 Abs. 1 Nr. 1–2 BWG)
Die gegebene Gesamtanzahl an Bundestagswahlkreisen wird mithilfe der Divisormethode mit Standardrundung (auch Sainte-Laguë/Schepers)-Verfahren genannt) auf die Bundesländer anhand ihrer Bevölkerungsanteile verteilt. Die angewendete Methodik sichert dabei (in einem gewissen Sinne) bestmögliche Proportionalität. Die Einteilung der Wahlkreise findet dann in jedem Bundesland statt.

(2) *Deutsche Bevölkerungszahl eines Wahlkreises* (§3 Abs. 1 Nr. 3, §3 Abs. 1 Satz 2 BWG)
Im Rahmen der Wahlgleichheit (Art. 38 Abs. 1 Satz 1 Grundgesetz) sind Abweichungen zwischen den Wahlkreisen bezüglich ihrer deutschen Bevölkerungszahl gering zu halten. Das Gesetz formuliert zwei Grenzen für die Abweichung von der durchschnittlichen Bevölkerungszahl der Wahlkreise: Die Toleranzgrenze von maximal 15% Bevölkerungsabweichung *soll* eingehalten werden und die Höchstgrenze von maximal 25% Abweichung *muss* eingehalten werden. Zusätzlich sind die Anzahl der Wahlberechtigten und zukünftige Bevölkerungsentwicklungen in den Blick zu nehmen (BVerfG 130, 212).

(3) *Zusammenhang eines Wahlkreisgebietes* (§3 Abs. 1 Nr. 4 BWG)
Das Gebiet eines jeden Wahlkreises soll ein zusammenhängendes Gebiet bilden.

(4) *Administrative Grenzen* (§3 Abs. 1 Nr. 5 BWG)
Bekannte Verwaltungsgrenzen der Gemeinden sowie (Land-)Kreisen und kreisfreien Städte sollen bei der Wahlkreiseinteilung nach Möglichkeit berücksichtigt werden. Die Praxis zeigt, dass dies auch für Gemeindeverbände und Regierungsbezirke gilt.

(5) *Kontinuität der Wahlkreise* (BVerfG 95, 335 und 130, 212)
Die Einteilung der Wahlkreise, d.h. die Gestalt ihre Abgrenzungen, soll im zeitlichen Verlauf möglichst stabil sein.

Der letztgenannte Grundsatz *Kontinuität* fällt in der behandelten Thematik weg, da komplette Neueinteilungen durchgeführt werden und vorherige Wahlkreise dabei keine Rolle spielen sollen. Alle anderen Vorgaben sind relevant.

11.2.2 Mathematische Modellierung: Bedingungen und Bewertungen

Bei der Überführung der rechtlichen Vorgaben in ein mathematisches Modell ist klar zwischen strikt einzuhaltenden Bedingungen sowie Bewertungskriterien zu unterscheiden. Die Eingliederung einer Vorgabe weicht evtl. von ihrer Formulierung als *Soll/Muss*-Vorschrift ab. Dies wird begründet.

Das Modell und somit die Grundlage der vorliegenden Arbeit lautet im Kern wie folgt. Details sowie die mathematisch vollständig ausformulierte Modellierung sind in den Arbeiten von Goderbauer und Winandy (2017) sowie Goderbauer und Lübbecke (2019a) zu finden.

(i) *Bedingungen, die jeder Wahlkreis ausnahmslos zu erfüllen hat*
- 25%-Höchstgrenze der Bevölkerungsabweichung einhalten
- zusammenhängendes Gebiet bilden
- Bundesländer- und (ggf.) Regierungsbezirksgrenzen nicht überschreiten
- Gemeindeverbände und „kleine“ Gemeinden nicht aufteilen

(ii) *Bewertungskriterien, um Wahlkreise bezüglich der Einteilungsziele zu beurteilen*
- Beachtung der Grenzen der Kreise und kreisfreien Städte
- Abweichung der deutschen Wahlkreisbevölkerung vom Durchschnitt

Strikt zu erfüllende Bedingungen

Der Zusammenhang eines jeden Wahlkreisgebietes ist als strikte Bedingung modelliert, trotz Soll-Formulierung im Wahlgesetz. Die Praxis zeigt, dass Wahlkreise in der Regel zusammenhängend sind (Goderbauer und Wicke, 2017). Ein begründetes Abgehen von dieser Vorgabe, z.B. im Falle von Nord- bzw. Ostseeinseln sowie Exklaven, wird durch Preprocessing der verwendeten Daten in Form von sogenannten virtuellen Benachbarungen (s. Abschnitt 11.4.1) abgefangen.

In der Praxis werden, falls im Rahmen der Höchstgrenze der Bevölkerungsabweichung möglich, Wahlkreise regierungsbezirksscharf eingeteilt (Goderbauer und Wicke, 2017). Besonders in Bayern hat dies traditionell einen hohen Stellenwert. Wir kommen dieser Praxis nach, indem in Nordrhein-Westfalen, Hessen, Bayern und Baden-Württemberg die Wahlkreise durch erneutes Anwenden der Zuteilungsmethode auf die Regierungsbezirke verteilt werden. Vereinzelt werden passend benachbarte Regierungsbezirke zusammengefasst (vgl. Tab. 11.5 und 11.6).

Dass Gemeindeverbände (auch Verbands-, Samtgemeinde oder Amt genannt) nicht und Gemeinden in Form von Großstädten nur in erzwungenen Fällen auf mehrere Wahlkreise aufgeteilt werden, geht aus unserer Sicht einher mit den rechtlichen Vorgaben und größtenteils der Umsetzung in der Praxis (Goderbauer und Wicke, 2017). Großstädte wer-

den basierend auf ihren Bezirken bzw. Stadtteilen bei der Wahlkreiseinteilung betrachtet (s. Abschnitt 11.4.1).

Bewertungsfunktionen der Einteilungsziele

Um (zulässige) Wahlkreise und schließlich Einteilungen anhand der Zielkriterien bewerten und vergleichen zu können, sind numerische Bewertungsfunktionen der Ziele zu definieren. Dabei wird die Ausprägung eines Einteilungsziels für einen Wahlkreis in Form einer reellen Zahl zwischen 0 (*Ziel ungenügend bzw. gar nicht ausgeprägt*) und 1 (*Ziel vollends ausgeprägt*) angegeben. Anhand einer vorgegebenen Gewichtung der Ziele berechnet sich die Bewertung eines Wahlkreises aus der gewichteten Summe der Zielbewertungen dieses Wahlkreises. Schließlich ist die Bewertung einer ganzen Wahlkreiseinteilung definiert als die Summe der Bewertungen der in der Einteilung enthaltenen Wahlkreise. Das Optimierungsziel besteht somit darin, eine zulässige Wahlkreiseinteilung mit maximaler Bewertung zu finden.

Bevölkerungsabweichung Die in Abbildung 11.1 dargestellte stückweise lineare Funktion rechnet die betragsmäßige Bevölkerungsabweichung eines Wahlkreises in eine Bewertung um. Dadurch werden kleine Abweichungen ähnlich gut bewertet und höhere Abweichungen überproportional stark bestraft.

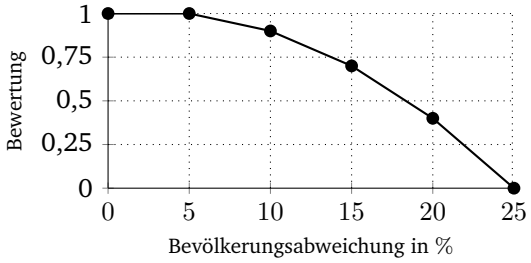


Abb. 11.1: Gewählte stückweise lineare Funktion für die Bewertung der Bevölkerungsabweichung.

Grenzen der Kreise und kreisfreien Städte einhalten Ein Wahlkreis erfüllt das Einteilungsziel der *administrativen Konformität* vollends (d.h. Bewertung 1), wenn einer der beiden folgenden Fälle erfüllt ist:

(i) Der Wahlkreis wird aus *genau einem oder genau mehreren* Kreisen und/oder kreisfreien Städten gebildet, oder

(ii) Der Wahlkreis liegt *vollständig* in *einem* Kreis oder *einer* kreisfreien Stadt und dieser Kreis bzw. kreisfreie Stadt muss *gezwungenermaßen* in mehr als einen Wahlkreis aufgeteilt werden, d.h. besitzt mehr als das $1{,}25$-fache der durchschnittlichen Wahlkreisbevölkerung.

In den restlichen Fällen ist die Bewertung der administrativen Konformität definiert als der *Längenanteil der Wahlkreisaußengrenze, die auch Grenze von Kreisen und/oder kreisfreien Städten ist*. D.h. in der Optimierung wird die Länge der Wahlkreisgrenze, die keine Grenze von Kreis/kreisfreier Stadt ist, minimiert. Dadurch wird ermöglicht, dass auf Grundlage der Kreise und kreisfreien Städte kompakte Wahlkreisgebiete berechnet werden. Im Falle der Stadtstaaten Berlin, Hamburg und Bremen wird die hier betrachtete administrative Ebene der

Kreise und kreisfreien Städte durch eine in diesen Städten entsprechende Untergliederung ersetzt (vgl. Abschnitt 11.4.1 und Tabelle 11.3).

Für die von uns durchgeführten Studien (Goderbauer et al., 2018a,b) gab das Büro des Bundeswahlleiters vor, bei der Anwendung der mathematischen Optimierung *beide Einteilungsziele als gleich gewichtig* anzusehen. Diese Gewichtung der Zielfunktionen ist auch die Grundlage sämtlicher Optimierungsergebnisse in diesem Artikel.

11.2.3 Über Graphpartitionierung zur optimalen Entscheidungsunterstützung



Abb. 11.2: Konstruktion eines mathematischen Graphen für die Wahlkreiseinteilung am Beispiel des Saarlandes: Gemeinden werden in sogenannte Knoten überführt, von denen jeweils zwei genau dann verbunden werden, wenn die zugehörigen Gebiete benachbart sind, also eine gemeinsame Grenze haben (Grenzverläufe: © GeoBasis-DE / BKG 2016).

Die Problemstellung der optimierungsbasierten Berechnung einer Wahlkreiseinteilung kann als eine *Partitionierungsaufgabe auf einem mathematischen Graphen* angesehen werden. Ein Graph ist eine abstrakte mathematische Struktur, die eine Menge von Objekten und bestehende Verbindungen zwischen diesen Objekten repräsentiert. Der hier relevante Graph wird aus geometrischen Daten des Wahlgebiets und dessen Untergebiete konstruiert (s. Abb. 11.2). Die repräsentierten Objekte (auch Knoten genannt) sind beispielsweise Gemeinden. Zwei solche Knoten sind miteinander verbunden, wenn die zugehörigen Gebiete benachbart sind. Zusätzlich werden jedem Knoten und jeder Verbindung weitere Informationen wie Bevölkerungszahl oder Zugehörigkeit zu einem Landkreis zugeordnet. Ein Wahlkreis wird durch eine Auswahl von Knoten des Graphen dargestellt. Eine solche Knotenmenge repräsentiert einen zulässigen Wahlkreis, wenn die genannten Bedingungen erfüllt sind: Die Knoten haben einen zusammenhängenden Teilgraphen zu bilden und die Summe der Bevölkerung der Knoten hat die gesetzlichen Schranken einzuhalten. Die Optimierungsaufgabe besteht nun darin, den Graphen in eine vorgegebene Anzahl an zulässigen Teilgraphen zu partitionieren, sodass die Einteilungsziele bestmöglich ausgeprägt sind.

Interaktive Software: Optimierungsbasierte Entscheidungsunterstützung

Zur Lösung des Optimierungsproblems haben wir passende Methoden entwickelt. Diese basieren primär auf Konzepten und Lösungstechniken der gemischt-ganzzahligen linearen Programmierung. Um von den optimierungsbasierten Lösungsmethoden berechnete

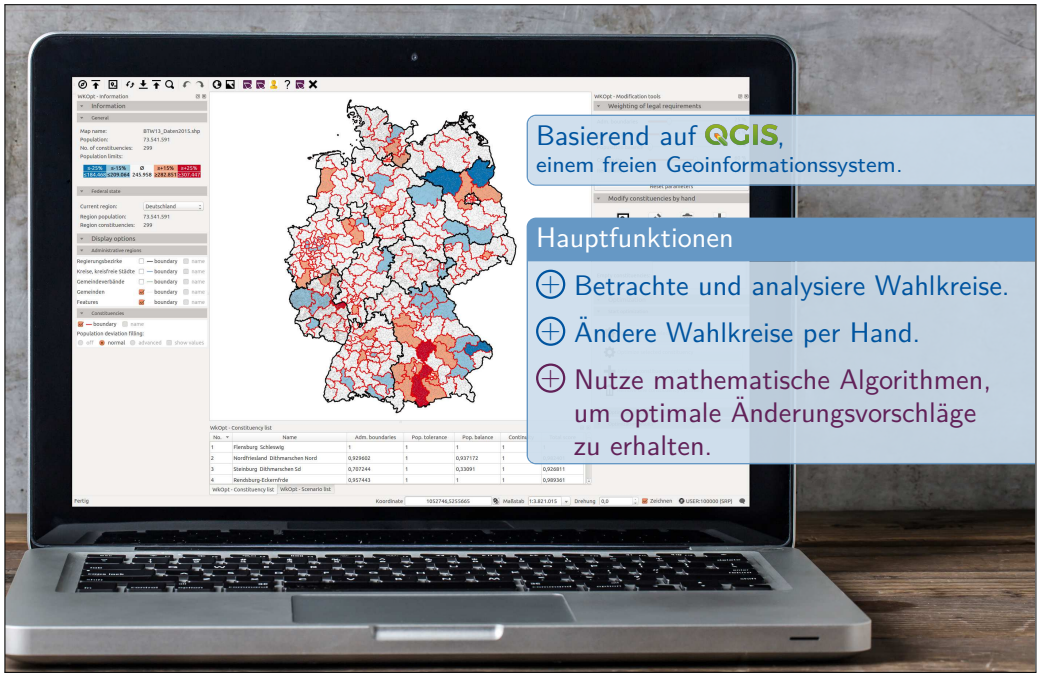


Abb. 11.3: Die Software zur Entscheidungsunterstützung bei der Einteilung von Wahlkreisen. U.a.: Interaktive Kartendarstellung mit ein- und ausblendbaren Grenzverläufen und Gebietsnamen sowie Einfärbung der Wahlkreise abhängig von dessen Bevölkerungsabweichung.

Wahlkreiskarten ansprechend darzustellen sowie bezüglich der Vorgaben analysieren zu können, haben wir zusätzlich eine spezielle *Software* entwickelt (s. Abb. 11.3). Neben der Visualisierung ist es auch möglich, per Mausklick Gebiete manuell umzusetzen und die Auswirkungen auf die Einteilungskriterien unmittelbar zu erfahren. Außerdem können Einteilungen miteinander verglichen werden, dabei werden umgesetzte Gebiete visuell hervorgehoben. Auch berechnete Einteilungen können per Hand modifiziert oder Vorschläge rückgängig gemacht werden. Somit behalten Nutzende der Software weiterhin die Hoheit über alle Entscheidungen – objektiv unterstützt. Die Software kann auch eingesetzt werden, um Wahlkreise auf anderen Ebenen einzuteilen, z.B. für Landtagswahlen oder Kommunalwahlen.

Weitere Details zum mathematischen Modell, den Lösungsmethoden und dem Software-Tool zur Entscheidungsunterstützung sind in den Arbeiten von Goderbauer und Lübbecke (2019a) sowie Goderbauer und Winandy (2017) zu finden.

11.3 Auf der Suche nach einer geeigneten Wahlkreisanzahl

In der aktuellen Debatte werden verschiedene Anzahlen an Bundestagswahlkreisen von Wissenschaftlern und Praktikern vorgeschlagen. Nach einem Überblick in Abschnitt 11.3.2 leiste wir einen eigenen Beitrag (Abschnitt 11.3.3): Basierend auf der gesetzlichen Vorgabe für die numerische Zuteilung der Wahlkreise auf die Bundesländer folgern wir Wahlkreisanzahlen, die bestmöglich auf die föderale Struktur Deutschlands abgestimmt sind. Diese

Argumentationslinie ist in der gegenwärtigen Debatte noch nicht vorzufinden – offenbart jedoch relevante Erkenntnisse. Beginnen tun wir zunächst mit einer Skizze der geschichtlichen Entwicklung der Anzahl der Bundestagswahlkreise in Deutschland.

11.3.1 Entwicklung der Wahlkreisanzahl

Eine Änderung der Anzahl der Bundestagswahlkreise ist in der Geschichte der Bundesrepublik Deutschland nicht ungewöhnlich (vgl. Tabelle 11.1).

Jahre der Bundestagswahlen	Anzahl Wahlkreise
1949, ’53	242
1957, ’61	247
1965, ’69, ’72, ’76, ’80, ’83, ’87	248
1990, ’94, ’98	328
2002, ’05, ’09, ’13, ’17	299

Tabelle 11.1: Anzahl der Bundestagswahlkreise von der ersten Bundestagswahl bis heute.

Bei der ersten Bundestagswahl 1949 war das Land in 242 Wahlkreise eingeteilt. Diese Anzahl kam zustande durch die gesetzliche Vorgabe der Mindestanzahl von 400 Abgeordneten und dem „ungefähren Verhältnis von 60 zu 40“ zwischen Wahlkreis- und Landeslistenmandaten (Bundesgesetzblatt, 1949). Das heute geltende 50:50-Verhältnis zwischen Direkt- und Listenmandaten gibt es seit der zweiten Bundestagswahl im Jahr 1953. Im Rahmen der Umsetzung dieser Änderung wurde bei unveränderter Wahlkreisanzahl die Mindestabgeordnetenanzahl angehoben (Bundesgesetzblatt, 1953). Außer durch die Wiedereingliederung des Saarlandes (1957, +5 Wahlkreise) und einer kleinen Anpassung (1965, +1 Wahlkreis), änderte sich die Wahlkreisanzahl bis zur Wiedervereinigung Deutschlands nicht. Zur Wahl 1990 kamen mit den fünf neuen Bundesländern 80 Wahlkreise hinzu. Somit waren es ab 1990 insgesamt 328 Bundestagswahlkreise. Seit der Wahl im Jahr 2002 gilt die aktuelle Anzahl 299. Diese letzte vollzogene Änderung von 328 auf 299 Wahlkreise wird im folgenden knapp dokumentiert, da sie auf der selben Motivation beruht wie die der aktuellen Reformdiskussion: Die Verkleinerung des Deutschen Bundestages.

In den 1990er Jahren galt die gesetzliche Mindestanzahl von 656 Abgeordneten (jeweils 328 Wahlkreis- sowie Listenmandate) und es entstanden nur bis zu 16 Überhangmandate. Eine Lösung zur Verkleinerung des Parlamentes war schnell gefunden: Die Verringerung der Wahlkreisanzahl unter Beibehaltung des geltenden Wahlrechts inkl. 50:50-Verhältnis zwischen Direkt- und Listenmandaten. Auf Empfehlung des Ältestenrates (BT-Drs. 13/1803, 1995) beschloss der Deutsche Bundestag (1995), das Parlament mit Wirkung ab dem Jahr 2002 „auf unter 600 Abgeordnete“ zu verkleinern. Weiter besagt der Beschluss, dass es nicht weniger als „heutiger Stand 672 minus höchstens bis 100 Abgeordnete“ und somit mindestens 572 sein sollen. Eine anschließend eingesetzte Reformkommission (BT-Drs. 13/4860, 1996) wählte aus der beschlossenen Menge möglicher Wahlkreisanzahlen $\{286, \ldots, 299\}$ die größte Alternative: 299. Man argumentierte mit der ansteigenden Bevölkerungszahl der einzelnen Wahlkreise bei jeder weiteren Verringerung der Wahlkreisanzahl. Eine weitere Reduktion

der Wahlkreisanzahl würde „die Möglichkeit einer intensiven Wahlkreisarbeit“ zwischen Abgeordneten und Bürgern „zu stark beeinträchtigen“ (BT-Drs. 13/4860, 1996).

Zugespitzt lässt der Vorgang den Schluss zu, dass die 299 simpel durch die obere Schranke des Ältestenrates (<300 Wahlkreise) und der Ausschöpfung dieses Spielraums durch die Reformkommission (sonst „zu große“ Wahlkreise) zustande gekommen ist. Dies widerspricht dem ersten Eindruck der „unrunden“ Zahl 299, die eine komplexere Argumentationskette vermuten lässt als lediglich die Begründung, dass sie die größte ganze Zahl unter 300 ist.

Aus heutiger Sicht erscheint die damalige Lage mit wenigen zusätzlichen Mandaten über der gesetzlichen Mindestgröße jedoch fast schon trivial. Die heutige Konfrontation mit allerhand aufschaukelnden Wechselwirkungen ist komplexer: Überhang- und Ausgleichsmandate, Auffächerung der Parteienlandschaft und damit einhergehende Abschwächung der Volksparteien, die dennoch überwiegend die Wahlkreisgewinner stellen. Dies alles führt zu dramatischen Abgeordnetenanzahlen in der Theorie (Funk, 2018) als auch Praxis in Form der letzten Bundestagswahl 2017.

11.3.2 Vorschläge in aktueller Reformdebatte

Einerwahlkreise	
270 WK	Schröder (2014)
250 WK	Bundeswahlleiter (Goderbauer et al., 2018a)
248 WK	*hier*
240 WK	Behnke (2013), Behnke (2017, ≤ 240 WK), Pukelsheim (2019)
200 WK	Grotz und Vehrkamp (2017), Pukelsheim (2018), Bundeswahlleiter (Goderbauer et al., 2018a), Hesse (2019)
Zweierwahlkreise	
150 WK	Behnke (2017), Grotz und Vehrkamp (2017)
149 WK	Grotz und Vehrkamp (2017)
145 WK	*hier*
125 WK	Bundeswahlleiter (Goderbauer et al., 2018b)
120 WK	Oppermann und Klecha (2018)

Tabelle 11.2: Vorgeschlagene Anzahlen an Einer- bzw. Zweierwahlkreisen und zugehörige Quellen.

Im Zuge der aktuellen Kontroverse über das Bundeswahlgesetz werden für Reformvarianten, die eine Reduktion der Wahlkreisanzahl beinhalten, konkrete Anzahlen vorgeschlagen. Einen Überblick bietet Tabelle 11.2. Urheber der Vorschläge sind Politikwissenschaftler, Mathematiker und Politiker. Die vom Bundeswahlleiter im Zuge der von Goderbauer et al. (2018a,b) durchgeführten Studien benannten Anzahlen werden auch berücksichtigt. Darüber hinaus schlagen wir in der noch folgenden Analyse selbst zwei Wahlkreisanzahlen vor; jeweils passend für den Bereich mit Anwendung von Einer- bzw. Zweierwahlkreisen.

11.3.3 Bewertung von Wahlkreisanzahlen auf Grundlage der Bevölkerungsanteile der Bundesländer

Aufgrund des im Grundgesetz unabänderlich festgeschriebenen bundesstaatlichen Gliederung der Bundesrepublik (Art. 20 Abs. 1 Grundgesetz) sind Bundestagswahlkreise bundesländerscharf einzuteilen. Die vorgegebene Gesamtanzahl an Wahlkreisen wird auf die Bundesländer verteilt. Das Bundeswahlgesetz (BWG) nennt diesbezüglich folgenden Grundsatz:

> *Die Zahl der Wahlkreise in den einzelnen Ländern muss deren Bevölkerungsanteil soweit wie möglich entsprechen.*
>
> **— § 3 Abs. 1 Punkt 2 Satz 1 BWG**

Das Gesetz gibt ein Verfahren vor (Divisormethode mit Standardrundung, vgl. Pukelsheim (2017)), mit dem die Verteilung durchzuführen und der genannte Grundsatz sichergestellt ist.

Bei Abänderung der Wahlkreisanzahl ist der zitierte Grundsatz – nach unser Interpretation – ebenfalls zu berücksichtigen, um eine auf die Bevölkerungsstruktur der Bundesländer passende Anzahl festzulegen. Daneben, dass die genannte und als Muss-Regel formulierte Vorgabe dies selbst und ebenso die im Grundgesetz postulierte Wahlgleichheit fordert, sind weitere wichtige Gründe zu nennen:

(1) *Überhangmandate*
Nach Behnke (2003, 2005, 2010a) ist eine unausgewogene Verteilung der Wahlkreise zwischen den Bundesländern ein Faktor (von weiteren), der das Entstehen von Überhangmandaten und somit die Vergrößerung des Bundestags begünstigen kann (vgl. auch Grotz (2000) und Schreiber et al. (2017, S. 184)).

(2) *Wahlkreiskontinuität*
Das Bundesverfassungsgericht urteilte wiederholt, dass die räumliche Gestalt der Wahlkreise möglichst stabil zu halten ist (BVerfGE 130, 212, 2012; BVerfGE 95, 335, 1997). In der Praxis wird dies primär als Begründung herangezogen, um lediglich die nötigsten Einteilungsänderungen von einer Wahl auf die nächste durchzuführen (Goderbauer und Wicke, 2017). Eine bezüglich der Bundesländerstruktur abgestimmte Wahlkreisanzahl ist maximal robust gegenüber Bevölkerungsentwicklungen und minimiert so das Risiko, dass sich die Zuteilung ändert. Jede Wahlkreisverschiebung zwischen den Ländern impliziert erzwungenermaßen einen massiven Eingriff in die Wahlkreisstruktur. Seit Einführung der Wahlkreisanzahl 299 im Zuge der Wahl 2002 änderte sich die Länderzuteilung zu jeder nachfolgenden Wahl.

(3) *Einteilungsfreiraum*
Um bezüglich der gesetzlichen Einteilungsziele (z.B. dem Orientieren an Landkreisgrenzen) nachhaltig gute Wahlkreise abgrenzen zu können, sind die durch die Zuteilung auf die Länder hervorgerufenen Bevölkerungsabweichungen so klein wie möglich zu halten. Werden hier schon hohe Abweichungswerte verursacht, ist der Einteilungsfreiraum in den Ländern aufgrund des gesetzlichen Höchstwerts von 25% eingeschränkt.

Im Folgenden führen wir aus, welche Wahlkreisanzahlen am besten zu der Bevölkerungsstruktur der Bundesländer passen (vgl. Goderbauer (2016a, Kapitel 7)). Die dafür durchgeführte numerische Evaluation bringt zusätzliche Erkenntnisse zum Vorschein.

Modellierung

Sei die Menge der Bundesländer mit B und die deutsche Bevölkerung (hier zum Stichtag 30.09.2017) eines Bundeslandes $b \in B$ mit $\text{bev}(b) \in \mathbb{N}$ bezeichnet. Zu einer Wahlkreisanzahl $k \in \mathbb{N}$ bezeichnen wir die durchschnittliche Bevölkerungszahl eines Wahlkreises in Deutschland mit

$$\varnothing\text{bevwk}^k := \frac{1}{k} \sum_{b \in B} \text{bev}(b).$$

Mithilfe der Divisormethode mit Standardrundung wird $k \in \mathbb{N}$ auf die Bundesländer verteilt. Sei die resultierende Anzahl der Wahlkreise eines Bundeslandes $b \in B$ unter Gesamtwahlkreisanzahl $k \in \mathbb{N}$ bezeichnet mit $\text{wk}^k(b) \in \mathbb{N}$; entsprechend gilt $\sum_{b \in B} \text{wk}^k(b) = k$. Zur Berechnung verwenden wir die Software BAZI (2018) von u.a. Pukelsheim. Davon ausgehend bezeichnen und berechnen wir die durchschnittliche Bevölkerungszahl eines Wahlkreises in Bundesland $b \in B$ mit

$$\varnothing\text{bevwk}^k(b) := \frac{\text{bev}(b)}{\text{wk}^k(b)}.$$

Daraus berechnet sich die relative Abweichung der durchschnittlichen Wahlkreisbevölkerung in Bundesland $b \in B$ von der in Deutschland:

$$\text{abw}^k(b) := \frac{\varnothing\text{bevwk}^k(b)}{\varnothing\text{bevwk}^k} - 1.$$

Die Verteilung dieser Werte diskutieren wir im Folgenden für sinnvolle Wahlkreisanzahlen $k \in \mathbb{N}$. Als Obergrenze der betrachteten k wählen wir 350. Dies begründen wir damit, dass ausschließlich eine Reduktion von 299 diskutiert wird, wir aber dennoch die Umgebung der aktuellen Wahlkreisanzahl begutachten können möchten.

Auswertung

Ab $k \geq 64$ erhält jedes Bundesland mindestens einen Wahlkreis. Abbildung 11.4 gibt die Verteilung der Werte $\text{abw}^k(b)$ für jedes $k \in \{64, \ldots, 350\}$ an. Abbildung 11.5 beschränkt sich auf die Darstellung der Maximalwerte $\max_{b \in B} |\text{abw}^k(b)|$.

Die Wahlkreisanzahl $k = 98$ ist die kleinste, bei der nach Verteilung auf die Bundesländer eine zulässige Einteilung möglich ist. Für $k = 98$ gilt: $\max_{b \in B} |\text{abw}^{98}(b)| = 24{,}6\% \leq 25\%$ (vgl. § 3 Abs. 1 Punkt 3 BWG). Bei Erhöhung von k zeigt sich, dass dieses Zulässigkeitsfenster zunächst nur spärlich, nämlich nur für $k = 98, 99, 100, 101, 102$ gegeben ist. Für $k \in \{103, \ldots, 123\}$ ist keine zulässige Wahlkreiseinteilung möglich, da der eine dem Saarland (SL) zugeteilte Wahlkreis um bis zu $49{,}7\%$ von der durchschnittlichen Bevölkerungszahl eines Wahlkreises abweichen würde. Erst für $k = 124$ werden dem Saarland zwei Wahlkreise zugeteilt und somit springt die saarlandspezifische Bevölkerungsabweichung auf (zulässige) $-24{,}6\%$.

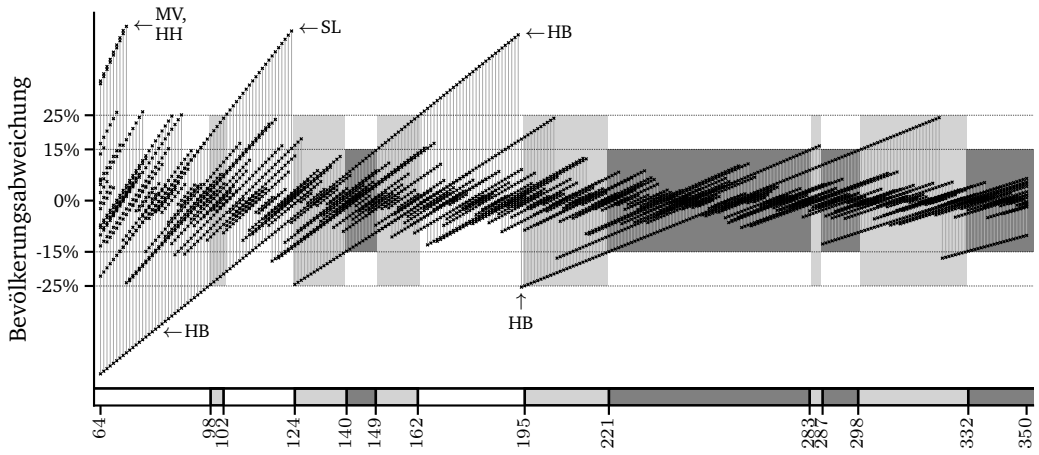


Abb. 11.4: Für jede Anzahl deutscher Bundestagswahlkreise $k \in \{64, \ldots, 350\}$ sind die resultierenden durchschnittlichen Bevölkerungsabweichungen $\text{abw}^k(b)$ der 16 Bundesländer $b \in B$ in einem schwarzen Dot-Plot aufgetragen.
Ein hellgrauer bzw. dunkelgrauer Werteschlauch repräsentiert, dass die im Gesetz genannten Abweichungsintervalle $\pm 25\%$ (hellgrau) bzw. $\pm 15\%$ (dunkelgrau) in dem Bereich eingehalten werden. Die Einfärbung spiegelt sich an der Abszissenachse wider. Die trennende Wahlkreisanzahl zwischen zwei Einfärbungen gehört jeweils zur dunkleren.
Zusätzlich ist notiert, welche Bundesländer die extremen Abweichungswerte verursachen.

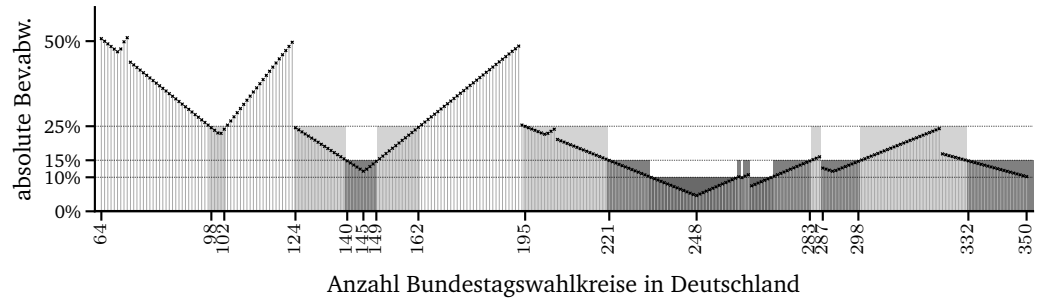


Abb. 11.5: Ergänzung zu Abb. 11.4: Hier ist lediglich die Maximalabweichung $\max_{b \in B} |\text{abw}^k(b)|$ für jede Anzahl k an Bundestagswahlkreisen dargestellt. Zusätzlich ist die vom Europarat empfohlene Soll-Schranke von 10% Bevölkerungsabweichung (Venedig-Kommission, 2002) abgetragen.

Wahlkreisanzahlen $k = 163, \ldots, 194$ sind ebenfalls nicht möglich, da in diesen Fällen Bremen (HB) Abweichungen von bis zu $48{,}6\%$ vorzuweisen hat. Anzahlen $k \geq 195$ sind zulässig, wenn auch im Fall $k = 323$ mit $\max_{b \in B} |\text{abw}^{323}(b)| = 24{,}3\%$ nur knapp.

Für $k = 299$ ergibt sich $\max_{b \in B} |\text{abw}^{299}(b)| = 15{,}07\%$. Somit wird die gesetzliche Soll-Grenze von maximal 15% Bevölkerungsabweichung aktuell schon durch die Zuteilung auf die Bundesländer gerissen. Bezüglich der Bewertung $\min_{k \in \{64,\ldots,350\}} \max_{b \in B} |\text{abw}^k(b)|$ ergibt sich als geeignetste Wahlkreisanzahl $k = 248$ mit $\max_{b \in B} |\text{abw}^{248}(b)| = 4{,}65\%$. Für den Anwendungsfall von Zweierwahlkreisen (etwa $k \leq 160$) ist Wahlkreisanzahl $k = 145$ am geeignetsten. Mit $\max_{b \in B} |\text{abw}^{145}(b)| = 11{,}78\%$ verursacht diese Anzahl die geringsten Abweichungen in dem Bereich.

Diskussion

Unter der Annahme, dass die 25%-Abweichungsgrenze sowie striktes Einhalten der Ländergrenzen weiterhin Bestand haben, können viele Wahlkreisanzahlen, insbesondere $k < 200$, nicht zulässig umgesetzt werden. Die Bevölkerungsschwäche der Bundesländer Bremen und Saarland verursacht dies. Im Besonderen sind die von Oppermann und Klecha (2018) angeregten 120 numerisch unzulässig. Alle anderen in Tabelle 11.2 genannten Vorschläge dagegen sind es, wenn auch in den Fällen von 200 und 125 nur knapp. Die Menge der zulässigen Wahlkreisanzahlen für die Anwendung von Zweierwahlkreisen ist sehr schmal. Nur für Anzahlen 140 bis 149 bleiben die Bevölkerungsabweichungen im 15%-Abweichungsintervall. Es gibt (internationale) Stimmen (vgl. OSCE (2009, 2013)), die die deutschen gesetzlichen Abweichungsgrenzen der Wahlkreisbevölkerung mit 15% bzw. 25% für zu hoch halten. Die Europäische Kommission für Demokratie durch Recht (Venedig-Kommission) empfiehlt in ihrem „Verhaltenskodex für Wahlen“ eine Soll-Grenze von 10% und eine Muss-Grenze von 15% (Venedig-Kommission, 2002). Obige Analyse zeigt, dass nur wenige Wahlkreisanzahlen (rund um $k = 248$) *nach* einer Verteilung auf die Bundesländer noch eine Wahlkreiseinteilung ermöglichen, die die europäische Soll-Schranke einhält.

Unsere aus der durchgeführten Analyse gewonnen Empfehlungen für Festlegung einer Wahlkreisanzahl lauten: 145 bei Zweierwahlkreisen und 248 bei Einerwahlkreisen. Bei letzteren 248 sind die erzielten Abweichungswerte von unter 5% nach Verteilung auf die Bundesländer beachtlich klein. Die Wahlkreisanzahl 248 ist somit genau diejenige, die zu Anzahlen in den einzelnen Bundesländern führt, sodass diese Anzahlen „deren Bevölkerungsanteil *soweit wie möglich* entsprechen“ – genau wie es der Grundsatz im Bundeswahlgesetz unter § 3 Abs. 1 Punkt 1 Satz 1 fordert. Interessant ist, dass genau diese Wahlkreisanzahl in den meisten bis heute in Deutschland durchgeführten Bundestagswahlen Bestand hatte (vgl. Tabelle 11.1).

Insgesamt zeigt sich, dass die Bevölkerungsanteile der Bundesländer mit in die Reformdebatte einzubeziehen sind. Diese haben eine gehörigen Einfluss auf den zulässigen Spielraum bei der Einteilung der Wahlkreise in den Bundesländern. Außerdem muss die Auswahl einer Wahlkreisanzahl filigran getroffen werden, damit Bewegungen in den Bevölkerungszahlen über die Zeit nicht zu gesetzwidrigen Abweichungswerten führen.

11.4 Objektive Wahlkreiseinteilung mittels mathematischer Optimierung

Unter Anwendung unserer Software zur Entscheidungsunterstützung sowie der entwickelten mathematischen Methoden der Optimierung (Abschnitt 11.2.3) haben wir Einteilungen Deutschlands in 299, 250, 200 und 125 Wahlkreisen sowie Einteilungen in die im vorherigen Abschnitt 11.3.3 motivierten Anzahlen 248 und 145 berechnet. Sämtliche Wahlkreiseinteilungen sind online in einer interaktiven Wahlkreiskarte (Abb. 11.6) verfügbar unter:

`http://www.or.rwth-aachen.de/wahlkreiskarte` (Goderbauer et al., 2019, online).

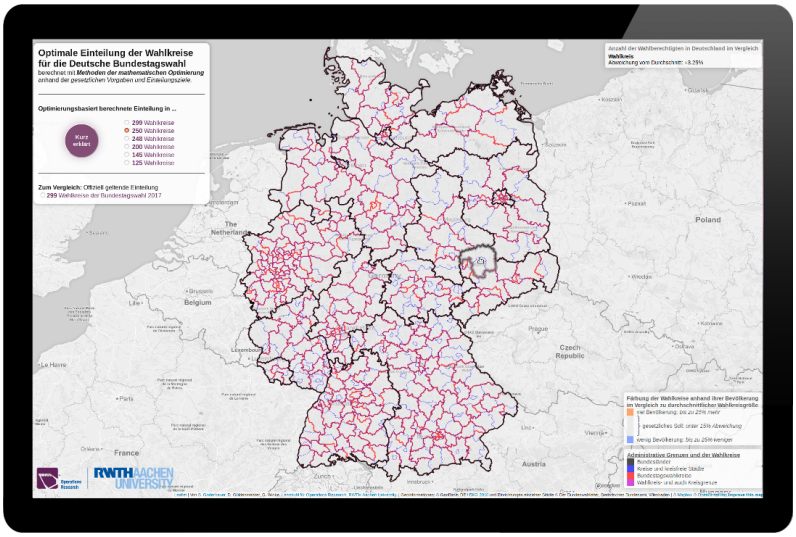


Abb. 11.6: Interaktive Wahlkreiskarte der optimierungsbasiert berechneten Einteilungen mit Zoom-Funktion, Bevölkerungsabweichungen und administrativen Grenzen.

In der interaktiven Online-Applikation können neben den Grenzverläufen der berechneten Wahlkreise auch vergleichend die der aktuell geltenden Einteilung Deutschlands studiert werden. Zusätzlich sind, im Zuge der gesetzlichen Einteilungsziele, relevante administrative Grenzen sowie Angaben zur Bevölkerung der Wahlkreise dargestellt.

Entsprechend dem zugrundeliegenden mathematischen Modell halten alle berechneten Wahlkreise die strikt zu erfüllenden Bedingungen ein. Die Gewichtung der beiden Zielfunktionen der Optimierung haben wir von den im Auftrag des Bundeswahlleiters durchgeführten Studien (Goderbauer et al., 2018a,b) übernommen: Gleichgewichtung der Ziele administrative Konformität und Bevölkerungsabweichung. Die Wahl der Zielpräferenzen kann bei der Durchführung von weiteren Berechnungen natürlich angepasst werden (vgl. Abschnitt 11.5).

Bevor in Abschnitt 11.4.3 die optimierungsbasiert eingeteilten Wahlkreise ausgewertet werden, wird in Abschnitt 11.4.1 die geschaffene und bei der Optimierung verwendete Datengrundlage vorgestellt und auf Einzelheiten hingewiesen.

11.4.1 Datengrundlage: Geometrie und Bevölkerung

Um Wahlkreise automatisiert mit mathematischen Methoden einteilen zu können, werden Bevölkerungsdaten und detaillierte Informationen zu Grenzverläufen, d.h. der Geometrie des Wahlgebiets benötigt. Beispielsweise bestimmen wir anhand von Grenzverläufen automatisiert die Nachbarschaftsbeziehungen zwischen Gemeinden. Diese Informationen werden benötigt um den mathematischen Graphen aufzustellen und so den Zusammenhang der Wahlkreisgebiete sicherzustellen. Daten der Grenzverläufe verschiedener Verwaltungsebenen werden außerdem benötigt, um die Zielfunktion der administrativen Konformität umzusetzen (vgl. Abschnitt 11.2).

Die in dieser Arbeit verwendeten Daten basieren hauptsächlich auf der vom Bundeswahlleiter (2017) zur Verfügung gestellten Basiskarte zum Stichtag 30.09.2017. Die im Dateiformat

Shapefile vorliegende Basiskarte enthält neben Geometrien auch Daten der Deutschen Bevölkerung zum angegebenen Stichtag. Die Basiskarte ist jedoch im Falle von bevölkerungsreichen Städte, die bei der Wahlkreiseinteilung auf mehr als einen Wahlkreis aufgeteilt werden müssen, *nicht* nutzbar. Diese bevölkerungsreichen Städte sind in der Basiskarte nicht detailliert auf der Ebene von Stadtteilen und/oder -bezirken angegeben. Wir haben daher die Basiskarte des Bundeswahlleiters um Geometrien und Bevölkerungsdaten von Stadtbezirken, -teilen o.ä. der 17 bevölkerungsreichsten deutschen Städte ergänzt. Die dabei verwendeten Daten erhielten wir auf Anfrage zumeist bei den Städten bzw. Landeswahlleitungen (Goderbauer et al., 2018a, Tabellen 11 und 12).

Ergänzung von virtuelle Gebietsbenachbarungen Wie erläutert berechnen wir Benachbarungen zwischen Gebieten automatisiert aus den Geometriedaten. Es gibt jedoch Gebiete, z.B. Inseln oder Exklaven, die nicht mit anderen Gebieten benachbart sind. Um auch diese nicht-angeschlossenen Gebiete in zulässige, d.h. zusammenhängende Wahlkreise einteilen zu können, haben wir in den Daten sogenannte virtuelle Benachbarungen ergänzt. Eine detaillierte Auflistung der hinzugefügten virtuellen Benachbarungen sowie eine jeweilige Begründung dafür sind in (Goderbauer et al., 2018a, Abschnitt A.4.2) angegeben.

Bevölkerungsreiche Städte

Die in Tabellen 11.3 und 11.4 angegebenen Städte sind diejenigen, um dessen Verwaltungsebenen unterhalb der Gemeindeebene wir die Basiskarte des Bundeswahlleiters ergänzt haben. Es sind die 17 bevölkerungsreichsten Städte Deutschlands. Die kleinste dabei betrachtete Stadt ist Wuppertal. Diese hat bei einer Gesamtwahlkreisanzahl von 250 (die größte betrachtete nach 299) aufgrund ihrer Bevölkerungszahl Anspruch auf knapp weniger als einen Wahlkreis. Wir haben festgelegt, dass dies das Kriterium sein soll, keine weiteren Städte in der Basiskarte mit Gebieten unterhalb der Gemeindeebene einzupflegen. Für die Vergleichseinteilung in 299 Wahlkreise nehmen wir Bevölkerungsabweichungen verschuldet durch die Nichtunterteilung von z.B. Bielefeld in Kauf.

Das Einteilungsziel bzgl. der administrativen Grenzen gibt vor, Grenzen der Kreise und kreisfreien Städte möglichst einzuhalten. In den Bundesländern Berlin, Hamburg und Bremen gibt es diese Ebene nicht. Die in Tabelle 11.3 für die Stadtstaaten jeweils angegebene 1. Verwaltungsebene sehen wir als diejenige Verwaltungsebene an, dessen Grenzen wir in den Stadtstaaten anstreben einzuhalten. Auf der 2. Verwaltungsebene der Stadtstaaten werden Wahlkreise eingeteilt.

		1. Verwaltungsebene		2. Verwaltungsebene	
Stadt	Dt. Bev.	#	Bezeichnung	#	Bezeichnung
Berlin	2.974.717	12	Bezirke	78	Abgeordnetenhauswahlkreise
Hamburg	1.534.643	7	Bezirke	104	Stadtteile
Bremen	469.087	5	Stadtbezirke	$19 + 4$	Stadt- + Ortsteile

Tabelle 11.3: Unterteilte Städte in den Stadtstaaten Berlin, Hamburg und Bremen.

Stadt	Dt. Bev.	Wahlkreisanspruch bei 250 Wahlkreisen	1. Verwaltungsebene #	1. Verwaltungsebene Bezeichnung
München	1.087.642	3,72	25	Stadtbezirke
Köln	871.136	2,98	9	Stadtbezirke
Frankfurt am Main	530.296	1,81	16	Ortsbezirke
Leipzig	527.270	1,80	10	Stadtbezirke
Dresden	511.939	1,75	10	Ortsämter mit zugeordneten Ortschaften
Düsseldorf	495.324	1,69	10	Stadtbezirke
Essen	494.207	1,69	9	Stadtbezirke
Dortmund	486.844	1,66	12	Stadtbezirke
Stuttgart	476.146	1,63	23	Stadtbezirke
Hannover	443.500	1,52	13	Stadtbezirke
Nürnberg	402.853	1,38	10	statistische Stadtteile
Duisburg	398.044	1,36	7	Stadtbezirke
Bochum	320.852	1,10	6	Stadtbezirke
Wuppertal	287.618	0,98	10	Stadtbezirke

Tabelle 11.4: Die bevölkerungsreichsten Städte wurden in den Daten unterteilt.

Bezüglich Berlin teilte uns das Büro des Bundeswahlleiters von der Landeswahlleitung Berlins mit (Goderbauer et al., 2018a), dass bei der Einteilung von Bundestagswahlkreisen in der Praxis die bezirksscharfen Wahlkreise für die Wahl zum Berliner Abgeordnetenhaus als Basis herangezogen werden (und nicht Ortsteile o.ä.). Dieser Vorgabe aus der Praxis kommen wir nach.

Melderegisterzahlen an amtliche Statistik anpassen

Den Statistischen Ämtern des Bundes und der Länder liegen Daten der Bevölkerungsfortschreibung auf Grundlage des Zensus 2011 bis zur Verwaltungsebene der Gemeinden in Deutschland vor – jedoch nicht unterhalb der Gemeindeebene. Diese Bevölkerungszahlen werden die *amtlichen Bevölkerungszahlen* genannt. Um in bevölkerungsreicheren Städten und insbesondere in den Bundesländern Berlin, Hamburg und Bremen Wahlkreise einteilen zu können, werden Bevölkerungdaten unterhalb der Gemeindeebene benötigt.

Grundsätzlich weichen die Bevölkerungszahlen der amtlichen Statistik und die der *Melderegister der Städte* voneinander ab. Um diesen Umstand zu bereinigen, ist es in der Praxis üblich, dass die Zahlen des städtischen Melderegisters genutzt werden, um die amtliche Bevölkerungszahl der Stadt anteilig auf die Stadtuntergebiete zu verteilen. Nach unserem Wissen ist nicht vorgeschrieben oder festgehalten, wie genau dies zu tun ist. Bei einer solchen Umrechnung wurden zuletzt bei der Wahlkreiseinteilung für die hessische Landtagswahl 2018 folgenschwere Fehler gemacht (vgl. Frankfurter Allgemeine (2018) und Staatsgerichtshof des Landes Hessen (2018)). Im Folgenden legen wir konkret dar, nach welchem Vorgehen wir Melderegisterzahlen an die amtliche Statistik angepasst haben und schlagen vor, diesen Prozess offiziell festzulegen.

(1) *Melderegisterdaten mit Stichtag 30.09.2017*
Einzelne Städte verfügen nicht über Melderegisterdaten zum Stichtag 30.09.2017, sondern lediglich über welche zu den Stichtagen 30.06.2017 und 31.12.2017. Wenn dies der Fall ist, bilden wir pro Stadtuntergebiet das arithmetische Mittel der Bevölkerungszahlen der beiden vorliegenden Stichtage und verwenden dieses Mittel als Bevölkerungszahl zum Stichtag 30.09.2017. Möglicherweise sind Werte nicht ganzzahlig; dies ist für den nachfolgenden Schritt jedoch nicht problematisch.

(2) *Zielgröße amtliche Bevölkerungszahl*
Ausgehend von Bevölkerungszahlen der Stadtuntergebiete zum Stichtag 30.09.2017 verwenden wir die Divisormethode mit Standardrundung um die Bevölkerung der Untergebiete zu erhalten, die in der Summe der amtlichen Bevölkerungszahl der Stadt entspricht.

11.4.2 Zuteilung der Wahlkreise auf Bundesländer

Das Bundeswahlgesetz sieht die Zuteilung der Wahlkreise auf die Bundesländer mittels der Divisormethode mit Standardrundung vor (§3 Abs. 1 Nr. 2 sowie §6 Abs. 2 Satz 2 bis 7 BWG). Tabellen 11.5 und 11.6 dokumentieren die Verteilung und die dabei zwangsläufig entstehenden Bevölkerungsabweichungen in den Bundesländern.

Im Vorliegen von Regierungsbezirken haben wir in einer weiteren Anwendung der Divisormethode die Wahlkreise auf die Regierungsbezirke verteilt. Es ist möglich, dass Abweichungen die 15%- oder gar 25%-Grenze reißen. Im Fall von dem hessischen Regierungsbezirk Gießen bei Wahlkreisanzahl 200 ist eine zulässige Einteilung von den zwei zugewiesenen Wahlkreisen *nicht* möglich. Somit werden in dem Szenario die Regierungsbezirke Gießen und Kassel gemeinsam betrachtet. Vergleichbares ist in Bayern bei 125 Wahlkreisen vorzufinden.

11.4.3 Auswertung der berechneten Wahlkreiseinteilungen

Im Folgenden werden die berechneten Einteilungen anhand der beiden Zielkriterien administrative Konformität und Bevölkerungsabweichung (vgl. Abschnitt 11.2.2) ausgewertet. Zuvor wird im Vergleich die aktuell geltende Einteilung Deutschlands in 299 Wahlkreise dahingehend begutachtet.

Zu jeder Wahlkreiseinteilung geben wir ein Streudiagramm an. Dabei repräsentiert jeder Punkt in einem Streudiagramm einen Wahlkreis der Einteilung und gibt die betragliche Bevölkerungsabweichung (Abszissenachse) sowie Konformität mit administrativen Grenzen (Ordinatenachse) des Wahlkreises an. Zusätzlich zu einem jeden Streudiagramm wird die Verteilung der Zielausprägungen in zwei Histogrammen ausgewertet.

Vergleichende Auswertung der aktuell geltenden Einteilung in 299 Wahlkreise

In der Auswertung der aktuell geltenden Bundestagswahlkreise (Abb. 11.7) wird deutlich, dass in der Praxis dem Zielkriterium der Einhaltung von administrativen Grenzen deutlich

	Wahlkreisanzahl							
	299		250		248		200	
Bundesland / RB	wk	abw	wk	abw	wk	abw	wk	abw
Schleswig-Holstein	11	−0,9%	9	1,3%	9	0,5%	7	4,2%
Meckl.-Vorpommern	6	5,1%	5	5,5%	5	4,7%	4	5,5%
Hamburg	6	4,5%	5	4,9%	5	4,0%	4	4,9%
Niedersachsen	30	−1,2%	25	−0,8%	25	−1,6%	20	−0,8%
Bremen	2	15,1%	2	−3,8%	2	−4,6%	2	−23,0%
Brandenburg	10	−2,1%	8	2,3%	8	1,5%	7	−6,5%
Sachen-Anhalt	9	−3,6%	7	3,6%	7	2,8%	6	−3,3%
Berlin	12	1,3%	10	1,6%	10	0,8%	8	1,6%
Nordrhein-Westfalen	64	−0,2%	54	−1,1%	53	−0,1%	43	−0,7%
RB Düsseldorf	18	0,5%	16	−5,5%	15	0,0%	12	0,8%
RB Köln	16	−1,6%	13	1,3%	13	0,5%	11	−4,3%
RB Münster	10	−4,0%	8	0,4%	8	−0,4%	6	7,1%
RB Detmold	7	8,3%	6	5,6%	6	4,8%	5	1,4%
RB Arnsberg	13	−1,1%	11	−2,3%	11	−3,1%	9	−4,5%
Sachsen	16	−0,4%	13	2,5%	13	1,6%	11	−3,1%
Hessen	22	−2,2%	18	0,0%	18	−0,8%	14	2,8%
RB Darmstadt	13	1,4%	11	0,2%	11	−0,6%	9	−2,0%
RB Gießen	4	−4,6%	3	6,4%	3	5,5%	~~2~~	~~27,6%~~
RB Kassel	5	−9,5%	4	−5,4%	4	−6,2%	~~3~~	~~0,9%~~
RB Gießen & Kassel	–	–	–	–	–	–	5	11,6%
Thüringen	8	5,1%	7	0,4%	7	−0,4%	6	−6,3%
Rheinland-Pfalz	15	−0,7%	13	−4,2%	12	3,0%	10	−0,4%
Bayern	46	0,9%	39	−0,5%	39	−1,3%	31	0,2%
RB Oberbayern	16	−1,2%	13	1,7%	13	0,8%	11	−3,9%
RB Niederbayern	4	13,7%	4	−4,9%	4	−5,7%	3	1,4%
RB Oberpfalz	4	3,7%	4	−13,3%	4	−14,0%	3	−7,6%
RB Oberfranken	4	1,4%	3	13,0%	3	12,1%	3	−9,6%
RB Mittelfranken	6	3,7%	5	4,0%	5	3,2%	4	4,0%
RB Unterfranken	5	−1,5%	4	2,9%	4	2,1%	3	9,8%
RB Schwaben	7	−4,0%	6	−6,3%	6	−7,1%	4	12,4%
Baden-Württemberg	38	0,7%	32	0,0%	32	−0,8%	25	2,4%
RB Stuttgart	14	0,3%	12	−2,1%	12	−2,9%	9	4,4%
RB Karlsruhe	10	−3,5%	8	0,9%	8	0,1%	7	−7,8%
RB Freiburg	8	−0,2%	7	−4,6%	7	−5,4%	5	6,8%
RB Tübingen	6	9,6%	5	10,0%	5	9,1%	4	10,0%
Saarland	4	−9,0%	3	1,4%	3	0,6%	2	21,7%
Deutschland	299		250		248		200	

Tabelle 11.5: Wahlkreisansprüche (wk) der Bundesländer und deren Regierungsbezirke (RB) sowie dadurch entstehende durchschnittliche Abweichung (abw) von gesamtdeutscher durchschnittlicher Wahlkreisbevölkerung für Wahlkreisanzahlen 299, 250, 248 und 200.

		Wahlkreisanzahl			
		145		125	
Bundesland / RB	Dt.Bev.	wk	abw	wk	abw
Schleswig-Holstein	2.668.573	5	5,8%	5	−8,8%
Meckl.-Vorpommern	1.543.746	3	2,0%	3	−12,1%
Hamburg	1.534.643	3	1,4%	3	−12,6%
Niedersachsen	7.256.379	14	2,7%	12	3,3%
Bremen	563.147	1	11,6%	1	−3,8%
Brandenburg	2.394.787	5	−5,1%	4	2,3%
Sachen-Anhalt	2.122.767	4	5,2%	4	−9,3%
Berlin	2.974.717	6	−1,7%	5	1,6%
Nordrhein-Westfalen	15.627.774	31	−0,1%	26	2,7%
RB Düsseldorf	4.424.694	9	−2,6%	7	8,0%
RB Köln	3.852.775	7	9,1%	7	−6,0%
RB Münster	2.349.929	5	−6,9%	4	0,4%
RB Detmold	1.854.532	4	−8,1%	3	5,6%
RB Arnsberg	3.145.844	6	3,9%	5	7,5%
Sachsen	3.898.328	8	−3,4%	7	−4,9%
Hessen	5.267.135	10	4,4%	9	0,0%
RB Darmstadt	3.225.903	6	6,6%	5	10,2%
RB Gießen	933.875	2	−7,5%	2	−20,2%
RB Kassel	1.107.357	2	9,7%	2	−5,4%
Thüringen	2.056.954	4	1,9%	3	17,1%
Rheinland-Pfalz	3.645.395	7	3,2%	6	3,8%
Bayern	11.358.690	23	−2,1%	19	2,1%
RB Oberbayern	3.867.666	8	−4,2%	6	10,1%
RB Niederbayern	1.112.718	2	10,3%	2	−4,9%
RB Oberpfalz	1.014.600	2	0,5%	2	−13,3%
RB Oberfranken	992.187	2	−1,7%	~~2~~	~~−15,2%~~
RB Mittelfranken	1.521.839	3	0,5%	~~2~~	~~−30,0%~~
RB Ober- und Mittelfranken	2.514.026	–	–	4	7,4%
RB Unterfranken	1.204.659	3	−20,4%	2	2,9%
RB Schwaben	1.645.021	3	8,7%	3	−6,3%
Baden-Württemberg	9.362.146	19	−2,3%	16	0,0%
RB Stuttgart	3.436.715	7	−2,7%	6	−2,1%
RB Karlsruhe	2.362.123	5	−6,4%	4	0,9%
RB Freiburg	1.953.568	4	−3,2%	3	11,3%
RB Tübingen	1.609.740	3	6,3%	3	−8,3%
Saarland	890.308	2	−11,8%	2	−23,9%
Deutschland	73.165.489	145		125	

Tabelle 11.6: (Ergänzung von Tab. 11.5) Aufschlüsselung der deutschen Bevölkerung der Bundesländer und Regierungsbezirke sowie Zuteilung von 145 und 125 Wahlkreisen und dadurch entstehende Bevölkerungsabweichungen.

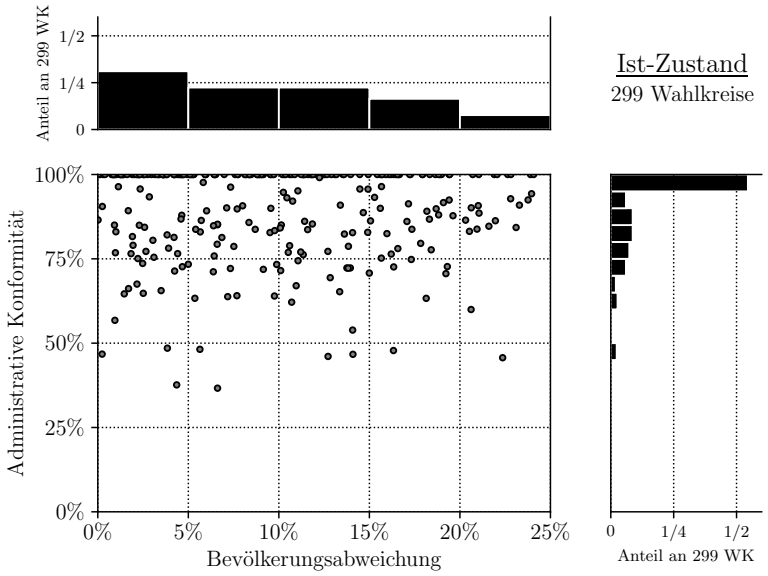
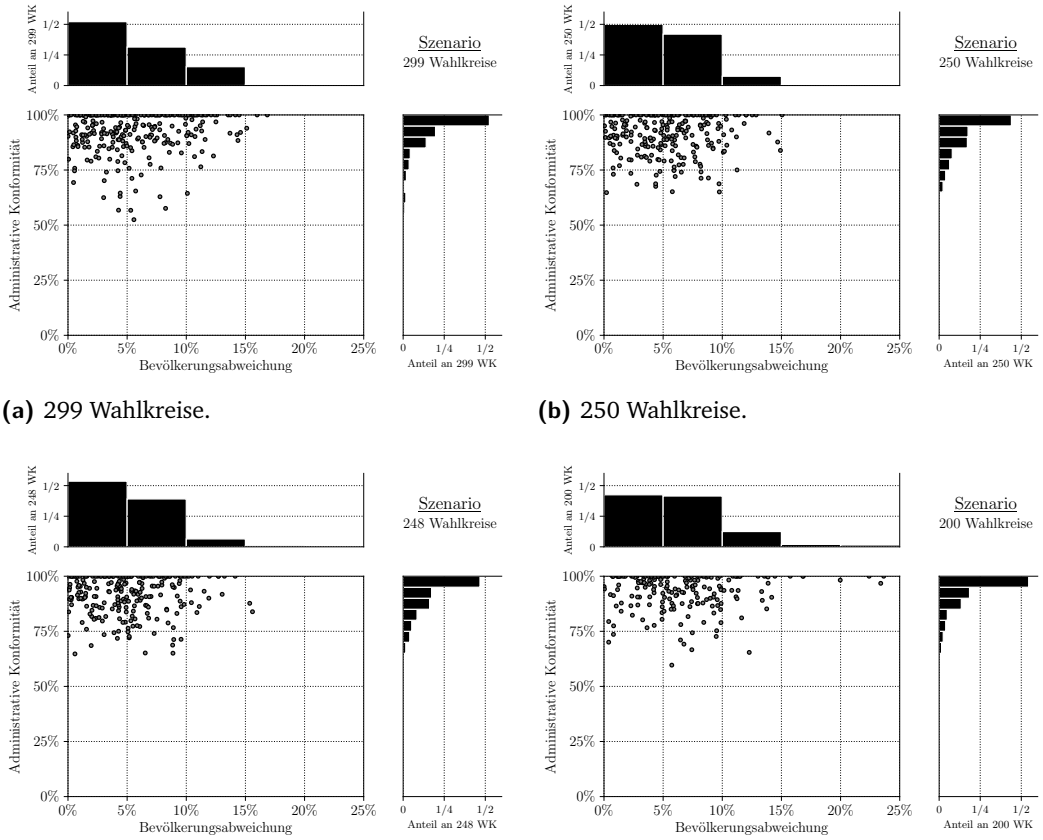


Abbildung 11.7: Ist-Zustand: Auswertung der *aktuell geltenden Einteilung* in 299 Bundestagswahlkreise, die auch Anwendung bei der Bundestagswahl 2017 fand.

mehr Gewicht zugesprochen wird als einer Minimierung der Bevölkerungsabweichung (vgl. auch Goderbauer und Wicke (2017)). Es liegt für über der Hälfte der Wahlkreise eine vollständige (oder nahezu vollständige) Übereinstimmung mit den Grenzen der Kreise und kreisfreien Städte vor. Im Gegensatz dazu sind die Ausprägungen der Bevölkerungsabweichungen über das gesamte Zulässigkeitsintervall $[-25\%, 25\%]$ verteilt. Anhand der Verteilung der Abweichungen ist nicht eindeutig zu verifizieren, dass im Wahlgesetz die Sollgrenze von 15% gefordert wird.

Einerwahlkreise

299 Wahlkreise Die Auswertung der optimierungsbasierten Einteilung in 299 Wahlkreise (Abb. 11.8a) beweist, dass durch die Anwendung von Mathematik eine 299er Einteilung möglich ist, die das hohe Maß an administrativer Konformität gleichermaßen wie die geltende Einteilung (vgl. Abb. 11.7) vorweist, jedoch bezüglich der Wahlkreisbevölkerung sehr viel ausgeglichener ist. Mehr als die Hälfte der Bundestagswahlkreise weicht weniger als 5% von der durchschnittlichen Bevölkerungszahl eines Wahlkreises ab. Mehr als $4/5$ der 299 Wahlkreise halten eine 10%-Schranke ein. Lediglich drei Wahlkreise weichen über 15% und um bis zu 17% vom Durchschnitt ab. Diese sind: (1) Einer der zwei Wahlkreise in Bremen; das Reißen der 15%-Sollabweichungsgrenze ist hier jedoch durch die Zuteilung auf die Bundesländer erzwungen (vgl. Tabelle 11.5). Beide Bremer Wahlkreise halten dafür perfekt die angestrebten Grenzen der Stadt- und Ortsteile ein. (2) Ein Wahlkreis im bayrischen Regierungsbezirk Niederbayern weicht $15{,}1\%$ vom Durchschnitt ab, wobei eine regierungsbezirksscharfe Einteilung hier schon eine Abweichung von $13{,}7\%$ erzwingt (vgl. Tabelle 11.5). (3) Ein Wahlkreis in Nordrhein-Westfalen, der genau aus der kreisfreien Stadt Bielefeld besteht und somit perfekte administrative Konformität vorweist, umfasst $16{,}8\%$ mehr Bevölkerung als ein Durchschnittswahlkreis.



(a) 299 Wahlkreise.

(b) 250 Wahlkreise.

(c) 248 Wahlkreise.

(d) 200 Wahlkreise.

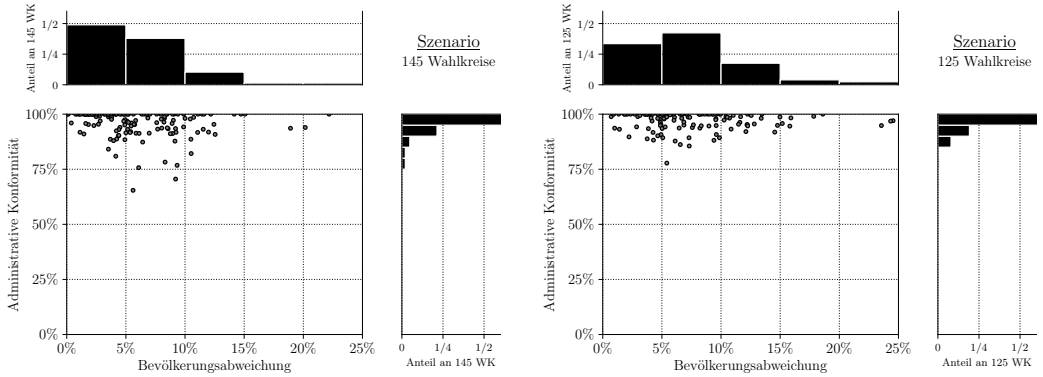
Abbildung 11.8: Auswertung der berechneten Einteilungen in 299, 250, 248 bzw. 200 Wahlkreise.

250 und 248 Wahlkreise Berechnete Einteilungen in 250 und 248 Wahlkreise werden in Abbildungen 11.8b und 11.8c ausgewertet. Das Erscheinungsbild ist ähnlich: Größtenteils hohe bis perfekte administrative Konformität und überwiegend Bevölkerungsabweichungen unter 10%. Die Ergebnisse in den Szenarien 250 und 248 sind ähnlich, da sich die Einteilungsaufgaben nur in der Wahlkreisanzahl des Regierungsbezirks Düsseldorf und Bundeslandes Rheinland-Pfalz sowie in der durchschnittlichen Wahlkreisbevölkerung unterscheiden. Die zwei Wahlkreise mit über 15% betraglicher Abweichung im Szenario 248 Wahlkreise liegen im bayrischen Regierungsbezirk Oberpfalz, der mit einer durchschnittlichen Abweichung von -14% aus der Zuteilung der Wahlkreise hervorgeht.

200 Wahlkreise Abbildung 11.8d zeigt die Auswertung der berechneten Einteilung in 200 Wahlkreise. Das Vorliegen von vier Wahlkreise mit über 20% Bevölkerungsabweichung ist der Verteilung der Wahlkreise auf die Bundesländer geschuldet. Im Saarland bzw. Bremen ist es nicht möglich, Wahlkreise mit durchschnittlich besseren Abweichungswerten als $21{,}7\%$ bzw. -23% einzuteilen (vgl. Tabelle 11.5).

Zweierwahlkreise

145 und 125 Wahlkreise Die berechneten Einteilungen in 145 sowie 125 Wahlkreise werden in Abbildung 11.9 anhand der Zielkriterien ausgewertet. Die administrativen Grenzen der u.a. Kreise und kreisfreien Städten werden in der berechneten Einteilung überaus gut beachtet. Die in wenigen Fällen vorliegenden extremen Bevölkerungsabweichungen sind der Verteilung der Wahlkreise auf die Bundesländer bzw. Regierungsbezirke geschuldet (vgl. dazu Tabelle 11.6).



(a) 145 Wahlkreise. **(b)** 125 Wahlkreise.

Abbildung 11.9: Auswertung der berechneten Einteilungen in 145 bzw. 125 Wahlkreise.

11.5 Mehr Transparenz in der Debatte durch Mathematik

Die Mathematik bietet nicht nur Objektivität in Folge transparenter Modelle und Methoden, sondern gleichzeitig auch das Handwerkszeug um praxisrelevante Lösungsalternativen für komplexe (Planungs-)Probleme zu liefern. Dies beinhaltet insbesondere die Möglichkeit, die mathematische Optimierung entscheidungs*unterstützend* einzusetzen. Dabei kann die Entscheidungsmacht bei den zuständigen Personen bzw. Gremien verbleiben und optimierungsbasiert berechnete Lösungen können als objektive Diskussionsgrundlage unterstützend zur Hilfe genommen werden.

In dem vorliegenden Artikel wurden Wahlkreiseinteilungen für die Deutsche Bundestagswahl vorgestellt, die mit objektiven Methoden der mathematischen Optimierung unter Verwendung von aktuellen und detaillierten Daten berechnet wurden. Die dabei zugrundeliegenden Bedingungen zur Charakterisierung von zulässigen Wahlkreisen sowie Zielkriterien zur Definition der Optimierungsrichtung wurden transparent aus den rechtlichen Vorgaben gefolgert. Die Ergebnisse dieses Artikels basieren zum Teil auf für den Bundeswahlleiter im Rahmen der Debatte einer Wahlrechtsreform durchgeführten Studien (Goderbauer et al., 2018a,b).

Die Flexibilität der angewandten Optimierungsmethoden ermöglicht es, falls gewünscht, die Gewichtung der konkurrierenden Einteilungsziele z.B. zugunsten der Einhaltung von administrativen Grenzen zu verschieben und auf dieser Basis weitere Berechnungen durchzuführen.

Falls, wie z.B. bei der alljährlichen Revision der Wahlkreise vor einer Wahl, eine Einteilung vorliegt, kann auch die Zielvorgabe der Wahlkreiskontinuität (vgl. Abschnitt 11.2.1) in die Optimierung einbezogen werden. Die Kontinuität einer Wahlkreiseinteilung kann an dem Anteil der „umgesetzten“ bzw. neu zugeordneten Bevölkerung gemessen werden. Eine Verschiebung der Präferenzen zwischen den Einteilungszielen modifiziert die Zielfunktion des Optimierungsproblems. Dementsprechend ändert sich die numerische Bewertung der Einteilungen und ggf. auch optimale Lösungen. Die strikt zu erfüllenden Bedingungen bleiben davon natürlich unberührt. Es ist auch möglich zusätzliche Bedingungen hinzuzufügen, wie z.B. die strengeren von der europäischen Venedig-Kommission (2002) geforderten Bevölkerungsschranken von maximal 10% bzw. 15% Abweichung vom Durchschnitt.
Für die Entscheidungsfindung bei der Wahlkreiseinteilung können berechnete Lösungen in einer interaktiven Software (vgl. Abb. 11.3) studiert werden und bei Bedarf per Mausklick einzelne Gemeinden oder Stadtteile umgesetzt werden. Die Prüfung auf Zulässigkeit sowie Auswertungen der Zielkriterien erfolgt unmittelbar. Die nutzende Person behält weiterhin sämtliche Entscheidungsmacht.

Zusätzlich zu der Anwendung der mathematischen Einteilungsmethodik und Auswertung der Ergebnisse liefert der vorliegende Artikel einen weiteren Beitrag für die Debatte, in der eine Reduktion der Bundestagswahlkreise diskutiert wird. Es wird eine numerische und auf Gesetzesgrundsätze stützende Argumentationslinie vorgestellt, die zu favorisierende als auch unzulässige Anzahlen an Bundestagswahlkreisen hervorbringt. Dabei zeigte sich, dass die genaue Wahl einer Wahlkreisanzahl nicht unerheblich ist und z.T. sogar filigran getroffen werden sollte. Das Intervall an umsetzbaren Anzahlen für die Anwendung von Zweierwahlkreisen stellte sich als besonders limitiert heraus.

Die dargestellte Bestimmung von geeigneten Wahlkreisanzahlen für Deutschland kann noch erweitert werden. Auf der einen Seite können zeitliche Entwicklungen der Bevölkerungsverteilung berücksichtigt werden, um nicht nur eine für den Status quo passende Anzahl zu erhalten, sondern ggf. auch eine in der Zukunft stabile Wahlkreiszuteilung auf die Bundesländer zu ermöglichen. Auf der anderen Seite können, falls von Seiten der Praxis weiterhin gewünscht, auch die auf der Ebene der Regierungsbezirke entstehenden Bevölkerungsabweichungen mit in die Analyse einbezogen werden.

Wir sind davon überzeugt, dass, falls die Anzahl der Bundestagswahlkreise angepasst wird, die Wahl der Anzahl fundiert zu treffen ist. Bezogen auf die Einteilung der Wahlkreise und dem zugehörigen Entscheidungsprozess sind wir der festen Ansicht, dass die Mathematik und insbesondere ihr Teilgebiet der mathematischen Optimierung praxisnahe Entscheidungsunterstützung für eine objektive Wahlkreisreform bieten kann.

12 Concluding Remarks

The contribution of this thesis to optimal political (re)districting and decision support according to legal and judicial requirements is summarized in the following. Future research perspectives are also outlined.

To summarize briefly With a focus on elections in Germany, the political districting problem is studied: Starting from legal texts and their interpretation in practice, leading to a mathematization of the German political districting problem, optimization-based solution methods and a geovisual decision support system are developed, both of which are equipped with a comprehensive collection of data. The research makes it possible to deliver practically relevant solutions and thereby to offer objective decision support with a transparent approach not only in politically sensitive issues.

Towards optimization-based decision support

Based on a unified mathematical definition of the political districting problem (Sec. 8.2.1 and 8.2.2), the problem's computational complexity is analyzed (Sec. 8.2.3). A comprehensive literature survey on proposed solution approaches (Sec. 8.4) is presented. The review contains models and optimization-based methods from the early 1960s to recent years (cf. Fig. 8.4). In addition, available software tools are gathered (Sec. 8.4.2). These includes implementations that have emerged from science, as well as tools offered by professional software companies.

In order to obtain a suitable formalization of the German problem, the electoral law and jurisdictions are studied (e.g., Sec. 7.2). Furthermore, a detailed numerical evaluation of electoral districts applied in the last German elections is conducted (Sec. 7.3 and 7.4). It is analyzed how the legal requirements on German electoral districts are implemented in practice. Based on that, numerical measures are defined which quantify the observance of districting criteria.

The applicability of approaches mentioned in the literature to the German variant is discussed and examined (Sec. 8.5). Thus, open research topics have been identified: The German version of the considered problem is not yet fully covered by the literature.

A MILP formulation is developed that meet all German requirements and criteria (Sec. 9.4.1). Additionally, it is the very first time that actually well-known a,b-separator inequalities are applied in political districting as connectivity model. Based on the proposed MILP, start

and improvement heuristics are developed (Sec. 9.4.3). All research carried out is packed into a ready-to-use decision support system (Sec. 9.5). The scope of the features of the software covers interactive visualization and descriptive analytics as well as the ability to automatically determine optimally adjusted electoral districts. The software tool is designed to offer the user the best possible support during the regular revision of districting plans.

Furthermore, a link between apportionment methods and the political districting problem is studied and extended (Chapter 10). A generalization of well-studied apportionment methods is developed and first efforts have been made to apply these in the districting process. This leads to a primal heuristic specific to the German version of administrative conformity (Sec. 10.4). These preliminary approaches look promising for further research.

Further research perspectives

The underlying problem of partitioning a territory into connected subareas is not only relevant in an electoral context as studied in this thesis. Other applications have been identified in geography (Duque et al., 2018; Jafari and Hearne, 2013), medicine/healthcare (Kong et al., 2010; Lin et al., 2018), sales (Haase and Müller, 2014), and police control (Chen et al., 2018). A recent survey on the districting problem is provided by Kalcsics (2015). In addition to application-specific conditions and criteria, districts need to be connected. This calls for a general framework able to cover most applications. We are working on such a customizable framework with a standardized solution strategy based on a branch-and-price approach (Krott, 2018; Krott, Goderbauer, et al., 2019). The connectivity of the determined subgraphs is ensured by the framework. Custom objectives or conditions on the districts can be added.

The connectivity model used in this thesis is based on separator inequalities (cf. Sec. 9.4.1.1). As outlined in the mentioned section, a lot more models are proposed to ensure connected subgraphs. A comprehensive computational study to compare connectivity models on the studied political districting problem can be performed. It would be interesting to investigate whether the theoretical advantages of the model used (no additional variables needed, facet defining property, cf. Sec. 9.4.1.1) are also computationally verifiable.

When evaluating alternative connectivity models, a special focus should be set on the one given by Williams (2002a,b) and Validi and Buchanan (2018). The proposed connectivity model is applicable on planar graphs. It may be worth exploiting this property. Can the German criterion of administrative conformity be implemented using the primal/dual scheme of planar graphs (Williams, 2002b)?

Independent of this, general research needs to be done on the implementation of administrative conformity (cf. Sec. 9.4.1.2). The computational studies conducted in this thesis illustrate that the slow improvement of the dual bound is due to the objective function of administrative conformity. Can the formulation be strengthened?

The developed MILP formulation is based on assignment variables $X_{i\ell} \in \{0, 1\}$ (Sec. 9.4.1). For most combinations of unit $i \in V$ and electoral district $\ell \in [k]$ its variable $X_{i\ell}$ equals zero

in feasible solutions. Preliminary studies showed that a domain reduction of the assignment variables is effective, i.e., not all variables are considered in the model anymore. One should research on the best approach to thinning out these variables. For the sake of exactness, the domain can possibly be adjusted during the solving process.

The heuristic approach outlined on the basis of proportional apportionment for connected coalitions (Sec. 10.4) can be further explored. It may even be possible to convert the procedure into an exact solution method. Instead of apportioning the electoral districts among connected coalitions of rural/urban districts only once, we consider all feasible connected coalitions. Assuming an optimal political districting of each connected coalition, i.e., subproblem, an optimal selection of connected coalition partitioning the initial contiguity graph can be performed via a set partitioning problem. This approach may be implemented in the from of a column generation and branch-and-price procedure.

Efforts to reform the electoral law of Germany

After the German federal elections of 2017, the president of the parliament, Wolfgang Schäuble, convened a cross-party working group to develop a reform of the electoral law. This reform has become necessary because the parliament seems to be growing in size with each election. This weakness of the German electoral system needs to be addressed.

As documented in Chapter 11, the research in this theses contributed to the official debate. On behalf of the Federal Returning Officer, we apply solution methods and software presented in Chapter 9 to compute new electoral districts for Germany. To achieve this goal, a comprehensive collection of geographical and demographic data was created (Section 11.4.1). Based on the districting plans we provided, the working group discussed various reform scenarios.

> *Die optimierungsbasierten Wahlkreiseinteilungen von Herrn Goderbauer und seinem Team sind ein essentieller Bestandteil der bisherigen Bemühungen um eine Wahlrechtsreform gewesen. Die gelieferten Einteilungen konnten unmittelbar für die Diskussion verwendet werden.*
>
> **— Dr. Georg Thiel, Bundeswahlleiter**
> (Federal Returning Officer of Germany)

In April 2019, few days before the submission of this dissertation, it became known that the efforts of the non-public parliamentary working group had ended without any result (Funk, 2019). The political factions could not agree on a reform option. The views of what a reform should look like were contradictory. In addition to a change in the number of electoral districts, discussions also focused on amendments in the way votes are converted into representatives. A modified calculation of overhang mandates and clearing mandates was also debated. However, all participants agreed that an adjustment of the electoral law is still necessary and has to be performed as soon as possible.

In the end, decisions about the electoral system are of highly political nature. In such a deadlocked situation, however, the theory of mathematical optimization can provide the following simple advice: If a problem does not contain any feasible solution, constraints must be relaxed to obtain feasibility.

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