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Computational Optimization for Solving Complex Location Problems

(Collection of thematically cohesive articles and studies)

Doctoral dissertation

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1 Computational Optimization in Location Analysis

1.1 Introduction

Facility location decisions play a crucial role in strategic management for the organizations in both private and public sectors (Ghosh & Craig, 1983; Owen & Daskin, 1998; Schilling, 1982). Location analysis (or location science) supports businesses in making informed decisions about where best to locate their facilities. It is essential in such areas as supply chain management (Melo et al., 2009), chain store development (Gonzalez-Benito et al., 2005; Karande & Lombard, 2005) or market entry decisions (Arnold & Narang Luthra, 2000). Good location can help companies achieve sustainable competitive advantage by providing access to necessary resources and talent pools, and the proximity to key markets. This, in turn, can lead to cost reduction and improvements in flexibility and responsiveness. It can fuel innovation and provide opportunities for brand differentiation. When it comes to operations management, location is key for lowering transportation costs and supporting supply chain management.

Although the classical approach to management, with its focus solely on efficiency and scientific method, is considered a relic of the past, its legacy is still alive and relevant in many successful organizations of today. A never-ceasing need for efficiency and effectiveness drives companies to make use of scientific tools and technologies, which in turn allow them to make smarter, faster decisions, especially in a competitive environment. In today's data-driven world, companies must compete at the highest level of decision analysis, frequently called *prescriptive analytics*, which uses advanced tools and technologies to recommend the best actions to be taken, with a deep understanding of risks, restrictions, and opportunities. Finding optimal solutions to problems within specific constraints facilitates the decision-making process at all levels of management and frequently determines obtaining and maintaining competitive edge. By their nature, these methods are quantitative and, frequently, highly complex. Being able to apply them effectively however, has become essential for many organizations.

In their raw form, many location problems are overly complex. Therefore, to be able to provide mathematically-justified solutions, feasible computational implementation and usable managerial insights, many location problems are often articulated in their simplified form. However, such a pragmatic approach also has its pitfalls as it has led to less desirable and sometimes impractical outcome solutions in a number of managerially-relevant use cases. In an attempt to rectify some of these weaknesses, this dissertation proposes several new methods in a collection of five journal articles.

The proposed methods utilize recent developments in solving techniques, emergence of powerful optimization software, as well as the advances in high-performance computing. Each of the included articles introduces an original solution and makes useful contributions to the field of management science. Extensive experiments are run to demonstrate the results of each proposed approach. The introduced methods strive to close the gap that emerged from the limitations of the existing approaches which provide insufficient managerial insights in support of the decision-making process related to facility location.

Location analysis falls under the discipline of management science. The definition of management science, also referred to as operations research or decision science, states that it is "an approach to decision-making based on the scientific method" (Anderson et al., 2000). The opening of the discipline of management science is attributed to Frederic W. Taylor (1856–1915), who in the 1880s began promoting the use of quantitative methods in management and introduced the *theory of scientific management* (Taylor, 1911). Despite the fact that it has been vastly criticized for its disregard for a human factor and focus only on increasing productivity, this classical approach to management laid grounds for the development of many useful methods supporting the decision-making process. Stemming from the need for a more scientific approach, location analysis has been supplying both theory and practice of management science with a wide range of valuable decision-making tools. Although it has theoretical roots in mathematics, economics, geography, and computer science, one of its major functions is managerial decision support on both strategic and operational levels. Its many applications stem from high practicality of location problems, which is also the reason why they draw a lot of attention from the industry, the military, and government agencies. Sample applications of facility location include locating bank branches, chain stores or logistics parks, designing hospital layouts, conducting a sustainable forest management or wildfire prevention, or locating pipe leak sensors.

A facility location problem is at the core of location analysis. It is an optimization problem which involves finding an optimal location for a facility, or multiple facilities, to serve the existing requirements. Different decision-makers' objectives determine the constraints and the optimality criteria.

Computational optimization constitutes an overarching, generic method utilized in this dissertation. It consists of other well established methods, such as mathematical modeling, data analysis, linear and non-linear optimization, and simulation.

Note that in this dissertation, the term "method" is more general than the term "technique". Methods can comprise other methods as well as various techniques, e.g., non-linear formulations or re-formulations, mixed integer programming (MIP), etc. Techniques, in turn, can involve a variety of tools and technologies, such as mathematical models, optimization methods, software or hardware.

The five journal articles included in this dissertation are the fruit of scholarly work produced by the candidate since 2019. The journals that became outlets for the included publications are all peer-revived and highly ranked in the field of management science and operations research. In Poland, all these journals have been classified as relevant to the discipline of *management and quality studies* (Instytut Rozwoju Szkolnictwa Wyższego, 2024).

Included articles are thematically cohesive, not only when it comes to the field of study that bonds them together, i.e., location analysis, but also through the type of methods they propose to close research gaps that emerged from the limitations of the existing solution techniques. The articles are interconnected in multiple ways. Figure 1.1 depicts these connections. *Computational Optimization for Facility Location* at the center of the graph represents the overarching, generic method, encompassing all individual areas of focus. These five focus areas, represented as light-gray disks, are *Carpooling*, *Hub Location in Carpooling*, *Restricted Obnoxious Facility Location*, *Competitive Facility Location*, and *Multi-purpose Competitive Facility Location*. In carpooling, computational optimization methods enable solving the non-linear carpooling problem that involves hub locations (Miklas-Kalczynska & Kalczynski, 2021). In restricted obnoxious facility location, these methods allow for a more practical representation of protected areas (Miklas-Kalczynska & Kalczynski, 2024). Furthermore, computational optimization methods make it possible for a trajectory method to be added to a set of available solution techniques for unconstrained problems (Z. Drezner & Miklas-Kalczynska, 2023). Finally, in competitive facility location, these methods facilitate locating multiple chain facilities by considering multi-purpose customer behavior. The techniques utilized in the dissertation papers, shown on the graph as oval shapes, along with the common field of study (location analysis), bond the papers together and create a cohesive structure.

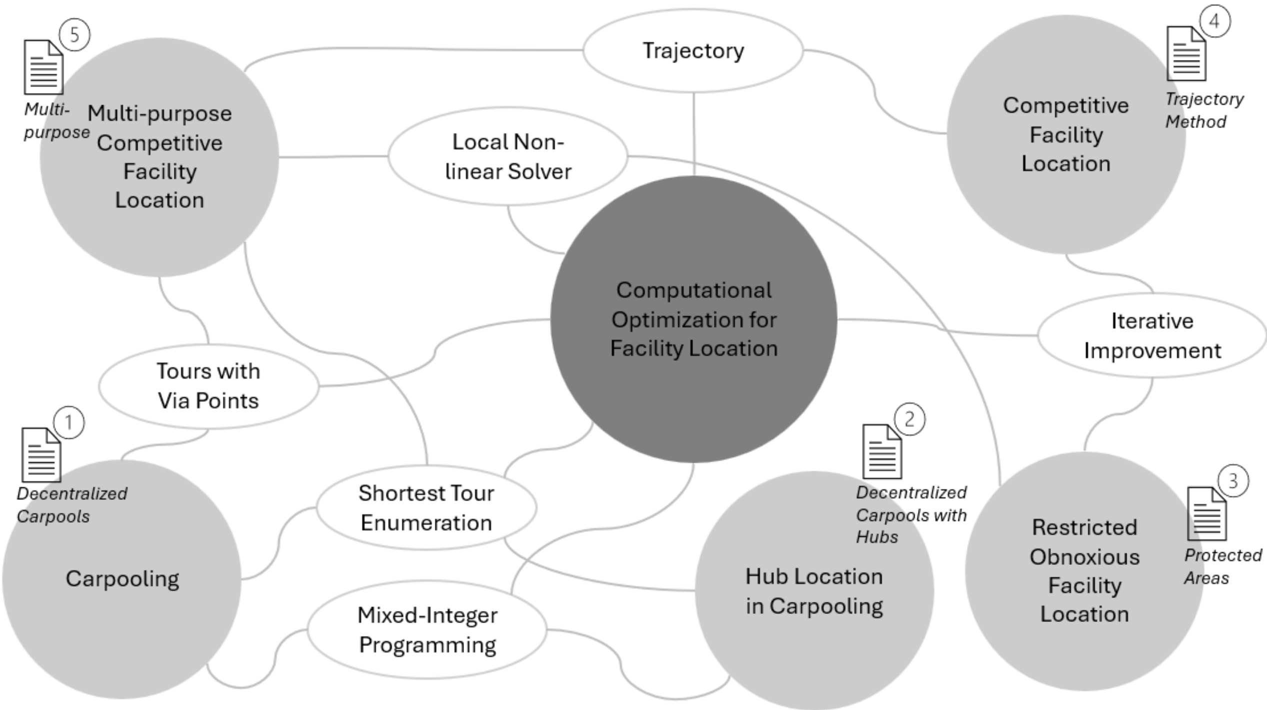

Figure 1.1: Connections between key dissertation concepts and research approaches, along with the corresponding research papers.

The first contribution of this dissertation, covered in the first two papers in the collection, (1) "A decentralized solution to the carpooling problem" (Kalczynski & Miklas-Kalczynska, 2019) and (2) "Self-organized Carpools with Meeting Points" (Miklas-Kalczynska & Kalczynski, 2021), deals with carpooling. Carpooling is one of the forms of a more general phenomenon, called ride-sharing. It differs from public transportation, in that people make long-term arrangements to commute together using their private vehicles. This sequence of papers investigates the benefits of two different carpool organization methods: centralized and self-organized. It explores the recent issue of low carpool participation rates, observable world-wide despite a global push towards lowering traffic congestion and fuel emissions. From the managerial standpoint, carpooling can reduce the need for parking space, increase employee productivity and improve morale. It can also be a source of financial and tax benefits for the companies (Shaheen et al., 2024).

The next area of focus, and the subject of the third paper in the collection, (3) "Multiple Obnoxious Facility Location - the Case of Protected Areas" (Miklas-Kalczynska & Kalczynski, 2024), is the problem of obnoxious facilities, i.e., the facilities that, although needed, are usually not wanted in proximity of *sensitive regions*, such as neighborhoods or recreational areas. A wind turbine or a power plant is not a welcome site when it is located too close to one's home or a vacation spot. Organizations that need to locate such facilities, are interested in building good models that help them avoid potential legal issues and bad optics when it comes to customer relations. Motivated by the shortcomings of the existing solutions, the paper proposes a new method for locating obnoxious facilities that takes into account the actual boundary of a sensitive area and not just its simplified point-based representation.

Another contribution of this dissertation is the trajectory principle, which is a technique that can be used to solve complex, non-linear unconstrained optimization problems, with a guarantee of optimality in case of convex problems. The fourth dissertation paper, (4) "Solving Non-Linear Optimization Problems by a Trajectory Approach" (Z. Drezner & Miklas-Kalczynska, 2023) utilizes recent computational optimization developments to propose new models that enable the trajectory principle to be applied to support the managerial decision-making process in facility location and other fields, supplementing the existing optimization toolkit.

The final contribution of this dissertation, presented in the fifth paper, (5) "Extensions to Competitive Facility Location with Multi-purpose Trips" (Miklas-Kalczynska, 2024), focuses on locating a new chain facility or facilities in a way that captures maximum market share, while taking into account multi-purpose customer behavior. Customers sometimes decide to make multiple stops to purchase various goods or services, instead of traveling to just one place, which adds a new dimension into the optimization process. Due to high mathematical complexity, earlier multi-purpose models limit the number of purposes to two. The paper proposes an extension that eliminates this restriction and enables maximizing the market share captured by the chain.

Table 1.1 shows the connections between the focus areas and the techniques, along with the related managerial insights. All focus areas as well as all the techniques depicted in Figure 1.1 and Table 1.1 are covered in more detail in the subsequent sections.

Four of the articles included in this dissertation were written in collaboration with another (single) co-author, which is common practice in the field of management science. The candidate's involvement in each of these articles was substantial, as detailed below. The last (and

Table 1.1: Connections between key dissertation concepts and research approaches, along with the corresponding managerial insights.

Focus area	Managerial insights	Methods and techniques					
		Computational optimization for facility location					
		Tours with via points	Shortest tour enumeration	Mixed-integer programming	Local non-linear solver	Trajectory	Iterative improvement
Carpooling	Organization's employee carpooling strategy support: - Increased productivity and morale - Financial and tax benefits (incentives) - Satisfied local zoning/emission requirements - Reduced employee parking costs	X	X	X			
Hub location in carpooling			X	X			
Restricted obnoxious facility location	Operational- and tactical- level decision support (obnoxious facilities): - Adherence to local policies and regulations - Improved public relations				X		X
Competitive facility location	Strategic-level decision support (retail facilities): - Support for location assessment teams - Objective analysis supporting intuition and field visits					X	X
Multi-purpose competitive facility location		X	X		X	X	

the most recent) paper is the candidate's single-authorship work.

In particular, the candidate's contributions to the co-authored scholarly output presented in this dissertation are as follows:

- The decentralized carpooling paper (Kalczynski & Miklas-Kalczynska, 2019): conceptualization and literature review, investigation and formal analysis, method development and modeling, analysis of the results and validation, interpretation of the results and formulation of conclusions, preparation and editing of the manuscript

- The carpooling with hubs paper (Miklas-Kalczynska & Kalczynski, 2021): conceptualization and literature review, investigation and formal analysis, method development and modeling, computational optimization, analysis of the results and validation, interpretation of the results and formulation of conclusions, preparation and editing of the manuscript

- The protected areas paper (Miklas-Kalczynska & Kalczynski, 2024): conceptualization and literature review, investigation and formal analysis (including running experiments), method development and modeling, analysis of the results and validation, interpretation of the results and formulation of conclusions, preparation and editing of the manuscript

- The trajectory approach paper (Z. Drezner & Miklas-Kalczynska, 2023): investigation and formal analysis (including running experiments), computational optimization, analysis of the results and validation, interpretation of the results and formulation of conclusions, generating graphs for the manuscript

- The multi-purpose shopping paper (Miklas-Kalczynska, 2024) is a single-authorship paper.

1.2 Research Problem

Location analysis has applications in many fields, such as production, transportation, logistics, routing, and telecommunications, to name a few. From the managerial perspective, beginning in the 1990s, the increasing complexity of business environment and rapid developments in information technology reintroduced the concept of the scientific method and mathematical modeling into the decision making process. Managerial activities became increasingly complex and the dynamic nature of the business environment put pressure on the decision makers to make the right decisions to avoid heavy losses. When it comes to new store location decisions, for example, the quantitative approach turned out to be indispensable in support of the traditional qualitative method, as making decisions based solely on experience or intuition proved too risky (Curry & Moutinho, 1992; Reynolds & Wood, 2010). Using the scientific process in decision making allows managers to state their objectives in an explicit and unambiguous way. It can also improve the effectiveness of their decisions. In the past decade, it became apparent that businesses must reevaluate and reshape their strategy and business model as data-driven decision making needs to be introduced into all levels of management. It became a widespread opinion that analytics must become an integral part of the organizational culture. It needs to be promoted by the decision makers and adopted by all employees (Bumblauskas et al., 2017; Carillo et al., 2019; Chatterjee et al., 2024; Müller & Jensen, 2017).

And so, although its beginnings are traced to purely mathematical problems, over time location science transformed into an important managerial tool, especially supporting long-term decision-making and allowing companies to obtain and sustain competitive advantage. Beginning with a French mathematician Pierre de Fermat (1607-1665) in the seventeenth century, the field of location analysis has been developing steadily until this day. A thorough review of the discipline can be found in (Laporte et al., 2019) or (Marianov & Eiselt, 2024) for example.

In his letter to the Italian scientist Evangelista Torricelli (1608-1647), Fermat described a purely theoretical problem of finding a point in a triangle, such that the sum of distances between this new point and the three vertices is the smallest. This seemingly simple question attracted much discussion among the researchers of the time. It was eventually solved by Torricelli. In geometry this problem is still known as the *Fermat's problem*, sometimes also called the *geometric median*. It became the foundation of many location problems.

Applying location analysis to the business-related decision-making for the first time is attributed to Johann Heinrich von Thünen (1783-1850), a German agriculturalist whose work proved crucial to the development of econometrics. His *theory of land use*, also known as the *ring theory*, investigated the relationship between the volume of agricultural production and the distance to the markets.

In today's business world, determining a location of a facility remains one of the most important types of strategic decisions managers have to make, whether it is production, distribution and storage, or delivering goods or services to the consumers. Any mistakes made in locating a facility are extremely difficult and costly, if not impossible, to correct. On the other hand, a good location can help a company get ahead of the competition and obtain considerable savings.

Whether concerning the corporate or the public sector, facility location problems can have a variety of different research objectives which determine the constraints and the optimality criteria. The goals of the decision makers may be very different, depending on the problem type, such as minimizing travel distance, attracting customers in an area, placing a facility of strategic importance, or ensuring service coverage. The below description of the key concepts of the field is not exhaustive, but limited to the issues that provide background to the content of this dissertation.

Fermat's problem was placed in the context of a market for the first time by a German scientist Alfred Weber (1868 – 1958) (Weber, 1909), alongside the concepts of supply, demand, and transportation cost. Weber constructed an example which became one of the classical problems in the field of location analysis, known as the *location triangle* or simply, the *Weber problem*. In this first prescriptive rather than descriptive location model, a factory acquires raw materials from two sources and delivers a final product to the market. Optimal location for the factory needs to be found with the goal of minimizing total transportation cost. The Weber problem has been researched and expanded on extensively over the years (Church, 2019; Church et al., 2022; Z. Drezner, 2024; Kalczynski & Drezner, 2024). In its original form, it minimizes the sum of weighted Euclidean distances, with the transportation costs as weights.

A Hungarian mathematician Endre Weiszfeld (1916–2003) was the first one to propose the solution algorithm to the Weber problem for more than the original three points (Weiszfeld, 1937), which later led to numerous further extensions, including the one proposed in the trajectory paper, which is part of this dissertation (Z. Drezner & Miklas-Kalczynska, 2023).

It is said that location science became a full-fledged scientific discipline in the 1960s, when the Weber problem was extended to include multiple facilities and the p-median problem was formulated by an Iranian-American mathematician L.H. Hakimi (Hakimi, 1964). The p-median problem became another fundamental problem in the field inspiring many further studies (Daskin & Maass, 2015; Mladenović et al., 2007). The objective of the p-median problem is to minimize the sum of weighted distances between each demand point and its closest facility. Finding a solution to this problem typically involves solving the Weber problem iteratively.

Apart from the p-median problem (minisum), among the core formulations originating from the Weber problem are the p-center problem (minimax), and the covering problem. The p-center problem, which is a minimax problem, minimizes the maximum distance between a demand point and its nearest facility. In a covering problem customers can be served by their closest facilities only when they are within a certain distance to them.

Going beyond the core location concepts, we can distinguish further, more contemporary extensions of location models. They include, but are not limited to, hub location, competitive, obnoxious, restricted and stochastic facility location. Hub location problems locate hub facilities with the goal of reducing the network's complexity, and thus, the total cost of the network. Competitive facility location assumes the existence of the competing facilities on the market. The goal is to maximize the market share. Obnoxious facility location deals with locating the facilities that produce nuisance and wants to minimize their impact. Restricted facility location assumes the existence of forbidden regions or barriers, while stochastic facility location considers uncertainty in location models.

Figure 1.2 depicts a general classification of the facility location problems based on (Fischer, 2011). The scope of this dissertation is restricted to the following specific facility location areas: hub location in carpooling, the Weber problem, competitive facility location, obnoxious facility location, restricted facility location, multipurpose trips in competitive facility location. The key concepts of these areas are presented below, with the scope of this dissertation emphasized.

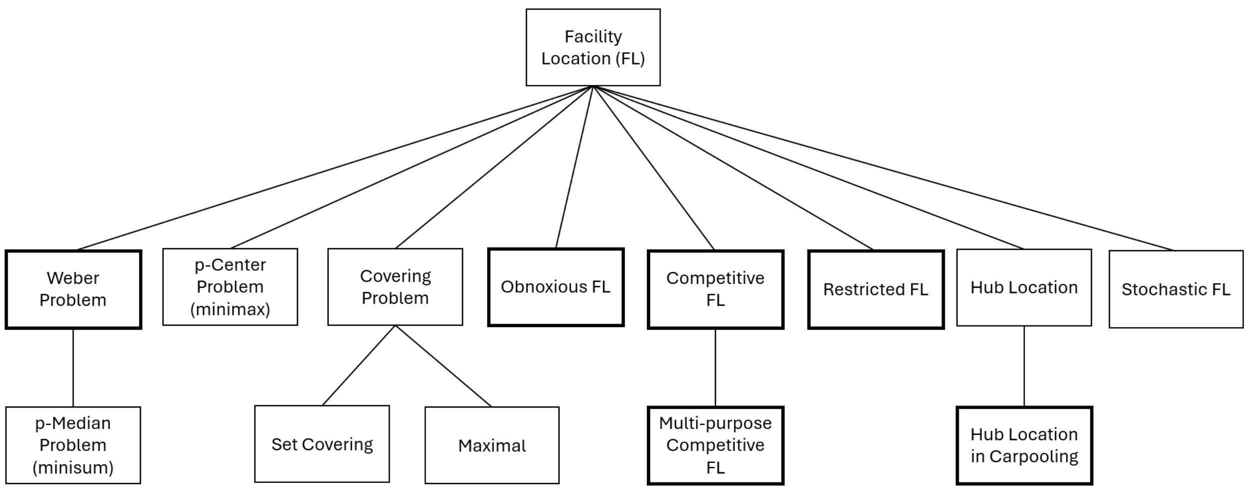

Figure 1.2: Classification of the facility location models based on (Fischer, 2011).

Key Concept 1: Carpooling

Carpooling belongs to a more general category of modes of transportation called ride-sharing (Agatz et al., 2012; Furuhata et al., 2013). In ride-sharing, a group of commuters with similar original locations agrees to travel together to reach a common destination. There have been many studies devoted to ride-sharing. An extensive ride-sharing literature review and model classification can be found in (Furuhata et al., 2013).

Carpooling involves the participants' private vehicles and is characterized by recurring trips (Baldacci et al., 2004). It usually involves no more than five participants, restricted by the number of seats in a typical private vehicle. This shared mobility is typically conducted without an explicit profit to the participants and costs are shared as the participants take turns driving.

Carpoolers, however, can have certain preferences when it comes to the length of the detour and the number of extra stops they are willing to add to their trip (Stiglic et al., 2015).

As carpooling is believed to be one of the effective options to reduce environmental impact of car ownership, such as traffic congestion or greenhouse gas emissions, it has been promoted by the governments around the globe. In various countries, government incentives are being offered, both for employees and employers. Some populated urban areas offer lanes for high occupancy vehicles (HOV), preferred parking, or even subsidies to private car owners who engage in carpooling. Some countries even develop national plans, like France's *National Daily Carpooling Plan* (*Plan national du covoiturage du quotidien*) (Government of France, 2023). Various carpooling platforms or apps are proposed and utilized by numerous organizations. The examples are Pave Commute in the U.S. (Pave Commute, 2024), or BlaBlaCar (BlaBlaCar, 2024) in Europe. Still, these attempts are not gaining as much traction as expected.

The two commonly distinguished types of carpool are the pick-up/drop-off carpool (PDC) and the to/from carpool (TFC) (Kalczynski & Miklas-Kalczynska, 2019). The pick-up/drop-off carpool model (PDC) is frequently associated with families driving their children to and from school or extracurricular activities. This type of carpool is typically an informal consumer-to-consumer arrangement among the families in the suburbs whose children participate in activities located some distance from home. The driver picks up passengers on the way to a common destination (e.g., a school), drops them off, and then returns to the point of origin. The passengers are later picked up by the driver, who again starts at the origin, and returns there after dropping everyone off at their own locations. In the to/from carpool model (TFC) the driver picks up passengers on the way to a destination (typically a workplace), they all stay at the location for a certain amount of time, and then the same driver drops everyone off at their original locations before returning home. This type of transportation arrangement, frequently called "corporate carpooling", is commonly employed by larger organizations that, after a short period of COVID-related telecommuting, began to require their employees to be present at the worksite every day again.

The existing carpool optimization techniques focus largely on system-wide (centralized) objectives, such as minimizing total distance traveled by all commuters. The goal may be to improve parking, reduce gas consumption or traffic (Bruck et al., 2017; Ferrari et al., 2003; Guidotti et al., 2017; Mallus et al., 2017). These centralized arrangements, however, frequently struggle with attracting willing participants (Agatz et al., 2012; Furuhata et al., 2013; Stiglic et al., 2016) as the benefits for individual carpoolers (reduced commuting time or distance) can be insignificant. A successful carpooling model, however, requires high participation and a high matching rate for the riders. The lack of effective solutions in this area has determined the first research gap and a corresponding research question of the dissertation, in which the focus is shifted from global policy goals to the individual carpool participant's perspective. A new carpool organization system is developed (Kalczynski & Miklas-Kalczynska, 2019), and later extended with meeting points in (Miklas-Kalczynska & Kalczynski, 2021), to determine whether this change of focus can influence carpool participation. From the managerial perspective, this information is key, as it may prompt appropriate adjustments of the carpool program strategies. Introduction of meeting points (hubs) has been shown to benefit carpool participation (Aissat & Oulamara, 2014; Aivodji et al., 2016; Kaan & Olinick, 2013; Stiglic et al., 2015). Carpool members may be picked up from well-located meeting points, including one of the participants' original locations. In such a model, the number of feasible carpools increases, as drivers no longer need to cover extra distance or stop multiple times along the way to pick-up riders.

Key Concept 2: Protected Areas in Obnoxious Facility Location

Obnoxious facility location involves facilities which, although needed, are not wanted in close proximity to the demand points. These facilities, sometimes referred to as *not-in-my-backyard* (NIMBY) facilities, generate some kind of negative effect (nuisance), such as noise, smell, traffic, lack of aesthetics, etc. Some examples include waste disposal sites, power plants, missile silos, or emergency rooms. In the context of the obnoxious facility location problems, the goal is to locate one or more such facilities while minimizing the negative impact on the established *sensitive* areas, such as neighborhoods or recreation sites.

Some of the existing models (discrete or network) locate facilities in a subset of available locations (Church & Garfinkel, 1978; Erkut & Neuman, 1989), while others find optimal locations for the facilities anywhere in a given region (continuous planar models) (Berman et al., 2003; Hansen & Cohon, 1981). An extensive review of the obnoxious facility location models can be found in (Church & Drezner, 2022).

Non-obnoxious location problems with protected areas (forbidden regions) have been a popular topic among location researchers (Canbolat & Wesolowsky, 2010; Carrizosa & Plastria, 1999; Hamacher & Nickel, 1995). These problems are relatively easy to solve in a discrete form by simply removing the locations inside the protected regions. The continuous models however, present a much greater challenge since there exist many potential locations for facilities to consider.

In the literature and in practical applications, protected (sensitive) areas tend to be represented as points (Carrizosa & Plastria, 1998). One popular point-based representation is a centroid (center of gravity). Given the irregular shapes of some sensitive regions however, such a representation may not be suitable. It may result in locating a facility near the boundary or even inside the protected region, even though it will be far from the centroid. To remedy this problem, some studies represent protected regions as geometric shapes (Fernández et al., 2000), or convex polygons (Byrne & Kalcsics, 2022) but, due to the increased complexity, only a few studies use non-convex polygons (Aneja & Parlar, 1994; Hamacher & Nickel, 1995; Hamacher & Schöbel, 1997). These deficiencies determine the second research gap and provide motivation for the second research question of this dissertation. The objective is to improve the effectiveness of the optimization models when protected areas are present. The method introduced in the protected areas paper included in this dissertation (Miklas-Kalczynska & Kalczynski, 2024) is suitable for any shape of a protected region. From the managerial standpoint, the improved quality of location decisions resulting from these novel models may be indispensable. Potential violations of the boundaries of protected areas may have serious consequences, such as severe fines or the loss of the trust of the community.

It should be noted that in the literature, forbidden regions are distinguished from barriers. The difference is the possibility of travel through a forbidden region, while barriers are impassable (Canbolat & Wesolowsky, 2010). Such distinction is not needed in this study however, since travel through protected areas does not need to be considered. Instead, the focus is on locating obnoxious facilities outside of the protected regions.

Key Concept 3: Competitive Facility Location

Competitive facility location models focus on attracting the maximum market share that can be gained by locating one or more new chain facilities in the presence of competitors. Research shows that during their site assessment process firms increasingly rely on highly quantitative methods rather than on traditionally used intuition and experience of operational managers (Reynolds & Wood, 2010). Market share gains are measured as a fraction of realized demand, or buying power, that is attracted by a facility from each demand point.

The competitive location model was first proposed in 1929 by an American economist Harold Hotelling (1895-1973). In Hotelling's model, a customer selects a facility to patronize based on price and transportation cost. When the competitors charge the same price, a customer will patronize the closest facility (Eiselt & Laporte, 1993). This premise became known as the *proximity rule*. Utility-based models later extended the original proximity rule by incorporating facility attractiveness levels (T. Drezner, 1994). Customers patronize the facilities with the highest subjectively perceived utility. As a result, customers residing at the same demand point may not patronize the same facility. In 1931, another American economist, William J. Reilly, proposed a different approach, which became known as *Reilly's law of retail gravitation* or *the gravity model* (Reilly, 1931). In Reilly's model the facilities in the nearby cities are patronized proportionally to each city's size and inversely-proportionally to the square of distance. This notion, which in the literature is referred to as *distance decay*, became the key element of the competitive location model. There are two most commonly used extensions of the model: power decay and exponential decay. In the power decay function (Huff, 1964, 1966), which is a generalization of the gravity model, the probability that a customers will patronize a facility is proportional to its attractiveness and to the distance decay function $f(d) = d^{-\lambda}$, where d is the distance and $\lambda > 0$ is the decay parameter that depends on retail category. (T. Drezner & Drezner, 2004) provided an optimal solution to this model in a single-facility scenario. The exponential decay function (Wilson, 1974), $f(d) = e^{-\lambda \mathrm{d}}$, assumes that the probability of patronizing a facility declines exponentially. Both functions were tested on real data (T. Drezner, 2006; Z. Drezner & Zerom, 2024), with the exponential decay model showing a better fit. These models provided a foundation for the new models developed in the multi-purpose shopping paper included in this dissertation (Miklas-Kalczynska, 2024). They are also used in the trajectory paper (Z. Drezner & Miklas-Kalczynska, 2023), which proposes a new generic method for solving them.

One key characteristic of competitive location models is their focus on customer behavior. Such class of models, called *customer choice models* or *shopping models*, is different from the class of *demand allocation models* or *shipping models*. In demand allocation models, the firm determines which customer is served by which facility, while in customer choice models, that decision is made by a customer. The multi-stage decision-making process that takes place (involving the facility choice, allocation of the demand at that facility, and a quantity to purchase) has lead to many versions of the model (Z. Drezner & Eiselt, 2024).

Multipurpose models introduce a new aspect into the competitive facility location. Factoring in the possibility that a customer can make multiple stops during a single shopping trip adds complexity, especially when the number of stops is greater than two. Thus, the two research questions in this dissertation that are related to competitive facility location stem from the lack of sufficient solving methods.

Managerial implications of location decisions in a competitive environment are significant. The absence of appropriate resources, such as state-of-the-art commercial solvers or a high-performance computing environment, may negatively impact the quality of location decisions. Therefore, the existence of methods that help the decision-makers to achieve their goals without the need for significant hardware or software expenditures can be advantageous. The trajectory paper (Z. Drezner & Miklas-Kalczynska, 2023) included in this dissertation closes this gap, proposing the trajectory method.

Among other competitive location models (beyond the scope of this dissertation) are cover-based models and flow interception models. In cover-based models, the original single-facility competitive location problem is converted into a single-facility max-covering problem. This is based on the observation that competing facilities have their *spheres of influence* related to the attractiveness levels. Flow interception models assume that a customer makes purchases on the way to a fixed destination, e.g. a workplace. The goal is for the competing chains to capture the maximum flow of customers passing by when traveling their origins and their destinations. (Z. Drezner & Eiselt, 2024) provide a detailed review of these research areas.

Key Concept 4: Multi-purpose Shopping

When multi-purpose shopping behavior exists on the competitive market, ignoring it during model building can lead to sub-optimal location decisions and cause profit loss. Hence the importance of the methods that incorporate this aspect of customer behavior in the decision-making process. The multi-purpose paper (Miklas-Kalczynska, 2024) included in this dissertation proposes a method that extends the existing models factoring in more than two possible stops.

When shopping or running errands, at times people choose to visit multiple locations during one trip (Federal Highway Administration, 2017). Various studies have been reporting very different results as to how many people choose multi-purpose trips, ranging between 25% and even 74% (Méndez-Vogel et al., 2023; O'Kelly, 1981; Popkowski-Leszczyc et al., 2004). The results of 2017 National Household Travel Survey, conducted by the US Department of Transportation (Federal Highway Administration, 2017), are reported in Table 1.2 (along with the 2005 results). According to this study close to 26% of trips were multi-purpose, with 20.8% two-purpose (2P), 4.5% three-purpose (3P), and 1.5% four-purpose (4P). Trips with more than four stops accounted for the remaining 0.7%. Note that in this context the term *multi-purpose*, unlike purchasing multiple types of goods in a single location (e.g., a supermarket), means also multi-stop.

Table 1.2: Percentage of multi-purpose trips.

Year	1P	2P	3P	4P	more
2005	72.5%	20.8%	4.5%	1.5%	0.7%
2017	74.1%	19.2%	4.5%	0.5%	0.3%

Source: NHTS Survey (Federal Highway Administration, 2017)

Studied broadly in various fields (Arentze et al., 2005; Ghosh & McLafferty, 1984; McLafferty & Ghosh, 1986; O'Kelly, 1981; Oppewal & Holyoake, 2004; Thill & Thomas, 1987), multi-purpose behavior, sometimes referred to as "trip-chaining", is related to the *theory of central places*, developed in the context of location science and dating back to 1950s (Eaton & Lipsey, 1982). It was proposed by W. Christaller and A. Lösch in the 1930s (Lösch, 1938) as an attempt to explain why firms offering different goods or services tend to cluster together. In the field of economics, the first mention of this trend may be traced back to Alfred Marshall and his agglomeration theory. It was developed further by Michael Porter and became known as *cluster theory* (Porter, 1998). It has been vastly studied ever since, e.g., (Gorynia & Jankowska, 2008; Kowalski, 2020; Kuah, 2002; Swords, 2013; Wolman & Hincapie, 2015). According to these theories, companies are able to increase their market shares when they set up their locations in proximity to other retailers, either providing easier access to non-competing goods, or facilitating comparison shopping.

The multipurpose shopping paper (Miklas-Kalczynska, 2024), which is part of this dissertation, contributes to this body of research. As mentioned in the previous section, the research problem stems from the lack of appropriate models to factor in a possible multi-purpose customer behavior. A staple example of practical applications are managerial decisions of locating a new chain facility or facilities in such a way that they are convenient for customers shopping not only for goods or services offered by the chain, but running multiple errands.

Note that the concept of trip-chaining is related to the pick-up/drop-off carpooling problem, and it can be considered as a "reversed carpool".

1.3 Research Gap

As mentioned in Section 1.2, there are two main streams in facility location research: discrete and continuous. In the discrete models, facilities can be located only in certain predetermined places. The continuous models on the other hand, allow for locating a facility anywhere in a given region. When it comes to optimization, discrete models are relatively easy to solve, but their practical applications are limited. Continuous location models entail much more complexity, and are frequently a better fit for real world applications.

In his Institute for Operations Research and the Management Sciences (INFORMS) Fellowship induction interview in 2018 (INFORMS, 2018) a renowned location scholar, Zvi Drezner, spoke of an important gap in continuous location research, which is the lack of standardized solution techniques. He said that most of his career has been devoted to developing computational optimization methods for these types of problems.

This dissertation intends to close the gap articulated by Drezner for areas of continuous facility location. Therefore, the included articles are tightly connected through the novel computational optimization methods applied to location problems. The introduction of these methods was possible thanks to the recent developments of mathematical modeling techniques in location, the emergence of efficient solvers, and the advancements in high-performance computing. Finding these new methods is significant because of the fact that most continuous optimization problems in location analysis present considerable challenges to managerial decision making. They are extremely difficult to solve due to the non-linear and non-convex nature of their mathematical formulations in terms of the objectives and constraints. The tools and technologies needed to solve such types of problems, such as efficient solvers, have not existed until very recently and are still difficult to apply, hence they are relatively rarely utilized. Instead, practical location problems need to be frequently simplified, i.e., solved as linear, convex, or discrete problems. New methods proposed in this dissertation, that allow solving continuous non-linear and non-convex versions of the problems, help alleviate the restrictions on practical applications of the obtained solutions. Consequently, the capacity for solving real-world problems increases, which facilitates quality decisions, as managers can make use of better information, and enhanced models.

The specific research gap addressed by the first two papers, "A decentralized solution to the carpooling problem" (Kalczynski & Miklas-Kalczynska, 2019) and "Self-organized Carpools with Meeting Points" (Miklas-Kalczynska & Kalczynski, 2021), is the absence of carpool organization methods that focus on the benefits to the individual carpoolers rather than system-wide gains. The paper intends to introduce the models that shift that focus. Such an approach may result in higher carpool participation without any additional external incentives. Managerial appli-

Table 1.3: Original contributions of the dissertation papers

Research paper	Research gap	Original contribution
"A decentralized solution to the carpooling problem"	Absence of carpool organization methods that focus on the benefits to the individual carpoolers rather than system-wide gains.	A new decentralized, self-organized carpool optimization model that optimizes individual participants' savings.
"Self-organized carpools with meeting points"	Limited number of centralized (and the lack of decentralized) carpool optimization models considering hubs.	Extending centralized and self-organized carpool models with hubs that are either mandated or optional.
"Multiple obnoxious facility location - the case of protected areas"	Insufficient representation of protected areas in the obnoxious facility location models (points or basic convex shapes).	A new iterative optimization approach that considers actual (potentially non-convex) boundaries of sensitive areas when locating obnoxious facilities.
"Solving non-linear optimization problems by a trajectory approach"	Limitations of local solvers when solving unconstrained non-linear differentiable location problems.	A new method for using trajectory principle to solve complex unconstrained problems, demonstrated on selected facility location problems.
"Extensions to competitive facility location with multi-purpose trips"	Lack of multi-purpose multi-facility competitive location models that consider more than two stops.	Multi-purpose multi-facility competitive location model, where trips with more than two stops are considered.

cations of the proposed methods are of particular significance to policy-makers interested in increasing carpool use and hence, limiting traffic congestion or emissions. The studies can benefit the private sector as well, proposing solutions that can lead to reduced parking costs and environmental impact, as well as improving employee productivity and workplace culture.

The third paper, "Multiple Obnoxious Facility Location - the Case of Protected Areas" (Miklas-Kalczynska & Kalczynski, 2024) attempts to fill the gap in obnoxious facility location research related to insufficient representation of protected areas. The paper intends to develop a new method that allows for limiting nuisance affecting the entire protected area using its actual boundary rather than only a point-based representation or an approximate shape. Models enhanced with this new method may lead to better location decisions when placing obnoxious facilities, like garbage dumps, airports, or polluting factories. When it comes to such facilities, inadequate location decisions may have serious consequences for public and private sector firms alike, when they lead to violations of existing regulations or cause public outrage.

The fourth paper, "Solving Non-Linear Optimization Problems by a Trajectory Approach" (Z. Drezner & Miklas-Kalczynska, 2023) intends to be a response to the lack of suitable tools (specifically, the limitations of local solvers) that would enable the use of the trajectory principle - a method first developed in late 1970s (Z. Drezner & Wesolowsky, 1978). The proposed new general computational optimization model can be used to solve many complex unconstrained optimization problems. Thanks to computational optimization, the method can be added to the collection of viable solving options. Many practical optimization problems that facilitate managerial decision-making can benefit from this method, as long as they are unconstrained and have differentiable objective functions. Applications may extend beyond location analysis, however the example used is competitive facility location. Long-term location decision of a new chain facility (or multiple facilities) placement can be found when the trajectory method is applied and results in finding a satisfactory solution or a good starting solution for other methods. The trajectory method has recently been applied to solve the multi-purpose competitive facility location model which is also part of this dissertation.

The fifth paper, ”Extensions to Competitive Facility Location with Multi-purpose Trips” (Miklas-Kalczynska, 2024) intends to close the gap in multi-purpose competitive facility location which is restricting the number of stops customers make to two. The extension of the two-purpose models to multi-purpose is challenging in terms of formulation, implementation, and computational complexity. The goal is to maximize market share captured while introducing the possibility of more than two stops made by customers shopping for non-competing goods or services. Strategic decisions of where to locate new chain facilities are of great importance to managers. Factoring in a realistic multi-purpose shopper behavior can lead to better location decisions that result in more market share captured by the chain.

1.4 Research Objectives

The purpose of this work is to propose novel computational optimization methods that can be employed to find solutions to hard optimization problems, making them suitable managerial tools. Each method involves mathematical modeling to formulate or reformulate the original problem. Such computational optimization models must be tailored specifically to the problem at hand and employ novel ways of utilizing the existing state-of-the art technology: software (solvers) and hardware (high-performance computers). New models can be built to harness the capabilities of computational optimization. Extensive computational experiments can be used to evaluate the models and demonstrate their usability. The objective of this research is to close the gaps identified in Section 1.3, specifically:

- In carpooling research, the objective is to find appropriate methods that would enable efficient solution of the non-linear carpooling problem that could also incorporate meeting hubs (Kalczynski & Miklas-Kalczynska, 2019; Miklas-Kalczynska & Kalczynski, 2021). The subsequent objective is to discover if self-organized carpools, whether with mandatory or optional hubs, influence carpool participation.

- In the area of restricted facility location, the objective is to develop a more viable representation of protected areas (Miklas-Kalczynska & Kalczynski, 2024). Based on this new representation, the subsequent goal is to develop a workable method for locating obnoxious facilities in the presence of sensitive regions.

- When it comes to the optimization methods, in the trajectory paper the objective is to introduce a method that would allow for finding solutions to unconstrained differentiable problems in an efficient manner (Z. Drezner & Miklas-Kalczynska, 2023).

- In competitive facility location, the objective is to close a gap in a particular line of research in competitive facility location, dedicated to multi-purpose, multi-stop shopping for non-competing goods (Miklas-Kalczynska, 2024). A related objective is to verify whether the model incorporating multi-purpose trips allows for capturing more market share than a single-purpose or a two-purpose model.

The scope of this work is limited to the field of location science. In particular, the included papers are nested in the following location research areas: hub location in carpooling, the Weber problem, obnoxious facility location, restricted facility location, and competitive facility location, as shown in Figure 1.2.

1.5 Theoretical Background and Research Questions

Decision-making is an essential part of management. The quality of managerial decisions, especially the long-term, strategic ones, can impact the well-being of an organization. Incorrect decisions can put it in serious trouble or even jeopardize its existence. Therefore, decision-makers are interested in obtaining the best possible, most accurate information, as fast as possible, to be able to make good decisions. The study of management science offers a variety of methods that facilitate decision-making. One of the methods that has been gaining on importance is computational optimization which became a valuable tool in today's research and practical applications (Koziel & Yang, 2011). The reason for its growing popularity in management science is that it enables solving problems that otherwise are impossible to solve efficiently due to their complexity. In a real business environment resources are limited, which makes optimization necessary. In most real-world applications, objectives and constraints are highly complex, therefore finding optimal solutions in reasonable time and with reasonable resources becomes a challenge, while settling for sub-optimal solutions or relying on simplified models can be risky. Therefore, managerial implications of computational optimization are indispensable.

Location science is one of the research fields that benefit from computational optimization, because of the non-linear, non-convex nature of their objective functions and constraints. Finding a global optimum for larger instances of such problems is not guaranteed in a reasonable amount of time. Recent emergence of new optimization tools and technologies, such as efficient general non-linear solvers, has opened a window of opportunity to deal with certain uncharted research areas in location analysis and enhance some existing models, making them more relevant to practice.

The subsections below present this dissertation's research questions, provide their theoretical foundations, and demonstrate their emergence from each corresponding body of research.

Theoretical Foundation 1: The Carpooling Problem (CPP)

Today, the majority of people worldwide still prefer to drive their own car to work, frequently being the only person in the vehicle. In the US and Western Europe, this number has been held steady for years, at around 70% (Brutel & Pages, 2021; Burrows & Burd, 2024; Federal Statistical Office of Germany, 2021). While there are places where ride-sharing systems, such as public transportation, are widely utilized, they are unpopular in many other locations. The reasons are typically cultural or organizational in nature, mostly related to an insufficient level of comfort or flexibility compared to that offered by a private vehicle.

As a consequence, the increased number of commuter trips during peak hours, paired with the low vehicle occupancy rates, leads to severe traffic congestion, high greenhouse gas emissions, or problems with parking. In response to these issues, many organizations encourage their members to pick up colleagues when driving to or from the workplace to minimize the number of private cars on site. Carpools are especially encouraged in places where parking is scarce, such as college campuses or companies located in big cities. These efforts however, have brought mixed results. One of the reasons may be the fact that carpool optimization techniques are largely based on the centralized approach, that is, focused on system-wide goals, such as the minimization of the total distance traveled, the reduction of pollution or traffic (Baldacci et al., 2004; Calvo et al., 2004; Ferrari et al., 2003; Yan & Chen, 2011). Although it may serve policy-makers' goals, it can produce unsatisfactory results for the individual participants (Agatz et al., 2012). This in turn, may discourage participation or necessitate additional incentives or regulations. While the centralized approach to the carpooling problem assumes that public policy objectives will be enough to motivate the individuals to carpool, studies evaluating commuting habits contradict these assumptions. For example, after several years of increasing popularity in the 1970s, the carpooling practices in the U.S. have declined, despite governmental incentives (Ferguson, 1997; Li et al., 2007). According to the *U.S. Census Journey to Work Data*, the percentage of workers commuting by carpool was 8.9% in 2019. During the COVID pandemic a drop to 7.8 % was observed in 2021, after which the numbers returned to the pre-pandemic levels in 2022 (8.6%) (Burrows & Burd, 2024), still almost three times as popular as public transportation. Considering the above findings, the first research question can be formulated as follows:

> *Research Question 1: How to shift focus from global policy goals to individual carpool participant's perspective and will this shift increase carpool participation?*

The answer can be obtained through the development of a decentralized approach to carpool organization, initially without the meeting points (Kalczynski & Miklas-Kalczynska, 2019), and then with the meeting points (hubs) incorporated into the model (Miklas-Kalczynska & Kalczynski, 2021). Such a strategy allows for a shift of focus from the global policy goals to the individual carpool participant's perspective. This approach is based on the idea that any attempts of carpool organization should enable potential participants to interact and make arrangements freely rather than impose compliance measures or regulations.

Theoretical Foundation 2: Obnoxious Facility Location Problem With Protected Areas

While the discrete (or network) obnoxious facility location models are relatively easy to solve, their practical applications are limited. The goal is to find an optimal location out of a predetermined finite set. Any spots that violate the restrictions, i.e., are too close to, or inside, the protected regions, can simply be eliminated. Continuous or planar models on the other hand, assume that the number of location possibilities is infinite, which makes such problems much more complex (Church & Drezner, 2022).

Traditionally, in continuous location problems the region over which a facility can be feasibly located is assumed to be the entire region considered in the analysis. Many real world problems, however, make this assumption unrealistic. Whether in urban areas or in nature, there are often obstacles that restrict the placement of facilities (or travel through them), such as rivers, lakes, highways, or railroad tracks.

Restricted areas in facility location are frequently represented as points (Carrizosa & Plastria, 1998; Z. Drezner & Wesolowsky, 1995) or basic geometric shapes, such as circles (Brimberg & Juel, 1998; Fernández et al., 2000; Melachrinoudis & Cullinane, 1986). Studies that represent forbidden regions as polygons typically use convex shapes (Bischoff & Klamroth, 2007; Byrne & Kalcsics, 2022; Canbolat & Wesolowsky, 2012; Dearing et al., 2005; Hamacher & Klamroth, 2000; Klamroth, 2001; McGarvey & Cavalier, 2005; Plastria et al., 2013; Savaş et al., 2002). Only a limited number of authors study non-convex polygonal forbidden regions (Aneja & Parlar, 1994; Hamacher & Schöbel, 1997; Oğuz et al., 2016) due to the complexity of such models. When it comes to the real-world protected areas however, their geometric representations are usually unions of geo-polygons, which can be projected onto a plane as convex or non-convex polygons. A polygon that does not have any “holes” or does not intersect with itself is called a simple polygon. If a geographic region has holes, a polygon that represents it can be easily divided into simple polygons.

As mentioned earlier, a popular centroid-based representation of a forbidden region proves unsuitable in practical applications. Although neighborhoods or carefully landscaped green parks in urban areas tend to have rather regular shapes, this is certainly not the case when considering wilderness areas or national parks. These may be very irregular, usually determined by the landscape they are created to preserve. In some cases, the centroids of such irregularly-shaped regions may be located outside of the boundaries of such regions. As a result, locating an obnoxious facility far from the centroid may, in fact, place it on the actual boundary, or even inside, of the region we want to protect. These observations lead to the second research question of this dissertation which can be formulated as follows:

Research Question 2: How to improve the effectiveness of the optimization models for *locating obnoxious facilities when polygonal protected areas are present?*

The answer to this research question can be found through the development of models that allow for considering the entire protected region and, consequently, prevent obnoxious facilities from being located too close to the actual boundary of the protected area, even an irregular one. Starting from the point-based problem, two different models can be considered. The first one, called maximin, focuses on maximizing the minimum distance between a facility and a protected area. In the second model, called cooperative, facilities "cooperate" in inflicting nuisance on the protected points. Such an approach aims at minimizing the cumulative negative impact of all the located facilities on the most affected sensitive point. The proposed method, based on iterative improvement, is meant to go beyond a point-based representation. For the maximin model this means locating a facility as far as possible from the protected area's boundary. For the cooperative model, negative impact on the entire protected area is to be minimized.

Theoretical Foundation 3: The Trajectory Method

Effective methods for solving practical location problems are not easy to find. The complexity of the models requires either considerable simplifications of realistic problems, or developing novel approaches. When practical location problems are simplified, or when their constraints are relaxed, there is a considerable risk of drifting too far from reality. This in turn, reduces usability of the developed models in decision making. Competitive facility location deals with such complex non-linear, non-convex problems. Maximizing market share captured by locating a new facility using a gravity model described in Section 1.2 requires measuring the distances to the demand points and utilizing one of the distance decay functions (Huff, 1964; Reilly, 1931). As noted in Section 1.2, distance decay is widely used in these types of models (Z. Drezner & Eiselt, 2024).

When it comes to such complex optimization problems, one significant obstacle when solving them comes from the limitations of the existing solvers. In the case on non-linear, non-convex problems, local (non-exact) solvers need to be used, as such problems may have multiple local optima. Local solvers however, do not guarantee finding an optimal solution. All we can hope for is finding a "good" solution, i.e., such that will not be too far from the unknown optimum. Local solvers are also challenging to use in terms of the need of proper parametrization and establishing an appropriate starting solution, which may greatly influence the quality of the obtained solution. These limitations lead to the third research question of this dissertation:

Research Question 3: How to solve unconstrained non-linear location problems with differentiable objectives, overcoming the limitations of local solvers?

A new method, that involves solving a set of ordinary differential equations numerically to trace a trajectory between the starting solution and the best-known or optimal solution, may be an answer to this question (Z. Drezner & Miklas-Kalczynska, 2023). It can be a good alternative to other methods, which necessitate using a solver. The trajectory approach is a purely analytical methods which, for some cases, can be implemented in a spreadsheet (e.g., Microsoft Excel) with basic algebraic manipulations. Ever since the trajectory idea was first introduced by Drezner and Wesolowsky in 1978 (Z. Drezner & Wesolowsky, 1978), it has not been utilized much due to the lack of techniques to formulate known models in terms of this approach. The field of facility location, in particular the Weber problem and the competitive facility location problem provide good grounds for the development of these techniques, but potential applications go well beyond the ones mentioned above. They can include many other differentiable, unconstrained problems, such as the multi-purpose shopping model proposed in (Miklas-Kalczynska, 2024), but also other problems outside of the location science field.

Theoretical Foundation 4: Competitive Facility Location With Multi-purpose Trips

In recent years, the concept of multi-purpose shopping has been attracting a lot of attention in the field of facility location. Depending on the type of goods customers shop for, there are two kinds of models: those concentrating on non-competing goods, and those focusing on substitutes. When considering shopping for non-competing goods (T. Drezner et al., 2023; Z. Drezner et al., 2023; Kalczynski et al., 2024; Lüer-Villagra et al., 2022; Marianov et al., 2018; Méndez-Vogel et al., 2023), it is assumed that multiple such goods (or services) exist on the market. It is also assumed that the chain and its competitors sell one of these goods. Customers can make separate shopping trips to purchase each good (single-purpose). They can also make multiple stops to purchase different goods during a single trip (multi-purpose).

Note that as opposed to shopping for non-competing goods, comparison shopping is a different behavior, in which a customer may revisit the locations to compare substitute products before making a purchase. This class of problems, which deals with substitute rather than non-competing products, constitutes a separate research gap in the area of multi-purpose shopping in facility location (Marianov & Méndez-Vogel, 2023; Méndez-Vogel et al., 2024) and is beyond of the scope of this dissertation.

The competitive location models assume that the chain's new facility (or facilities), offering a particular kind of retail products or services (e.g., a coffee shop), is being located in an area. The chain aims at attracting the maximum possible market share, while competing with other chains in the area that offer a similar product or service. One must consider that there is a proportion of customers who combine purchasing a product or service offered by the chain with a visit to one or more other retailers offering non-competing goods, such as groceries or gas. These other facilities do not compete with the chain or one another. They are often located close together, creating retail-rich areas. Taking such multi-purpose customer behavior into consideration may provide a more suitable model and thus, allow for capturing more of the available market share. This observation leads to the fourth and final research question of this dissertation:

> *Research Question 4: Considering the possibility of multi-purpose customer behavior, how to locate a new facility or facilities so that the chain captures the maximum possible market share?*

Existing competitive location multi-purpose models reduce the number of stops to two (T. Drezner et al., 2023; Z. Drezner et al., 2023; Kalczynski et al., 2024; Lüer-Villagra et al., 2022; Marianov et al., 2018; Méndez-Vogel et al., 2023). Incorporating the possibility of more than two stops requires determining the order of visited locations. This could be the shortest tour, or perhaps additional constraints might be necessary. For example, when running errands, customers might prefer to purchase perishable goods at the very end, before returning home. Based on multiple studies in cognitive psychology, when arranging their multi-purpose trips, human beings are able to intuitively and almost effortlessly solve small instances of the Traveling Salesman Problem (TSP) to near optimality (Dry et al., 2006; MacGregor & Chu, 2011; MacGregor & Ormerod, 1996; Vickers et al., 2001), especially when the difference between the shortest and the longest path is significant (O'Kelly & Miller, 1984).

1.6 Research Methods and Data Sources

Research methods used in this work fall under an umbrella of computational optimization. The techniques include mathematical modeling, linear and non-linear optimization, as well as simulation.

When it comes to the tools utilized in the papers, Wolfram's Mathematica (versions 12-14) (Wolfram Research, Inc., 2024) was used for the derivations, generation of the starting solutions for local search, visualization, as well as small-scale testing. The global solver (global optimum guaranteed) used in the studies was Gurobi (versions 10-11) (Gurobi Optimization, LLC, 2024), with up to 32 CPUs. Local non-linear solver (global optimality not guaranteed) used was SNOPT 7.7.4 (Gill et al., 2005) with no parallelism. High performance computing environment that was utilized included virtualized Linux Ubuntu 22.04 LTS environment with up to 38 vCPUs and up to 374GB of vRAM. The physical server utilized was a VxRail V570F with Intel Xeon Gold 6248 @ 2.5GHz (2 socket, 20 cores per processor, 80 logical processors), 748GB RAM, and VMware vSAN storage. A total of three physical servers were at the candidate's disposal, and were utilized depending on the task at hand. Some of the tools by default are set to use many or all available resources (such as Gurobi or Mathematica), some can use only one CPU at a time (e.g. SNOPT).

Following are the details of the research approaches, along with the data sources, and the methodology adopted in the dissertation.

Research Approach 1: Enumeration and Mixed Integer Linear Programming

One of the major obstacles when solving the carpool problem is the number of possible carpools to consider. As it grows faster than exponentially with the increase in the number of carpool participants, it can considerably slow the optimization process, making larger real-world problems impossible to solve in reasonable time. To help overcome this issue, a carpool enumeration technique is introduced in (Kalczynski & Miklas-Kalczynska, 2019) that incorporates individual preferences on minimum savings and maximum extended distance traveled per trip. The technique allows to enumerate feasible carpools in a relatively short time and is useful for a wide range of practical problems. The following paper, (Miklas-Kalczynska & Kalczynski, 2021), improves the enumeration technique by introducing elliptical neighborhoods. These neighborhoods are calculated using a baseline distance (without carpooling) and a maximum detour a carpool participant is willing to drive. The neighborhood concept allows for a significant reduction of analyzed carpools, including only those that are rational and practical. In order for the participants to be considered neighbors, their neighborhoods must overlap when it comes to the original locations or the meeting points. In other words, neighbors must be within a reasonable detour distance from one another and must have enough available passenger seats to be placed in each other's carpools. Figure 1.3 depicts the concept of the elliptical neighborhood for the to/from carpool model (TFC). It shows 100 original locations on a 20×20 unit square.

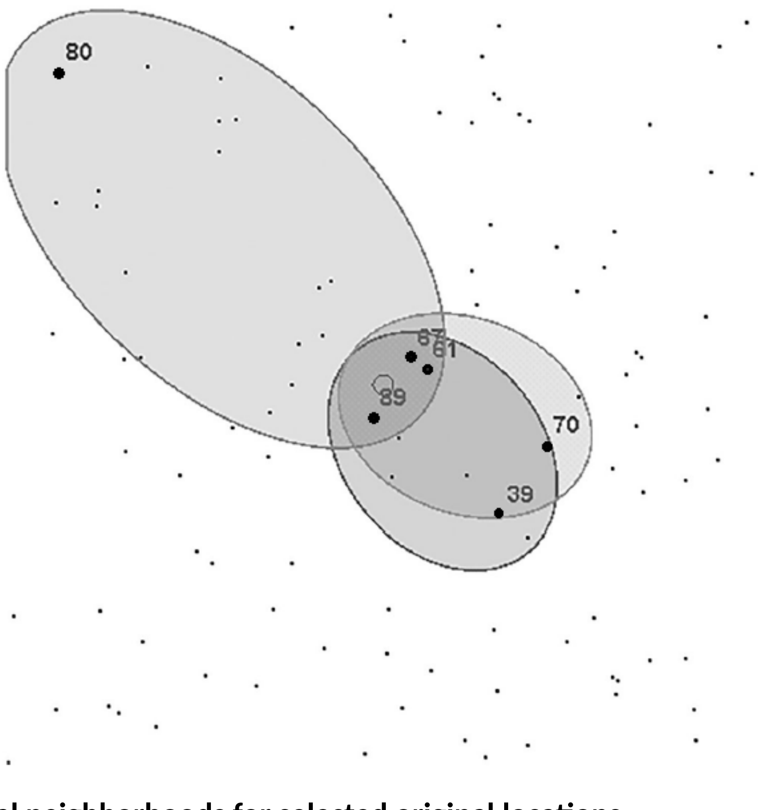

Figure 1.3: Elliptical neighborhoods for selected original locations.
Source: (Miklas-Kalczynska & Kalczynski, 2021)

The destination is represented by a small circle in the middle. The three ellipses are constructed based on the established constraints for original locations f_{39},f_{70} and f_{80}.

Out of the three original locations, only f_{39} and f_{70} are neighbors in the TFC model without hubs because the elliptical region of f_{39} contains the original location f_{70} and vice versa. However, the situation changes when we assume that any of the three original locations within the intersection of the three elliptical regions, namely f_{61},f_{67},f_{89}, may become hubs (TFC model with hubs, or TFCH). In such case, all three original locations f_{39},f_{70} and f_{80} are considered neighbors because their potential hubs are in the intersection of their elliptical neighborhoods.

The shortest tour enumeration algorithm introduced in the carpool papers was later utilized in the multi-purpose shopping paper (Miklas-Kalczynska, 2024) to establish the shortest multi-purpose shopping trips. Similarly, the concept of "via distances", necessary to form the enumeration of carpools, was re-used in the multi-purpose shopping for establishing the multi-stop trip distances. This was made possible by treating multi-purpose trips as "reverse carpools" (see Figure 1.1).

The carpooling papers use two solving techniques: centralized (maximizing system-wide benefits) and decentralized (focused on individual participant preferences). The formulation of the centralized problem is equivalent to a well-known set partitioning problem. The objective is to maximize total (system-wide) savings from car pooling, while the constraints ensure that one and only one carpool is selected for each participant. This problem can be solved to optimality for large practical instances by global solvers, such as Gurobi (Gurobi Optimization, LLC, 2024). The decentralized approach is a new heuristic and is one of the major contributions of the carpooling paper. The neighborhoods are generated before the carpool enumeration is applied, which substantially reduces the number of multi-participant carpools in the enumeration. In each iteration of the heuristic, the carpools with the highest savings for their respective participants are selected. Next, the selected participants and all remaining potential carpools, along with their original locations, are removed from further analysis. A simple tie-breaking technique is used. The algorithm terminates when all participants are assigned to carpools. The heuristic is described in detail in (Kalczynski & Miklas-Kalczynska, 2019).

The efficient carpool enumeration technique enabled the use of mixed-integer programming (MIP) in both carpool papers. It is an optimization model in which some or all of the variables are integers. Appropriate formulation of the carpooling problems enabled the use of this model, and the application of the corresponding solution technique supported by global solvers.

As far as the data is concerned, both simulated and real-world instances were utilized. Figure 1.4 shows the real-world instance utilized in both carpooling studies. The data comes from a private U.S. school (pre-K to 8th grade) located in Orange County, California. The figure shows the school's location (marked with an arrow), as well as the locations of 187 family homes, based on the street addresses. Most families use their private vehicles to drop off and pick up their children. To reduce commuting costs, many families choose to enter into carpooling arrangements with their neighbors (pick-up/drop-off carpool model or PDC model). There is no centralized planning, rather, the system is organized by the parents. Matching is based on individual preferences. Potential carpools are limited by the number of participants and available seats. The driving distance matrix was created for the study using Google Maps API (Google, 2016).

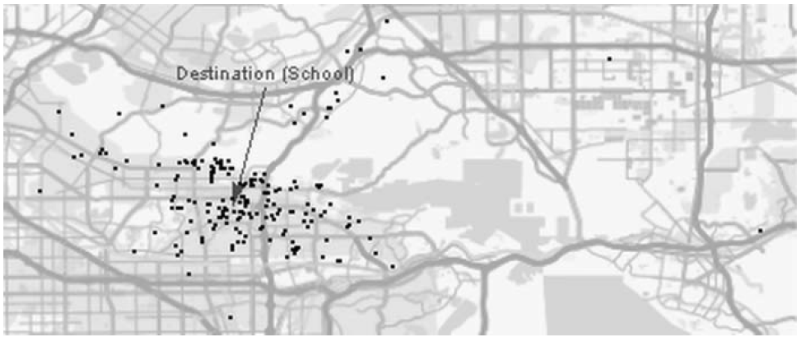

Figure 1.4: A real-world carpool instance.
Source: (Kalczynski & Miklas-Kalczynska, 2019)

In addition to the above real world instance, 1,000 random instances were generated, each with 100 different origins distributed on a 40 by 40 units square. Moreover, 35 problem instances from the study by Baldacci, Maniezzo and Mingozzi (Baldacci et al., 2004) are used, incorporating between 50 and 250 original locations.

Research Approach 2: Iterative Application of Local Non-Linear Solver

The iterative approach used in (Miklas-Kalczynska & Kalczynski, 2024) for locating multiple obnoxious facilities around protected areas was inspired by the iterative improvement concept used in the decentralized carpooling (Kalczynski & Miklas-Kalczynska, 2019; Miklas-Kalczynska & Kalczynski, 2021) and the iterative trajectory technique (Z. Drezner & Miklas-Kalczynska, 2023), which are part of this dissertation. It starts with the selection of the initial set of protected (sensitive) points that represent protected areas in the original point-based model. These initial points can be polygon vertices, centroids or other selected points, as long as they are part of the protected area they represent. Next, the method in (Miklas-Kalczynska & Kalczynski, 2024) is as follows:

1. *Set the best area-based objective to positive infinity (for minimization models) or negative infinity (for maximization models).*

2. *Solve the point-based continuous obnoxious facility location problem using the set of sensitive points and a point-based objective.*

3. *If any of the facilities is located inside (or on a border of) any of the protected areas, then add new sensitive points at these locations and go to Step 2.*

4. *Add new model-specific sensitive points and calculate the area-based objective.*
5. *If no new sensitive points are added or additional stopping criteria are met then STOP. Otherwise, set the best area-based objective to be the new area-based objective, and go to Step 2.*

The approach is applied to two continuous obnoxious facility location models: maximin (Z. Drezner et al., 2019) and cooperative (T. Drezner et al., 2020). The maximin model aims at maximizing the minimum distance between a facility and its nearest protected area. In the cooperative model, multiple facilities contribute to producing some kind of negative effect on sensitive points, i.e., nuisance. A non-linear formulation of a cooperative point-based model represents nuisance using the *inverse square law*, which is commonly applied when some type of energy is evenly radiated outward from a point source. The objective is to minimize the cumulative negative impact of all the facilities on the most affected sensitive point.

In the iterative approach developed in this dissertation, new sensitive points are added using different strategies, depending on the model. In the maximin model, we define the minimum distance from an outside point to the polygon as the minimum distance to the boundary of that polygon. This may be a distance to the nearest vertex or a perpendicular distance to the nearest edge. In the cooperative model, each time a point-based solution is obtained, a point that receives the most nuisance is calculated and added to the list of sensitive points. Thanks to the proof presented by (Coletti et al., 2024), the search for the most-affected sensitive point can be restricted to the boundaries of the protected areas.

An efficient local non-linear solver is used iteratively to solve the problem. The main advantage of the new approach developed in this dissertation is that it does not require any modifications to the existing point-based models, but relies on applying them iteratively, while adjusting input data at each iteration. The concept of iterative improvement, which is a commonly used approach in decision-making, connects the protected-areas study with the trajectory paper (Z. Drezner & Miklas-Kalczynska, 2023) and the carpooling papers (Kalczynski & Miklas-Kalczynska, 2019; Miklas-Kalczynska & Kalczynski, 2021). The techniques based on incremental improvement involve applying a certain process repeatedly until a desired outcome is achieved or a satisfactory solution is found.

Both generated and real-world instances are used in this research. 100 large instances in the 100×100 square with randomly-generated protected areas were created using the technique described in the paper's Appendix (Miklas-Kalczynska & Kalczynski, 2024). The real-world instance was the southwest region of the state of Colorado. Figure 1.5 shows the protected areas in the state and the selected region, which is marked gray.

The geo-polygon data representing the protected areas were extracted from the publicly-available source (UNEP-WCMC, IUCN, 2021). As a result, 133 protected areas were identified, with the total of 3075 vertices. Next, the existing multi-polygonal areas were split into simple polygons. The "holes" existing in some polygons were ignored. GeoPandas (van den Bossche

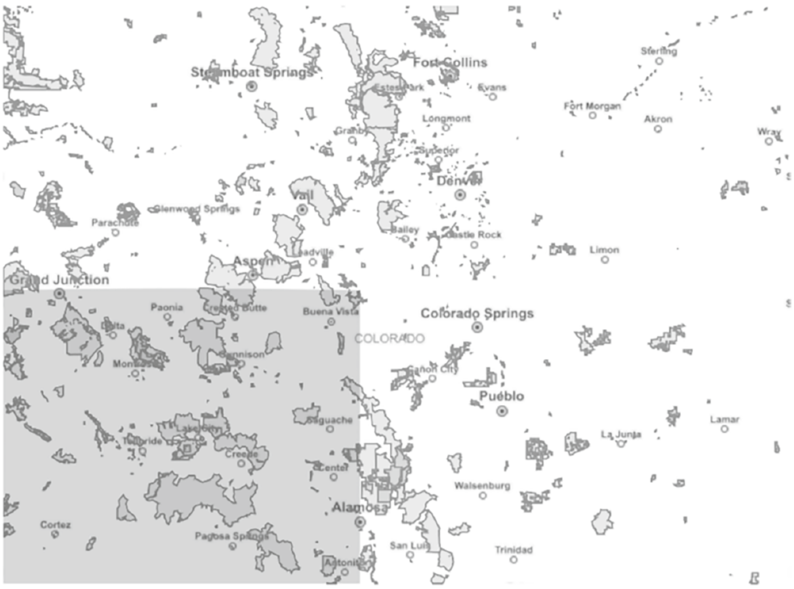

Figure 1.5: Protected areas of the state of Colorado and the selected region.
Source: (Miklas-Kalczynska & Kalczynski, 2024)

et al., 2021) was used to extract geo-polygon data of the area, compute polygon centroids, and simplify geo-polygons (with 0.005 degree tolerance). When it comes to the quality of the data, the source, which is the U.N. List of Protected Areas is recognized as "the only global list of protected areas recognised by governments and mandated by the U.N." (UNEP-WCMC, IUCN, 2021) and undergoes regular quality checks. All transformations of geographic data were done in Mathematica (Wolfram Research, Inc., 2024), with all geo-locations projected onto the two-dimensional Cartesian space using the azimuthal equidistant projection, a tool used by geographers.

Research Approach 3: Ordinary Differential Equations

In the trajectory paper (Z. Drezner & Miklas-Kalczynska, 2023), the trajectory principle (Z. Drezner & Wesolowsky, 1978) is revisited and applied utilizing novel computational optimization techniques for solving unconstrained optimization problems with differentiable objective functions. The trajectory method requires a parameter to be introduced into the optimization problem and an objective function to be expressed in terms of this parameter. The parameter needs to be introduced in such a way that its starting value allows for obtaining an optimal solution relatively easily. Next, a trajectory, formulated as a set of ordinary differential equations, will connect the obtained solution to the desired solution within a specified precision. The fourth order Runge-Kutta method (RK4), which is a convenient numerical integration procedure (Abramowitz & Stegun, 1968; Ince, 1956; Kutta, 1901; Runge, 1895) is used to find the trajectories for the selected problems.

As mentioned earlier, the trajectory method can be applied to solve a variety of other unconstrained optimization problems, as long as the derivatives of the objective functions can be found. The multi-purpose competitive location model introduced in (Miklas-Kalczynska, 2024) is a good example. Currently, the techniques introduced in the paper have led to the trajectory method applications to at least three other complex location models.

In the trajectory paper, computational experiments for the competitive location model were run using the real-life data from Orange County, California. The data, originally presented in (T. Drezner, 2006), were collected from 3,112 customers residing at 81 zip codes, who were intercepted at seven existing malls in the area. Table 1.4 shows the shopping malls along with their corresponding attractiveness levels (A_j).

Table 1.4: Shopping Malls in Orange County, CA, and their corresponding attractiveness levels (T. Drezner, 2006).

j	Shopping Mall	Zip Code	A_j
1	Orange Mall	92865	0.177
2	Laguna Hills Mall	92653	0.595
3	Westminster Mall	92683	1.011
4	Main Place	92701	1.154
5	Brea Mall	92821	1.529
6	Fashion Island	92660	2.367
7	South Coast Plaza	92626	2.484

Source: (Z. Drezner & Miklas-Kalczynska, 2023)

Wolfram's Mathematica (Wolfram Research, Inc., 2021) was used to solve the above seven instances with the trajectory method developed in this dissertation and - for comparison - with the Nelder-Mead method (with default settings). The RK4 method was implemented in Mathematica from scratch to calculate the trajectories. Nelder-Mead, which is readily available in Mathematica, is a direct search method for global optimization which can also be used for local search in non-convex optimization.

Research Approach 4: Large-scale Non-linear Optimization With Embedded Small-scale Optimization

The continuous competitive facility location problem is non-linear and non-convex. Extending the existing two-purpose models with a scenario in which a customer can visit more than two locations during a single trip complicates them further. Such models are very challenging in terms of the formulation, implementation, and computational complexity.

The multi-purpose shopping paper, included in this dissertation (Miklas-Kalczynska, 2024), develops a multi-purpose (MP) competitive facility location model. It builds upon the original gravity model described in Section 1.2, as well as on the single-facility (T. Drezner et al., 2023) and the multi-facility two-purpose (2P) models (Kalczynski et al., 2024). The objective function represents the relative increase in market share captured by the chain when adding a new facility or facilities. The development of this new model comes from an observation that a MP trip can be considered as a “reversed carpool”. This property enables applying the “via distance” concept from carpooling in the context of MP shopping (see Figure 1.1).

The computational optimization model, developed in this dissertation, uses an efficient non-linear solver. The possibility of a customer making more than two stops requires calculating the shortest path. Therefore, the method includes the embedded shortest tour computation as part of the objective function calculation. This task is accomplished through the total enumeration of multipurpose shopping trips, similar to (Miklas-Kalczynska & Kalczynski, 2021). However, in this case, the enumeration is embedded in the non-linear optimization process and not used to formulate the problem.

When considering a three-purpose (3P) model for example, what adds to the complexity is the fact that not all customers are assumed to embark on a three-purpose trip. Rather, some proportion of trips will be single-purpose (1P) and some two-purpose (2P). Moreover, two different options of 2P trips need to be considered, because in a 3P model, a customer can chose two out of three types of non-competing facilities (NCFs) to visit during a 2P trip. For example, apart from coffee, one customer can choose to purchase gas, while another customer can decide on a visit at a grocery store. Proportions of those preferences, i.e., details about how many trips are 3P, how many 2P and how many 1P, are not possible to determine without collecting additional information or making some additional assumptions. The same is true for any MP model with more than two purposes.

The experiments were run on randomly generated instances incorporating 100 to 5000 demand points and up to 15 facilities. Figure 1.6 shows a sample instance of the 3P model with 100 demand points, 10 competing facilities, and two NCF types with 10 facilities each. Gray discs represent the demand points, circles represent competing facilities, while triangles and squares represent the locations of two different types of NCFs, each with ten locations. Different sizes of the demand points represent the buying power weights.

Note that each multi-purpose (MP) instance incorporates a set of demand points with corresponding weights, locations and types of NCFs, locations of the competing facilities, all corresponding attractiveness levels, and the proportions of MP trips. For example, continuing the example of the chain locating a new coffee shop, an instance may include two types of NCFs (gas stations and grocery stores), and three other coffee shops that compete with the studied chain. The definition of an instance becomes important when comparing two different MP models. Details on valid comparison criteria can be found in (Miklas-Kalczynska, 2024).

1.7 Results and Discussion

The research papers included in this dissertation provided interesting results and valuable insights that supplied answers to all research questions. They also closed the research gap for the areas under study and opened avenues for future research, both by the author and by other

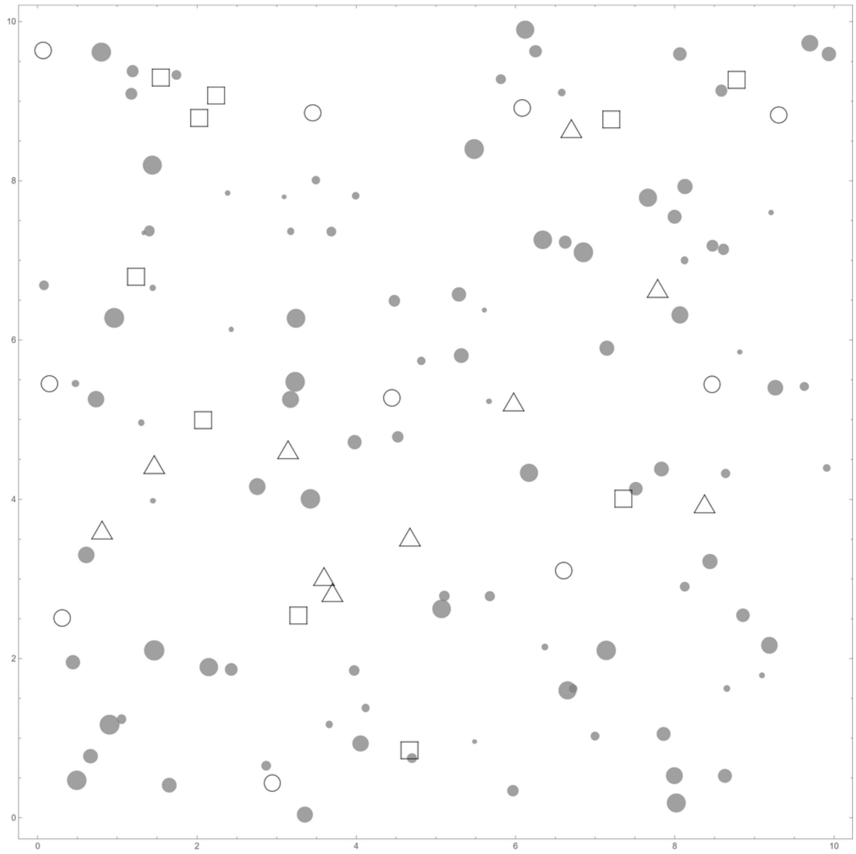

Figure 1.6: 3P instance with 100 demand points (grey discs), 10 competing facilities (circles), 2 NCF types (triangles and squares), and 10 facilities per each NCF type.
Source: (Miklas-Kalczynska, 2024)

researchers, some already resulting in publications, see (Coletti et al., 2024), for example. The results obtained in each study, along with the responses they provide to the corresponding research questions, are presented below.

Result 1: Decentralized carpools with optional hubs increase carpool participation.

The sequence of two closely related papers dealing with the carpooling problem provided valuable insights into carpool organization. The new carpool enumeration technique introduced in (Kalczynski & Miklas-Kalczynska, 2019), and later improved in (Miklas-Kalczynska & Kalczynski, 2021), is based on the minimum average savings and maximum extra distance preferences of each individual carpool participant. The method proved efficient in a wide range of test problems.

In the decentralized solution of the real-world study included in (Kalczynski & Miklas-Kalczynska, 2019), which used the data from the school located in Orange County, California, the carpool enumeration method resulted in 23 518 potential carpools. Table 1.5 compares the results obtained with the decentralized and the centralized solutions. Both solutions offer substantial savings over the baseline (no carpooling). The centralized solution generated 3.59% more system-wide savings compared to the decentralized solution and was able to eliminate 4 more vehicles off the streets. However, compared to the decentralized solution, 90 families (37.43%) had to sacrifice a portion of their individual savings while 51 families (27.27%) gained in individual savings. This means that, compared to the decentralized solution, the centralized approach had to redistribute a significant portion of individual savings in order to achieve a relatively small improvement in system-wide savings. We can suspect that those who lost individual savings might want to seek alternative, more beneficial arrangements, thus destabilizing the entire carpool system.

Table 1.5: Real-World Instance System-Wide Results

	Baseline	Decentralized Solution	Centralized Solution
Number of vehicles per trip	187	90	86
Number of 2+ Carpools	0	53	59
Families Assigned to Carpools	0	150.0 (80.21%)	160.0 (85.56%)
Savings Per Trip (miles)	0	1042.5 (49.72%)	1117.8 (53.31%)

When it comes to the simulated instances, the median of additional savings from the centralized approach to the TFC problem was only 1.53%. 10% of the participants would benefit from the centralized carpooling arrangements, while 16% would be motivated to form alternative carpools. This is because we assume that in their decision-making process, carpool participants tend to focus on their own neighborhood. In this way, they can avoid adding too many extra miles to their trip. A central planner on the other hand, will ignore individual preferences by design, instead focusing on system-wide goals, which may lead to the solutions that may prove disadvantageous to some carpool participants.

The centralized approach to the PDC problem generated a median of 3.87% in additional savings. 25% of the participants would benefit from the centralized carpooling arrangement and 34% would be motivated to form alternative carpools, which in reality means a possible refusal to participate in a carpool. Figure 1.7 shows a solution to a sample simulated CPP instance. The empty circle in the middle is the destination, and the original locations are marked with black dots. Two-participant carpools are depicted as lines, while three-participant carpools are gray triangles (unless the origins are collinear).

The results obtained from 35 University of Bologna instances (Baldacci et al., 2004) showed that for the TFC type, the system-wide savings obtained by the decentralized method were only 0.23% - 6.95% lower than the maximum savings obtained with the centralized approach. 16.4% of the participants would benefit from the centralized solution while 20% would lose savings. In the PDC arrangement, the system-wide savings obtained by the decentralized method were only 0.02% - 5.66% lower than the maximum savings obtained with the centralized method. 10% of the participants would benefit from the centralized solution and 17.5% would lose savings.

All experiments yielded consistent results. The pattern that emerged indicates that the decentralized solutions result in relatively minor decrease in system-wide savings compared to the

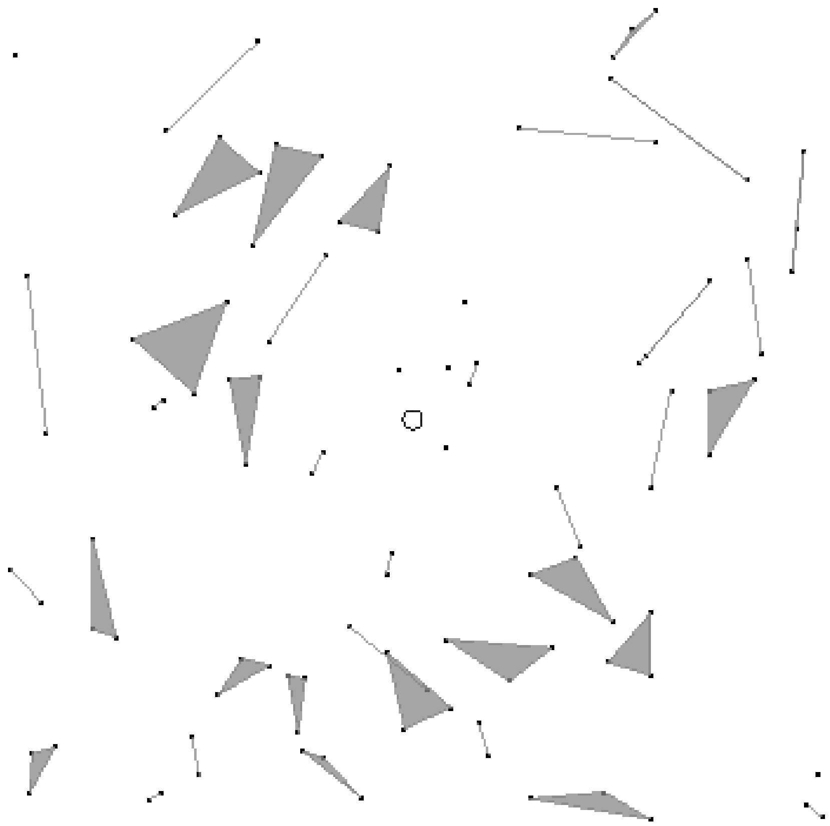

Figure 1.7: A solution to a simulated CPP instance.
Source: (Kalczynski & Miklas-Kalczynska, 2019)

centralized solutions, while bringing an advantage in reduced reallocation of individual participants' savings.

In the carpool with hubs study (Miklas-Kalczynska & Kalczynski, 2021), the original (PDC, TFC) problems were solved along with their versions with hubs (PDCH, TFCH) and the mixed models (PDC/PDCH and TFC/TFCH), where hubs were optional. Both, the self-organizing and the centralized techniques were applied and the carpools were generated with the improved enumeration technique based on elliptical neighborhoods. An instance consisted of a destination and 100 original locations. Figure 1.8 shows sample centralized and decentralized solutions to the PDCH problem with three available seats. The empty circle in the middle marks the destination, the original locations are shown as black dots, and hubs are marked with larger black discs. Two-participant carpools are depicted as lines, while three-participant carpools are gray triangles (unless the origins are collinear). Although the self-organized solution focuses on maximizing individual savings instead of system-wide savings, the system-wide savings of the self-organized solution are only 2.65% lower than the savings from the centralized solution for this instance. Noticeably, in both cases, the closest origins are not included in carpools, which is a result of the minimum savings and maximum additional distance constraints.

Consistent with earlier results (Kalczynski & Miklas-Kalczynska, 2019), self-organized solutions that focus on maximizing individual participant savings, achieve system-wide savings sim-

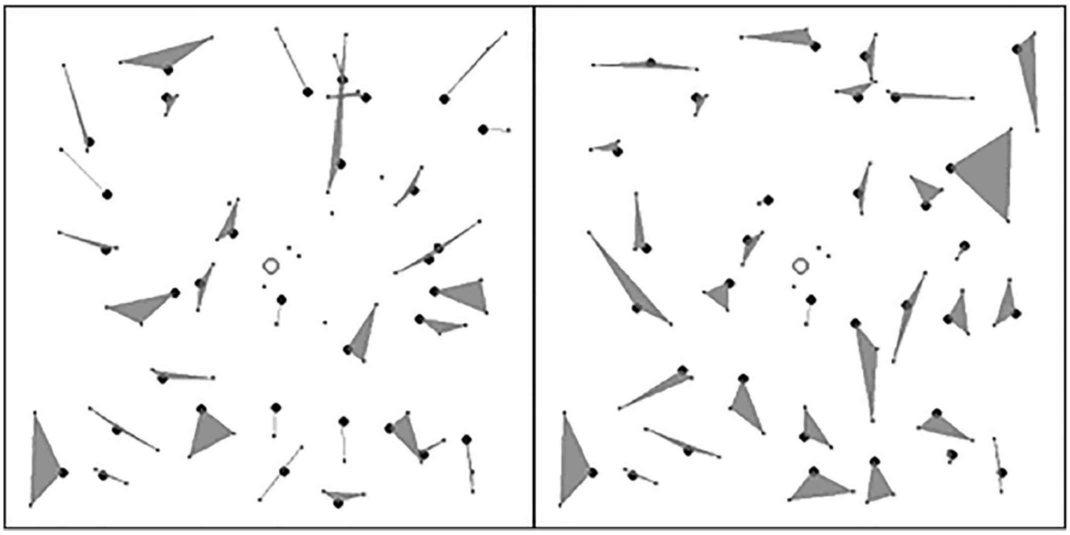

Figure 1.8: Centralized (left) and self-organized (right) solutions to PDCH with the maximum of 3 seats.
Source: (Miklas-Kalczynska & Kalczynski, 2021)

ilar to the centralized approach, yet can increase carpool participation. In case of the TFC model for example, these increases were 15% - 24%. Table 1.6 shows carpool participation rates for all models.

Table 1.6: Carpool participation rates
Source: (Miklas-Kalczynska & Kalczynski, 2021)

	PDC		PDCH		PDC/PDCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	88%	94%	94%	96%	92%	96%
3	88%	93%	93%	97%	94%	96%
4	88%	91%	89%	97%	92%	97%
	TFC		TFCH		TFC/TFCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	70%	72%	86%	96%	86%	96%
3	73%	74%	93%	96%	93%	96%
4	73%	74%	88%	97%	88%	97%
5	73%	74%	90%	97%	90%	97%

In all cases, the results indicate that hubs increase system-wide savings from carpooling. These savings become more prominent when hubs are introduced as an option instead being imposed on participants by a central planner. Table 1.7 shows system-wide savings for the TFC carpool. The introduction of hubs increased savings by 9.38%- 24.87%. In all models types, savings rose as the maximum carpool size grew. Complete results are available in (Miklas-Kalczynska & Kalczynski, 2021).

The above findings provide the answer to the first research question of this dissertation:

Table 1.7: TFC carpool system-wide savings
Source: (Miklas-Kalczynska & Kalczynski, 2021)

	TFC		TFCH		TFC/TFCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	31.36%	32.89%	40.79%	44.40%	40.74%	44.40%
3	37.37%	38.16%	52.69%	55.47%	52.91%	55.50%
4	37.98%	38.32%	57.50%	60.69%	57.50%	60.69%
5	37.98%	38.32%	59.95%	63.19%	59.95%	63.19%

How to shift focus from global policy goals to individual carpool participant's perspective and will this shift increase carpool participation? (see Section 1.5). The decentralized solution to carpooling with optional hubs shifts focus from global to individual, and improves carpool participation.

Result 2: Iterative improvement and polygonal protected areas in obnoxious facility location improve the effectiveness of location models.

In the protected areas study, computational experiments were run on both, generated and real-world instances. The results show that the iterative approach developed in the study leads to much better solutions than the point-based optimization.

One hundred generated instances included a 100 × 100 square with randomly generated protected areas. Both the maximin and the cooperative versions of the problems were solved on these instances, with the number of facilities ranging from two to ten. This resulted in the total of 900 instances studied. The table presented in Table 1.8 reports average percentage of improvement obtained by iterative approach as compared to the centroid approach on simulated instances.

When it comes to the maximin model, where minimum distance to protected areas is maximized, the overall improvement was 225.6% for 610 (67.7%) problem instances for which a feasible solution was obtained with both methods. In the cooperative model, where maximum nuisance for protected areas is minimized, the overall improvement was 34.3% for 674 (74.9%) instances.

The iterative method was able to obtain a feasible solution for additional 213 (23.67%) instances in case of the maximin model, and 86 (9.56%) instances in case of the cooperative model. Except for the last row, which is based on a small number of instances, the overall improvement increases as protected areas cover more and more of the square.

When protected areas cover from 20% to 39.99% of the area, compared to the centroid-based approach, the iterative approach to the maximin model locates the nearest obnoxious facility 1.5 to 24 times farther from the protected area, while the iterative approach to the cooperative model reduces the overall nuisance on the most-affected point by 51–96%.

Southwest part of the state of Colorado was selected as a real-life example. 133 protected

Table 1.8: Average percentage of improvement by the percentage of the total area covered by the protected areas — iterative versus centroid approach on simulated instances.
Source: (Miklas-Kalczynska & Kalczynski, 2024)

Maximin: average improvement (%)—iterative versus centroid on simulated instances

Prot. areas	*p*									Overall
	2	3	4	5	6	7	8	9	10	
0–9.99%	4.1	3.5	5.3	6.0	4.4	11.4	9.8	8.7	9.6	7.0
10–19.99%	17.4	24.6	41.8	31.5	44.6	62.9	138.7	182.7	193.7	79.8
20–29.99%	448.0	389.7	479.3	159.0	308.5	328.8	2474.2	542.1	149.5	544.3
30–39.99%	534.5	696.0	499.5	184.5	217.7	316.0	1391.4		379.8	559.3
40% and more	54.1	121.2								76.5
Overall	255.4	247.8	218.4	71.8	118.3	119.6	702.0	188.6	95.0	225.6

Cooperative: average improvement (%)—iterative versus centroid on simulated instances

Prot. areas	*p*									Overall
	2	3	4	5	6	7	8	9	10	
0–9.99%	4.9	7.2	7.5	6.8	4.8	17.1	10.6	6.2	4.9	7.8
10–19.99%	16.8	11.8	18.9	13.6	31.3	21.3	1.7	1.0	32.8	16.9
20–29.99%	51.4	56.4	63.2	63.2	60.8	59.2	70.5	57.2	74.5	60.9
30–39.99%	74.4	70.2	81.6	79.8	73.8	89.3	38.8	52.6	96.2	72.6
40% and more	38.2	26.8	43.1	91.0	96.0	96.8	49.9	99.9	6.8	55.1
Overall	36.7	35.9	37.9	33.6	37.2	37.1	25.9	25.2	35.6	34.3

areas were identified using publicly-available geo-polygon data, resulting in 3075 vertices. Even after the necessary adjustments, 4.6% of the centroids were located outside of the boundaries of the corresponding areas. Figures 1.9 and 1.10 show sample results for both models. The circles indicate the located facilities. In case of the cooperative model, the radius of each circle is proportional to the weight of the corresponding facility. The reason why there are only eight distinct facilities in Figure 1.10 is that three areas are co-located in the lower left corner.

In the minimax example, centroid-based optimization failed to produce a feasible solution, and the iterative approach yielded the maximum minimum distance to the most-affected area over 17 times larger (7.6235 mi.) than the solution based on polygon vertices (0.4419 miles).

In the cooperative example, the iterative approach produced the objective that was over 172 times better than the centroid-based result and 4.5 better than the vertex-based result.

Table 1.9 presents the results for both models. Mapping software was used to obtain the original 133 centroids (one per each protected area). Center of gravity formula was applied to compute the secondary 279 centroids (one per each simple polygon). The results for the maximin model show that the new iterative heuristic found the best area-based objective (the

Figure 1.9: Maximin iterative optimization results for 14 facilities and 50-mile minimum distance between the facilities.
Source: (Miklas-Kalczynska & Kalczynski, 2024)

Figure 1.10: Cooperative iterative optimization results for 10 facilities (8 distinct).
Source: (Miklas-Kalczynska & Kalczynski, 2024)

maximum minimum distance from an obnoxious facility to a protected area) for all analyzed cases. The centroid-based results were improved for all numbers of facilities (p). For a larger number of points, our approach resulted in the same objective as the point-based approach in four cases. For $p = 12$, only our method was capable of finding a feasible solution, and the objective was improved for $p = 4$ and $p = 14$. The objectives reported for the cooperative model are the area-based objectives multiplied by 10 000. They show the total negative effect of all p facilities on the most-affect point. The iterative approach was superior in all cases. In almost all other cases, our approach improved the point-based objectives. Only for $p = 2$, our method yielded the same objective as the point-based method with the high number of points.

Table 1.9: Maximin and Cooperative results for SW Colorado.
Source: (Miklas-Kalczynska & Kalczynski, 2024)

Maximin results for SW Colorado

p	Point-based optimization						Iterative optimization		
	133 centroids		279 centroids		3075 vertices		279 polygons		
	Obj.	Time (s)	Obj.	Time (s)	Obj.	Time (s)	Obj.	Iters.	Time (s)
2	0.8639	4.46	14.4515	2.79	**22.8937**	40.83	**22.8937**	1[a]	40.83
4	4.3765	8.46	8.7879	17.29	11.0795	505.31	**18.0710**	2	1171.16
6	4.3199	49.28	7.4957	156.15	**10.6417**	6211.34	**10.6417**	1[a]	6211.34
8	0.9215	78.98	1.8812	413.63	**9.3575**	13,740.30	**9.3575**	1[a]	13,740.30
10	2.1605	235.38	INSIDE	640.58	**8.9262**	35,684.20	**8.9262**	1[a]	35,684.20
12	1.6756	411.59	INSIDE	1651.76	INSIDE	42,019.00	**8.4077**	7	340,925.00
14	INSIDE	600.71	INSIDE	1672.73	0.4419	92,977.60	**7.6235**	15	1,334,468.17

[a]The first iteration is equivalent to point-based optimization on 3075 vertices
The best-known objective values are emphasized

Cooperative (minimization) results for SW Colorado

p	Point-based optimization						Iterative optmization		
	133 centroids		279 centroids		3075 vertices		279 polygons		
	Obj.	Time (s)	Obj.	Time (s)	Obj.	Time (s)	Obj.	Iters.	Time (s)
2	13.3180	2.53	24.5783	4.66	**13.2579**	913.70	**13.2579**	1[a]	913.70
4	2916.5800	6.44	208.7210	12.36	162.4499	1443.59	**68.9154**	3	4395.60
6	428.2080	8.72	163.4090	46.30	134.9716	2249.89	**99.7552**	2	5033.24
8	354.0690	18.26	352.6990	47.51	300.4981	2384.59	**144.8193**	2	4234.73
10	27,718.3000	26.85	2035.1900	77.55	733.4072	3487.06	**160.9980**	7	23,486.40
12	2623.0200	42.48	279.4490	112.46	INSIDE	3774.56	**222.9809**	14	64,052.90
14	364.3410	37.63	626.7380	124.96	693.7988	7634.78	**329.2254**	13	113,096.00

[a]The first iteration is equivalent to point-based optimization on 3075 vertices
Objective values multiplied by 10,000 and the best-known objective values are emphasized

SNOPT (Gill et al. 2005) starting from the same 100 random solutions was used for both point-based and iterative approaches. The results show that the approach based on iterative application of an efficient local non-linear solver can indeed facilitate solving an obnoxious planar facility location problem involving polygonal protected areas. It delivers solutions that are more effective than the point-based models, hence providing an answer to the second research question: *How to improve the effectiveness of the optimization models when polygonal protected areas are present?* (see Section 1.5). The optimization models become more effective when the iterative improvement technique, combined with polygonal representation of protected areas, is used. The CPU processing times for the iterative method are offset by the fact that the point-based method was unable to find satisfactory solutions (or found no solutions at all for some of the cases). CPU times can be shortened by adjusting the optimization parameters.

Result 3: Trajectory approach can be applied to solve complex location problems.

The competitive location model was solved for the problem of locating a mall facility in Orange County, California (T. Drezner, 2006), which is a competitive facility location problem based on the classical Weber problem. Seven instances, each based on a different attractiveness level, were solved in Mathematica 13 (Wolfram Research, Inc., 2021) by Nelder-Mead (a direct search methods for global optimization) and the trajectory method developed in this dissertation. The attractiveness levels of the existing malls were used. They resulted in different locations for the new mall.

Table 1.10: Calculated locations and percent market shares.
Source: (Z. Drezner & Miklas-Kalczynska, 2023)

	Best	Nelder-Mead (One Run)			Nelder-Mead (25 Runs)			Trajectory		
A	known	x	y	M	x	y	M	x	y	M
0.177	**3.098%**	20.172	10.682	2.139%	5.369	25.025	**3.098%**	5.343	25.024	3.094%
0.595	**9.087%**	19.380	10.846	5.651%	7.004	24.495	**9.087%**	7.004	24.495	**9.087%**
1.011	**13.917%**	18.742	11.452	8.163%	7.288	24.157	**13.917%**	7.288	24.157	**13.917%**
1.154	**15.388%**	18.557	11.638	8.899%	7.286	23.988	**15.388%**	7.286	23.988	**15.388%**
1.529	**18.918%**	7.314	23.127	**18.918%**	7.314	23.127	**18.918%**	7.314	23.127	**18.918%**
2.367	**25.473%**	7.458	22.839	**25.473%**	7.458	22.839	**25.473%**	7.458	22.839	**25.473%**
2.484	**26.271%**	7.511	22.789	**26.271%**	7.511	22.789	**26.271%**	7.511	22.789	**26.271%**

The bold values are the best known results obtained for each row.

Table 1.10 shows the results obtained by a single run of Nelder-Mead for each instance, along with the best result obtained by solving each instance 25 times. Note that the problem is non-convex, so Nelder-Mead acts as a local rather than a global solver. The trajectory approach does not involve a random component, therefore it was run only once. The CPU times were not reported because the environments used were not comparable.

For six out of the seven instances the trajectory method obtained the best known solution. A very close value of the market share was found for the seventh instance. Decreasing the step size (h) in the Runge–Kutta method will result in converging to the best known value.

A single application of Nelder-Mead resulted in the best known solutions found in three out of seven instances, while in the remaining four cases the market share was significantly lower, located in a different region of Orange County. When the number of Nelder-Mead runs was increased to 25 (each with a random start), the best known solution was found at least once for all instances.

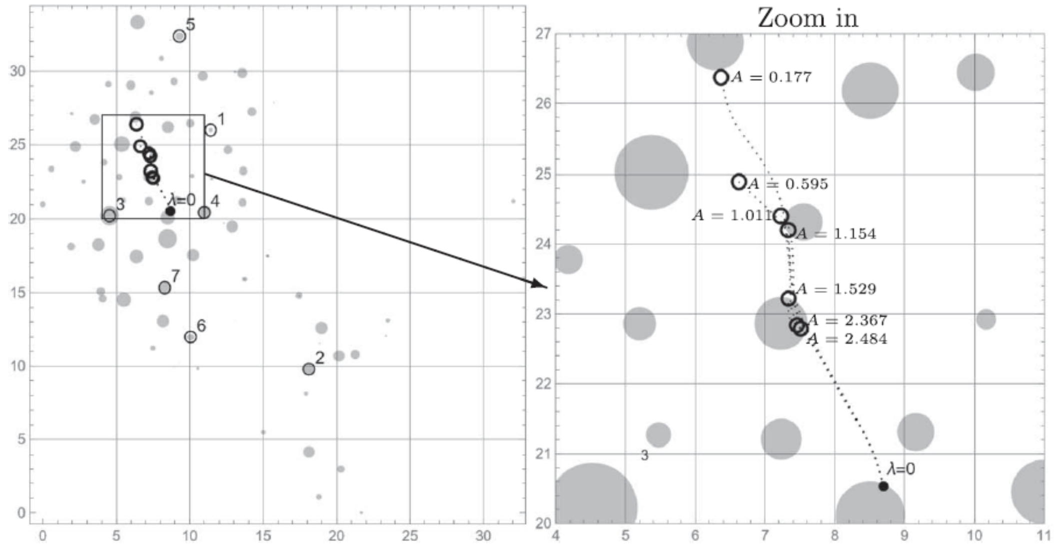

Figure 1.11: Trajectories for seven instances.
Source: (Z. Drezner & Miklas-Kalczynska, 2023)

Figure 1.11 shows the trajectories for all seven instances. Grey circles represent demand points. Their sizes are proportional to the corresponding population counts. The seven existing malls are depicted with black circles and numbered. All trajectories start at $\lambda = 0$. The locations of the new facilities placed at the end of their respective trajectories are marked with empty circles with the attractiveness levels shown next to each of them.

For small values of λ the trajectories almost coincide. Larger attractiveness values (A) result in shorter trajectories. Consequently, for larger values of A, the location of the new facility is closer to the $\lambda = 0$ location. All seven instances resulted in the locations of a new facility in the same region of the county, depicted in the square that is magnified to the right of the figure. The four single-run Nelder-Mead locations with significantly lower market share (not shown) were located in a different region, near the existing facility 2.

The obtained results show that the trajectory method can be applied to solve a competitive location problem with good results, which is an answer to the third research question of this dissertation: *How to solve unconstrained non-linear location problems with differentiable objectives, overcoming the limitations of local solvers?* (see Section 1.5). As long as the analytical derivatives and their initial values can be found, the trajectory method can be applied to many complex location problems.

Result 4: A new multi-purpose shopping model for maximizing market share in competitive facility location.

Simulation experiments were run on randomly generated instances with up to 15 facilities and up to 5000 demand points. The experiment design is based on instances solved in related papers (T. Drezner et al., 2023; Kalczynski et al., 2024). The SNOPT solver with 100 random starts was used for each instance.

Initially, the proportions of trips from (Federal Highway Administration, 2017) were assumed, with 75% of 1P, 20% of 2P, and 5% of 3P trips. In addition, the proportions of 2P trips were split evenly between the two trip options (i.e., two different NCF types). The comparisons were conducted between the 1P, 2P, and 3P models on the same instance. The reported MP model market shares were the best-known solutions to the model instances with 100% MP trips.

The market share improvements between the 1P and the 2P model reach 178.99% and 180.8% between the 1P and 3P trips. The single-facility 3P model improves the 2P model slightly, but the improvements become more prominent when more facilities are added (see Table 1.11).

Table 1.11: Model comparisons for n=100 demand points assuming 100% MP trips in the 2P and 3P models.
Source: (Miklas-Kalczynska, 2024)

	n = 100, 3P obj. based on			Relative impr. in obj.		
p	1P	2P	3P	2P/1P	3P/1P	3P/2P
1	0.0934	0.2606	0.2623	178.99%	180.83%	0.66%
2	0.1938	0.4064	0.4110	109.69%	112.04%	1.12%
3	0.2784	0.5187	0.5367	86.32%	92.79%	3.48%
4	0.3993	0.5474	0.6430	37.10%	61.03%	17.46%
5	0.4121	0.6543	0.6810	58.77%	65.26%	4.09%
10	0.6404	0.7264	0.8086	13.43%	26.27%	11.32%
15	0.6970	0.8064	0.8633	15.70%	23.86%	7.06%

Figure 1.12 shows the locations of the solutions to the single-facility 1P, 2P, and 3P models for different configurations of MP proportions. The magnified areas show larger concentrations of solutions. Selected 3P locations are labeled. They are the solutions that yielded the largest increase in market share captured over 2P and 1P models. The result suggest that when MP trips exist, different services tend to locate close to each other, which confirms earlier findings (T. Drezner et al., 2023; Kalczynski et al., 2024; Marianov et al., 2018).

Finally, the experiments were extended to different combinations of proportions. The extensive results are reported in the paper (Miklas-Kalczynska, 2024). For p = 1, 2, 3, 4, and 5 show the maximum improvement of the 3P model over the 1P model of 180.83%, 112.04%,

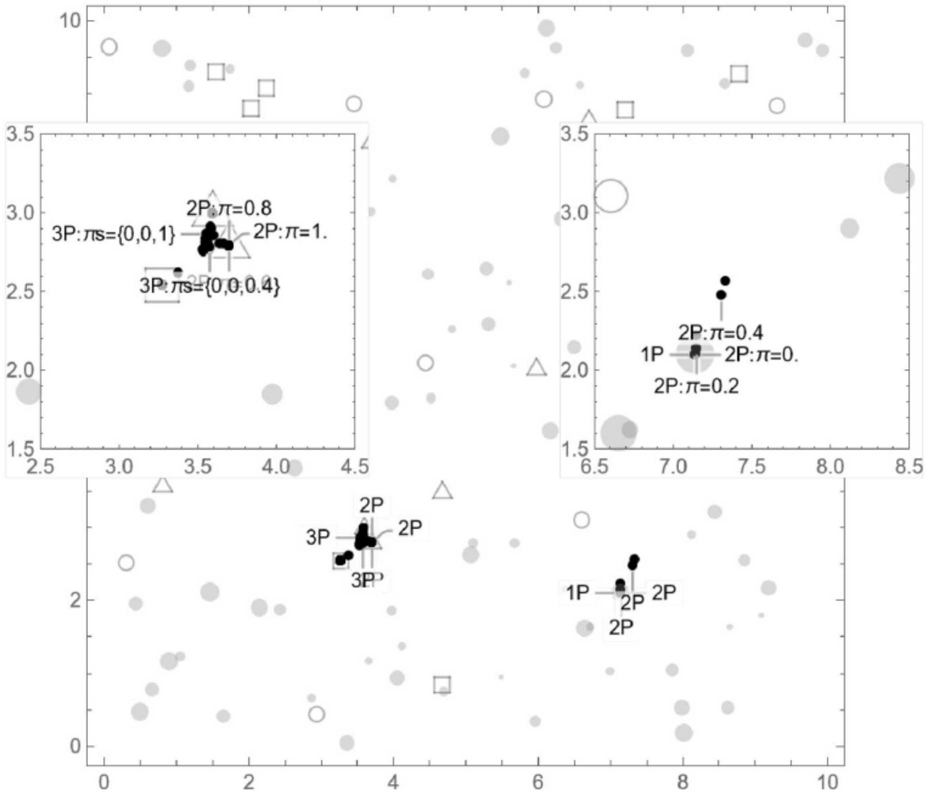

Figure 1.12: Locations of the solutions to 1P, 2P, and 3P models with different proportions of MP trips when locating a single chain facility.
Source: (Miklas-Kalczynska, 2024)

92.79%, 64.23%, and 65.26% respectively. The corresponding maximum improvements of the 3P model over the 2P model were 15.6%, 16.24%, 26.49%, 25.27%, and 20.93%. When the number of added facilities increases, these gains tend to diminish. This may be due to cannibalization of the market share in which chain facilities compete against each other because they compete for a fixed demand (Z. Drezner & Eiselt, 2024).

The average improvement over the 1P model was 42.99% for the 2P model and only 6.87% for the 3P model. In addition, changes in locations for different proportions of MP trips were small, which suggests that expanding the model beyond three purposes may not be justifiable.

New formulation of the MP model made it suitable for computational optimization. Application of an efficient local non-linear solver produced valuable results, hence providing the answer to the fourth research question posed in this dissertation: *Considering the possibility of multi-purpose customer behavior, how to locate a new facility or facilities so that the chain captures the maximum possible market share?* (see Section 1.5). The new model, which factors in a possibility of more than two stops during a shopping trip, is a better representation of customer behavior than the previous models and can capture the maximum possible market share. It can also provide the chain with valuable insights about the best new locations.

1.8 Conclusions

The contributions of this dissertation relate to a group of problems that recently have been attracting a lot of attention from the facility location research community. Each of these problems is also relevant to practice and has important managerial implications. These problems share the same characteristic: due to their high complexity, they are not possible to solve without novel computational optimization methods. Applying such methods however, requires creating new formulations and innovative solution techniques. Following is a summary of each of the contributions, along with encountered limitations and future research avenues.

Carpooling

The carpooling problem studies introduce tools for optimizing the existing carpooling systems. These findings, made possible with novel computation optimization techniques, can facilitate the development of more effective and sustainable uses of transportation resources.

The original decentralized heuristic solution introduced in (Kalczynski & Miklas-Kalczynska, 2019) models a self-organizing carpooling system, based on the preferences of individual participants. The heuristic is able to achieve system-wide savings that are comparable to a centralized system, yet it is well suited to promote carpool participation. This idea provides an alternative to the decision-makers who, instead of having to design additional incentives to ensure a stable carpooling system, can introduce a carpool system that is perceived as a fair and advantageous solution for a larger number of participants.

The carpool with hubs study (Miklas-Kalczynska & Kalczynski, 2021) reveals that the introduction of hubs not only improves system-wide savings from carpooling (Stiglic et al., 2015), but also that introducing meeting hubs as an option can lead to further improvements. The original efficient carpool enumeration technique enables solving optimization problems in reasonable time for any type of carpool models and their combinations. Managerial implications involve an ability to build better carpooling systems that improve carpool participation. The societal benefits include reduced carbon footprint and reducing traffic congestion. Consequently, organizations can demonstrate their commitment to environmental issues and care for their employees. Individuals benefit by having their preferences met, which leads to a more comfortable and efficient commute.

There are certain practical limitations to both studies. It is assumed that all participants are in possession of a car and that the maximum number of seats in a vehicle is limited to five. Participants are not able to switch carpools on different days. In the long run, it is assumed that the driving is evenly distributed among all participants. Also, our solution does not consider bargaining or the possibility for the participants to be compensated for giving up their top choices.

Another limitation of the first of the carpool papers (Kalczynski & Miklas-Kalczynska, 2019) was remedied in the following carpool with hubs study (Miklas-Kalczynska & Kalczynski, 2021).

The disadvantage of the first enumeration technique was the fact that it was expensive in terms of the allocation of computational resources, which might be prohibitive for larger numbers of origins or available passenger seats.

Future research could investigate sensitivity of the solution to changes in problem parameters. Weighted average savings could be used in the self-organized model and carpool participants could be able to use some of their driving days as an incentive to attract others to carpool with them. Moreover, fairness in carpooling could be approached from the economic games theory standpoint by considering the distance each carpool participant drives rather than the number of times they drive. Also, future extensions could attempt to incorporate various tie-breaking techniques for the decentralized approach.

Finally, the introduced model is an important consideration for the companies developing autonomous car fleets (e.g., Waymo, Tesla). The impact of this emerging technology, however, has not yet been investigated, which creates another potential future research avenue. Such an impact could be both positive and negative. Potential positive changes might include increased participation rates resulting from an improved safety, convenience and reliability due to removing human drivers from an arrangement. Fewer accidents, timely pickups, and an ability to navigate complex routes, can reduce the burden on carpool participants. Moreover, self-driving cars could make carpool participation possible for those who are unable to drive, such as seniors, people with disabilities, etc. Potential negative consequences include safety and privacy concerns, especially when the carpools involve minors. User behavior and preferences is one of the crucial aspect in carpooling. It remains to be seen how people respond to self-driving carpool opportunities.

Obnoxious Facility Location with Protected Areas

The work included in the dissertation (Miklas-Kalczynska & Kalczynski, 2024) introduces an original iterative computational optimization model for planar multiple obnoxious facility location with protected areas represented as convex and non-convex polygons, which also works for any closed shape. These models, and the corresponding solution techniques, are the main contributions of this paper. Managerial implications involve a better and more effective decision-making process. Since the study shows that the most affected point will always be on the boundary of the protected area, the task of locating obnoxious facilities is made easier. Other managerial implications pertain to regulatory compliance. Violations of environmental regulations may lead to significant costs and worsen community relations. Reducing the negative impact of obnoxious facilities, for both the environment and the communities in proximity of the facilities, has become a crucial factor in location decisions. Mitigating the risk of potential legal issues or complaints is a factor influencing operational efficiency. In today's world, companies are expected to demonstrate their dedication to the idea of reducing their environmental impact. Decision-makers must also show their concern for the residents' quality of life, especially when it comes to such long-term commitments as the location decisions.

The original iterative approach considers the negative impact of an obnoxious facility on the entire protected regions rather than only on its point-based representation. The formulation leverages a conjecture that has become a recently-proven theorem (Coletti et al., 2024) that greatly simplifies the optimization process by demonstrating that in 2D and 3D inverse-square models, the most affected point will always be on the boundary of the protected area, and never inside of it. This original result is a major contribution to management science.

Novel computational optimization techniques are applied to run computational experiments on generated and large-scale real-world instances. The results show that the iterative approach provides better solutions than point-based optimization, which has implications for the location theory and practice.

A limitation of the method is the fact that the existing solvers can solve only small problem instances to optimality. Larger, practical instances can be solved by means of multi-start local search methods. Consequently, we can only say that our method will yield a solution that is never worse than the one obtained through a point-based approach. The trade-off between the length of the optimization process and the quality of the obtained solution presents a challenge for decision-makers in this type of approach.

Facilities in location analysis are traditionally represented as points. Representing them as polygons could be an interesting future research avenue to investigate but it would fall outside of the location science field. In addition, sensitivity analysis of the solution in regards to the number of starting points and the stopping criteria could be conducted.

Trajectory Approach

The major contribution of the work related to the trajectory approach is proposing an original set of techniques for applying this method to solving complex optimization problems in the field of location analysis. The benefits of using this method are not restricted to the location theory, but can be applied to any unconstrained optimization problems with a differentiable objective function. Managerial implications of this method stem from its relative ease of use, which allows for saving resources while speeding up the decision-making process. Since the method is purely analytical, it can often be implemented with the use of a common spreadsheet tool, without a need for costly commercial solvers. Before the trajectory method can be applied, however, a problem at hands needs certain adjustments. The work in (Z. Drezner & Miklas-Kalczynska, 2023) shows how to reformulate common location problems to make them suitable for the method. To demonstrate the benefits of the trajectory method, computational experiments were run for the problem involving the location of a new shopping mall in Orange County, California, a Weber-based competitive facility location problem.

Computational optimization played a crucial role in this research. It enabled the trajectory approach to be added to the field as an efficient method for solving problems with defined convexity or generating starting solutions for non-convex problems. The quality of a starting solution has been shown to greatly improve the optimization results.

The fact that explicit derivatives of the objective function have to exist is an obvious limitation of the trajectory method. Moreover, certain objective functions, although differentiable, can prove too complex for the derivatives to be computed in reasonable time.

Future research includes applying the trajectory approach to a variety of unconstrained optimization problems, such as the multi-purpose problem (Miklas-Kalczynska, 2024), and comparing the results with those obtained by other solution techniques.

Multi-purpose Shopping in Competitive Facility Location

This work is the first study in the area of competitive facility location that considers more than two stops in multi-purpose shopping trips. The original models introduced in (Miklas-Kalczynska, 2024), which assume various proportions of single-and multi-purpose trips, are formulated for both, single- and multi-facility scenarios.

In addition, a novel comparison method is developed to compare the results. The study shows that the multipurpose model with more stops captures at least as much market share as a model with fewer stops and, in most cases, yields substantial gains. The results confirm earlier findings that proximity to non-competing facilities offering non-competing products or services can influence customers' decision whether to patronize the chain facility (Eaton & Lipsey, 1982).

Managerial implications of being able to better locate a new chain facility or facilities are significant. The opening a new store in a spot that is convenient for customers shopping not only for goods or services offered by the chain, but running multiple errands, can increase market share and can help the chain gain competitive advantage.

Computational optimization techniques employed in this and related research included in the dissertation were indispensable in extending the multi-purpose scenario beyond two stops, which is arguably a closer representation of customers' shopping habits. Also, the results indicate that due to diminishing returns, the 3P model with a mix of 1P, 2P, and 3P trips seems to be sufficient to reflect the reality and extending it further may not be justifiable.

Arbitrary assignments of the proportions for trips with different numbers and combinations of stops is a limitation of this study. Future research could incorporate a survey or approximate proportions instead. Some of the proportions could become variables having particular constraints, e.g., staying within a 5% margin.

This study is limited to shopping for non-competing goods and services. An interesting future research avenue could involve shopping for substitute goods instead where comparison-shopping takes place and the customer may choose to return to previously visited locations (Marianov et al., 2020).

To sum up, this collection of thematically cohesive articles introduces the original solutions to each of the presented problems. These solutions in the field of location analysis, obtained through computational optimization methods, techniques, and tools, close the corresponding research gaps for the studied areas and constitute significant contributions to the field of location analysis, as well as to a broader field of management science. The included papers have opened new research avenues, inspired other researchers, and have been referenced in various publications. Their findings provide useful insights for strategic planning and decision-making. Recent trends suggest that location is becoming one of key factors in corporate strategy worldwide (Florida & Adler, 2022). Smart location decisions can enhance the firm's competitiveness and efficiency and bring about long-term success and profitability. These decisions, however, because of their long-lasting consequences and high costs of potential relocations, require quantifiable objectives, constraints, and outcomes. Not surprisingly, location analysis has become one of the key tools in management. Trends such as the transition towards a dynamic rather than static efficiency, as well as the persistently growing dominance of the knowledge-based economy over the industrial one, indicate that in years to come, locational decisions can become more and more important for strategic decision-making and computation optimization will be indispensable in these efforts.

1.9 List of Component Articles

1. Kalczynski, P., Miklas-Kalczynska, M. (2019) *A decentralized solution to the car pooling problem*, International Journal of Sustainable Transportation, Taylor & Francis, 13(2), pp. 81–92,
   https://doi.org/10.1080/15568318.2018.1440674
   [70 points on the list by the Ministry of Science]

2. Miklas-Kalczynska, M., Kalczynski, P. (2021) *Self-organized Carpools with Meeting Points*, International Journal of Sustainable Transportation, Taylor & Francis, 15(2), pp. 140-151,
   https://doi.org/10.1080/15568318.2019.1711468
   [70 points on the list by the Ministry of Science]

3. Miklas-Kalczynska, M., Kalczynski, P. (2024) *Multiple Obnoxious Facility Location - the Case of Protected Areas*, Computational Management Science, Springer Nature, 21(1), p. 23,
   https://doi.org/10.1007/s10287-024-00503-4
   [70 points on the list by the Ministry of Science]

4. Zvi Drezner, Malgorzata Miklas-Kalczynska (2023), *Solving non-linear optimization problems by a trajectory approach*, IMA Journal of Management Mathematics, Oxford University Press, 35(3), pp. 537–555,
   https://doi.org/10.1093/imaman/dpad011
   [40 points on the list by the Ministry of Science]

5. Miklas-Kalczynska, M. (2024) *Extensions to Competitive Facility Location with Multi-purpose Trips*, Networks and Spatial Economics, Springer Nature, 24, pp. 565-588, https://doi.org/10.1007/s11067-024-09625-3
   [100 points on the list by the Ministry of Science]

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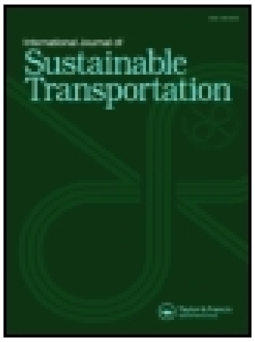

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A decentralized solution to the car pooling problem

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ABSTRACT
Existing carpool optimization techniques based on the centralized approach serve policy-makers' goals, but neglect the realities of participants. Moreover, absent strict enforcement, participants often ignore centralized solutions and maximize their own savings. We present a new heuristic, formulated and tested on real-world, and simulated car pooling problem instances, that mimics a decentralized carpool self-organization process. Our findings reveal system-wide savings similar to centralized models, and a potential strategy for improving carpool utilization.

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1. Introduction

In general, the car pooling problem (CPP) can be defined as sharing a private vehicle by a certain number of users to reach one or more destination points. In this paper, we consider two common types of carpools:

1. To/from carpool (TFC) in which the vehicle operator picks up passengers on the way to a common destination (e.g., a workplace) and later drops them off at their locations before returning to the origin, and
2. Pick up/drop off carpool (PDC) in which the vehicle operator picks up passengers on the way to a common destination (e.g., school), drops them off at the destination, and returns to the origin (or goes to the destination to pick up the passengers and drops them off on the way back to the origin).

In each of these carpools, participants take turns in using their vehicles to complete the assignment.

In the subject literature, e.g., (Baldacci, Maniezzo, & Mingozzi, 2004; Calvo, de Luigi, Haastrup, & Maniezzo, 2004; Ferrari, Manzini, Pareschi, Persona, & Regattieri, 2003; Yan & Chen, 2011), carpool optimization techniques are usually based on the centralized approach, such as the minimization of the system-wide total distance traveled. While such an approach serves policy-makers' goals (e.g., the reduction of pollution or traffic), it may produce unsatisfactory results for the participants (Agatz, Erera, Savelsbergh, & Wang, 2012). Moreover, absent strict enforcement, such centralized solutions may prove to be unstable because participants will try to maximize their individual savings.

To illustrate the differences between decentralized and centralized solutions, let us consider a simple problem with three origins f_1, f_2, f_3 and a common destination z. Let us assume that each origin has one vehicle with an operator and only one seat available for a passenger. There is only one passenger to be picked up from each origin. Consequently, the only possible car pooling arrangements are $\{f_1, f_2\}$, $\{f_2, f_3\}$, and $\{f_1, f_3\}$. The distances are shown in Figure 1.

The baseline round trip commute distance for the participant originating from f_1 is 6 units ($f_1 \rightarrow z \rightarrow f_1$). In the TFC arrangement with a passenger from f_2, the round trip distance increases to 10 units ($f_1 \rightarrow f_2 \rightarrow z \rightarrow f_2 \rightarrow f_1$). However, participants in this carpool will drive every other day, so the *average* carpool distance for the participant from f_1 is 5 units. The baseline round trip commute distance for the participant originating from f_2 is 8 units ($f_2 \rightarrow z \rightarrow f_2$). When car pooling to and from the destination with a passenger from f_1, the distance does not change ($f_2 \rightarrow f_1 \rightarrow z \rightarrow f_1 \rightarrow f_2$). However, the *average* carpool distance for the participant from f_2 is 4 units. In the PDC arrangement with the participant commuting from f_2, the round trip distance for the participant fromf_1 is 8 units ($f_1 \rightarrow f_2 \rightarrow z \rightarrow f_1$), and the average commute distance is 4 units (it is also 4 units for the participant from f_2). Potential carpool configurations with the corresponding average round trip distances are presented in Table 1.

The centralized solution to the three-origin instance is $\{f_2, f_3\}$, with the system-wide total commute distance of 16.12 (15.12) units for the TFC (PDC) model and 5.00 (6.00) units of system-wide savings, as compared to the total baseline distance. The centralized solution, however, is not the first choice of any participant. The decentralized solution to the three-origin instance is $\{f_1, f_2\}$, which provides the minimum average distance for both participants. With the system-wide total distance of 17.25 (16.25) units, the decentralized solution still provides savings of 5.00 (6.00) units and it does not require additional incentives to coerce participants commuting from f_1 and f_2 to sacrifice their individual savings for the common good.

The rest of the paper is organized as follows. The carpool optimization literature review is presented in the next section. Section 3 presents the formal model of the car pool problem and proposed solution techniques. Computational experiments

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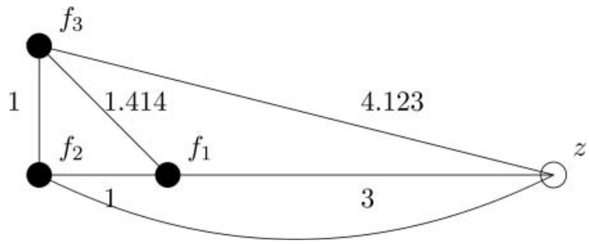

Figure 1. A three-origin car pooling problem instance.

involving real-world and simulated problem instances are presented in Section 4, and followed by the summary of the results.

2. Background

The majority of research dealing with the car pooling problem focuses on centralized solutions, aimed mostly at such environmental benefits as reducing traffic congestion or lowering fuel emissions (Agatz, Erera, Savelsbergh, & Wang, 2012; Ferrari, Manzini, Pareschi, Persona, & Regattieri, 2003). In the most popular approach, a carpool is usually considered as a transportation service organized by a company for its employees to encourage them to share a ride to and/or from work and—as a consequence—reduce the number of cars on the road, gasoline consumption, pollution, traffic, etc.

The centralized approach to the car pooling problem assumes that global public policy objectives will be sufficient motivators for the individuals to participate in the car pooling systems. These factors however have proven ineffective in North America, where—after a short period of carpool popularity in 1970s—the practice declined considerably by 1990s, despite the introduction of favorable government incentives (Ferguson, 1997; Li et al., 2007). According to the *U.S. Census Journey to Work Data*, carpool participation went down from 19.7% in 1980 to 13.4% in 1990 and in 2015 only 11% (13.5 million out of 123.3 million) of those who drove to work by car, truck, or van, carpooled (U.S. Census Bureau, 2015). While the popularity of all other alternatives to driving alone fell down in the eighties, carpool's decline was deeper and faster (Ferguson, 1997).

Studies aimed at identifying factors influencing carpool participation have been based mostly on survey research or case studies, often offering conflicting results. In general, researchers name demographic, economic, and socioeconomic factors that motivate people to carpool (Ferguson, 1997). In their meta-analysis of the field literature, Neoh, Chipulu, & Marshall (2015) distinguish internal and external factors. Internal factors are individual characteristics, such as demographics or subjective preferences, while external factors involve policy measures, available incentives, or various situational aspects, such as the availability of public transportation.

In general, socio-demographic factors are not believed to have a strong influence on car pooling decisions (Canning, Hughes, Hellawell, Gatersleben, & Fairhead, 2010; Ferguson, 1997; Teal, 1987), although it was shown that, in the U.S., younger people (Garling, Garling, & Johansson, 2000) and immigrants (Blumenberg & Smart, 2010; Cline, Sparks, & Eschbach, 2009) are more likely to carpool.

Car pooling is more popular when public transportation is not available, especially when longer distances are involved (Eriksson, Friman, & Garling, 2008). Whether longer travel distances encourage or discourage car pooling is unclear, as the results of the studies are contradictory (Cervero & Griesenbeck, 1988; Jacobson & King, 2009; Kocur & Hendrickson, 1983).

Travel time is another factor of importance in car pooling decisions. On one hand, carpool can save time in the long run (Giuliano, Levine, & Teal, 1990). On the other hand, travel time can extend due to necessary detours, which can potentially discourage commuters from participating (Tsao & Lin, 1999). According to Rietveld, Zwart, Van Wee, & van den Hoorn (1999), car pooling could increase commuting time by up to 17%. In some countries however (such as the U.S.), the ability to use the carpool lane can greatly reduce travel time and seems to be one of the major factors encouraging carpool participation (Li et al., 2007).

Researchers generally agree that psychological factors are dominant in car pooling decisions (Gardner & Abraham, 2007). As typical factors they name convenience (Horowitz & Sheth, 1977), privacy and comfort (Correia & Viegas, 2011; Dueker, Bair, & Levin, 1977), lack of control (Huang, Yang, & Bell, 2000; Ozanne & Mollenkopf, 1999; Stradling, Meadows, & Beatty, 2000), necessity to socialize (Bonsall, Spencer, & Tang, 1984; Gardner & Abraham, 2007), differences in cultural background or values (Charles & Kline, 2006; Morency, 2007). Not surprisingly, however, one of the most important incentives is the willingness to reduce cost (Canning, Hughes, Hellawell, Gatersleben, & Fairhead, 2010; Cools, Tormans, Briers, & Teller, 2013; DeLoach & Tiemann, 2012; Horowitz & Sheth, 1977; Washbrook, Haider, & Jaccard, 2006).

The car pooling problem is considered one of the variants of the more general class of ride-sharing problems, in particular the "single driver, multiple rider arrangement" (Agatz, Erera, Savelsbergh, & Wang, 2012; Furuhata et al., 2013). Typically, the objective of the car pooling problem is either to maximize

Table 1. Carpool arrangements for the three-origin instance.

		Average distance (TFC)			Average distance (PDC)		
Origin	Baseline distance	$\{f_1, f_2\}$	$\{f_2, f_3\}$	$\{f_1, f_3\}$	$\{f_1, f_2\}$	$\{f_2, f_3\}$	$\{f_1, f_3\}$
f_1	6.00	5.00*	6.00	5.54	4.00*	6.00	4.27
f_2	8.00	4.00*	5.12	8.00	4.00*	4.56	8.00
f_3	8.25	8.25	5.00	4.41*	8.25	4.56	4.27*
Total	**22.25**	**17.25**	**16.12**†	**17.95**	**16.25**	**15.12**†	**16.54**
Savings	NA	5.00	6.13	4.30	6.00	7.13	5.71

*Participant's first choice.
†Policy-maker's first choice.

the number of participants, to minimize the total distance driven, or to minimize the total travel time. Each of the participants has their own preferences or constraints as to the earliest time they want to leave home or arrive at the destination, and maximum time they are willing to travel. Classification of the optimization literature according to the objectives and constrains can be found in Agatz, Erera, Savelsbergh, & Wang (2012).

Baldacci, Maniezzo, & Mingozzi (2004) separate the *to-work* carpool problem (different origins, same destination) from the *from-work* problem (single origin, multiple destinations). They further distinguish several carpool problem forms, depending on how the drivers for the carpool are identified. There are two versions of the problem per each problem form, depending on whether the to-work and from-work carpools are to be considered together or separately. Focusing on the problem form in which the drivers and cars are known in advance, and considering a separate to-work variant, Baldacci, Maniezzo, & Mingozzi (2004) give grounds to the to-work car pooling problem (CPP). According to Lawler, Lenstra, Kan, & Shmoys (1993); Baldacci, Maniezzo, & Mingozzi (2004), the CPP is NP-hard, "as it contains the Vehicle Routing Problem with unit customer demands, which is known to be NP-hard in the strong sense."

Agatz, Erera, Savelsbergh, & Wang (2012) classify the carpool problem as a special case of the "pickup and delivery problem," thoroughly covered in the operations research literature. A special case of such a problem, where all cars have the same capacity, is known as a *Dial-A-Ride Problem* (DARP) (Baldacci, Maniezzo, & Mingozzi, 2004; Berbeglia, Cordeau, Gribkovskaia, & Laporte, 2007; Cordeau & Laporte, 2007; Savelsbergh & Sol, 1995).

A considerable portion of research in the area focuses on the notion of *fair share* in the carpool problem (Ajtai et al., 1998; Fagin & Williams, 1983; Naor, 2005). The issue was first introduced by Fagin & Williams (1983), who defined the fairness of the algorithm that if, on a certain day, g people participate in carpool, each of them owes the driver $1/g$ of a ride. The unfairness at a given moment is then defined as the maximum number of owed rides that any participant has accumulated or that any participant owes the rest of the group. Consequently, a scheduling algorithm is fair if there is a bound on the unfairness, which is a function of the number of drivers.

As mentioned before, when it comes to the proposed solutions, the researches usually approach the carpool problem from the system rather than an individual perspective. Calvo, de Luigi, Haastrup, & Maniezzo (2004) propose a centralized, integrated car pooling system, utilizing communication technologies, such as SMS and GIS. They define the *Daily Car Pooling Problem* (DCPP) as a special case of DARP. Ferrari, Manzini, Pareschi, Persona, & Regattieri (2003) present several heuristic algorithms based on savings functions, including temporal condition and a geographic location. Baldacci, Maniezzo, & Mingozzi (2004) show two integer programming formulations to solve their to-work CPP, using both the exact and the heuristic method. Yan & Chen (2011) develop a many-to-many carpool problem, with multiple origins and destinations. They define it as the "integer multiple commodity network flow problem" and use the time-space network method to solve it. Yan, Chen, & Chang (2014) develop a stochastic carpooling model that uses stochastic travel times. Stiglic, Agatz, Savelsbergh, & Gradisar (2015) consider the advantages of meeting points introduced into the system. Stiglic, Agatz, Savelsbergh, & Gradisar (2016) show that increased participant flexibility influences matching rates. Wang, Agatz, & Erera (2017) focus on the stability of a ride-sharing system in a dynamic setting, in which the participants can refuse a proposed solution.

While these centralized system-wide optimization solution techniques attempt to achieve societal or environmental goals, they may not necessarily lead to the solutions preferred by each individual carpool participant (Agatz, Erera, Savelsbergh, & Wang, 2012; Wang, Agatz, & Erera, 2017). In this paper, we take a look at the car pooling problem from the individual participant's perspective. Furthermore, we illustrate the differences between centralized and decentralized solutions to the CPP with the real-world and simulated instances of the problem.

3. Problem formulation and solution techniques

We consider a car pooling problem (CPP) (Baldacci, Maniezzo, & Mingozzi, 2004) wherein participants residing at different origins frequently commute to a common destination such as a workplace, school, or an activity in a to/from (TFC) or pick-up/drop-off (PDC) arrangement. Each origin provides a vehicle with a certain number of passenger seats available. The schedule is fixed, known in advance, and common for all participants. Each participant is willing to carpool by sharing available passenger seats with others in order to reduce the distance driven in the long run. However, a participant will consider car pooling only if the long-term savings exceed a certain minimum distance (time) and if the extended distance (time)—due to detours taken to pick up or drop off others—remains below a certain threshold. These constraints are used to determine the set of potential carpools. Each participant ranks all potential carpools according to their individual long-term savings and chooses the best available arrangement.

3.1. *Distance*

Let $d(a, z) = d(z, a)$ be the distance (e.g., Euclidean, shortest driving, quickest driving, etc.) between origin a and destination z.

Let $h(a, \{v_1, v_2, \dots\}, z)$ be the shortest total distance between a and z via $\{v_1, v_2, \dots\}$ such that each via point is visited once and only once. And so, when there are no via points, $h(a, \emptyset, z) = d(a, z)$, for one via point $h(a, \{v_1\}, z) = d(a, v_1) + d(v_1, z)$, while for two via points,

$h(a, \{v_1, v_2\}, z) = min(d(a, v_1) + d(v_1, v_2) + d(v_2, z); d(a, v_2) + d(v_2, v_1) + d(v_1, z))$ which is the shortest distance.

Let $F = \{f_1, f_2, \dots, f_n\}$ be the set of n origins of participants interested in car pooling to a common destination. Each participant commuting from f_k has $p_k \geq 0$ passengers and a vehicle with q_k passenger seats available ($q_k > p_k$).

Commute distances depend on the carpool type. In the special case of no car pooling (empty carpool), the baseline distance for a participant commuting from origin f_k is

$$b_k = h(f_k, \emptyset, z) + h(z, \emptyset, f_k) = 2\, d(f_k, z).$$

For a non-empty carpool, $C = \{f_i, f_j, \ldots\}$, the commute distance for a participant starting from $f_k \in C$ is

$$c_k(C) = 2\, h(f_k, C \setminus f_k, z)$$

for the TFC model, and

$$c_k(C) = h(f_k, C \setminus f_k, z) + d(z, f_k)$$

for the PDC model.

The extended commute distance (due to detours taken to pick up or drop off others) for a participant commuting from f_k to z in carpool C is

$$e_k(C) = c_k(C) - b_k.$$

Because in the long run carpool participants divide driving fairly (Fagin & Williams, 1983) among themselves, the commute distance for each participant is divided by the number of carpool participants $|C|$. Then, the average savings for a participant commuting from f_k to z in carpool C are

$$s_k(C) = b_k - c_k(C)/|C|$$

Additional commute distances and average savings for the instance presented in Figure 1 and the PDC arrangement are shown in Tables 2 and 3.

Consider a decentralized solution to the PDC, $\{f_1, f_2\}$. For the participant originating from f_1, the extended commute distance per trip $e_k(C)$ and the average savings $s_k(C)$ are both equal to 2 units. In other words, the participant at f_1 agrees to extend his or her commute from 6 to 8 units to pick up or drop off passengers at f_2 but, in the long run, this participant drives every other day, so his or her average commute distance is 8/2 = 4 units (2 units saved over the baseline distance of 6 units). The ultimate winner of this arrangement is the participant at f_2, who saves 50% at no additional cost, and the loser is the participant at f_3, who is left out of any car pooling arrangement, despite having the longest baseline distance.

Table 2. Additional commute distance $e_k(C)$ per trip for the three-origin instance (PDC).

Origin	Baseline distance	Additional absolute (relative) commute distance per trip		
		$\{f_1, f_2\}$	$\{f_2, f_3\}$	$\{f_1, f_3\}$
f_1	6.00	2.00 (33.3%)	0.00 (0.00%)	2.53 (42.2%)
f_2	8.00	0.00 (0.00%)	1.12 (14.0%)	0.00 (00.0%)
f_3	8.25	0.00 (0.00%)	0.88 (10.7%)	0.29 (3.5%)

Table 3. Average savings $s_k(C)$ for the three-origin instance (PDC).

Origin	Baseline distance	Average absolute (relative) savings		
		$\{f_1, f_2\}$	$\{f_2, f_3\}$	$\{f_1, f_3\}$
f_1	6.00	2.00 (33.3%)	0.00 (00.0%)	1.735 (28.9%)
f_2	8.00	4.00 (50.0%)	3.44 (43.0%)	0.000 (00.0%)
f_3	8.25	0.00 (00.0%)	3.69 (44.7%)	3.985 (48.3%)

3.2. *Carpool enumeration*

The number of carpools for n origins and q passenger seats available is bound from above by the total number of subsets of size 1, 2, …, q one can create out of n elements, i.e.,

$$\sum_{r=1}^{q} \binom{n}{r} = \sum_{r=1}^{q} \frac{n!}{r!(n-r)!}. \tag{1}$$

Reducing the number of potential carpools to be analyzed is necessary because the shortest distance function is applied to each carpool and the number of potential carpools determines the number of variables in the optimization problem.

In practice, 95% of the to-work carpools are three-passenger ($q = 3$) or smaller and 77% of carpools have only one passenger ($q = 1$) (U.S. Census Bureau, 2015), while most cars have four passenger seats, so q will be much smaller than n. For example, when $q = 4$, the upper bound on the number of carpools is 4,087,975 (66,018,450) for $n = 100$ (200) but not all of these carpools are rational.

In this paper, we assume that carpool participants are rational, i.e., each will select carpools with positive savings. In addition, each participant may specify constraints pertaining to the minimum average distance saved by car pooling (σ_i) and maximum extended distance for carpool detours (ε_i).

We propose a simple carpool enumeration technique to determine the set of potential carpools P. Because carpools are sets of origins, P is a superset of origins.

First, for each origin f_i in F, a complete set of one-participant "carpools" $\{f_i\}$ is created and added to P. Next, for each carpool $\{f_i\}$ in P, a two-participant carpool $C = \{f_i, f_j\}$, such that $i < j$, is created and added to a temporary set P' if all of the following criteria are met:

- Enough seats: $p_i + p_j \leqslant \min(q_i, q_j)$
- Rational savings: $s_\ell(C) > 0$ for each f_ℓ in C
- Extended distance: $e_\ell(C) \leqslant \varepsilon_\ell$ for each f_ℓ in C

and all carpools in P', which also meet the minimum savings criteria, $s_\ell(C) \geq \sigma_\ell$ for each f_ℓ in C, are added to P.

A special set of neighbors N_i is created for each origin f_i in F. N_i contains all origins f_j for which a carpool $\{f_i, f_j\}$ exists in P'. This set will be used to reduce the number of potential carpools in the following steps. For each carpool $\{f_i, f_j\}$ in P', a three-participant carpool $C = \{f_i, f_j, f_k\}$, such that $i < j < k$, is created and added to P'' if all of the following criteria are met:

- Enough seats: $p_i + p_j + p_k \leqslant \min(q_i, q_j, q_k)$
- Neighborhood: $f_k \varepsilon N_\ell$ for each f_ℓ in C/f_k
- Rational savings: $s_\ell(C) > 0$ for each f_ℓ in C
- Extended distance: $e_\ell(C) \leqslant \varepsilon_\ell$ for each f_ℓ in C

and all carpools in P'', which also meet the minimum savings criteria, $s_\ell(C) \geq \sigma_\ell$ for each f_ℓ in C, are added to P.

Other car pooling tuples (quadruples, etc.) are generated in an analogous manner and the resulting set of potential carpools P is used to obtain solutions to the CPP.

Recall that the set of potential carpools $P = \{C_j\}_{j=1,2,\ldots,m}$ is a superset of origins F that consists of m non-empty carpools, i.e., $\{f_1\}, \{f_2\}, \ldots, \{f_k, f_\ell, \ldots\}$. Any subset S of P such that:

$$S \subseteq P \text{ and } \bigcup_{C_j \in S} \{C_j\} = F \text{ and } \cap_{C_j \in S} \{C_j\} = \emptyset \tag{2}$$

is a *feasible solution* to the carpool problem, regardless of the chosen optimality criteria.

Because P contains a complete set of one-participant "carpools," $\{f_1\}, \{f_2\}, \ldots, \{f_n\}$, which meets the criteria (2), a feasible solution to our carpool problem always exists.

The proposed enumeration of all potential carpools as set P is common for the TWC and PDC models and it incorporates the minimum savings (σ_k) and maximum extended distance (ε_k) constraints in such a manner that they do not need to be considered at later stages.

We consider two techniques for solving the car pooling problems: (1) centralized—with a single system-wide objective and (2) decentralized—based on matching participants' preferences.

3.3. *Centralized solution*

The proposed centralized solution maximizes the system-wide savings, which is equivalent to minimizing the total distance traveled. If one assumes the same fuel efficiency of all participating vehicles, it is also equivalent to minimizing the fuel consumption and emissions of gaseous pollutants.

Let $y_{ij} = 1$ if $f_i \in C_j$, otherwise $y_{ij} = 0$. We also define the total savings for carpool C_j as

$$w_j = \sum_{f_k \in C_j} s_k(C_j).$$

Then, the 0-1 integer linear programming formulation of the proposed problem is

$$\text{maximize}\left\{\sum_{j=1}^{m} x_j w_j\right\} \tag{3}$$

Subject to :

$$\sum_{j=1}^{m} x_j y_{ij} = 1 \text{ for } i = 1, 2, \ldots, n, \tag{4}$$

$$x_j \in \{0, 1\}. \tag{5}$$

The objective (3) is to maximize the total (system-wide) savings from car pooling, while the constraints (4) ensure that one and only one carpool is selected for each participant. The binary variable x_j (5) will be assigned the value of 1 when carpool C_j is selected by all its participants.

Note that this formulation is equivalent to the set partitioning problem, which is one of the classical NP-hard problems (Garfinkel & Nemhauser, 1969).

3.4. *Decentralized solution*

In this approach, we attempt to find a solution which reflects the real-world matching of participants' car pooling preferences. We assume that, given a choice of two potential carpools, a participant will prefer the carpool which results in more savings. Formally, for a participant commuting from f_k to z, such that $f_k \in C_i$ and $f_k \in C_j$, $C_i \succcurlyeq_k C_j$ if $s_k(C_i) \geq s_k(C_j)$.

The following heuristic is applied to obtain a decentralized solution to the CPP.

Let F' be the subset of F representing all participants interested in and available for car pooling, and let S^* be the solution set.

Step 1: IF F' is empty THEN stop ELSE for each participant's origin $f_k \in F'$, determine the subset of carpools $P_k = \{C_j\} \subset P$ such that $f_k \in C_j$, find one carpool C^*_k in P_k that gives the participant starting from f_k the highest savings $s_k(C_j)$, add it to a temporary set P^* and proceed to Step 2.
Step 2: IF P^* contains at least one carpool C^* such that it gives the highest savings to each of its participants THEN add <u>all</u> such carpools to S^* and go to Step 3 ELSE proceed to the impasse-breaking Step 4.
Step 3: Remove all C^* participants' origins from F' and remove all potential carpools which include any of these origins from P; repeat for all C^*, remove all carpools from P^*, and go to Step 1.
Step 4: For each participant's origin $f_k \in F'$ and their potential carpool arrangements P_k, rank the carpools by the decreasing order of savings $s_k(C_j)$. For each carpool C_ℓ in P, calculate the average rank across all participants in C_ℓ, select <u>one</u> carpool C^* with the minimum average rank (or the minimum maximum rank), add it to S^*, and go to Step 3.

The proposed decentralized optimization process is based on limited information about the neighbors available to each participant. In each iteration, each participant selects the best carpool from the remaining arrangements, which becomes fixed only if it is also the best for all other participants in this carpool. This matching process does not require any special incentives.

An *impasse* occurs when there are no more carpools providing the best choice for each participant. The proposed impasse-breaking Step 4 is based on the assumption that—faced with the choice of being left out of car pooling—at least one participant will select his or her next-best option.

Per (2) a participant belongs to one and only one active carpool. Because the sum of individual savings from all active carpools is equal to the total (system-wide) savings from car pooling and the total savings do not decrease in each iteration, our decentralized approach can be classified as a greedy heuristic when overall system savings are the objective of the optimization process. The centralized solution (3) is the upper bound on the system-wide savings.

The following section describes the results of computational experiments involving a real-world instance and random instances for both the TFC and PDC car pooling problems, in which the centralized and decentralized solutions are compared in terms of system-wide, as well as individual savings.

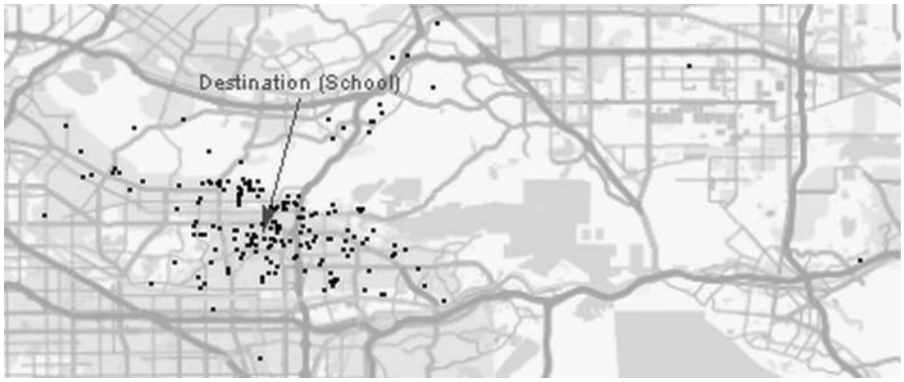

Figure 2. A real-world car pooling problem instance.

4. Computational results

We implemented the decentralized method in Java and used IBM ILOG CPLEX Optimization Studio 12.6 running on a virtualized server with 16 vCPU cores and 128GB of vRAM for the centralized solution. The decentralized solution was developed with the worst-case computational complexity of $O(nm\log(m))$ determined by the initial ranking of each row of the sparse $n \times m$ savings matrix. The task of determining the shortest distances for each participant of each carpool is a part of the initial setup for both the decentralized and centralized solutions; its worst-case computational complexity is $O(mq_{\max}^3)$, where $q_{\max}$ is the maximum number of passenger seats available. In practice, m is much larger than n and $q_{\max}$ is equal to 4 for most cars.

4.1. *Real-world instance*

We obtained data from a private “pre-K to 8” school located in Orange County, California. Most families use their private vehicles to commute to that school two times per day: to drop off and to pick up their non-driving children. Many families choose to reduce the commuting cost (time) by car pooling with their neighbors. These self-organized carpools are based on matching individual preferences rather than on centralized planning. Fairness in Fagin and Williams' (Fagin & Williams, 1983) sense is assumed, i.e., in the long run, each family participating in a carpool will drive the same number of times. The choice of potential carpools is limited by the number of participating children and the number of seats available. Each family chooses to participate in a carpool only if it maximizes their individual savings. If the top choice is not available, the family will choose the next-best arrangement. The worst-case scenario for each family is the status-quo, i.e., no car pooling.

At the time of writing this paper, 281 children from 195 families attended the aforementioned school. Over 37% of these families had multiple children attending: one family had four, 12 had three, and 60 had two children. Figure 2 shows the locations of the school (marked by an arrow) and the origins of the 187 families, for which the street addresses were available. The (symmetric) driving distance matrix was created using Google Maps API (Google, 2016).

The average baseline travel distance for a family commuting to the school is 11.2 miles (11 km). The total baseline driving distance for all 187 families is 2 096.7 miles (3374.3 km) per trip. Assuming the standard two trips per day, 180 school days per year, and the average fuel efficiency of 20 mpg (11.8 L/100 km), the school families drive approximately 754,812 miles (1,214,752 km) and burn approximately 37740.6 gallons (142863.7 liters) of gasoline per school year.

For the purpose of this study, we made the following assumptions:

- Each family owns and operates a vehicle with 4 passenger seats available
- Each family would like to save at least 2 miles (3.2 km) and no less than 25% of the baseline distance on the average
- Each family is willing to extend their daily commute due to carpool detours by at most 50%, but no more than 10 miles (16.1 km).

Our carpool enumeration method resulted in 23,518 potential carpools added to P. The decentralized heuristic solution was obtained with the Java implementation in 2.9 seconds and the centralized solution was obtained with IBM's CPLEX after 163.07 seconds.

Table 4 shows the comparison of the results obtained with the decentralized and centralized solutions. Both solutions offer substantial savings over the baseline. The centralized solution shows 3.59% more in system-wide savings than the decentralized solution and takes 4 more vehicles off the streets. However, compared to the decentralized solution, 90 families (37.43%) sacrificed a portion of their individual savings (9.14% on the average and up to 57.2%) and 51 families (27.27%) gained and average of 21.2% (up to 64.99%) in individual savings.

Thus, compared to the decentralized solution, the centralized approach significantly redistributed individual savings in order to achieve a relatively small improvement in system-wide

Table 4. Real-world instance system-wide results.

	Baseline	Decentralized solution	Centralized solution
Number of vehicles per trip	187	90	86
Number of 2+ carpools	0	53	59
Families assigned to carpools	0	150.0 (80.21%)	160.0 (85.56%)
Savings per trip (miles)	0	1042.5 (49.72%)	1117.8 (53.31%)

savings. Such a solution may destabilize the entire car pooling system because it is relatively easy for groups of families who lost individual savings to realize that they could create alternative arrangements which would benefit them more (such as $\{f_1, f_2\}$ in Table 1).

4.2. Random instances

In this section, we will further illustrate the differences between decentralized and centralized solutions using randomly generated instances. For these instances, we additionally assumed that each odd-numbered origin has one non-driving passenger and each even-numbered origin has two non-driving passengers.

We generated 1,000 random instances of the CPP problem, each with 100 different origin points distributed on a 40 by 40 units square, and used Euclidean distance function. Figure 3 shows a solution to a sample instance of the problem. The destination is located in the center of the square and the origins of participants in carpools are connected with lines and polygons.

Next, for each of the 1,000 random instances, we determined the set of potential carpools P for the TFC and PDC arrangements, respectively, and solved them using both the decentralized and centralized approaches.

4.2.1. To/from carpool (TFC)

For each instance of the problem, we compared system-wide savings achieved by decentralized and centralized solutions. Figure 4 shows the boxplot with additional system-wide relative savings achieved from applying the centralized approach. The median additional savings from the centralized approach were only 1.53% and Q1 and Q3 were 0.96% and 2.21%, respectively.

Next, we studied the redistribution of individual savings by measuring the percentage of those participants whose individual savings decreased, did not change or increased as a result of applying the centralized instead of the decentralized approach. The boxplots in Figure 5 indicate that only 10% participants would benefit from centralized car pooling arrangements. Others (16%) would be motivated to form alternative carpools, thus destabilizing the whole system.

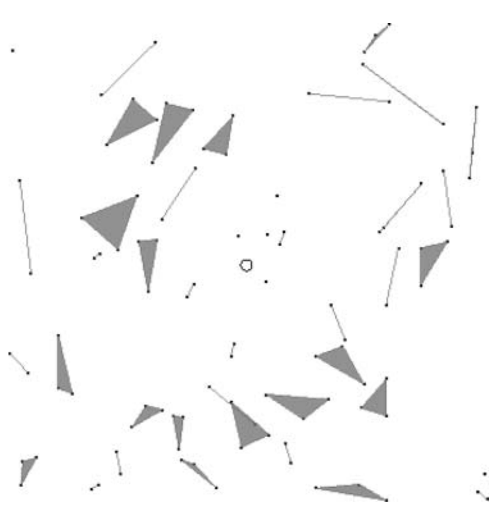

Figure 3. A simulated car pooling problem instance.

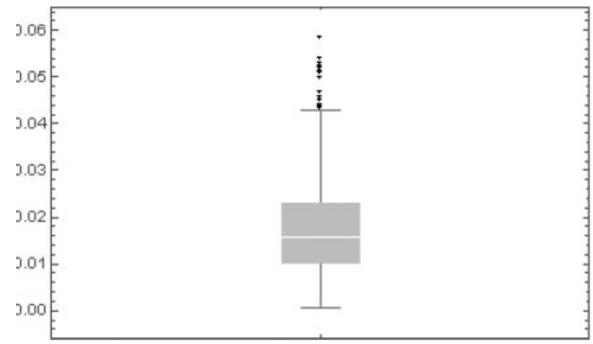

Figure 4. Additional relative savings from the centralized approach (TFC).

4.2.2. Pick-up/drop-off carpool (PDC)

We applied the same approach to test the PDC model. Figure 6 shows the boxplot with additional system-wide relative savings achieved from applying the centralized approach. The median additional savings were only 3.87% and Q1 and Q3 were 3.13% and 4.63%, respectively.

The boxplots in Figure 7 indicate that only 25% participants would benefit from centralized car pooling arrangements. Others (34%) would be motivated to form alternative carpools, thus destabilizing the whole system.

4.3. University of Bologna daily car pooling problem instances

In a new set of experiments, we used the coordinates of the destinations and origins as well as distances from the 35 problem instances used in Baldacci, Maniezzo, & Mingozzi

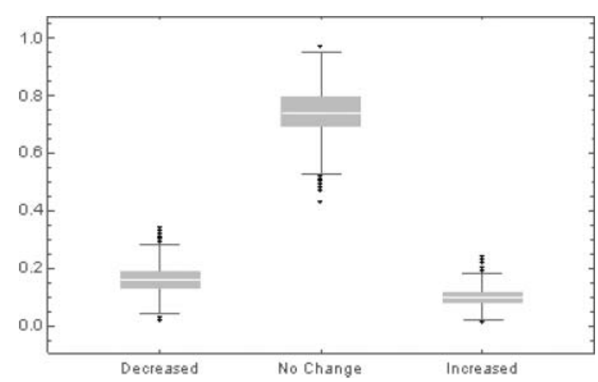

Figure 5. Individual savings redistributed by the centralized approach (TFC).

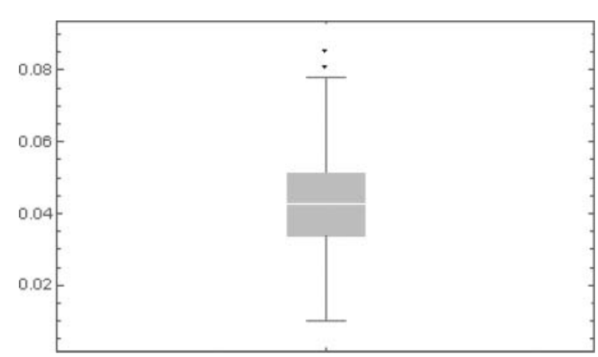

Figure 6. Additional relative savings from the centralized approach (PDC).

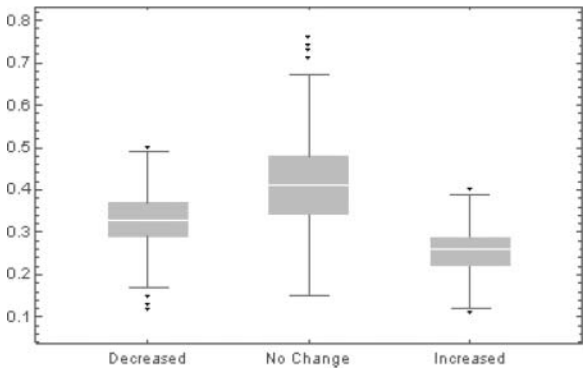

Figure 7. Individual savings redistributed by the centralized approach (PDC).

(2004) and available at the University of Bologna website http://astarte.csr.unibo.it/data/. Each instance consists of one destination and between 50 and 250 origins. Similarly to Baldacci et al., we assumed that each origin has one passenger ($p = 1$) and all vehicles have four available passenger seats ($q = 4$). However, unlike Baldacci et al., we did not designate 25% of the origins as drivers but we assumed that all carpool participants will serve as drivers. Also, we did not use the earliest leaving and latest arrival times for each participant. Instead, we used the minimum savings of 25% of the baseline distance or 2 units, and maximum additional driving distance of 50% of the baseline or 10 units for each participant.

Tables 5 and 6 show the results for the TFC and PDC arrangements with original distances: the problem code (Prob.), the number of origins (n), the average baseline distance (Avg. Base), the total baseline distance (Base), the number of feasible carpools (m), the feasible carpools enumeration time (Enum. Time) in seconds, maximum system savings obtained by set partitioning (Ctr. Sav.), optimization time (Cplex Time) in seconds, system savings from the decentralized solution (Dec. Sav.), decentralized solver time (Heur. Time) in seconds, percentage of participants whose individual savings decreased (Dec.), did not change (No Ch.) or increased (Inc.) in centralized solution, and the additional system-wide savings from the centralized solution (Add. Sav.).

According to (1) the total number of subsets with at least 1 and no more than 4 elements is 251,175 and 161,487,125 for $n = 50$ and $n = 250$, respectively, but the average number of feasible pools was only 1,561 (2,081) for the TFC (PDC) arrangement. The maximum enumeration time for the 35 instances was 25.33 (24.05) seconds and the average was 7.15 (5.77) seconds. The average time to obtain a heuristic solution was < 0.01 (0.11) s and it took CPLEX 0.82 (2.85) seconds on average to obtain a centralized solution.

For the TFC arrangement, the system-wide savings obtained by the decentralized method were 0.23%–6.95% (median = 1.58%) lower than the maximum savings obtained with the centralized method. 16.4% of the participants would benefit from the centralized solution while 20% would lose individual

Table 5. University of Bologna instances (original distances)—TFC.

Prob.	n	Avg. Base.	Base	m	Enum. time (s.)	Ctr. sav.	Cplex time (s.)	Dec. sav.	Heur. time (s.)	Dec. %	No ch. %	Inc. %	Add. sav. %
A1	50	49.16	2,458	173	0.17	1427.00	0.13	1333.00	0.00	22.0	64.0	14.0	3.82
A2	75	49.57	3,717	338	0.39	2232.00	0.14	2150.50	0.00	24.0	54.7	21.3	2.19
A3	100	50.98	5,098	694	0.51	3160.50	0.45	2889.00	0.00	19.0	64.0	17.0	5.33
A4	120	103.03	12,363	1,394	1.10	8793.00	0.50	8621.00	0.00	30.8	45.9	23.3	1.39
A5*	120	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—
A6	134	72.93	9,772	4,562	2.86	6706.00	1.00	6640.50	0.01	17.2	65.6	17.2	0.67
A7	150	50.16	7,524	1,449	2.90	4960.00	0.72	4815.50	0.00	20.0	65.3	14.7	1.92
A8	170	92.64	15,748	1,976	5.97	11029.00	0.50	10868.50	0.01	28.2	48.9	22.9	1.02
A9	170	74.45	12,656	1,657	5.33	8707.50	0.28	8293.50	0.00	26.5	50.0	23.5	3.27
A10	195	92.19	17,977	2,648	10.01	12572.00	1.76	12163.00	0.01	23.6	54.3	22.1	2.28
A11	199	49.36	9,822	2,544	9.74	6595.00	0.73	6473.50	0.02	25.6	54.8	19.6	1.24
A12	225	50.04	11,259	3,097	16.69	7610.50	1.26	7431.50	0.01	18.7	64.9	16.4	1.59
B1	100	227.28	22,728	500	0.64	14862.50	0.27	14093.00	0.01	29.0	52.0	19.0	3.39
B2	100	234.08	23,408	452	0.27	15162.00	0.52	14360.00	0.00	19.0	67.0	14.0	3.43
B3	100	236.96	23,696	438	0.34	15346.00	1.09	14275.50	0.00	27.0	52.0	21.0	4.52
B4	100	238.70	23,870	474	0.27	15723.67	0.31	15261.00	0.00	24.0	58.0	18.0	1.94
B5	100	235.72	23,572	425	0.26	15664.50	0.20	14515.00	0.00	11.0	79.0	10.0	4.88
B6	100	236.16	23,616	492	0.29	15259.50	0.44	13617.50	0.00	31.0	47.0	22.0	6.95
B7	100	238.76	23,876	410	0.28	15371.67	0.30	15017.50	0.00	17.0	75.0	8.0	1.48
B8	150	250.52	37,578	1,046	1.75	25568.00	0.34	25482.50	0.00	8.7	86.0	5.3	0.23
B9	150	249.52	37,428	918	2.77	25382.50	0.37	25173.00	0.00	21.3	64.0	14.7	0.56
B10	150	251.78	37,767	930	1.54	25578.50	0.28	24516.50	0.00	26.0	56.0	18.0	2.81
B11	150	249.17	37,375	1,029	2.41	25418.67	0.27	25171.50	0.00	14.7	76.6	8.7	0.66
B12	150	249.31	37,396	1,256	2.74	25241.00	0.45	24790.00	0.00	20.7	62.7	16.6	1.21
B13	200	257.44	51,488	1,746	9.74	36036.00	0.36	35590.50	0.00	16.0	70.5	13.5	0.87
B14	200	253.97	50,794	1,843	8.92	35446.33	0.70	34746.50	0.00	18.5	67.0	14.5	1.38
B15	200	257.03	51,406	1,646	9.33	35864.33	1.47	34960.00	0.00	21.0	64.5	14.5	1.76
B16	200	255.88	51,176	1,705	9.16	35782.67	0.55	35177.50	0.00	13.5	75.5	11.0	1.18
B17	200	258.06	51,612	1,744	9.51	36093.00	1.47	35690.50	0.00	16.5	70.0	13.5	0.78
B18	200	257.05	51,410	1,673	9.14	35568.00	0.50	34011.50	0.00	19.5	63.5	17.0	3.03
B19	250	274.34	68,586	2,823	25.33	47726.50	1.39	46935.00	0.01	19.6	64.0	16.4	1.15
B20	250	277.58	69,396	2,780	24.71	48289.83	2.14	47174.00	0.01	22.8	61.6	15.6	1.61
B21	250	274.96	68,740	2,869	24.85	47785.50	5.21	46699.50	0.00	18.8	68.0	13.2	1.58
B22	250	275.66	68,914	2,763	25.25	48127.33	0.97	47523.00	0.00	18.0	66.8	15.2	0.88
B23	250	275.86	68,964	2,761	24.06	48077.17	1.20	47273.0	0.00	15.2	72.4	12.4	1.17

*A5 has the same structure as A4.

savings. For the PDC arrangement, the system-wide savings obtained by the decentralized method were 0.02%–5.66% (median = 1.13%) lower than the maximum savings obtained with the centralized method. 10% of the participants would benefit from the centralized solution while 17.5% would lose individual savings.

A quick inspection of the average baseline (individual round-trip) distances in Tables 5 and 6 reveals that they are unlikely to be real-world commuting distances in miles or kilometers. In order to make the distances more realistic in the context of school/work commuting, we divided them by 10 and repeated the experiment. The results for the TFC and PDC arrangements are presented in Tables 7 and 8.

Our enumeration technique resulted in the average number of 10,218 (65,473) feasible pools for the TFC (PDC) arrangement. The maximum enumeration time was 34.44 (30.98) seconds and the average was 9.03 (9.16) seconds. The average time to obtain the heuristic solution was 0.06 (92.14) seconds and, despite being run on a machine with 128GB RAM and 16 parallel cores, CPLEX was unable to obtain solutions to 4 of the PDC problems (A10, B17, B21, and B22) within 36,000 seconds.

As in the case of the original distances, the TFC model for the scaled distances yielded smaller/easier problems than the PDC model, the Java implementation of the decentralized heuristic was faster than CPLEX (except for two PDC instances: B16 and B23), system-wide savings obtained by the decentralized method were only slightly lower than the maximum savings obtained with the centralized method, and the percentages of participants whose individual savings decreased as a result of the centralized optimization were larger than the corresponding percentages of participants whose individual savings increased (except for two PDC instances: A12 and B23).

In sum, the results for the University of Bologna instances were consistent with those obtained on the real-world and randomly generated instances described earlier in this section.

4.4. Additional numerical simulation experiments

We conducted additional experiments in order to test the impact of the assumptions on the results.

First, we re-solved all 1,000 random instances using the minimax impasse-breaking technique. The results were different from the average-based technique by approximately 1%.

Next, we reduced the number of origins to n = 50, eliminated the maximum extended distance constraints (ε), and reduced the minimum savings (σ) to a very small positive number. We generated 10,000 random instances, solved and compared them using the same approach as for the 1,000 random instances. In the TFC arrangement, 32% of participants lost individual savings (28% gained) for the median improvement in system-wide savings of only 3.85%. In the PDC arrangement 40% of participants lost individual savings (32% gained) for the median improvement in system-wide savings of only 3.87%.

Table 6. University of Bologna instances (original distances)—PDC.

Prob.	n	Avg. base.	Base	m	Enum. time (s.)	Ctr. sav.	Cplex time (s.)	Dec. sav.	Heur. time (s.)	Dec. %	No ch. %	Inc. %	Add. sav. %
A1	50	49.16	2,458	104	0.80	900.33	0.05	852.33	0.00	4.0	92.0	4.0	1.95
A2	75	49.57	3,717	221	0.54	1580.67	0.22	1466.33	0.00	26.7	52.0	21.3	3.08
A3	100	50.98	5,098	815	1.04	2437.75	0.23	2278.83	0.03	32.0	46.0	22.0	3.12
A4	120	103.03	12,363	2,398	2.21	8575.25	25.65	8110.50	0.07	35.8	33.4	30.8	3.76
A5*	120	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—
A6	134	72.93	9,772	27,361	3.47	5584.17	19.84	5414.67	2.83	26.1	53.0	20.9	1.73
A7	150	50.16	7,524	1,860	4.46	4421.58	0.25	4136.33	0.04	39.3	26.0	34.7	3.79
A8	170	92.64	15,748	2,868	4.76	10246.00	18.40	9746.83	0.08	30.0	42.4	27.6	3.17
A9	170	74.45	12,656	3,794	6.65	8271.83	0.30	7555.58	0.10	27.1	41.1	31.8	5.66
A10	195	92.19	17,977	3,333	7.06	11643.33	1.93	10974.75	0.09	30.8	39.5	29.7	3.72
A11	199	49.36	9,822	4,383	7.33	6200.33	1.62	5668.16	0.08	34.2	31.6	34.2	5.42
A12	225	50.04	11,259	5,512	11.55	7266.41	1.76	6693.33	0.12	33.8	35.1	31.1	5.09
B1	100	227.28	22,728	285	0.98	4364.83	0.08	4341.25	0.00	14.0	78.0	8.0	0.10
B2	100	234.08	23,408	462	0.80	3571.33	0.38	3566.33	0.00	8.0	91.0	1.0	0.02
B3	100	236.96	23,696	279	0.94	3482.16	0.14	3118.16	0.02	19.0	72.0	9.0	1.54
B4	100	238.70	23,870	370	0.79	4193.75	0.06	3790.33	0.00	17.0	73.0	10.0	1.69
B5	100	235.72	23,572	364	0.78	3879.00	0.03	3869.00	0.01	5.0	93.0	2.0	0.04
B6	100	236.16	23,616	373	0.82	3502.00	0.06	3438.00	0.01	18.0	71.0	11.0	0.27
B7	100	238.76	23,876	233	1.35	4296.83	0.03	4247.67	0.01	6.0	86.0	8.0	0.21
B8	150	250.52	37,578	838	2.70	10873.67	0.17	10831.42	0.01	16.7	75.3	8.0	0.11
B9	150	249.52	37,428	485	3.08	11818.33	0.08	11446.25	0.01	17.3	72.7	10.0	0.99
B10	150	251.78	37,767	528	2.33	10175.00	0.09	10084.17	0.01	16.7	76.0	7.3	0.24
B11	150	249.17	37,375	780	3.19	9435.00	0.19	9407.42	0.01	12.7	81.3	6.0	0.07
B12	150	249.31	37,396	1,059	2.45	9728.42	0.34	9597.00	0.02	12.7	79.3	8.0	0.35
B13	200	257.44	51,488	1,091	6.67	16652.75	0.13	16228.08	0.01	14.0	74.5	11.5	0.82
B14	200	253.97	50,794	1,352	6.04	16230.00	0.25	15844.58	0.02	17.0	72.0	11.0	0.76
B15	200	257.03	51,406	881	6.82	15797.00	0.19	14984.33	0.04	17.5	71.0	11.5	1.58
B16	200	255.88	51,176	967	7.90	16282.41	0.09	16098.42	0.01	8.5	86.0	5.5	0.36
B17	200	258.06	51,612	1,107	6.49	15224.00	0.27	15123.50	0.01	16.0	75.0	9.0	0.19
B18	200	257.05	51,410	715	7.70	13717.42	0.11	13248.67	0.01	18.5	74.0	7.5	0.91
B19	250	274.34	68,586	1,147	16.75	24799.50	0.48	24021.83	0.02	20.8	68.0	11.2	1.13
B20	250	277.58	69,396	1,042	24.05	21442.83	0.30	21268.08	0.01	19.2	72.4	8.4	0.25
B21	250	274.96	68,740	1,184	16.09	22603.25	0.23	21808.58	0.01	12.4	80.4	7.2	1.16
B22	250	275.66	68,914	981	14.20	24277.25	0.14	23624.33	0.01	19.2	72.0	8.8	0.95
B23	250	275.86	68,964	1,274	16.88	22809.00	0.14	21708.58	0.01	16.0	76.0	8.0	1.60

*A5 has the same structure as A4.

Table 7. University of Bologna instances (0.1-scaled distances)—TFC.

Prob.	n	Avg. base.	Base	m	Enum. time (s.)	Ctr. sav.	Cplex time (s.)	Dec. sav.	Heur. time (s.)	Dec. %	No ch. %	Inc. %	Add. sav. %
A1	50	4.92	245.80	67	0.16	66.45	0.00	59.95	0.00	4.0	92.0	4.0	2.64
A2	75	4.96	371.80	126	0.83	124.10	0.14	124.1	0.00	0.0	100.0	0.0	0.00
A3	100	5.10	509.80	168	0.54	181.10	0.14	160.90	0.00	13.0	75.0	12.0	3.96
A4	120	10.30	1236.40	12,508	2.03	818.60	4.18	804.80	0.04	24.2	58.3	17.5	1.12
A5*	120	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—	—″—
A6	134	7.29	977.20	2,921	2.56	541.73	0.44	536.10	0.00	9.7	80.6	9.7	0.58
A7	150	5.02	752.40	393	2.21	328.10	0.13	318.15	0.00	7.3	87.4	5.3	1.32
A8	170	9.26	1574.80	13,444	7.66	1007.55	2.98	994.85	0.02	20.0	62.4	17.6	0.81
A9	170	7.44	1265.60	9,196	6.77	731.05	4.35	715.95	0.03	16.5	69.4	14.1	1.19
A10	195	9.22	1797.80	15,321	13.31	1151.15	4.26	1129.80	0.03	19.0	65.6	15.4	1.19
A11	199	4.94	982.20	718	10.76	450.75	0.14	432.25	0.00	11.6	77.8	10.6	1.88
A12	225	5.00	1125.80	948	18.60	539.20	0.25	505.90	0.00	10.7	80.0	9.3	2.96
B1	100	22.73	2272.80	997	0.91	1459.57	0.48	1388.95	0.01	22.0	69.0	9.0	3.11
B2	100	23.41	2340.80	946	0.54	1500.05	0.44	1451.65	0.01	8.0	86.0	6.0	2.07
B3	100	23.70	2369.60	1,089	0.36	1505.85	0.59	1376.90	0.00	19.0	71.0	10.0	5.44
B4	100	23.87	2387.00	1,460	0.36	1534.72	0.87	1458.80	0.01	17.0	72.0	11.0	3.18
B5	100	23.57	2357.20	779	0.36	1520.40	0.22	1505.55	0.00	12.0	77.0	11.0	0.63
B6	100	23.62	2361.60	1,240	0.40	1486.10	0.62	1341.10	0.00	23.0	59.0	18.0	6.14
B7	100	23.88	2387.60	997	0.39	1529.27	0.53	1480.00	0.00	11.0	82.0	7.0	2.06
B8	150	25.05	3757.80	5,701	2.39	2570.55	0.58	2412.30	0.01	13.3	75.4	11.3	4.21
B9	150	24.95	3742.80	6,299	3.00	2548.23	0.69	2421.45	0.02	18.0	67.3	14.7	3.39
B10	150	25.18	3776.80	5,586	1.91	2570.02	0.69	2382.30	0.01	22.7	60.6	16.7	4.97
B11	150	24.92	3737.60	4,644	3.05	2559.73	0.50	2538.35	0.01	10.7	83.3	6.0	0.57
B12	150	24.93	3739.60	3,621	3.02	2546.37	0.34	2507.95	0.01	15.3	73.4	11.3	1.03
B13	200	25.74	5148.80	11,269	11.10	3561.18	1.08	3473.40	0.02	15.5	70.5	14.0	1.70
B14	200	25.40	5079.40	14,562	10.69	3498.23	2.89	3367.00	0.03	21.5	62.0	16.5	2.58
B15	200	25.70	5140.60	10,744	10.83	3522.20	8.57	3491.20	0.18	18.0	70.5	11.5	0.60
B16	200	25.59	5117.60	10,829	10.98	3508.70	1.47	3420.55	0.01	15.5	72.5	12.0	1.72
B17	200	25.81	5161.20	18,378	11.32	3552.10	2.34	3505.55	0.06	15.5	72.5	12.0	0.90
B18	200	25.70	5141.00	12,180	11.48	3513.67	1.86	3378.30	0.09	18.5	65.5	16.0	2.63
B19	250	27.43	6858.60	26,803	33.49	4794.85	14.52	4739.85	0.13	12.8	74.4	12.8	0.80
B20	250	27.76	6939.60	41,401	32.22	4859.10	17.50	4792.65	0.25	20.4	64.8	14.8	0.96
B21	250	27.50	6874.00	35,343	32.44	4800.08	23.87	4621.15	0.13	16.4	73.2	10.4	2.60
B22	250	27.57	6891.40	30,824	34.44	4838.22	4.49	4778.55	0.45	20.8	60.4	18.8	0.87
B23	250	27.59	6896.40	43,613	32.88	4822.95	14.95	4744.80	0.33	22.8	60.4	16.8	1.13

*A5 has the same structure as A4.

We also adapted Beasleys p-median test problem instances from the OR-Library (Beasley, 2004) to the car pooling problem by making the following additional assumptions:

- The destination is located at the 1-median location and all the remaining locations are considered participants' origins.
- All transportation costs (distances) are divided by 10 (to make them more realistic commuting distances).
- Each odd-numbered location has one non-driving passenger and each even-numbered location has two non-driving passengers.

We solved the first 10 problems (problems 1–5 had 100 participants and problems 6–10 had 200) and compared them using the same approach. The results indicate that the centralized policy causes a large proportion (30.3%–44.44%) of participants to lose individual savings in order to achieve a relatively small improvement (1.53%–6.37%) in the system-wide savings.

All the results follow the same pattern, i.e., centralized solutions offer a relatively small increase in system-wide savings over decentralized solutions, in exchange for a substantial redistribution of individual savings.

5. Discussion

Our decentralized solution technique assumes that participants at each origin can serve as either drivers or passengers, which is typical for a car pooling environment with privately owned vehicles. This approach is different from the one presented in Baldacci, Maniezzo, & Mingozzi (2004) in which a certain percentage (e.g., 25%) of participants is designated as permanent drivers for carpools.

We chose the maximization of the savings (minimization of the distance traveled) over the minimization of an artificial penalty because such a criterion can be easily interpreted for individual participants as well as for the entire system.

The usability of our carpool enumeration technique relies on the assumptions of the minimum average savings and maximum extra distance traveled per trip. We showed that we can enumerate feasible carpools in seconds for a wide range of practical problems. The output from our enumeration can be used to obtain both the centralized and decentralized solutions. These solutions can be compared using both system-wide and individual savings.

Our heuristic uses self-organization by matching individual preferences until an impasse is reached. An impasse is broken by forcing one or more participants of a single carpool to give up their most-preferred choices. This impasse-breaking technique attempts to simulate a real-world decision-making process in which participants are likely to settle for a less-preferred choice in order to be included in any carpool rather than being left out.

Although our decentralized solution was designed to maximize individual participants' savings, it also yields very

Table 8. University of Bologna instances (0.1-scaled distances)—PDC.

Prob.	n	Avg. base.	Base	m	Enum. time (s.)	Ctr. sav.	Cplex time (s.)	Dec. sav.	Heur. time (s.)	Dec. %	No ch. %	Inc. %	Add. sav. %
A1	50	4.92	245.80	71	0.19	70.28	0.03	68.98	0.00	6.0	92.0	2.0	0.53
A2	75	4.96	371.80	186	0.79	108.86	0.05	90.90	0.00	10.7	82.7	6.6	4.83
A3	100	5.10	509.80	260	1.28	191.61	0.06	135.13	0.01	26.0	55.0	19.0	11.08
A4	120	10.30	1236.40	90,125	8.27	823.15	95.71	803.15	23.02	30.0	48.3	21.7	1.62
A5*	120	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—	—"—
A6	134	7.29	977.20	13,501	5.00	538.81	14.43	507.02	0.88	17.9	67.9	14.2	3.25
A7	150	5.02	752.40	1,764	3.49	348.96	4.15	318.25	0.05	20.0	65.3	14.7	4.08
A8	170	9.26	1574.80	99,271	9.64	1005.93	981.51	983.89	74.48	31.8	42.9	25.3	1.40
A9	170	7.44	1265.60	41,857	7.37	737.88	676.72	714.64	8.09	24.1	56.5	19.4	1.84
A10	195	9.22	1797.80	128,360	12.51	1174.68–1175.32	36,000**	1150.85	274.22	NA	NA	NA	NA
A11	199	4.94	982.20	5,624	10.68	472.53	881.67	434.23	0.19	21.6	62.8	15.6	3.90
A12	225	5.00	1125.80	9,353	14.98	566.24	9.56	523.09	0.37	21.3	56.9	21.8	3.83
B1	100	22.73	2272.80	3,652	1.53	1416.98	1.14	1362.58	0.09	24.0	61.0	15.0	2.39
B2	100	23.41	2340.80	3,693	1.10	1339.91	1.69	1267.69	0.21	36.0	39.0	25.0	3.09
B3	100	23.70	2369.60	3,663	1.24	1358.99	2.40	1302.45	0.06	21.0	64.0	15.0	2.39
B4	100	23.87	2387.00	4,091	1.19	1368.61	57.39	1313.89	0.21	23.0	65.0	12.0	2.29
B5	100	23.57	2357.20	3,122	1.24	1352.02	1.06	1302.10	0.11	30.0	49.0	21.0	2.12
B6	100	23.62	2361.60	3,742	1.24	1344.21	8.28	1248.38	0.06	26.0	56.0	18.0	4.06
B7	100	23.88	2387.60	3,247	1.12	1360.23	2.12	1309.92	0.08	29.0	59.0	12.0	2.11
B8	150	25.05	3757.80	21,454	3.58	2456.49	67.25	2370.58	4.58	24.0	58.7	17.3	2.29
B9	150	24.95	3742.80	20,286	2.96	2330.20	18.00	2288.78	2.80	21.3	62.7	16.0	1.11
B10	150	25.18	3776.80	23,604	3.91	2478.68	19.53	2399.42	5.04	30.0	48.0	22.0	2.10
B11	150	24.92	3737.60	19,623	3.58	2456.76	30.55	2389.21	4.96	28.7	54.6	16.7	1.81
B12	150	24.93	3739.60	20,184	3.52	2444.21	203.54	2376.87	1.51	29.3	44.0	26.7	1.80
B13	200	25.74	5148.80	83,257	10.96	3454.60	471.95	3414.14	35.36	27.5	49.0	23.5	0.79
B14	200	25.40	5079.40	79,598	11.26	3506.40	962.90	3364.48	74.93	28.0	51.0	21.0	2.79
B15	200	25.70	5140.60	65,262	12.13	3439.85	53.41	3297.65	41.53	29.5	43.5	27.0	2.77
B16	200	25.59	5117.60	69,412	10.56	3519.62	28.83	3376.60	38.00	28.0	48.5	23.5	2.79
B17	200	25.81	5161.20	79,320	11.42	3468.18–3470.09	36,000**	3339.77	86.68	NA	NA	NA	NA
B18	200	25.70	5141.00	77,286	12.34	3438.97	1667.21	3318.48	62.89	33.5	44.5	22.0	2.34
B19	250	27.43	6858.60	227,486	29.88	4709.03	836.24	4463.91	314.85	44.0	25.2	30.8	3.57
B20	250	27.76	6939.60	262,949	22.95	4783.42	1183.63	4625.09	820.61	30.0	43.6	26.4	2.28
B21	250	27.50	6874.00	246,142	28.89	4726.06–4727.62	36,000**	4499.78	236.14	NA	NA	NA	NA
B22	250	27.57	6891.40	236,588	30.98	4753.49–4756.35	36,000**	4598.32	500.33	NA	NA	NA	NA
B23	250	27.59	6896.40	253,413	30.45	4750.78	289.62	4623.13	589.46	31.6	35.2	33.2	1.85

*A5 has the same structure as A4.
**unable to obtain an optimal solution.

good system-wide solutions. Centralized techniques are intended to optimize the entire system, without matching individual preferences. As such, centralized solutions may motivate individual participants to seek other solutions. Our decentralized solution may reduce or eliminate such actions and still provide very good system-wide savings.

One limitation of this study is the necessity of enumerating feasible carpools, which might be prohibitive for a large number of origins (n) and a large number of passenger seats per vehicle (q). Also, the lack of reasonable assumptions on the minimum savings and maximum extra distance per trip may lead to very large values of feasible carpools (m), which determine the number of variables in the formulation of the set-partitioning problem. Another limitation of the proposed solution is the greedy way of braking impasses in the decentralized heuristic. Each impasse may result in ties which may lead to different solutions. Lastly, our solution technique does not consider bargaining, i.e., compensating participants for giving up their most-preferred choices. The planned extensions of this research will address some of the above-mentioned limitations.

6. Concluding remarks

We presented a new decentralized approach to solving carpool problems of the two common types: to/from (TFC) and pick-up/drop-off (PDC). Our decentralized heuristic solution, which is based on matching participants' preferences, mimics carpool self-organization. Compared with the centralized approach, our heuristic achieves similar system-wide savings but does not require additional incentives, i.e., it is perceived by participants as a fair market solution by participants.

The results suggest a potential strategy for improving carpool utilization. This strategy requires policy-makers to give up a small portion of the *planned* system-wide savings to increase the *actual* savings due to an improved car pooling utilization.

One way for organizations to implement the proposed approach would be to offer a ranked list of potential available carpools to each participant instead of a pre-defined assignment. Selecting one or prioritizing more carpools would send an invitation to other participants and the first arrangement accepted by all interested parties would make the carpool permanent.

Future research will address improving the carpool enumeration technique, incorporating various tie-breaking techniques for the decentralized approach, and introducing meeting points (hubs) for commuters, which may be different from their origins. Furthermore, the concept of fairness in car pooling will be analyzed from the economic games theory perspective by considering the distance driven by each carpooler rather than the number of times they drive.

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Self-organized carpools with meeting points

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Self-organized carpools with meeting points

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ABSTRACT

Carpooling promises benefits to the environment and consumers alike, but research has shown that there are multiple practical challenges to realizing these benefits. One possible solution is the addition of meeting points (hubs) in the design of carpooling systems. Recent studies indicate that introducing hubs increases both carpool participation and system-wide savings. Little to no research has been conducted, however, to understand the origin of these savings, determine their utility in different carpooling models, or detailing how hubs should be introduced (i.e. as a mandate or option). Additionally, we know nothing about the impact of hubs on self-organizing carpools (the primary means of creating carpooling systems). To address these gaps, we studied the impact of meeting points on two types of carpooling models (pick-up/drop-off and to/from), using two solution paradigms (centralized and self-organized), with hubs that were either mandated or optional. Our findings show that adding the option of meeting hubs improves system-wide savings from carpooling. These findings, along with our introduction of a new efficient carpool enumeration technique, have important practical implications for the design of modern carpooling systems in the development of more effective and sustainable uses of transportation resources.

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1. Introduction

Carpooling can be defined as sharing a private vehicle by a certain number of people to reach one or more destination points. According to a Census Bureau report released in 2015 (McKenzie, 2015), most people in the U.S. (85%) used private vehicles to commute to work, and 76% of them drove alone. Only 9% of commuters reported carpooling with their neighbors or coworkers and a little over 5% used public transportation. After increasing consistently over the previous decades, these numbers have remained relatively stable in recent years. These trends lead to traffic congestion, a personal cost of commuting, and high emissions of gaseous pollutants (even if electric vehicles are used). The most frequently cited reasons why carpooling is not more popular include the lack of effective methods to encourage carpool participation and the need to coordinate ride schedules (Furuhata et al., 2013).

The majority of carpool optimization techniques focus on centralized (system-wide) objectives, such as the minimization of the total distance traveled by all commuters (Agatz, Erera, Savelsbergh, & Wang, 2012; Ferrari, Manzini, Pareschi, Persona, & Regattieri, 2003). While such an approach serves the community's goals (e.g. reducing pollution and traffic), it may produce unsatisfactory results for individual carpoolers (Agatz et al., 2012) which, in turn, may reduce participation in carpooling. Recently, Kalczynski and Miklas-Kalczynska (2019) showed that self-organized carpools, motivated by individual preferences, produce savings similar to centralized carpools and are both easier to implement and do not require additional incentives to encourage participation. Furthermore, while the majority of carpooling literature and government reports consider the "To/From" models associated with commuting to and from work, Kalczynski and Miklas-Kalczynska (2019) studied "Pick-up/Drop-off" models inspired by parents driving their children to and from school or activities.

This current study builds upon and extends the models presented in Kalczynski and Miklas-Kalczynska (2019) by introducing meeting points (hubs) to carpools of both the Pick-up/Drop-off (PDC) and To/From (TFC) types, comparing the savings from self-organized (decentralized) and centralized (system-wide) solutions, and utilizing simulated instances of carpooling problems.

The main contribution of this research is to provide evidence that meeting points introduced as options, rather than imposed, result in additional system-wide savings. This discovery has important implications to policy-makers, organizations, and communities who design and implement carpooling systems. Other important contributions of this paper include the provision of a theoretical explanation of why the introduction of hubs increases system-wide savings and revealing the extent of these savings in different types of carpooling models (i.e. PDC and TFC) and for different solution objectives (i.e. self-organized and centralized). Our main results apply to all models and objectives studied.

The remainder of the paper is organized as follows. The relevant literature review is presented in the next section.

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Section 3 describes relevant concepts illustrated with examples. Section 4 presents the formal model of the carpool with meeting points along with the theoretical definition of the carpooling "neighborhood," improved carpool enumeration, and solution techniques. Computational experiments involving simulated problem instances are presented in Section 5, followed by the concluding remarks.

2. Background Studies

2.1. Context and definitions

Carpooling belongs to a broader category of problems, called ridesharing (Agatz et al., 2012; Furuhata et al., 2013), which is a general term used to describe shared trips between a group of commuters with similar original locations and/or destinations. Ridesharing differs from services such as Lyft or Uber in that the planned trip would occur regardless of a passenger match. In ridesharing, a person who acts as a driver is willing to pick-up and drop-off riders along the way, despite the need to make detours and extra stops. The length of the detour and the number of extra stops depend on the driver's willingness to extend his or her trip time/distance (Stiglic, Agatz, Savelsbergh, & Gradisar, 2015).

There have been many studies of traditional ridesharing, which detail, review and classify ridesharing models (Furuhata et al., 2013), provide a survey of the dynamic ridesharing models, in which drivers and riders are matched on short notice (Agatz et al., 2012), and describe past, present and future ridesharing trends in North America (Chan & Shaheen, 2012). This and similar lines of research distinguish three different categories of ridesharing: acquaintance-based, organization-based, and ad hoc (Stocker & Shaheen, 2017). In acquaintance-based ridesharing, people who organize themselves to travel together know each other, whereas in the organization-based ridesharing, the participants need to sign up for the service. Finally, ad hoc ridesharing refers to an incidental shared trip.

Carpooling is a form of ridesharing, in which people travel together on recurring trips (Baldacci, Maniezzo, & Mingozzi, 2004; Calvo, de Luigi, Haastrup, & Maniezzo, 2004). Whereas, ridesharing includes carpooling and vanpooling, depending on the number of passengers traveling together in a vehicle, carpooling involves less than seven passengers while vanpooling seven to 15. In practice, however, most passenger cars have five seats.

The most extensively researched version of the carpooling problem is the centralized (system-wide) approach, in which a carpool is organized as a transportation service by a company for its employees in order to improve a parking situation, or to reduce traffic congestion, gasoline consumption, and/or pollution, etc. (Agatz et al., 2012; Bruck, Incerti, Iori, & Vignoli, 2017; Ferrari et al., 2003; Guidotti, Nanni, Rinzivillo, Pedreschi, & Giannotti, 2017; Mallus, Colistra, Atzori, Murroni, & Pilloni, 2017; Yu, van den Berg, & Verhoef, 2019). In contrast with the aforementioned studies, Kalczynski and Miklas-Kalczynska (2019) propose a decentralized carpool self-organization process which shows savings similar to centralized models, yet can also increase carpool utilization. The model, which focuses on individual savings instead of focusing only on system-wide savings challenges inefficiencies in carpool participation. This paper, a continuation of the work of Kalczynski and Miklas-Kalczynska (2019), focuses on the decentralized carpool approach and proposes a way of further improving carpool participation by incorporating meeting points into the model.

2.2. Meeting points in carpooling literature

High participation in any carpooling system is key to its success. High participation has proven difficult to maintain, however, since factors such as the need to coordinate carpool schedules or the lack of effective incentives, are considered challenging to overcome (Agatz, Erera, Savelsbergh, & Wang, 2011; Furuhata et al., 2013; Kleiner, Nebel, & Ziparo, 2011; Lee & Savelsbergh, 2015; Stiglic et al., 2015, Stiglic, Agatz, Savelsbergh, & Gradisar, 2016). Additionally, in order to function effectively over the long haul, carpooling systems require high matching rate for riders. Several solutions to this problem have been put forward. For example, Lee and Savelsbergh (2015) propose dedicated drivers for unmatched riders, while Kleiner et al. (2011) suggest a sealed-bid second price auction approach. Less researched option is the addition of meeting points (hubs). Carpool participants may be picked up at well-placed meeting points, including one of the participants' original locations. With hubs, it is no longer necessary for drivers to increase the number of stops along the way to pick-up riders, so the number of feasible carpools increases. Stiglic et al. (2015) discuss the idea of meeting points in a carpooling problem and discover that meeting points in the centralized model can indeed increase the number of matched participants and produce considerable system-wide driving distance savings. They present an algorithm that matches drivers and riders with meeting points and use a simulation utilizing real-life traffic patterns.

In other relevant work, Kaan and Olinick (2013) consider meeting points in a vanpooling model. Their paper explores the problem of assigning the vanpool participants and the vehicles to the park-and-ride locations. They use mixed integer programing and provide a number of solution heuristics. In contrast, Aissat and Oulamara (2014) focus on finding the best meeting points once a match between a single driver and a single rider has been established. They provide the exact and heuristic approaches to identify meeting points, based on minimizing total travel cost of both the driver and rider. Aïvodji, Gambs, Huguet, and Killijian (2016) further expand the utility of meeting points as a means of protecting the privacy of user location data. To incorporate the privacy-protection mechanisms into a ridesharing system, they use secure multiparty computation and multimodal routing algorithms. Finally, Chen, Mes, Schutten, and Quint (2019) consider a multi-hop ridesharing problem that incorporates meeting points and provide a greedy heuristic utilizing linear programing. In their research, they introduce return restrictions and incorporate a backup transportation service, such as taxi, as an option

Table 1. Carpooling models.

Acronym	Model
PDC	Pick-up/drop-off carpool
TFC	To/from carpool
PDCH	Pick-up/drop-off carpool with hubs
TFCH	To/from carpool with hubs
PDC/PDCH	Pick-up/drop-off carpool with optional hubs
PDC/TFCH	To/from carpool with optional hubs

for carpool participants. Based on their results they conclude that ridesharing creates more benefits in the case of high participation and when the original locations and the destinations are closer to each other.

The concept of meeting points in ridesharing is sometimes utilized in the context of "slugging." In slugging, passengers walk to predetermined locations and wait for their rides to pick them up. Some potential problems with determining suitable meeting points include safety considerations related to both meeting points themselves as well as the passengers' routes from their original locations to the meeting points. Weather can also be a problem (Stiglic et al., 2015). In order to better understand the complexities of the slugging problem, Ma and Wolfson (2013) provide a formal definition of a slugging problem and propose a quadratic algorithm to solve it. They also discuss dynamic slugging and introduce several heuristics. As helpful as this research is, the authors do not consider the problem of choosing suitable meeting points. This neglect was rectified by Czioska and Sester (2015) who devote their work to determining suitable meeting points in the context of slugging and compare five optimization methods to identify meeting point locations on a street network. Their model focuses on balancing of travel times between a single driver and a single rider, so that they meet simultaneously at the meeting point.

In this paper, we build upon this research to offer a comprehensive theoretical analysis of the carpooling neighborhood concept and explain the increase in carpooling options when hubs are utilized. Through this process, we develop a new carpool enumeration technique and reveal how savings from meeting points depend on both the type of carpooling model and the solution technique.

3. Savings from carpooling and meeting points

In both PDC and TFC carpool models, participants take turns using their private vehicles to pick-up and drive others in carpools to a common destination. In the PDC model (e.g. driving children to school), the driver and vehicle return to the original location, whereas in TFC model (e.g. commuting to work), the driver and vehicle remain at the destination, after dropping off the passengers. Both PDC and TFC models complete the cycle for the driver and driver's vehicle, i.e. they return to their point of original location. The difference between the PDC and TFC models is that, in PDC, the driver and vehicle do not stay at the destination with the passengers but return directly to the original location.

We extend both of the TFC and PDC carpooling models by using participants' original locations as meeting points

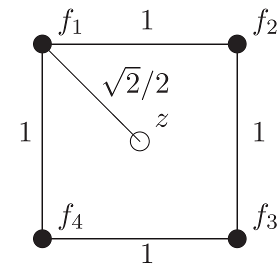

Figure 1. A four-origin carpooling problem instance.

(hubs) for carpools. In the remainder of the paper, these new models will be referred to as the "To/From Carpool with Hubs" (TFCH) and "Pick-up/Drop-off Carpool with Hubs" (PDCH). Although any location could serve as a carpool hub, we chose to use participants' original locations because this arrangement is attractive for the participants (because there is no additional driving distance). As a result, the first choice of every participant is a carpool in which their original location is a meeting point.

In TFCH, participants arrive at a meeting point in their private vehicles before departing to the destination in a carpool. All vehicles except for one remain at the hub. The participants take turns driving others from the hub to the destination and then back to the hub. Next, they use their private vehicles to return from the hub to their respective original locations.

In PDCH, riders are dropped off at a meeting point. Then, drivers and vehicles return to their original locations, except for the driver, whose turn it is to drive the riders to the destination. After dropping off the passengers at the destination, the carpool driver returns directly to his or her original location.

Table 1 summarizes the carpooling models described in the remainder of this paper.

3.1. Minimum savings and maximum additional distance

Not all carpools which are rational, i.e. result in positive savings for all participants, are practical. Consider an example in Figure 1, in which four original locations are located on the corners of a unit square with the destination in the middle. To maximize their individual savings, the participants consider forming a PDC carpool $\{f_1, f_2, f_3, f_4\}$. We use braces to represents unordered sets in the remainder of this paper.

In this arrangement, each participant drives every fourth day. On that "driving day," the driver picks up the remaining three participants on the way to school, drops them off at school and then returns to the original location. The baseline (no carpooling) distance, $b_k = \sqrt{2}$ for $k = 1, \ldots, 4$ for the example in Figure 1, is the same for all participants.

On the driving day, the participant originating from f_k drives three distance units to pick-up others, plus $\sqrt{2}/2$ to get to school, and then, $\sqrt{2}/2$ more to return home. Consequently, the total distance traveled on a driving day will be $3 + \sqrt{2} = 4.41$ units. However, the same distance will be zero on the non-driving day. Hence, the average driving distance in this carpool is 1.10 units, which yields

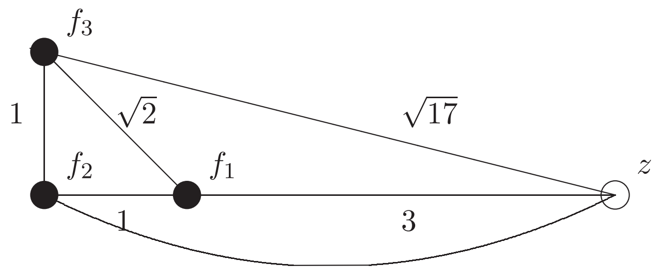

Figure 2. A three-origin carpooling problem instance.

the average savings of 0.31 units or about 22% of the baseline.

Despite positive individual and system-wide savings, this arrangement requires each participant to drive three additional units (212.13% of the baseline) every 4 days. Depending on the unit size (e.g. 1 mile vs. 10 miles), this arrangement may be impractical from the savings and/or extended driving distance perspective. Thus, for practical applications, participants must specify their minimum savings (e.g. 2 miles or 25% of the baseline, whichever is larger) and maximum additional distance (e.g. 10 miles or 50% of the baseline, whichever is smaller) constraints. If the baseline distance, b_k, is known, the combination of absolute and relative constraints can be converted for each participant to either absolute or relative.

This maximum extended driving distance constraint is of particular importance to the new enumeration technique presented later in this paper.

3.2. Meeting points (hubs)

To illustrate carpools with hubs, let us reuse a simple instance with three original locations f_1, f_2, f_3 and a common destination z, originally presented by Kalczynski and Miklas-Kalczynska (2019). As in the original illustration, we assume that each original location has one vehicle with a driver and only one seat available for a passenger. There is only one passenger to be picked up from each original location. We also assume that each original location can serve as a meeting hub.

Given these assumptions, the following carpooling arrangements are possible in TFCH and PDCH models: $\{f_1,f_2\}_{f_1}$, $\{f_1,f_2\}_{f_2}$, $\{f_2,f_3\}_{f_2}$, $\{f_2,f_3\}_{f_3}$, $\{f_1,f_3\}_{f_1}$, and $\{f_1,f_3\}_{f_3}$, in which the subscript of each set denotes the hub.

The distances for all carpool arrangements are shown in Figure 2.

In addition to the average system-wide distance traveled by all participants, Kalczynski and Miklas-Kalczynska (2019) considered average distances for each participant. This distance is a measure of commute cost for carpooling with the assumption that in the long run, each participant drives the same number of times (this should not be difficult to achieve with about 250 work days and 180 school days or 360 trips in a year).

Let us consider the $\{f_1,f_3\}_{f_1}$ case for the TFCH model in which f_3 carpools with f_1 using the original location of f_1 as a hub. The average commute distance for the participant at f_1 is simply half of the participant's baseline (because they drive every other day). The average commute distance for f_3 in this arrangement is $\left(\sqrt{2}+3+3+1.41+2\sqrt{2}\right)/2 = 5.83$. This includes the distance driven on a driving day and the cost of getting to the hub on the non-driving day. The average cost for f_3 is 29.4% less than their baseline. The average cost for f_2 (not in any carpool) is equal to their baseline. As a result, the average total cost (distance) for all commuters in the $\{f_1,f_3\}_{f_1}$ case is $3+5.83+8=16.83$ which is 24.4% less than the baseline.

All potential carpool configurations for the TFCH and PDCH models with corresponding average round trip distances and savings are presented in Tables 2 and 3.

Tables 2 and 3 show some interesting results:

- $\{f_1,f_3\}_{f_3}$ (TFCH) will not be selected by a rational participant at f_1 because it results in negative individual savings for this participant. However, it shows positive total savings, which makes it a rational solution from a centralized perspective.
- The $\{f_2,f_3\}_{f_2}$ shows the maximum total savings of 6.25 for TFCH and 6.69 for PDCH and would be the system-wide first choice. These savings are higher than 6.13 for the original TFC problem but lower than 7.13 for the original PDC problem reported in (Kalczynski & Miklas-Kalczynska, 2019).
- The first choices of individual participants are the ones in which their original locations serve as hubs. This means that a carpool which is the first choice for all its members does not exist, so participants will have to settle for lower savings in order for the self-organized carpooling to work.

4. Problem formulation

In this section, we present the mathematical formulation for the proposed model. First, we extend the framework introduced by Kalczynski and Miklas-Kalczynska (2019) for PDC and TFC to incorporate mandatory meeting points. We call these extended models PDCH and TFCH. Then, we further extend the models to incorporate hubs as an option rather than a mandate. We call these PDC/PDCH and TFC/TFCH. Finally, we apply a theoretical analysis of the carpooling neighborhood concept. This process led to a complete redesign of the carpool enumeration technique presented by Kalczynski and Miklas-Kalczynska (2019). This new technique, which is based on elliptical neighborhoods, is applicable to all models and provides theoretical foundations to understand why introducing meeting points results in system-wide savings and increased carpool participation.

Moreover, our new models are compatible with the existing self-organized and centralized solution techniques, so we briefly describe these techniques in the last subsection. The self-organized solution concept, first introduced by Kalczynski and Miklas-Kalczynska (2019), attempts to maximize savings of each individual participant, in contrast with the "classical" centralized (system-wide) solution concept which maximizes savings from the policy-makers

Table 2. Carpool arrangements for the three-origin instance – TFCH.

		Average distance for to/from carpools with hubs					
Original location	Baseline distance	$\{f_1,f_2\}_{f_1}$	$\{f_1,f_2\}_{f_2}$	$\{f_1,f_3\}_{f_1}$	$\{f_1,f_3\}_{f_3}$	$\{f_2,f_3\}_{f_2}$	$\{f_2,f_3\}_{f_3}$
f_1	6.00	3.00[a]	6.00	3.00[a]	6.95	6.00	6.00
f_2	8.00	5.00	4.00[a]	8.00	8.00	4.00[a]	6.12
f_3	8.25	8.25	8.25	5.83	4.12[a]	6.00	4.12[a]
Total	**22.25**	**16.25**	**18.25**	**16.83**	**19.07**	**16.00**[b]	**16.24**
Savings	NA	6.00	4.00	5.42	3.18	6.25	6.01

[a]Participant's first choice.
[b]System-wide optimal solution.

Table 3. Carpool arrangements for the three-origin instance – PDCH.

		Average distance for pick-up/drop-off carpools with hubs					
Original location	Baseline distance	$\{f_1,f_2\}_{f_1}$	$\{f_1,f_2\}_{f_2}$	$\{f_1,f_3\}_{f_1}$	$\{f_1,f_3\}_{f_3}$	$\{f_2,f_3\}_{f_2}$	$\{f_2,f_3\}_{f_3}$
f_1	6.00	3.00[a]	5.00	3.00[a]	5.68	6.00	6.00
f_2	8.00	5.00	4.00[a]	8.00	8.00	4.00[a]	5.56
f_3	8.25	8.25	8.25	5.68	4.12[a]	5.56	4.12[a]
Total	**22.25**	**16.25**	**17.25**	**16.68**	**17.80**	**15.56**[b]	**15.68**
Savings	NA	6.00	5.00	5.57	4.45	6.69	6.57

[a]Participant's first choice.
[b]System-wide optimal solution.

Table 4. Summary of notation used.

Symbol	Meaning	Description
i,j,k,ℓ,r	Index	Reusable indices used in iterations and summations
a_k	Semi-major axis	Semi-major axis of the elliptical neighborhood
b_k	Baseline distance	Baseline travel distance (to and from z) starting at f_k
$c_k()$	Cost of commute	Average daily cost of commute from original location f_k
C	Carpool	Set of participants' original locations in a carpool
C_{f_ℓ}	Carpool with a hub	Carpool with a hub at original location f_ℓ
$d()$	Distance function	Distance between two points
$e_k()$	Extended distance	Total detour for participant at f_k on the driving day
ε_k	Max. extended distance	Maximum total detour for participant at f_k
F	Set of original locations	A set of n original locations $\{f_1,f_2,...,f_n\}$
f_k	Original location	Original location of participant k
m	Number of carpools	The number of potential (feasible) carpools
n	Number of original locations	The number of participants' original locations
N_ℓ	Neighborhood	The potential carpoolers of original location or hub
P	Set of carpools	A set of m potential carpools
p_k	Number of passengers	The number of passengers traveling from f_k
q_k	Number of seats	The number of seats in the vehicle at f_k
q_{max}	Max. number of seats	The maximum number of passengers per vehicle
$s_k()$	Savings from carpooling	The average distance saved by participant at f_k
z	Destination	Carpooling destination such as school or work

perspective. Table 4 shows the summary of notation used in the remainder of this paper.

4.1. Cost and savings

The shortest path algorithm is not needed for models with hubs imposed. The entries from the distance matrix are sufficient to determine both the carpooling cost and the savings. This is because participants travel individually to and from the hub, and carpooling occurs only between the hub and the destination.

Let $d(a,z)=d(z,a)$ be the distance (e.g. Euclidean, shortest driving, quickest driving, etc.) between location a and destination z.

Let $F=\{f_1,f_2,...,f_n\}$ be the set of n original locations of participants interested in carpooling to a common destination. Each participant commuting from f_k has $p_k\geq 0$ passengers and a vehicle with q_k seats available $(q_k>p_k)$.

For a non-empty carpool using f_ℓ as a hub, $C_{f_\ell}=\{f_i,f_j,...\}$, the average daily cost of commute for a participant starting from $f_k\in C_{f_\ell}$ is

$$c_k(C_{f_\ell})=2\ d(f_\ell,z)+2\ d(f_k,f_\ell)+2\ (|C_{f_\ell}|-1)\times d(f_k,f_\ell) \tag{1}$$

for the TFCH model, and

$$c_k(C_{f_\ell})=d(f_k,f_\ell)+d(f_\ell,z)+d(z,f_k)+2\ (|C_{f_\ell}|-1)\times d(f_k,f_\ell) \tag{2}$$

for the PDCH model. The main difference between the models is that, in the PDCH model the driver returns to the point of original location after dropping off passengers at destination z (e.g. school) while, in TFCH, the driver remains with passengers at destination z (e.g. work) and then returns to the hub f_ℓ with passengers before going back to original location f_k.

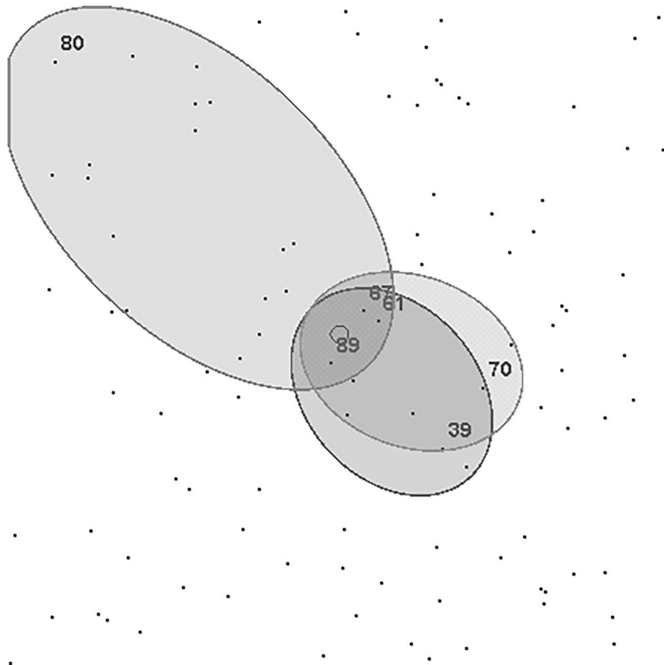

Figure 3. Elliptical neighborhoods for selected original locations.

The extended commute distance (due to detours taken to pick-up or drop-off others on the driving day) and average savings for a participant commuting from f_k to z in carpool C_{f_ℓ} are:

$$e_k(C_{f_\ell}) = c_k(C_{f_\ell}) - 2\ (|C_{f_\ell}| - 1) \times d(f_k, f_\ell) - b_k \tag{3}$$

$$s_k(C_{f_\ell}) = b_k - c_k(C_{f_\ell})/|C_{f_\ell}| \tag{4}$$

Note that the extended driving distance (3) pertains only to participants on their driving days and does not include commuting to and from the hub on non-driving days. Also, if the participant's original location serves as a hub, the extended driving distance for this participant is zero which acts as an additional incentive for participants located close to destination z.

The savings from carpooling are averaged over a long period (e.g. 250 work days or 180 school days). We make a practical assumption that participants divide driving days equally among themselves over the long period of time. For example, in a three-family carpool, each family will drive for 60 out of 180 school days.

Because of the introduction of the hubs into the original models, a new carpool enumeration technique is needed.

4.2. Carpool enumeration

The total enumeration of carpools (with or without hubs) is not practical as the number of carpooling arrangements grows faster than exponentially.

For carpools with n participants, with each participant's original location potentially serving as a hub and q_{max} maximum seats in a vehicle, the maximum number of carpools depends on the number of subsets, no larger that q_{max}, one can create from a set of n participants. Therefore, we can extend the classic combination formula to find the total number of carpools in the system:

$$\sum_{r=1}^{q} r \binom{n}{r} = \sum_{r=1}^{q} \frac{n!}{(r-1)!(n-r)!}. \tag{5}$$

And so, for 100 participants and four seats, the number of carpools with hubs is 66,018,450 however, only a small portion of them will be rational and practical. Note that, single-participant "carpools" are also included in this calculation.

The number of analyzed carpools can be significantly reduced by taking into account individual constraints, such as the number of passengers and seats, maximum extended driving distances, or minimum savings.

Kalczynski and Miklas-Kalczynska (2019) presented an enumeration technique in which a set of "neighbors," i.e. participants willing to form a carpool, is created and extended in a greedy manner. Carpools generated by this technique are non-empty and collectively exhaustive subsets of the set of original locations, F. In this paper, we present an improved version of this approach. We redefine and extend the set of neighbors for each participant and then use this set to enumerate carpools for models with or without hubs.

A neighbor of a participant traveling from f_i is another participant who is willing to form such a carpool C with f_i which is rational for both of them. Intuitively, neighbors must have enough available passenger seats in their vehicles, and they must be within a reasonable detour distance from one another. This distance can be quantified by specifying the maximum extended distance, ε_k, that participant k is willing to travel on a driving day.

And so, a participant traveling from f_j is a neighbor of a participant traveling from f_i if $p_i + p_j \leq min(q_i, q_j), e_i(C) \leq \varepsilon_i$, and $e_j(C) \leq \varepsilon_j$. The former inequality ensures that enough seats are available in vehicles used to carpool and the latter limits the maximum detour on the driving day to ε_j.

Note that in models with hubs we look for potential meeting points (not participants' original locations) which are within the neighborhood of f_i. For a given hub f_ℓ, we identify sets of original locations whose respective neighborhoods contain this hub. These original locations are used to form carpools with f_ℓ serving as the hub.

On the plane with all distances measured with the Euclid formula, the region in which neighbors (or hubs) of f_k are located is bound by an ellipse with foci at the destination z and original location f_k. The size and eccentricity of this ellipse depend on the type of the carpooling problem, and relative extended distance, ε_k/b_k. However, for any model, these elliptical regions have to mutually include their original locations (or a common hub) in order to be considered neighbors.

An ellipse can be fully defined by its foci and the semi-major axis a. The foci of the neighborhood ellipses are at the destination z and the original location f_k. Therefore, we used general ellipse representations to derive the lengths of semi-major axes of the neighborhood regions of f_k:

$$a_k = 0.25\ b_k(1 + 2\ \varepsilon_k/b_k) \tag{6}$$

for the PDC and PDCH models, and

$$a_k = 0.25 \ b_k(1 + \varepsilon_k/b_k) \tag{7}$$

for the TFC and TFCH models.

With these parameters, it is relatively easy to check whether a given point is contained within the elliptical region defined for f_k. And so, on the plane, f_j is a neighbor of f_i if it is within f_i's elliptical neighborhood.

Formally, let N_i be the set of neighbors for a participant traveling from f_i. For the models without hubs,

$$N_i = \{f_j\} : d(f_i, f_j) + d(f_j, z) \leq 2a_i \ \cap \ d(f_j, f_i) + d(f_i, z) \leq 2a_j \tag{8}$$

and for the models with hubs, where f_ℓ is a hub,

$$N_\ell = \{f_j\} : d(f_j, f_\ell) + d(f_\ell, z) \leq 2a_j \tag{9}$$

Equations (8) and (9) define the sets of original locations or meeting points on the plane which are contained within the elliptical regions defining car-pooling neighborhoods.

Figure 3 illustrates the concept of the elliptical neighborhood for the TFC-type models. It shows 100 original locations on a 20×20 unit square (see the Appendix). The small circle in the middle represents the destination. The three ellipses shown are based on the ε_k constraints for original locations f_{39}, f_{70}, and f_{80}. For each original location, the maximum extended driving distance is either 50% of the baseline, or 10 units, whichever is smaller. The baseline driving distances are 18.66, 18.43, 47.71 for f_{39}, f_{70}, and f_{80}, respectively, which means that the maximum extended driving distances, ε_k, are 9.33, 9.22, and 10 units.

Of these three original locations, only f_{39} and f_{70} are neighbors in the original TFC model (no hubs) because the elliptical region of f_{39} contains f_{70} and vice versa. However, when we consider any of the three original locations contained within the intersection of the three elliptical regions (f_{61}, f_{67}, f_{89}) as potential hubs (TFCH), all three original locations f_{39}, f_{70}, and f_{80} are neighbors from the maximum extended driving distance perspective. For PDC models, the elliptical regions are simply larger for the same values of ε_k.

Note that, unlike in Kalczynski and Miklas-Kalczynska (2019), the neighborhoods N_i and N_ℓ are generated before any carpools are enumerated and they do not include the minimum savings constraints.

Such a set of neighbors substantially reduces the number of multi-participant carpools in the enumeration. Because the ellipses for PDC models are larger, the neighborhoods for these models are expected to be larger than neighborhoods of TFC models. Also, neighborhoods of models with hubs are expected to be much larger than those of models without hubs. Larger neighborhoods result in larger sets of potential carpools. This explains increased participation in carpools with hubs and increased savings from such carpools.

We use the new neighborhood to enumerate carpools. Our improved enumeration algorithm involves generating all subsets of N_i of size $q = 1, 2, 3, \ldots, q_{max}$ for each $i = 1, 2, \ldots, n$ (without creating duplicate subsets) for carpools without hubs (PDC, TFC). For carpools with hubs (PDCH and TFCH), we assume that f_ℓ is fixed as the hub and we generate subsets of size $q - 1$ from all neighbors in N_ℓ. For all types of models, carpools which do not meet the criteria of available passenger seats, maximum extended driving distance or minimum savings are eliminated.

The above approach to building the set of potential carpools P is more exhaustive than the greedy one presented by Kalczynski and Miklas-Kalczynska (2019), yet it still enables the enumeration of rational and practical carpools in a reasonable time.

4.3. Solution techniques

Our formulations allow applying the existing self-organized and centralized solution techniques without any modifications. This section offers just a brief description of these techniques. The reader is referred to Kalczynski and Miklas-Kalczynska (2019) for all details needed to implement these techniques.

The set P of m potential carpools created with our new enumeration technique is transformed into a (sparse) $n \times m$, matrix of individual savings using (4). Each column of this matrix represents participants' individual savings corresponding to a potential carpool from P. A total for each column represents the contribution of each carpool C_j in P ($j = 1, \ldots, m$) to system-wide savings.

A feasible solution to the carpooling problem consists of such an assignment of participants to carpools in which each participant is assigned to one and only one carpool. This is possible because P contains all single-participant "carpools." Also, it does not matter what carpool model (PDC, PDCH, TFC, or TFCH) is used to create carpools in P. P can contain carpools from various models, as long as one keeps track of the models corresponding to columns in the savings matrix.

This approach allows us to append potential carpools (and corresponding columns of saving matrices) from various models. We utilize it to formulate and solve mixed PDC/PDCH and TFC/TFCH problems. In such mixed models, designating original locations as hubs is optional.

Both solution techniques (centralized and decentralized) described by Kalczynski and Miklas-Kalczynska (2019) can be applied to solving both the new problems with hubs and the mixed problems.

The centralized approach can be considered a special case of the Generalized Assignment Problem (GAP) or a multi-dimensional 0–1 Knapsack Problem with the capacity of each knapsack equal to 1 and forced equality constraints. This formulation is also known as the Set Partitioning Problem and is modeled as a Binary Linear Program (BLP).

The self-organizing (decentralized) approach is based on matching participants' preferences (savings) and does not directly consider system-wide savings. Still, this technique yields very good system-wide solutions, is much less complex compared to finding the centralized solution, and maximizes individual participant's savings. In each iteration of the self-organizing technique, the carpools with the highest savings for their respective participants are selected. Next, the selected participants and all remaining potential carpools, including their original locations, are removed from

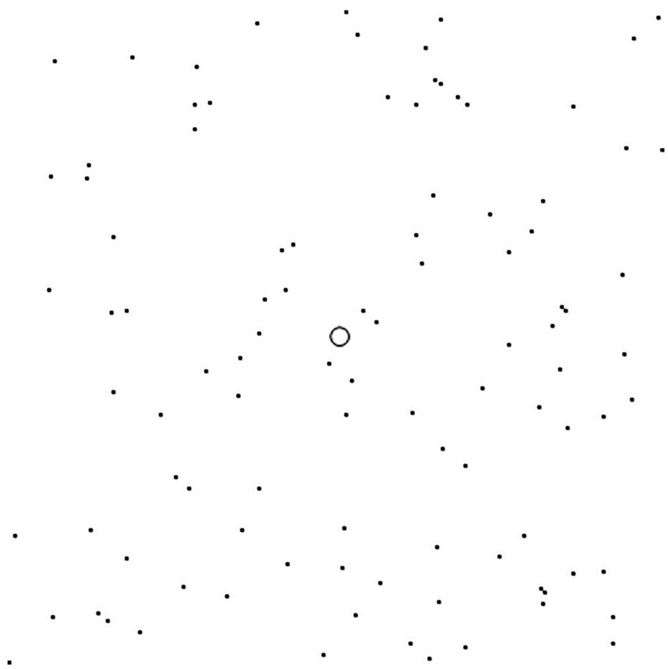

Figure 4. A simulated carpooling problem instance.

further consideration. The algorithm uses a simple tie-breaking technique and stops when all participants are assigned to carpools. The readers are referred to Kalczynski and Miklas-Kalczynska (2019) for detailed descriptions of both the decentralized and centralized solution techniques for carpooling problems.

5. Computational experiments

Kalczynski and Miklas-Kalczynska (2019) conducted extensive simulation experiments with the PDC and TFC formulations using real-world and simulated carpooling problem instances. Their results were consistent across instances and problem types. The primary focus of this paper is to study the impact of introducing meeting points to carpools, i.e. studying PDCH, TFCH and mixed PDC/PDCH and TFC/TFCH models. For this reason, we use a pseudo-random instance described in the Appendix and shown in Figure 4, which can be easily replicated. And so, data for these experiments are generated rather than acquired. This way, anyone with a spreadsheet can accurately replicate the entire data set and create additional ones if needed. All simulation experiments described in this paper were conducted with *Mathematica* 11.3 running on a virtualized Windows environment with 16 vCPUs and 64GB of RAM.

The total baseline distance (no carpooling) for the problem shown in Figure 4 is 3049.12 units. The instance consists of the destination, marked with a small circle in the middle, and 100 original locations.

We assume that all cars in the PDC-type models have at most four available seats (one is reserved for the driver), all vehicles in the TFC-type models have five seats, and that each original location has exactly one participant.

Table 5. The number of potential PDC carpools.

	Problem type		
q_{max}	PDC	PDCH	PDC/PDCH
2	413	625	1,038
3	665	5,379	6,044
4	764	34,019	34,783

Table 6. PDC Carpool Participation Rate.

	PDC		PDCH		PDC/PDCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	88%	94%	94%	96%	92%	96%
3	88%	93%	93%	97%	94%	96%
4	88%	91%	89%	97%	92%	97%

Table 7. PDC/PDCH carpool hub utilization.

q_{max}	SELFORG	CENTR
2	66.24%	3.84%
3	62.98%	22.08%
4	66.24%	53.35%

We solved the original (PDC, TFC) problems, their versions with hubs (PDCH, TFCH), and the mixed models (PDC/PDCH and TFC/TFCH) for the maximum carpools sizes: $q_{max} = 2$, 3, 4, and 5 using the self-organizing (SELFORG) and centralized (CENTR) techniques applied to potential carpools generated with our new enumeration technique. The mixed models make the use of hubs optional, i.e. the solver can choose the best carpool arrangement from the set of potential carpools with and without hubs.

5.1. The pick-up/drop-off carpools

Table 5 shows the number of potential PDC carpools resulting from our new enumeration technique. The original PDC problem has 413 single-participant and two-participant carpools, and 764 carpools with 1, 2, 3, or 4 participants to choose from. These numbers increase to 625 and 34,019, respectively, when hubs are introduced. The number of potential carpools for the mixed PDC/PDCH model is the sum of the carpools from PDC and PDCH models.

Table 6 shows carpool participation rates for the PDC-type models. For q_{max}=4, the participation rate in carpools optimized with the self-organized and centralized techniques were 88% and 91%, respectively for the original PDC model. Introducing hubs as an option (PDC/PDCH) increased participation to 92% and 97% for the self-organized and centralized carpools, respectively.

Table 7 shows carpool hub utilization in the PDC/PDCH model for self-organized and centralized solutions. For this model, when hubs are offered as an option, they were selected by 62.98%–66.4% of carpoolers in self-organized carpools and only for 3.84%–53.35% in centralized carpools. In all instances, optional hubs resulted in more system-wide savings as indicated in Table 8.

Table 8 shows the system-wide savings from carpooling for the PDC-type models. The savings increase with the increase of the maximum carpool size, regardless of the type of model and the solution technique. The savings also increase by 0.55%–3.79% when hubs are introduced as an option in the mixed PDC/PDCH model. The system-wide savings are lower for the self-organized carpools than for the centralized carpools (by 4.36% for the PDC/PDCH with q_{max}=4).

Figure 5 shows the self-organized and centralized solutions to the PDCH problem with q_{max}=3. The destination is marked with a small circle, the original locations – with small points, and hubs – with large points. Carpools with two participants are connected with a line, and three-participant carpools are marked with triangles unless they are on a straight line.

Table 8. PDC carpool system-wide savings.

	PDC	PDCH	PDC/PDCH			
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	40.65%	45.00%	43.20%	44.92%	43.35%	45.55%
3	52.15%	57.08%	54.14%	56.79%	55.42%	58.88%
4	55.53%	60.45%	57.91%	62.11%	59.32%	63.68%

The self-organized carpools maximize individual savings and do not consider system-wide savings, so the two solutions consist of different pools. Still, for q_{max}=3 the system-wide savings of the self-organized solution are only 2.65% lower than the savings from the centralized solution.

One can also observe that, in both solutions, the original locations closest to the destination are not in carpools. This is expected when minimum savings and maximum additional distance constraints are used. For original locations participating in carpools, some of the hubs are not the closest to the destination in the pool.

Figure 6 shows the self-organized and centralized solutions to the mixed PDC/PDCH model for q_{max}=3. Allowing

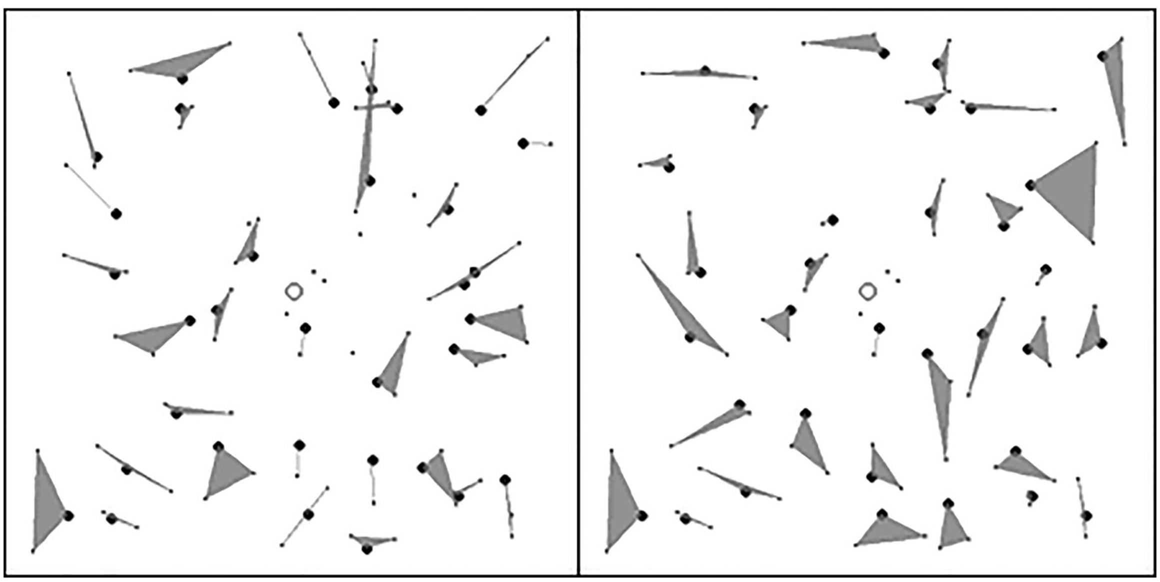

Figure 5. SELFORG and CENTR solutions to PDCH with q_{max}=3.

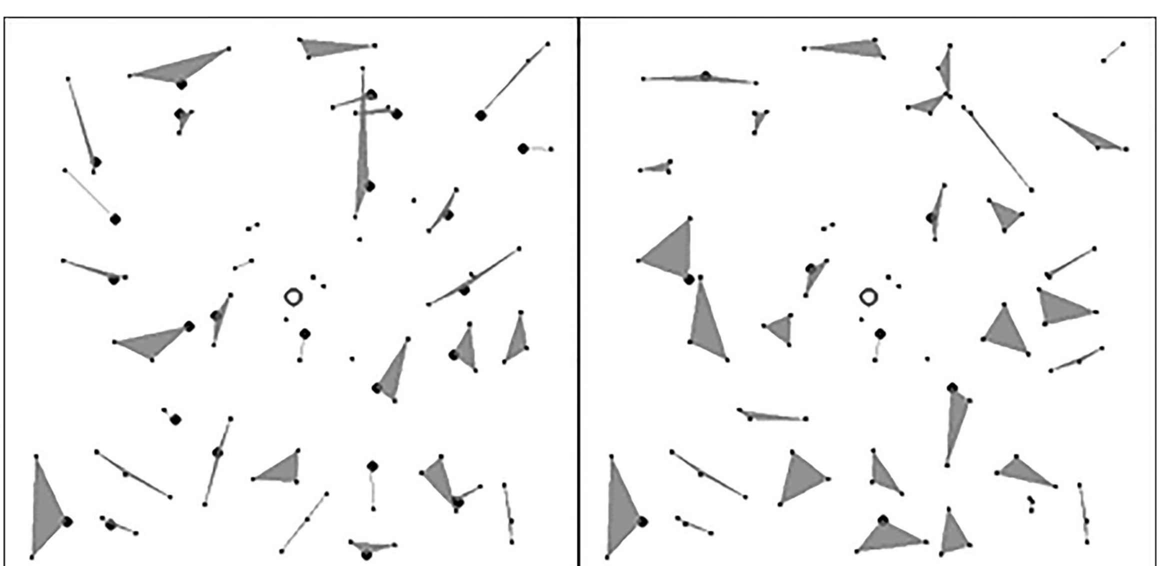

Figure 6. SELFORG and CENTR solutions to PDC/PDCH with q_{max}=3.

Table 9. The number of potential TFC carpools.

	Problem type		
q_{max}	TFC	TFCH	TFC/TFCH
2	180	476	656
3	201	2,866	3,057
4	204	13,798	14,002
5	204	56,691	56,895

Table 10. TFC carpool participation rate.

	TFC		TFCH		TFC/TFCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	70%	72%	86%	96%	86%	96%
3	73%	74%	93%	96%	93%	96%
4	73%	74%	88%	97%	88%	97%
5	73%	74%	90%	97%	90%	97%

Table 11. TFC/TFCH carpool hub utilization.

q_{max}	SELFORG	CENTR
2	65.36%	92.16%
3	75.33%	89.28%
4	75.68%	94.09%
5	81.00%	94.09%

the solvers to choose from a combination of carpools with and without hubs improved savings by 1.31% and 2.09% for the self-organized and centralized solutions, respectively. Carpools with hubs were preferred by the self-organized solver. Still, the difference between the self-organized and centralized savings is only 3.46%.

5.2. The to/from carpools

Recall that the TFC-type models are inspired by commuting to and from work hence the addition of q_{max}=5.

Similar to the PDC models, Table 9 shows a significant increase in carpooling options when hubs are introduced. For q_{max}=5, the number of potential carpools is 204 and 56,691 for the TFC and TFCH models, respectively.

Table 10 shows that introducing hubs to the TFC model increases carpool participation by 15%–24%, which is considerably more than the 2%–6% increase for the PDC-type models.

Table 11 shows that, unlike for the PDC models, carpools with hubs are preferred by both the self-organizing and centralized solution techniques for the TFC-type models. Nearly all carpools selected in the mixed TFC/TFCH are carpools with hubs. Although carpools with hubs were selected less frequently (65.36%–81.00%) in self-organized carpools than in centralized carpools (89.28%–94.09%), offering carpools as an option still increased system-wide savings (with just one small exception of −0.05% for q_{max}=2) as seen in Table 12.

The difference in additional savings from hubs between the PDC and TFC-type models is evident in Table 12. In the TFC models, the savings from introducing hubs ranged from 9.38% to 24.87%. Similar to the PDC-type models, savings increase with the increase in the maximum carpool size.

Table 12. TFC carpool system-wide savings.

	TFC		TFCH		TFC/TFCH	
q_{max}	SELFORG	CENTR	SELFORG	CENTR	SELFORG	CENTR
2	31.36%	32.89%	40.79%	44.40%	40.74%	44.40%
3	37.37%	38.16%	52.69%	55.47%	52.91%	55.50%
4	37.98%	38.32%	57.50%	60.69%	57.50%	60.69%
5	37.98%	38.32%	59.95%	63.19%	59.95%	63.19%

Figure 7 shows the self-organized and centralized solutions to the TFCH problem with q_{max}=3. Similar to the PDCH model, the two solutions show very different carpool arrangements, but the system-wide savings from the self-organized solution are only 2.78% lower than the savings from the centralized solution.

The carpooling arrangements for the mixed TFC/TFCH model (not shown) are almost identical to the TFCH model.

6. Concluding remarks and future research

This paper extends the carpooling models defined by Kalczynski and Miklas-Kalczynska (2019) with meeting points (hubs), and improves carpool enumeration for all types of models, while presenting solutions to the new models, as well as the combination of the original and new carpooling models.

Our results show that the introduction of hubs improves system-wide savings from carpooling which is consistent with Stiglic et al. (2015). Additionally, however, we show that savings improve when hubs are introduced as an option rather than imposed on participants and these findings apply to all the different carpooling models considered (PDCH, TFCH, PDC/PDCH, TFC/TFCS) as well as solution objectives (self-organized and centralized).

We presented the theoretical background for our effective carpool enumeration by introducing elliptical neighborhood regions on the plane. These elliptical neighborhoods explain the significant increase in potential carpooling options when hubs are introduced into the system. We also extended the greedy carpool enumeration with a more exhaustive one and showed how various carpooling models could be combined to be more effective.

We also found that the existing self-organized (decentralized) solution technique introduced by Kalczynski and Miklas-Kalczynska (2019) could be used to effectively and efficiently solve the problems with imposed and optional hubs for both PDC and TFC types. The resulting self-organized carpools maximize individual participants' savings and still yield attractive system-wide savings, comparable with the centralized solutions. We conducted computational experiments using an easy-to-replicate problem instance presented in the Appendix.

Although our findings revealed new ways to achieve carpooling efficiency, there are limitations to our study. First, there are some practical limitations. These include not allowing participants to switch carpools on different days, enforcing equal division of driving on participants, and limiting the maximum number of seats in the vehicle to 5, thus

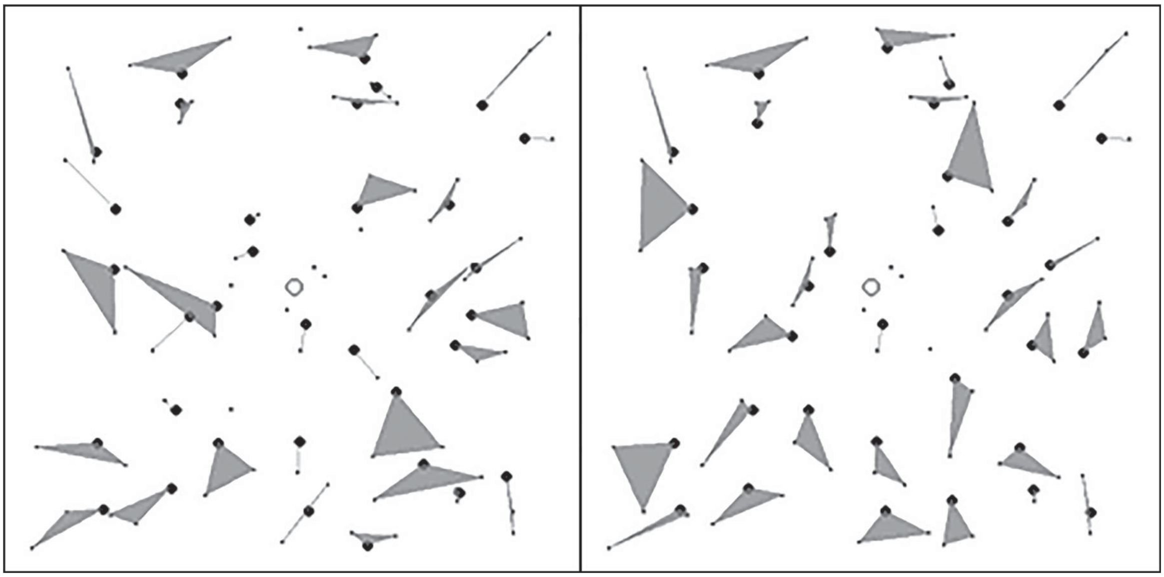

Figure 7. SELFORG and CENTR solutions to TFCH with q_{max}=3.

excluding, e.g. minivans and larger vehicles. Second, there are limitations to the research methodology. We studied the models on one instance and we assumed constant values of maximum additional distance and minimum savings. It would be interesting to check how sensitive the solutions are to these parameters. Future research could consider a self-organized carpooling model with weighted average savings. In such a model, participants will be allowed to offer a portion of their driving days as an incentive for others to carpool with them. It might be interesting to compare it to the centralized model with exogenous incentives.

Recent developments in self-driving vehicle technology (fully autonomous, driverless) indicate that the driver's role will be significantly diminished or eliminated in the near future. So far, very few studies exist that analyze the impact of this phenomenon on carpooling, which makes it another potential research avenue.

Despite the limitations, the results of this research have important practical implications to policy-makers, organizations, and communities organizing carpools. Not only does this work recommend using meeting points (hubs) as an option to increase system-wide savings, regardless of the model or solution technique, it also presents tools for optimization, testing, and improving carpooling systems in the real world.

Together, these solutions hold promise for a more effective and sustainable use of transportation resources.

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Appendix: Generating random instances

Pseudo-random numbers for our test instance were generated by the procedure originally used in Drezner, Kalczynski, and Salhi (2019), which was based on the idea of Law and Kelton (1991). We used this approach so that it can be easily replicated by others to verify the results reported in this paper.

We generate a sequence of integer numbers in the open range (0, 100,000). A starting seed r_1, which is the first number in the sequence, is selected. The sequence is generated by the following rule for $k \geq 1$:

- Set $\theta = 12,219 r_k$.
- Set $r_{k+1} = \theta - \lfloor \frac{\theta}{100,000} \rfloor \times 100,000$, i.e. r_{k+1} is the remainder of dividing θ by 100,000. It is also the last five digits of θ.

For the x-coordinates of the meeting points and original locations we used $r_1 = 97$ and for the y-coordinates we used $r_1 = 367$. We divided the coordinates by 2,500, so the points are in a 40 by 40 square. The coordinates of the first five original locations are: (0.0388, 0.1468), (34.0972, 33.7492), (33.6868, 21.4748), (19.0092, 0.5812), (33.4148, 21.6828). The destination z is in the middle of the square, i.e. at (20, 20).

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ORIGINAL PAPER

Multiple obnoxious facility location: the case of protected areas

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Abstract
Most of the existing obnoxious facility location models use points to represent locations of demand centers and facilities. These points are typically centroids of geographical regions, such as cities or protected wildlife areas. Representing areas as points is convenient for the development and analysis of location models, but it may hinder the models' practical applications. In continuous models, facilities may be located far from the centroid but close to (or even inside) the boundaries of the protected area. Also, some centroids may be located outside of the areas which they represent. We propose a heuristic that leverages the existing point-based models to locate multiple obnoxious facilities around protected areas and, at the same time, minimize the negative impact on those areas. The effectiveness of our approach is illustrated with both generated and real-world instances.

Keywords Location · Protected areas · Heuristics · Obnoxious facility

1 Introduction

Obnoxious facilities are sites, buildings, institutions, stationary objects, or devices that provide needed services but can also negatively impact the surroundings. Some examples of obnoxious facilities include power plants, communication towers, weather instruments, and missile silos. Obnoxious facility location problems deal with locating one or more such facilities while minimizing the negative impact of these facilities on the existing protected areas such as cities, national parks, or wildlife preservation areas.

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1.1 Background

Discrete or network obnoxious facility location models (Church and Garfinkel 1978; Erkut and Neuman 1989) generally focus on selecting a subset of available locations for facilities, while continuous planar models (Shamos and Hoey 1975; Hansen and Cohon 1981; Berman et al. 2003) focus on finding the optimal locations for facilities in the plane. The reader is referred to Church and Drezner (2022) for an in-depth review of obnoxious facility location models.

Nearly all protected areas in the world are represented by unions of geo-polygons, which are later projected onto the plane as polygons. In geometry, a simple polygon (convex or concave) is a polygon that does not have “holes” and does not intersect with itself. While self-intersections do not have practical applications in representing geographical regions, it is possible for some regions to have “holes.” Such polygons can be easily divided into simple polygons.

Most continuous obnoxious facility location models represent protected areas such as cities or national parks as centroids. A centroid (e.g., the center of gravity) is a point that can be determined for any simple polygon or a union of polygons. However, such a reduced representation may result in locating facilities far from the centroid but near the boundary or even inside the protected region. The problem of locating a facility outside of a forbidden region (restricted facility location) has been extensively studied in non-obnoxious facility location literature; see, e.g., Hamacher and Nickel (1995) or Canbolat and Wesolowsky (2010) for a review. It can be relatively easily solved in discrete (e.g., Hamacher and Klamroth 2000; Oğuz et al. 2018) or network (e.g., Drezner and Wesolowsky 1995) models by removing potential locations violating the restrictions, but it is difficult to solve in continuous models.

Restricted facility location literature distinguishes forbidden regions from barriers. While locating a new facility within a forbidden region or a barrier is not permitted, traveling through a forbidden region is possible, but it is not possible through a barrier (Canbolat and Wesolowsky 2010). Since our focus is solely on locating obnoxious facilities outside of protected areas, and since we do not consider transportation, this distinction is not needed. Furthermore, some papers use “semi-obnoxious” or “semi-desirable” terms for facilities that exhibit both desirable and undesirable qualities, such as landfills, airports, or hospitals. In this paper, we do not make such a distinction. Carrizosa and Plastria (1999) provide a thorough review of semi-obnoxious facility location literature.

When it comes to forbidden regions or barriers in the context of (semi-)obnoxious facility location, rectilinear (Manhattan) or Euclidean distance formulas are used most often, and research has mostly focused on locating a single facility. Munoz-Perez and Saameno-Rodriguez (1999) consider locating an obnoxious facility in the presence of polygonal zones. They identify a finite dominant set and use Euclidean distances. Melachrinoudis and Xanthopulos (2003) use Euclidean distance and define a bi-criterion problem to locate a single semi-obnoxious facility, while Plastria et al. (2013) introduce the repelling polygonal regions for restricted semi-obnoxious facility location. Brimberg and Juel (1998) propose a location model for a semi-desirable facility using an arbitrary distance function that accounts for the transportation costs. They consider both Euclidean and rectilinear distances.

Restricted areas are represented in various ways throughout the literature. Some earlier works use points (Carrizosa and Plastria 1998; Drezner and Wesolowsky 1995) or simple geometric shapes, such as circles (Fernández et al. 2000; Melachrinoudis and Cullinane 1986; Brimberg and Juel 1998). The majority of papers using polygons to represent forbidden regions focus on convex polygons. Klamroth (2001) proposes a general solution strategy for locating a facility where convex polyhedral barriers restrict travel that involves reducing a non-convex optimization problem to a finite number of related convex problems. Hamacher and Klamroth (2000) provide a discretization of the restricted location problem and use block norms. Butt and Cavalier (1996) minimize the sum of the weighted Euclidean distances from the new facility to existing facilities in the presence of convex polygonal forbidden regions. Batta et al. (1989) consider the existence of both convex forbidden regions and barriers and use the Manhattan distance to solve the p-median problem showing that a finite set of points is needed to find an optimal solution. Savaş et al. (2002) consider rectilinear distances and arbitrary barriers, which they enclose within polygonal shapes. Bischoff and Klamroth (2007) study a multi-facility location problem and propose two location and allocation heuristics. Dearing et al. (2005) develop a dominating set result for center location problems with polyhedral barriers using the Manhattan distance. Canbolat and Wesolowsky (2012) demonstrate an experimental approach based on the Varignon frame for the Weber problem in the presence of convex barriers. Byrne and Kalcsics (2022) propose partitioning of a convex region with multiple facilities and a polygonal barrier into convex polygonal cells to optimally locate a new facility. McGarvey and Cavalier (2003) apply a branch-and-bound algorithm to solve the 1-median problem with the forbidden regions represented as convex polygons. McGarvey and Cavalier (2005) use convex polygons as forbidden regions in the context of competitive facility location. Plastria et al. (2013) use convex polynomial forbidden regions in the context of obnoxious facility location. They define repelling areas and introduce the margin maximization model.

Among a limited number of authors who study non-convex polygonal forbidden regions are Aneja and Parlar (1994), who focus on the Weber problem and use Euclidean distance, Hamacher and Schöbel (1997), who study the restricted Euclidean center problem and provide an extension of polyhedral non-convex forbidden regions, and Oğuz et al. (2016), who propose a modeling framework for solving restricted location problems with regions represented as phi-objects (see Bennell et al. 2010). Hamacher and Nickel (1995) considered multiple location models and a generic distance metric, including models with non-convex polygonal forbidden regions and multiple obnoxious facilities. Their heuristic is based on a sequential application of solutions to a single-facility problem.

While some of the models in the literature are bi-objective (e.g., Ohsawa and Tamura 2003; Melachrinoudis and Xanthopulos 2003; Plastria and Carrizosa 1999) or multi-objective (e.g., Erkut and Neuman 1992), the majority of them are single-objective.

1.2 Our approach

In this paper, we consider polygonal protected areas, which can be either convex or non-convex, and we utilize the Euclidean distance to locate multiple obnoxious facilities in the plane so that the negative impact on the areas, expressed as a single objective, is minimized. Our optimization models are both non-linear and non-convex.

In addition to locating facilities outside of forbidden regions, we are also concerned with the impact of each obnoxious facility on the entire region and not just on its centroid. Therefore, we treat protected areas (Fernández et al. 2000) as an extension of forbidden regions. Facilities, on the other hand, are represented as points in the plane. To solve such problems, we propose a generic approach that leverages existing point-based obnoxious continuous multi-facility location models. Our approach does not require any modifications to the point-based models but relies on applying them iteratively, with external adjustments made to the input data in each iteration.

Our formulations take advantage of a recently-proven theorem that significantly simplifies the optimization process. The results of our experiments with locating multiple obnoxious facilities in simulated instances, as well as in Southwest Colorado, show major improvements to the objective as compared to the models with protected areas represented with centroids or other sets of points. Thus, the proposed models and the corresponding solution techniques are the main contributions of this paper to the location theory and practice.

The remainder of this paper is organized as follows. Section 2 presents our iterative approach to solving continuous planar multiple obnoxious facility location problems in the context of the maximin and cooperative models. Section 3 offers the results of computational experiments on simulated problem instances and the Southwest region of the State of Colorado. Section 4 offers a brief discussion of the proposed approach and the results, followed by concluding remarks in Sect. 5.

2 Iterative continuous obnoxious facility location

Since most nuisance (noise, light, heat) propagates "by air," we use Euclidean distances once the map is projected onto the plane.

While we consider all facilities to be points, protected areas are represented by polygons. Therefore, a clear distinction between *point-based* and *area-based* models, distances, objectives, etc. is assumed throughout.

We consider a model, distance, or objective to be point-based when each protected area is represented as a finite set of points such as a single centroid or a set of polygon vertices. On the other hand, a model, distance, or objective is area-based when each protected area is represented by the corresponding geometrical shape (polygon).

In point-based models, the minimum distance between a facility and a protected area is simply the shortest Euclidean distance to a point representing the area. In the area-based models the minimum distance between a facility (a point) and a polygonal protected area is the minimum point-to-region distance. The minimum distance is the length of a line segment drawn from the point to a perpendicular intersection with a polygon edge, if such a line segment exists. Otherwise, the minimum distance is the minimum of the distances from the point to polygon vertices.

2.1 The algorithm

We propose the following iterative approach for locating multiple obnoxious facilities around protected areas.

We choose the initial set of protected (sensitive) points to represent protected areas in the underlying point-based model. These could be, e.g., all polygon vertices, centers of gravity of convex areas, or other selected points.

1. Set the best area-based objective to positive infinity (for minimization models) or negative infinity (for maximization models).
2. Solve the point-based continuous obnoxious facility location problem using the set of sensitive points and a point-based objective.
3. If any of the facilities is located inside (or on a border of) any of the protected areas, then add new sensitive points at these locations and go to Step 2.
4. Add new model-specific sensitive points and calculate the area-based objective.
5. If no new sensitive points are added or additional stopping criteria are met then STOP. Otherwise, set the best area-based objective to be the new area-based objective, and go to Step 2.

Note that the initial execution of Step 2 may involve either specialized starting solutions or a set of random starting solutions. While we do not impose any requirements, starting from solutions for which all facilities are located outside of the protected areas may improve the algorithm's performance. Also, additional stopping conditions, such as the number of iterations without any improvement or the maximum total number of iterations, may be used.

Below we show how this approach can be applied to improve the results of the two continuous obnoxious facility locations models. We use the simplest planar formulations but our approach can be used for more complex models, e.g., weighted sensitive points, three-dimensional, etc.

Let (a_i, b_i) for $i = 1, \ldots, n$ be the known locations of sensitive points, and (x_j, y_j) for $j = 1, \ldots, p$ be the unknown locations of the p obnoxious facilities. In addition, some well-defined region-bounding constraints are necessary, otherwise the obnoxious facilities will be located at infinity. Therefore, we must define a bounding region (e.g., a square or polygon) $\mathcal{B} \in \mathbb{R}^2$.

2.2 Maximin models

In continuous obnoxious facility location, *maximin* models consider maximizing the minimum distance between a facility and its nearest protected area. Such point-based models are represented by the following (or a similar) non-convex QCP (Quadratically-Constrained Program) formulation (Drezner et al. 2019):

$$\begin{aligned} & \max \ \{L\} \\ \text{subject to: } & (x_j - a_i)^2 + (y_j - b_i)^2 \geq L & \text{for } i = 1, \dots, n; j = 1, \dots, p \\ & (x_i - x_j)^2 + (y_i - y_j)^2 \geq D^2 & \text{for } 1 \leq i < j \leq p \\ & (x_j, y_j) \in \mathcal{B} & \text{for } j = 1, \dots, p \end{aligned} \tag{1}$$

where L is the square of the objective function, D is the minimum required separation distance for facilities, and $\mathcal{B}$ is a bounding region.

For these types of models, the objective is to locate the facilities as far as possible from the protected points, and also at least D units apart from one another. The minimum distance D for facilities is required because without it all facilities will be located at the same point. Also, it is possible that facilities negatively impact one another.

With our proposed approach, the facilities will be located outside of the boundaries of the protected areas and as far as possible from these areas, which is a more practical outcome than maximizing the minimum distance from these regions' centroids.

2.3 Cooperative models

In cooperative models (Drezner et al. 2020), multiple facilities "cooperate" in inflicting nuisance on the protected points. A sample non-linear formulation of a cooperative point-based model is:

$$\begin{aligned} & \min \ \{L\} \\ \text{subject to: } & \sum_{j=1}^{p} \frac{w_j}{(x_j - a_i)^2 + (y_j - b_i)^2} \leq L & \text{for } i = 1, \dots, n \\ & (x_j, y_j) \in \mathcal{B} & \text{for } j = 1, \dots, p \end{aligned} \tag{2}$$

with the positive weights w_j given. Note that w_{ij} was used by Drezner et al. (2020), but here we use the weights only for the facilities, hence only one index.

The negative effect generated by a single facility follows the "inverse square law," which applies to a range of physical phenomena, such as light, sound, or electricity. Unlike in the maximin model, in the cooperative model the facilities "cooperate" in generating nuisance. The objective is to minimize the cumulative negative impact of all the facilities on the most affected sensitive point.

2.4 Adding new sensitive points

Our proposed approach has the following advantages over the centroid-based models: (1) the facilities will be located outside of the protected areas, and (2) the collective impact will be measured at the most affected point of the entire area rather than at its centroid, which may be located outside of the area itself. Below we describe the additional sensitive point selection processes for the two models.

2.4.1 Maximin model

Recall that nuisance (e.g., noise, light, radiation) typically propagates "by air," so we consider the minimum Euclidean distance between a facility and a protected area to be the minimum of the distances to the vertices and perpendicular distances to the edges of each protected area. We assume that planar polygons for the protected areas are available at the desired resolution. In our approach, the vertices of these polygons (rather than their centroids) and some additional special points are used to represent the protected areas.

Let P_k for $k = 1, \dots, m$ be the polygonal representations of the protected areas. Each simple polygon P (convex or non-convex) consists of an ordered list of vertices $v_1, v_2, \dots, v_{\ell_k}$. A closed chain of line segments (edges) is formed by these vertices. One can quickly determine whether a point is outside of the polygon by solving the point-in-polygon (PIP) problem using, e.g., the ray-casting algorithm (Shimrat 1962).

We define the minimum distance from point (x_0, y_0), located outside of the polygon to the polygon, as the minimum distance to the boundary of that polygon. This could be the distance to the nearest vertex or the perpendicular distance to the nearest edge (a line segment).

Consider a line segment defined by two distinct points (a_1, b_1) and (a_2, b_2). Let $A = a_1 - a_2$ and $B = b_1 - b_2$. The coordinates (x, y) of a point on a line that passes through these points that is nearest to (x_0, y_0) are $x = a_1$ and $y = y_0$ if $A = 0$, otherwise,

$$
\begin{aligned}
x &= \left(\frac{B\left(a_2\left(b_1 - y_0\right) + a_1\left(y_0 - b_2\right)\right)}{A^2} + x_0 \right) \Big/ \left(\frac{B^2}{A^2} + 1 \right) \\
y &= \frac{A\left(a_1 b_2 - a_2 b_1 + B x_0\right) + B^2 y_0}{A^2 + B^2}.
\end{aligned}
\tag{3}
$$

If point (x, y) is located between points (a_1, b_1) and (a_2, b_2), i.e., when the sum of distances from (x, y) to the endpoints of the segment is equal to the length of the segment, (x, y) is the nearest point to (x_0, y_0), otherwise, the nearest endpoint of the segment is the nearest point to (x_0, y_0).

Once the point-based maximin model (1) is solved, the area-based objective is the minimum distance between the facilities and polygons and the corresponding additional sensitive point. It is found by applying (3) to all pairs of facilities and polygon edges and identifying the point with the minimum distance.

2.4.2 Cooperative model

Once the point-based cooperative model (2) is solved, we can solve the following supporting problem:

$$\begin{aligned} & \max \ \{L\} \\ \text{subject to: } & \sum_{j=1}^{p} \frac{w_j}{(x_j^* - a_0)^2 + (y_j^* - b_0)^2} \geq L \\ & \{a_0, b_0\} \in P \end{aligned} \tag{4}$$

to find point (a_0, b_0) inside or on the boundary of a convex polygon P which has the most nuisance. Any non-convex protected area is represented by a union of convex polygons. Then, point (a_0, b_0) for the most affected polygon P is added to the list of sensitive points and the algorithm continues. However, the proof presented by Coletti et al. (2023) enables us to limit the search for the most-affected sensitive point to the boundaries of the protected areas.

Theorem 1 *In the planar multiple obnoxious facility location cooperative model* (2) *with protected areas represented as closed geometric shapes and all obnoxious facilities located outside of these shapes, the most affected point of any protected area will be located on the boundary of that area.*

Proof The proof of this theorem is the result obtained by Coletti et al. (2023) reduced to the two-dimensional case. In order for a local maximum of the following function of two variables, a and b:

$$\sum_{j=1}^{p} \frac{w_j}{(x_j - a)^2 + (y_j - b)^2} \tag{5}$$

to exist in the region of interest, the Hessian matrix must be negative semidefinite, i.e., both its eigenvalues must be non-positive. The Hessian of any function of two variables is:

$$\mathcal{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix},$$

and its two eigenvalues are:

$$\lambda_1 = \frac{1}{2}\left(H_{11} + H_{22} + \sqrt{4H_{21}^2 + \left(H_{11} - H_{22}\right)^2}\right)$$

and

$$\lambda_2 = \frac{1}{2}\left(H_{11} + H_{22} - \sqrt{4H_{21}^2 + \left(H_{11} - H_{22}\right)^2}\right).$$

In order for eigenvalue λ_1 to be non-positive, the sum of the second partial derivatives, $H_{11} + H_{22}$ must be non-positive. For our function, this sum simplifies to:

$$\sum_{j=1}^{p} \frac{4w_j}{\left(\left(x_j - a\right)^2 + \left(y_j - b\right)^2\right)^2},$$

which cannot be negative or zero because $w_j > 0$ for $j = 1, 2, \ldots, p$. Therefore, a local maximum of (5) cannot exist in the region of interest. □

Theorem 1 has very important implications for our area-based model. The supporting problem (4) can be changed to searching for additional sensitive points only on the boundaries of the protected areas. To avoid embedded optimization, we apply (3), but the area-based objective and the corresponding new sensitive point are identified as those with the maximum weighted reciprocal of the squared area-based distance rather than those with the minimum area-based distance. This approach provides good approximate locations of the most-affected sensitive points.

3 Computational experiments

3.1 Small generated instances

In order to illustrate our approach we considered a problem of locating two obnoxious facilities ($p = 2$) in a 100×100 square with two convex and two non-convex polygons.

3.1.1 Maximin

For the maximin model, we set the minimum distance between facilities to $D = 20$, otherwise all obnoxious facilities will be located at a single point. First, we solved the problem with the point-based model using the centers of gravity for each area.

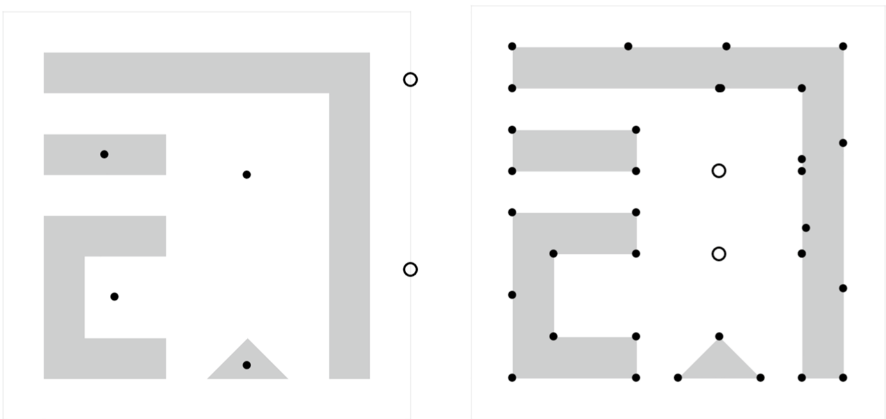

Fig. 1 Centroid-based and iterative solutions to the maximin problem

The left-hand side of Fig. 1 shows the solution with the facilities marked with open circles and sensitive points marked with dots. Note that the centers of gravity for the non-convex polygons are outside of the areas. The point-based objective (computed based on centroids) was 46.3081. However, the nearest sensitive point is actually on the edge of the nearest polygon, so the area-based maximin distance for this solution is 10 which is over 4 times worse than the point-based objective.

Next, we applied our approach with the maximum number of iterations set to 50 and the maximum number of iterations with no improvement in the objective (i.e., patience) set to 10. We used polygon vertices as the initial set of sensitive points. The solution with area-based objective equal to 20 (see the right-hand side of Fig. 1) was found after 15 iterations. One can see additional sensitive points added to the polygons in subsequent iterations. If only polygon vertices were used (no iterations), the point-based approach would result in a violation of the forbidden region constraints.

3.1.2 Cooperative

We used the same instance to illustrate the cooperative model with weights $w_j = j \times p / \sum_{k=1}^{p} k$. There is no minimum required distance between facilities in the cooperative model, which may result in co-located facilities. If two facilities are co-located, their weights are added.

Similarly to the previous experiment, we first solved the problem using the point-based models and centroids. The point-based optimization objective (multiplied by 10,000) was 5.338. However, the area-based objective for this configuration of facilities, was 67.0782, over 12.5 times worse than the point-based objective. This was because the facility with the largest weight (in the upper right corner) was as far away as possible from the nearest centroid but very close to the nearest polygon. The left-hand side of Fig. 2 shows the results for the centroid-based optimization. The radii of the circles are proportional to the weights of the facilities.

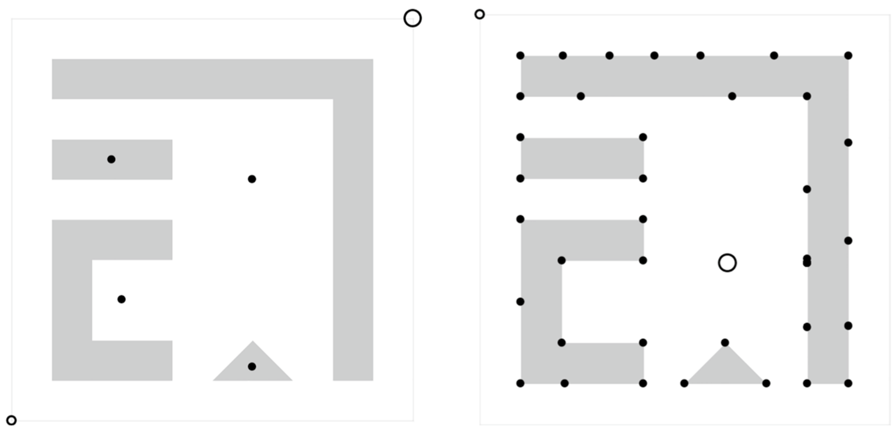

Fig. 2 Centroid-based and iterative solutions to the cooperative problem

The iterative approach applied to the same instance resulted in the best-known solution with the area-based objective of 35.9409 (nearly 2 times better than the area-based objective found with centroids) obtained after 27 iterations. The right-hand side of Fig. 2 shows the results with the additional sensitive points. If only polygon vertices were used (no iterations), the area-based objective would be 134.4205 which is 3.74 times worse than the area-based objective obtained with the iterative approach. In this case, the centroid-based approach yielded a better value of the objective function than the vertex-based approach by coincidence. The facilities and their weights are located according to the existing sensitive points and the area-based objective is measured after the optimization process is completed. For this instance, the vertices prevented the solver from locating the facilities at the opposite corners, and located them close to the polygon edges. This initial solution (not shown) was improved in subsequent iterations by adding sensitive points to the polygon edges.

The point-based solutions to both maximin and cooperative models were obtained with SNOPT (Gill et al. 2005), starting from 100 randomly generated solutions. In order to reduce the effect of randomness on the performance of the heuristic (heuristic gap), the same starting solutions were used in each iteration and the only input that changed between iterations was the set of sensitive points.

The above illustration shows that, for this small generated instance, our iterative area-based technique improves the results as compared to optimization based on centroids or on vertices with no iterations. In the following sections, we will demonstrate the effectiveness of our technique on simulated and large-scale real-world instances.

3.2 Simulated instances

We generated 100 instances in the 100×100 square with randomly-generated protected areas using the technique described in the Appendix. We solved the maximin and cooperative versions of the problems on these instances for $p = 2, 3, \dots, 10$ (a total of 900 problems), and compared the solutions obtained with our approach to those obtained with the existing centroid-based models. Similarly to the small instances, we used SNOPT starting from the same 100 random solutions for both centroid and iterative approaches.

Tables 1 and 2 show the average improvement in the objective obtained with our proposed iterative technique as compared to centroid-based models for the maximin and cooperative models, respectively. Instances are grouped according to the percentage of the square covered by the protected areas and by the number of obnoxious locations p.

Table 1 shows the overall improvement of 225.6% for the maximin model for 610 (67.7%) instances for which a feasible solution was obtained with both the iterative and centroid methods. However, the iterative method was able to obtain a feasible solution for additional 213 (23.67%) instances. With the exception of the last row, which is based on a small number of instances, the overall improvement appears to increase as protected areas cover more of the square. When protected

Table 1 Maximin: average improvement (%)—iterative versus centroid on simulated instances

Prot. areas	*p*									Overall
	2	3	4	5	6	7	8	9	10	
0–9.99%	4.1	3.5	5.3	6.0	4.4	11.4	9.8	8.7	9.6	7.0
10–19.99%	17.4	24.6	41.8	31.5	44.6	62.9	138.7	182.7	193.7	79.8
20–29.99%	448.0	389.7	479.3	159.0	308.5	328.8	2474.2	542.1	149.5	544.3
30–39.99%	534.5	696.0	499.5	184.5	217.7	316.0	1391.4		379.8	559.3
40% and more	54.1	121.2								76.5
Overall	255.4	247.8	218.4	71.8	118.3	119.6	702.0	188.6	95.0	225.6

Table 2 Cooperative: average improvement (%)—iterative versus centroid on simulated instances

Prot. areas	*p*									Overall
	2	3	4	5	6	7	8	9	10	
0–9.99%	4.9	7.2	7.5	6.8	4.8	17.1	10.6	6.2	4.9	7.8
10–19.99%	16.8	11.8	18.9	13.6	31.3	21.3	1.7	1.0	32.8	16.9
20–29.99%	51.4	56.4	63.2	63.2	60.8	59.2	70.5	57.2	74.5	60.9
30–39.99%	74.4	70.2	81.6	79.8	73.8	89.3	38.8	52.6	96.2	72.6
40% and more	38.2	26.8	43.1	91.0	96.0	96.8	49.9	99.9	6.8	55.1
Overall	36.7	35.9	37.9	33.6	37.2	37.1	25.9	25.2	35.6	34.3

areas cover between 20% and 39.99% of the overall area, our iterative approach locates the nearest obnoxious facility 1.5 to 24 times farther from the protected area than the centroid approach.

Table 2 shows the overall improvement of 34.3% for the cooperative model for 674 (74.9%) instances for which a feasible solution was obtained with both the iterative and centroid methods. However, the iterative method was able to obtain a feasible solution for additional 86 (9.56%) instances. With the exception of the last row, which is based on a small number of instances, the overall improvement also appears to increase as protected areas cover more of the square. When protected areas cover between 20% and 39.99% of the overall area, our iterative approach reduces the overall nuisance on the most-affected point by 51–96% compared to the centroid approach.

For both the maximin and cooperative models, the iterative approach yielded worse results for some instances. For the maximin model, there were 25 instances (2.78%) for which only the centroid approach produced a feasible solution. There were also 41 instances (4.56%) for which the centroid approach yielded a better objective for the average "improvement" of −12.34%. For the cooperative model, there were 92 instances (10.22%) for which only the centroid approach produced a feasible solution and 11 instances (12.33%) for which the centroid approach yielded a better objective for the average "improvement" of −16.90%. In practice, all these cases would be eliminated by using the centroid-based approach as one of the starting solutions for the iterative approach.

The results of the simulation experiments confirm the effectiveness of our iterative approach. The method is particularly useful when protected areas cover a between 20 and 40% of the overall area.

3.3 Case study: protected areas in Southwest Colorado

To further demonstrate the effectiveness of our approach, we chose the Southwest part of the State of Colorado because Colorado has multiple protected areas, and its geographical range, after the projection, can be approximated by a rectangle.

The geo-polygon data for protected areas were extracted from the WDPA database (UNEP-WCMC, IUCN 2021), available to the public. The data for the geo-polygon approximately covering the Southwest Colorado area, was extracted with GeoPandas (van den Bossche et al. 2021). The same tool was used to compute polygon centroids, and to simplify the geo-polygons with the 0.005 degree tolerance.

133 protected areas, which at least partially belong to Southwest Colorado, were identified with this process. These areas consisted of the total of 3075 vertices. A quick analysis of the geo-points revealed that 22 of the 133 centroids (16.5%) were located outside of protected regions because some of these areas consisted of multiple polygons and some were non-convex. Consequently, we split the multi-polygonal areas into 279 simple polygons (we ignored the "holes" in polygons). Still, for 13 of them (4.6%), the centroids were located outside of their boundaries. This means that, when the classical centroid-based approach is used to locate the obnoxious facilities, some of the areas are not protected at all because the optimization is based on points located outside of these areas.

We projected all geo-locations onto the two-dimensional Cartesian space using the azimuthal equidistant projection with the azimuth located at the center of the geographical bounding box. All transformations of geographical data were done in *Mathematica* (Wolfram Research, Inc. 2022). Figure 3 shows the protected areas and the analyzed region. The Cartesian coordinates were then used as inputs to the point-based maximin (Drezner et al. 2019) and cooperative models (Drezner et al. 2020) implemented in SNOPT (Gill et al. 2005).

3.3.1 Maximin

For the maximin model, we used the separation among facilities of approximately 50 miles, i.e., $D = 50$. First, we located the obnoxious facilities using the centroids. The original 133 centroids (one per each park) were obtained from the mapping software. The secondary 279 centroids (one per each simple polygon) were computed using the center of gravity formula. Next, we located the facilities with our proposed approach.

Table 3 shows the results. We report the first iteration separately (under the point-based models) in order to show the improvement from the iterative process and not just from using polygon vertices as points. Therefore, the first three optimization

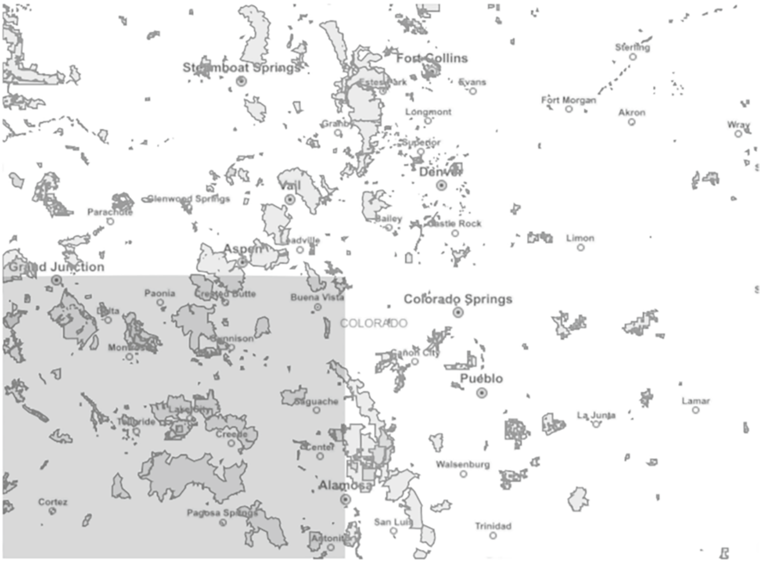

Fig. 3 Protected areas of the state of Colorado and the selected region

Table 3 Maximin results for SW Colorado

p	Point-based optimization						Iterative optimization		
	133 centroids		279 centroids		3075 vertices		279 polygons		
	Obj.	Time (s)	Obj.	Time (s)	Obj.	Time (s)	Obj.	Iters.	Time (s)
2	0.8639	4.46	14.4515	2.79	**22.8937**	40.83	**22.8937**	1[a]	40.83
4	4.3765	8.46	8.7879	17.29	11.0795	505.31	**18.0710**	2	1171.16
6	4.3199	49.28	7.4957	156.15	**10.6417**	6211.34	**10.6417**	1[a]	6211.34
8	0.9215	78.98	1.8812	413.63	**9.3575**	13,740.30	**9.3575**	1[a]	13,740.30
10	2.1605	235.38	INSIDE	640.58	**8.9262**	35,684.20	**8.9262**	1[a]	35,684.20
12	1.6756	411.59	INSIDE	1651.76	INSIDE	42,019.00	**8.4077**	7	340,925.00
14	INSIDE	600.71	INSIDE	1672.73	0.4419	92,977.60	**7.6235**	15	1,334,468.17

[a]The first iteration is equivalent to point-based optimization on 3075 vertices

The best-known objective values are emphasized

models used are point-based and the last one is iterative. Regardless, the area-based objectives are reported for all models, i.e., for the most affected points.

The results for the maximin model show that our iterative heuristic found the best area-based objective (the maximum minimum distance from an obnoxious facility to a protected area) for all analyzed cases. We improved the centroid-based results for all values of p. For a larger number of points, our approach resulted in the same objective as the point-based approach in four cases. For $p = 12$, only our method was capable of finding a feasible solution, and the objective was improved for $p = 4$

and $p = 14$. We chose the case with $p = 14$ as an illustration for which the centroid-based optimization failed to produce a feasible solution, and the solution based on polygon vertices yielded the maximum minimum distance of only 0.4419 miles. Our iterative approach resulted in a much better solution, with the maximum minimum distance to the most-affected area over 17 times larger (7.6235 mi.). Figure 4 shows the optimization results.

3.3.2 Cooperative

For the cooperative model, we did not use set any separation between facilities. Instead, we assumed weights $w_j = j \times p / \sum_{k=1}^{p} k$. Table 4 shows the results. Regardless of the model type used (point-based or iterative), all objectives reported in the table are the area-based objectives multiplied by 10,000, i.e., they show the total negative effect of all p facilities on the most-affect point found by (4).

Table 4 shows that the iterative approach produced the best results for all analyzed cases. For $p = 2$, our method produced the same objective as the point-based method with a large number of points. In all other cases, our approach improved the point-based objectives. We chose the case of $p = 10$ as an illustration. For this case, the centroid-based models produced poor solutions with the objective values of 27718.3 and 2035.19 for the 133 and 279 centroids respectively. The vertex-based optimization yielded the objective value of 733.4072. Our iterative approach resulted in 160.998, which is over 172 times better than the centroid-based result and 4.5 better than the vertex-based result. Figure 5 shows

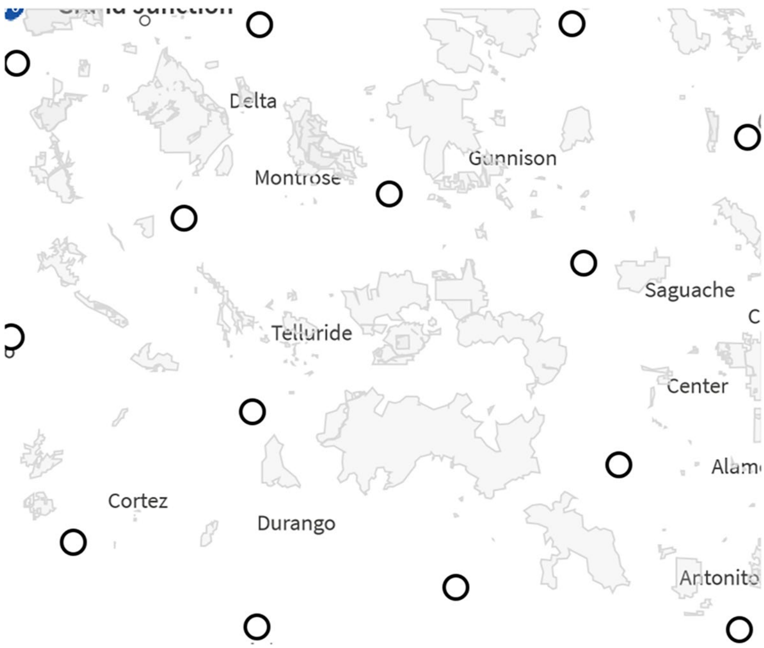

Fig. 4 Maximin iterative optimization results for $p = 14$ and $D = 50$

Table 4 Cooperative (minimization) results for SW Colorado

p	Point-based optimization						Iterative optmization		
	133 centroids		279 centroids		3075 vertices		279 polygons		
	Obj.	Time (s)	Obj.	Time (s)	Obj.	Time (s)	Obj.	Iters.	Time (s)
2	13.3180	2.53	24.5783	4.66	**13.2579**	913.70	**13.2579**	1[a]	913.70
4	2916.5800	6.44	208.7210	12.36	162.4499	1443.59	**68.9154**	3	4395.60
6	428.2080	8.72	163.4090	46.30	134.9716	2249.89	**99.7552**	2	5033.24
8	354.0690	18.26	352.6990	47.51	300.4981	2384.59	**144.8193**	2	4234.73
10	27,718.3000	26.85	2035.1900	77.55	733.4072	3487.06	**160.9980**	7	23,486.40
12	2623.0200	42.48	279.4490	112.46	INSIDE	3774.56	**222.9809**	14	64,052.90
14	364.3410	37.63	626.7380	124.96	693.7988	7634.78	**329.2254**	13	113,096.00

[a]The first iteration is equivalent to point-based optimization on 3075 vertices

Objective values multiplied by 10,000 and the best-known objective values are emphasized

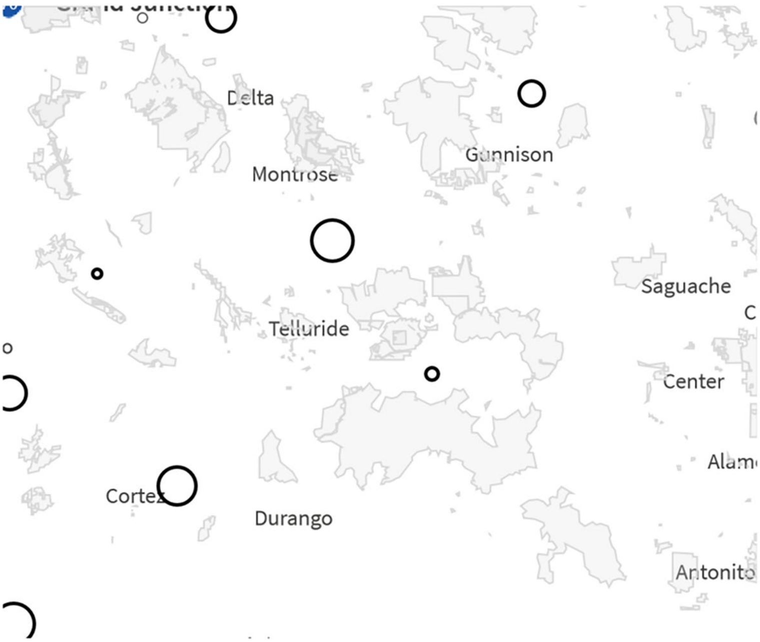

Fig. 5 Cooperative iterative optimization results for $p = 10$

the result for $p = 10$ with the radius of each circle proportional to the weight of the corresponding facility. Note that there are eight distinct facilities in this figure because three are co-located in the lower left corner.

4 Discussion

The cooperative obnoxious facility location problem, originally introduced by Drezner et al. (2020), is one way of representing the nuisance inflicted by multiple obnoxious facilities on sensitive points and it applies to multiple types of nuisance governed by the inverse square law, such as noise, radiation, etc. The proposed extension of the model to two-dimensional sensitive areas assumes that minimizing the overall negative impact of all facilities on a single most-affected point that belongs to one of the areas is the best solution for all sensitive areas collectively, as no other point in any area will get more nuisance. For example, some U.S. states have laws limiting the noise level near bird nesting sites. Suppose a lumber company wants to locate several facilities that emit considerable noise, such as sawmills. Our model can determine the number, size, and locations of such facilities, while keeping the noise level at nearby nesting sites below the legal threshold.

Our approach can be adapted to a wide range of obnoxious facility location models, such as the weighted demand points (Kalczynski et al. 2022) or max-sum problems (Kalczynski and Drezner 2019) and does not require any modifications to these models. Instead, it relies on iterative runs of the existing techniques, and adding sensitive points to the input data with each iteration. This approach allows for solving practical problems of locating obnoxious facilities around protected areas.

Only very small instances of the original point-based problems can be solved to optimality with the available solvers. Multi-start local search methods are typically used to solve practical instances of the maximin and cooperative models. Assuming that the same solver and the same *feasible* starting solution are used, our iterative approach will yield an area-based objective that is the same or better than a point-based approach (regardless of the number of points used to represent the protected areas).

Although for a large number of points the optimization times might be a concern, our approach works for any number of initial points (including a single point that belongs to any of the protected areas). On the other hand, obtaining a quality solution with a very limited set of initial points would likely require using more iterations, diversifying the starting solutions for a local non-linear solver, as well as changing the stopping criteria to allow for more patience, i.e., iterations with no improvement of the objective.

The trade-off between the optimization time and the quality of the obtained solution results in a decision problem that should be considered on a case-by-case basis. The iterative nature of the proposed method that leverages existing point-based models allows for saving the best-known results for an immediate application or as a starting solution to be improved later. Suppose the minimum distance of an obnoxious facility from a protected area is regulated by law. In Table 3, the best-known solution to the Maximin model with $p = 14$ was obtained after more than 15 days. However, neither of the centroid-based approaches resulted in a feasible solution (at least one facility was located inside one of the protected areas).

The best-known values of the objective function in the subsequent iterations were infeasible in iterations 1–4, 0.41805 in iteration 5, 1.9045 in iteration 6, 5.038 in iterations 7–14, and 7.6235 in iteration 15. After obtaining the first feasible solution, the decision maker could manually terminate the optimization process after any iteration.

5 Concluding remarks

We developed a new optimization model for planar multiple obnoxious facility location with protected areas represented as convex and non-convex polygons. Our model leverages a recently-proven theorem and existing point-based models (only the input to these models changes). The proposed approach considers the negative impact of obnoxious facilities on the entire protected regions rather than their point-based representations.

We implemented our iterative heuristic on the maximin and cooperative models. We demonstrated how to obtain feasible solutions with all facilities located outside of protected areas. We also showed how to find the most-affected point of a protected area for such solutions. In both the maximin and cooperative models, the most affected point is always on the boundary of the protected area, i.e., on the vertex or edge of the polygon.

Our computational experiments on generated and large-scale real-world instances show that the proposed iterative approach leads to much better solutions than point-based optimization, which has implications for the location theory and practice.

One of the potential future research avenues is to also consider facilities as polygonal regions rather than points. From a practical standpoint, one could also investigate the effect of choosing a smaller set of starting points and different stopping criteria on the optimization time and solution quality.

Appendix

Generating multiple instances, each with a set of random non-overlapping simple polygons (convex and non-convex) was necessary for our simulation. We used the following approach, which yields patterns similar to real-world protected areas.

First, we randomly generate 100 points in a 100 by 100 square and superimpose a Voronoi mesh on this square. Next, we randomly choose between 1 and 50 of the Voronoi mesh polygons and unionize them. If all the resulting polygonal areas are simple polygons, we consider an instance valid, otherwise the instance is rejected. The vertices of these polygonal protected areas are used to determine their centroids.

In our experiment, this process resulted in discarding 33 instances in order to generate 100 valid simulated instances. Figure 6 shows five examples of valid instances with protected areas (shown in black) covering between 1.3 and 48% of the total area of the square.

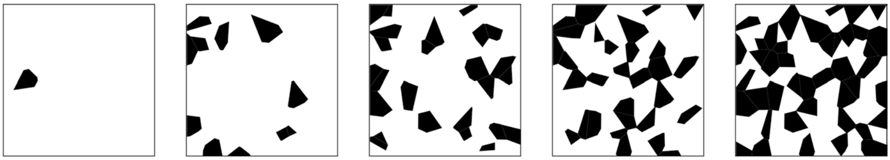

Fig. 6 Sample simulated instances

Author contributions M.M-K and P.K.: made substantial contributions to the conception or design of the work; drafted the work or revised it critically for important intellectual content; approved the version to be published; and agree to be accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

Data availability statement The data generated during and/or analysed during the current study are available in the *Open Science Framework* repository, https://osf.io/t65dr.

Declarations

Conflict of interest The authors declare no competing interests.

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Solving non-linear optimization problems by a trajectory approach

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We propose solving non-linear optimization problems by a trajectory method. A parameter is introduced into the optimization problem. For example, a variable in the original formulation is replaced by its squared value. The parameter is the power at which the variable is raised. For a particular value of the parameter (power of 2), the optimal solution is easily obtained. The original optimization problem is defined for another value of the parameter (power of 1). As another example, the means and standard deviations of a function based on a set of variables can be calculated. We multiply the standard deviations by a factor (the parameter) between 0 and 1. Suppose that the problem is easily solvable for zero standard deviations (factor of 0). If we 'slowly' increase the factor, the solution moves to the desired solution for a factor of 1. A trajectory connects the easily obtained solution to the desired solution. We trace the trajectory and the solution for the optimization problem is at the end of the trajectory. The procedure is applied for solving the single facility Weber location problem, and a competitive location problem with good results.

Keywords: non-linear optimization; trajectory; location.

1. Introduction

The trajectory principle was introduced in Drezner & Wesolowsky (1978a,b, 1982). We are not aware of follow-up papers that applied the trajectory approach to other problems. It is a general optimization technique that can be used to solve many optimization problems, not necessarily guaranteeing optimality unless the problem is convex.

Problems that can be solved by the trajectory method are minimization (or maximization) problems that can be parameterized by a parameter λ. Consider an objective function $F(X)$ and variables $X = \{x_1, x_2, \dots, x_p\}$. The optimal solution is known, or can be easily found, for some $\lambda = \lambda_0$, and the original problem is identical to the parameterized problem with $\lambda = \lambda_1$. There exists a trajectory of solutions $X(\lambda) = \{x_1(\lambda), \dots, x_p(\lambda)\}$ for $\lambda_0 \le \lambda \le \lambda_1$ connecting the solution $X(\lambda_0)$ to $X(\lambda_1)$. If the problem is not convex, the trajectory may by discontinuous. If we are able to calculate the trajectory starting at $\lambda = \lambda_0$, we can find the desired solution for $\lambda = \lambda_1$.

1.1 *Examples*

The examples listed below could be solved by the trajectory approach. Only three of them (references cited) were solved by the trajectory method. The other examples were not yet solved with this method. The formula for the trajectory needs to be derived for each example as detailed in Section 2.

- Consider the planar Weber problem (Church, 2019; Francis *et al.*, 1992; Love *et al.*, 1988; Weber, 1909).

  1. For Euclidean distances the objective function is: $\sum_{i=1}^{n} w_i\sqrt{(x-x_i)^2+(y-y_i)^2}$. It can be formulated as $\sum_{i=1}^{n} w_i\left\{(x-x_i)^2+(y-y_i)^2\right\}^{1-\lambda}$. The problem is defined for $\lambda = \frac{1}{2}$. For $\lambda = 0$ the solution is the centre of gravity. We know the solution for $\lambda = 0$ and are interested in the solution for $\lambda = \frac{1}{2}$. For more details and derivations see Section 3.
  2. The Weber problem with ℓ_p distances can be formulated as minimizing

$$\sum_{i=1}^{n} w_i\left((x-x_i)^{2+(p-2)\lambda}+(y-y_i)^{2+(p-2)\lambda}\right)^{1-(1-\frac{1}{p})\lambda} \tag{1}$$

     with $\lambda_0 = 0$ and $\lambda_1 = 1$ (that was solved by a trajectory approach in Drezner & Wesolowsky, 1978b). The solution for $\lambda = 0$ is the centre of gravity, and the solution for $\lambda = 1$ is the desired solution.

- These two problems with positive and negative weights (Chen *et al.*, 1992; Drezner & Suzuki, 2004; Drezner & Wesolowsky, 1991; Maranas & Floudas, 1993; Tellier & Polanski, 1989) can also be solved the same way. When the weights are non-negative the problem is convex. However, when the weights can be negative they may not be convex.

- Round-trip (that was solved by a trajectory approach in Drezner & Wesolowsky, 1982) is to find the best location for a facility that minimizes the maximum round-trip distance to pairs of demand points.

- Minimax problems (that was solved by a trajectory approach in Drezner & Wesolowsky, 1978a) are converted to minisum problems by the following property for any set of positive constants $c_1, \dots, c_n$: $\max\{c_1, \dots, c_n\} = \lim_{\theta\to\infty}\left[c_1^\theta + \dots + c_n^\theta\right]^{\frac{1}{\theta}}$. The trajectory to $\theta \to \infty$ is evaluated.

- Competitive location problem based on the gravity rule (Huff, 1964, 1966) is solved by a trajectory method in Section 4. For complete details please see Section 4.

- When the parameters of a model are stochastic, then the objective function is stochastic as well. When the parameters have fixed values, we normally minimize or maximize an objective function. When the parameters follow a random distribution, it was proposed to minimize the probability of failing to meet a threshold.

  1. Such an objective was first suggested by Kataoka (1963) in the context of a transportation problem. Similar models were introduced in the finance literature for minimizing the probability that a portfolio will fail to meet a given profit threshold (Finkelshtain *et al.*, 1999; Jacobs & Levy, 1996; Johansson *et al.*, 1999; Olsen, 1997).
  2. Drezner *et al.* (2002) proposed a competitive facility location model where the objective is to minimize the probability of failing to capture a market share threshold (to avoid loosing money) rather than maximizing the expected market share.

3. Drezner & Drezner (2011) minimized the probability of exceeding a cost threshold in the Weber location problem (Francis *et al.*, 1992; Love *et al.*, 1988; Weber, 1909).

- The trajectory for these three models can be constructed as follows. Let the mean of the expected cost for a given value of X be $\mu(X)$ and its variance be $V(X)$. For a given threshold T, the probability that the cost exceeds the threshold (to be minimized) is equivalent to finding the best solution X that maximizes $\lambda = \frac{T-\mu(X)}{\sqrt{V(X)}}$. Alternatively, for a given λ the objective is to minimize the necessary threshold $T(X) = \mu(X) + \lambda\sqrt{V(X)}$. If $\min\{T(X)\} \geq T$ this value of λ is achievable at that X. The solution for $\lambda = 0$ is available by 'standard' approaches that do not consider parameters' uncertainty. A trajectory of the best X that minimizes $T(X)$ can be constructed for λ between 0 and the value for which $\min\{T(X)\} = T$. A similar procedure can be constructed if the objective is maximizing profit. Many other models can be generalized this way. For example, the last mile logistics models (Demir *et al.*, 2022).

2. Finding the Trajectory

Once the derivatives of the optimal location by λ can be explicitly evaluated, the trajectory can be formulated as a set of ordinary differential equations. As suggested in Drezner & Wesolowsky (1978a,b, 1982), an efficient way to numerically solve a set of ordinary differential equations is the Runge-Kutta method (Abramowitz & Stegun, 1972; Ince, 1926; Kutta, 1901; Runge, 1895). There are many variants of this solution approach. Three commonly used approaches are detailed in Table 1. Suppose we integrate from $\lambda = \lambda_0$ to $\lambda = \lambda_0 + h$. At λ_0, $x = x_0$; $y = y_0$, and at $\lambda + h$ we estimate (x, y) as $(x_0 + \Delta x, y_0 + \Delta y)$. Estimating Δx, Δy can be accomplished by one of the numerical integration procedures listed in Table 1 (Abramowitz & Stegun, 1972).

An error term of the first two equations is $O(h^5)$ meaning that if h is halved the error is expected to drop by a factor of 32. Since the equations have to be applied twice to achieve the same h, halving h reduces the expected error by a factor of 16. When the error term is $o(h^4)$, the factor is 8.

The optimal point (it may be a local optimum) for a given λ satisfies $\frac{\partial F(X(\lambda))}{\partial X} = 0$, which can be written as: $\frac{\partial F(X(\lambda))}{\partial x_i} = 0$ for $i = 1, \ldots, p$. Differentiating by λ:

$$\frac{\partial^2 F(X(\lambda))}{\partial x_i \partial \lambda} + \sum_{j=1}^{p} \left\{ \frac{\partial^2 F(X(\lambda))}{\partial x_i \partial x_j} \frac{dx_j}{d\lambda} \right\} = 0 \text{ for } i = 1, \ldots, p$$

The matrix $\left\{ \frac{\partial^2 F(X(\lambda))}{\partial x_i \partial x_j} \right\}$ is the Hessian matrix $H(\lambda)$ (Casado-Izaga, 2010). We get in vector notation: $\frac{\partial^2 F(X(\lambda))}{\partial X \partial \lambda} + H(\lambda) \frac{dX(\lambda)}{d\lambda} = 0$ and thus:

$$\frac{dX(\lambda)}{d\lambda} = -H^{-1}(\lambda) \frac{\partial^2 F(X(\lambda))}{\partial X \partial \lambda} \equiv D[X(\lambda), \lambda] \tag{2}$$

which is a set of ordinary differential equations.

TABLE 1 *Numerical integration methods*

Fourth-order Runge-Kutta (Kutta (1901); Runge (1895))	
$fx_1 = hf_x(x_0, y_0, \lambda_0)$	$fy_1 = hf_y(x_0, y_0, \lambda_0)$
$fx_2 = hf_x(x_0 + \frac{1}{2}fx_1, y_0 + \frac{1}{2}fy_1, \lambda_0 + \frac{1}{2}h)$	$fy_2 = hf_y(x_0 + \frac{1}{2}fx_1, y_0 + \frac{1}{2}fy_1, \lambda_0 + \frac{1}{2}h)$
$fx_3 = hf_x(x_0 + \frac{1}{2}fx_2, y_0 + \frac{1}{2}fy_2, \lambda_0 + \frac{1}{2}h)$	$fy_3 = hf_y(x_0 + \frac{1}{2}fx_2, y_0 + \frac{1}{2}fy_2, \lambda_0 + \frac{1}{2}h)$
$fx_4 = hf_x(x_0 + fx_3, y_0 + fy_3, \lambda_0 + h)$	$fy_4 = hf_y(x_0 + fx_3, y_0 + fy_3, \lambda_0 + h)$
$\Delta x = \frac{1}{6}(fx_1 + 2fx_2 + 2fx_3 + fx_4) + O(h^5)$	$\Delta y = \frac{1}{6}(fy_1 + 2fy_2 + 2fy_3 + fy_4) + O(h^5)$
Runge-Kutta-Gill (Gill (1951))	
Define: $\alpha_1 = 1 - \sqrt{\frac{1}{2}}; \alpha_2 = 1 + \sqrt{\frac{1}{2}}; \alpha_3 = \sqrt{\frac{1}{2}} - \frac{1}{2}; \alpha_4 = \sqrt{\frac{1}{2}}.$	
$fx_1 = hf_x(x_0, y_0, \lambda_0)$	$fy_1 = hf_y(x_0, y_0, \lambda_0)$
$fx_2 = hf_x(x_0 + \frac{1}{2}fx_1, y_0 + \frac{1}{2}fy_1, \lambda_0 + \frac{1}{2}h)$	$fy_2 = hf_y(x_0 + \frac{1}{2}fx_1, y_0 + \frac{1}{2}fy_1, \lambda_0 + \frac{1}{2}h)$
$fx_5 = \alpha_3 fx_1 + \alpha_1 fx_2$	$fy_5 = \alpha_3 fy_1 + \alpha_1 fy_2$
$fx_3 = hf_x(x_0 + fx_5, y_0 + fy_5, \lambda_0 + \frac{1}{2}h)$	$fy_3 = hf_y(x_0 + fx_5, y_0 + fy_5, \lambda_0 + \frac{1}{2}h)$
$fx_6 = \alpha_2 fx_3 - \alpha_4 fx_2$	$fy_5 = \alpha_2 fy_3 - \alpha_4 fy_2$
$fx_4 = hf_x(x_0 + fx_6, y_0 + fy_6, \lambda_0 + h)$	$fy_4 = hf_y(x_0 + fx_6, y_0 + fy_6, \lambda_0 + h)$
$\Delta x = \frac{1}{6}(fx_1 + 2\alpha_1 fx_2 + 2\alpha_2 fx_3 + fx_4) + O(h^5)$	$\Delta y = \frac{1}{6}(fy_1 + 2\alpha_1 fy_2 + 2\alpha_2 fy_3 + fy_4) + O(h^5)$
No derivative required at the end of the integration segment (Heun (1900))	
$fx_1 = hf_x(x_0, y_0, \lambda_0)$	$fy_1 = hf_y(x_0, y_0, \lambda_0)$
$fx_2 = hf_x(x_0 + \frac{1}{3}fx_1, y_0 + \frac{1}{3}fy_1, \lambda_0 + \frac{1}{3}h)$	$fy_2 = hf_y(x_0 + \frac{1}{3}fx_1, y_0 + \frac{1}{3}fy_1, \lambda_0 + \frac{1}{3}h)$
$fx_3 = hf_x(x_0 + \frac{2}{3}fx_2, y_0 + \frac{2}{3}fy_2, \lambda_0 + \frac{2}{3}h)$	$fy_3 = hf_y(x_0 + \frac{2}{3}fx_2, y_0 + \frac{2}{3}fy_2, \lambda_0 + \frac{2}{3}h)$
$\Delta x = \frac{1}{4}(fx_1 + 3fx_3) + O(h^4)$	$\Delta y = \frac{1}{4}(fy_1 + 3fy_3) + O(h^4)$

For a function of two variables, $f(x, y, \lambda)$, equation (2) can be explicitly written as follows.

$$H(\lambda) = \begin{pmatrix} \frac{\partial^2 f}{\partial^2 x} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial^2 y} \end{pmatrix} \rightarrow H^{-1}(\lambda) = \frac{1}{\frac{\partial^2 f}{\partial^2 x}\frac{\partial^2 f}{\partial^2 y} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2} \begin{pmatrix} \frac{\partial^2 f}{\partial^2 y} & -\frac{\partial^2 f}{\partial x \partial y} \\ -\frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial^2 x} \end{pmatrix}$$

and

$$\frac{\partial^2 F(X(\lambda))}{\partial X \partial \lambda} = \begin{pmatrix} \frac{\partial^2 f}{\partial x \partial \lambda} \\ \frac{\partial^2 f}{\partial y \partial \lambda} \end{pmatrix}$$

leading to:

$$\frac{\partial x}{\partial \lambda} = \frac{\frac{\partial^2 f}{\partial x \partial y}\frac{\partial^2 f}{\partial y \partial \lambda} - \frac{\partial^2 f}{\partial^2 y}\frac{\partial^2 f}{\partial x \partial \lambda}}{\frac{\partial^2 f}{\partial^2 x}\frac{\partial^2 f}{\partial^2 y} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2}; \frac{\partial y}{\partial \lambda} = \frac{\frac{\partial^2 f}{\partial x \partial y}\frac{\partial^2 f}{\partial x \partial \lambda} - \frac{\partial^2 f}{\partial^2 x}\frac{\partial^2 f}{\partial y \partial \lambda}}{\frac{\partial^2 f}{\partial^2 x}\frac{\partial^2 f}{\partial^2 y} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2} \quad (3)$$

If $\frac{\partial^2 f}{\partial x \partial y} = 0$, the formulas are much simplified. $\frac{\partial x}{\partial \lambda} = -\frac{\frac{\partial^2 f}{\partial x \partial \lambda}}{\frac{\partial^2 f}{\partial^2 x}}$ and $\frac{\partial y}{\partial \lambda} = -\frac{\frac{\partial^2 f}{\partial y \partial \lambda}}{\frac{\partial^2 f}{\partial^2 y}}$. In order to obtain any desired accuracy, the interval h is halved, and halved again until the desired accuracy is achieved.

We demonstrate the trajectory method on two location problems: the Weber problem (Church, 2019; Weber, 1909), and the competitive location model (Drezner, 2019).

3. The Weber Problem

Consider the standard Weber problem with Euclidean distances. n demand points located at (x_i, y_i) with weights w_i are located in an area. By equation (1) for $p = 2$, the Weber problem can be formulated as minimizing:

$$f(x,y,\lambda) = \sum_{i=1}^{n} w_i \left[(x-x_i)^2 + (y-y_i)^2\right]^{1-\lambda} \tag{4}$$

for $\lambda = \frac{1}{2}$. The solution to minimizing (4) for $\lambda = 0$ is the centre of gravity (Francis *et al.*, 1992; Love *et al.*, 1988)

$$x_0 = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}; \quad y_0 = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i} \tag{5}$$

and for $\lambda = \frac{1}{2}$, the end of the trajectory is the desired Weber solution.

For $X = X(\lambda)$ which is an optimal solution point for λ:

$$\begin{aligned} \frac{\partial f}{\partial x} &= 2(1-\lambda)\sum_{i=1}^{n} w_i \left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda} (x-x_i) = 0 \\ \frac{\partial f}{\partial y} &= 2(1-\lambda)\sum_{i=1}^{n} w_i \left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda} (y-y_i) = 0 \end{aligned} \tag{6}$$

The second derivatives at $X = X(\lambda)$ incorporating identities (6) are:

$$\begin{aligned} \frac{\partial^2 f}{\partial x^2} &= 2(1-\lambda)\sum_{i=1}^{n} w_i \left\{-\lambda\left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda-1}(x-x_i)^2 + \left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda}\right\} \\ &= 2(1-\lambda)\sum_{i=1}^{n} w_i \left\{\left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda-1}\left[(1-\lambda)(x-x_i)^2 + (y-y_i)^2\right]\right\} \\ \frac{\partial^2 f}{\partial y^2} &= 2(1-\lambda)\sum_{i=1}^{n} w_i \left\{\left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda-1}\left[(x-x_i)^2 + (1-\lambda)(y-y_i)^2\right]\right\} \\ \frac{\partial^2 f}{\partial x \partial y} &= -4\lambda(1-\lambda)\sum_{i=1}^{n} w_i \left\{\left[(x-x_i)^2 + (y-y_i)^2\right]^{-\lambda-1}(x-x_i)(y-y_i)\right\} \end{aligned}$$

$$\frac{\partial^2 f}{\partial x \partial \lambda} = -2(1-\lambda)\sum_{i=1}^{n} w_i \left[(x-x_i)^2+(y-y_i)^2\right]^{-\lambda}(x-x_i)\ln\left((x-x_i)^2+(y-y_i)^2\right)$$
$$\frac{\partial^2 f}{\partial y \partial \lambda} = -2(1-\lambda)\sum_{i=1}^{n} w_i \left[(x-x_i)^2+(y-y_i)^2\right]^{-\lambda}(y-y_i)\ln\left((x-x_i)^2+(y-y_i)^2\right) \qquad (7)$$

The trajectory can be calculated by substituting equations (7) into equation (3).

3.1 *An approximate starting solution point*

We propose a new approximate starting solution point by calculating the derivatives for $\lambda = 0$, estimating the endpoint of the trajectory by these derivatives, and obtain a starting solution for iterative procedures such as the Weiszfeld algorithm (Weiszfeld, 1937). Assuming that the derivatives do not change much on the trajectory, and applying $\lambda_1 - \lambda_0 = \frac{1}{2}$, leads to the following approximations for the final point of the trajectory $(\hat{x}, \hat{y})$ which is the solution point of the Weber problem:

$$\hat{x} = x_0 + \Delta x \approx x_0 + \frac{1}{2}\left.\frac{\partial x}{\partial \lambda}\right|_{\lambda=0};\ \hat{y} = y_0 + \Delta y \approx y_0 + \frac{1}{2}\left.\frac{\partial y}{\partial \lambda}\right|_{\lambda=0}. \qquad (8)$$

The starting point (x_0, y_0) is given by equation (5).

For $\lambda = 0$: $\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial y^2} = 2\sum_{i=1}^{n} w_i$; $\frac{\partial^2 f}{\partial x \partial y} = 0$; $\frac{\partial^2 f}{\partial x \partial \lambda} = -2\sum_{i=1}^{n} w_i (x_0 - x_i)\ln\left[(x_0-x_i)^2+(y_0-y_i)^2\right]$; $\frac{\partial^2 f}{\partial y \partial \lambda} = -2\sum_{i=1}^{n} w_i (y_0 - y_i)\ln\left[(x_0-x_i)^2+(y_0-y_i)^2\right]$.

By equation (3)

$$\left.\frac{\partial x}{\partial \lambda}\right|_{\lambda=0} = \frac{\sum_{i=1}^{n} w_i (x_0-x_i)\ln\left[(x_0-x_i)^2+(y_0-y_i)^2\right]}{\sum_{i=1}^{n} w_i}$$

$$\left.\frac{\partial y}{\partial \lambda}\right|_{\lambda=0} = \frac{\sum_{i=1}^{n} w_i (y_0-y_i)\ln\left[(x_0-x_i)^2+(y_0-y_i)^2\right]}{\sum_{i=1}^{n} w_i}$$

By equation (8):

$$\Delta x \approx \frac{1}{2}\left.\frac{\partial x}{d\lambda}\right|_{\lambda=0};\ \Delta y \approx \frac{1}{2}\left.\frac{\partial y}{d\lambda}\right|_{\lambda=0}.$$

The estimated end of the trajectory and thus the estimate of the Weber solution is $(x_A, y_A) = (x_0 + \Delta x, y_0 + \Delta y)$ is:

$$
\begin{aligned}
x_A = x_0 + \Delta x &= \frac{\sum_{i=1}^{n} w_i \left\{ x_i + \frac{1}{2}(x_0 - x_i) \ln\left[(x_0 - x_i)^2 + (y_0 - y_i)^2\right] \right\}}{\sum_{i=1}^{n} w_i} \\
y_A = y_0 + \Delta y &= \frac{\sum_{i=1}^{n} w_i \left\{ y_i + \frac{1}{2}(y_0 - y_i) \ln\left[(x_0 - x_i)^2 + (y_0 - y_i)^2\right] \right\}}{\sum_{i=1}^{n} w_i}
\end{aligned} \tag{9}
$$

This point can serve as a starting solution to any iterative method such as the Weiszfeld procedure (Weiszfeld, 1937; Weiszfeld & Plastria, 2009) or other approaches (for example, Drezner, 2015) rather than the centre of gravity (x_0, y_0). The Weiszfeld algorithm is an iterative procedure. Let the current iteration point be $(\hat{x}, \hat{y})$. Define $\hat{w}_i = \frac{w_i}{\sqrt{(\hat{x}-x_i)^2+(\hat{y}-y_i)^2}}$, then the next iterate (x', y') is:

$$
x' = \frac{\sum_{i=1}^{n} \hat{w}_i x_i}{\sum_{i=1}^{n} \hat{w}_i}; \; y' = \frac{\sum_{i=1}^{n} \hat{w}_i y_i}{\sum_{i=1}^{n} \hat{w}_i}. \tag{10}
$$

3.1.1 *An Example.* We created a problem of 50 demand points with equal weights. In order to be able to replicate it we created a pseudo random configuration similar to the one proposed by Law & Kelton (1991), and applied in many recent papers such as Drezner *et al.* (2019). The coordinates are in (0, 1) with three decimal places. We selected $x_1 = 0.291, y_1 = 0.643$. For $k = 2, \ldots, 50$, $x_k = 413x_{k-1} - \lfloor 413x_{k-1} \rfloor$ and $y_k = 413y_{k-1} - \lfloor 413y_{k-1} \rfloor$, where $\lfloor a \rfloor$ is the largest integer less than a.

The trajectory and the approximate location are depicted in Figure 1. On the left panel of the figure the demand points are shown and the trajectory is depicted in a very small area near the centre of the square. This small area is magnified and depicted on the right panel of the figure. By the design of the approximate location, the line connecting the starting $\lambda = 0$ location (which is the centre of gravity) and the approximate location is the tangent to the trajectory curve at $\lambda = 0$.

3.1.2 *Analysis.* Let (x^*, y^*) be the optimal location to the Weber problem. The distance between the centre of gravity and the optimal location is $d_1 = \sqrt{(x_0 - x^*)^2 + (y_0 - y^*)^2}$. The distance between the location $(\hat{x}, \hat{y})$, obtained by (9), and the optimal location is $d_2 = \sqrt{(\hat{x} - x^*)^2 + (\hat{y} - y^*)^2}$. We compared these distances on 100 randomly generated problems with $n = 50$ demand points with equal weights in a square of side 1. We found that $d_2 < d_1$ for 96 instances out of 100. The four instances for which $d_2 > d_1$ had the smallest values of d_1 among the 100 d_1 distances. For these four instances the centre of gravity was very close to the optimal solution.

The relative distances for the 100 instances are depicted in Figures 2 and 3. The line in Figure 2 is the 45° line showing that except for the four points on the bottom left, all distances to $(\hat{x}, \hat{y})$ are shorter. The regression line in Figure 3 has a slope of 0.57 which means that on average the distances by (9) are

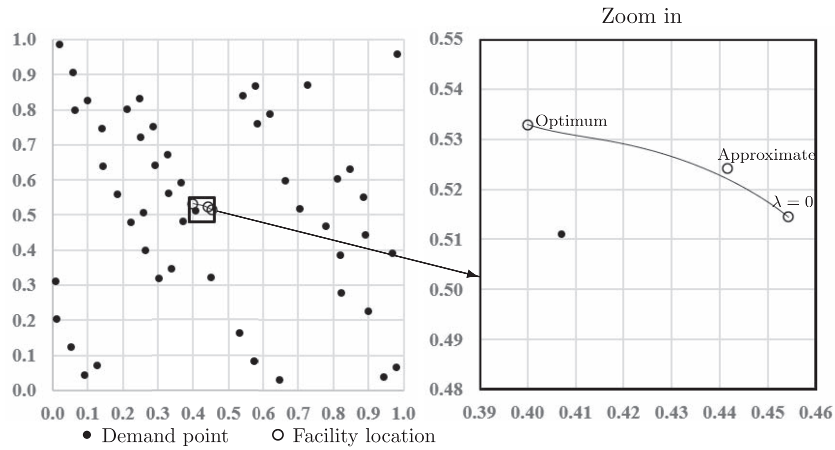

FIG. 1. The trajectory of solving the Weber problem.

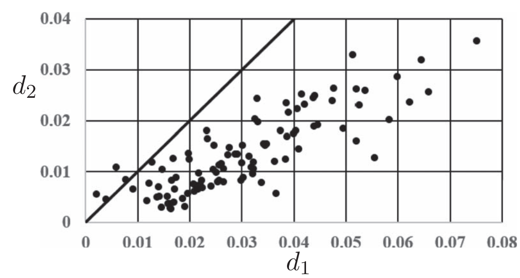

FIG. 2. Relationship between distances to the optimal solution.

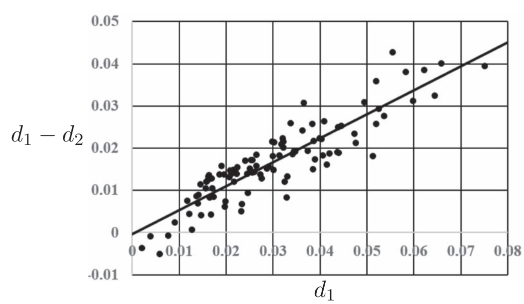

FIG. 3. The improvement in the distances to the optimal solution.

43% closer to the optimal location. The p-value of the regression line is 1.9×10^{-36}. The four exceptions are at the bottom left corner below the line $y = 0$.

3.1.3 *An improved approximate location.* As was found for the example problem in Section 3.1.1, the approximate solution is in the general direction of the optimal location. However, the point closest to the optimal location on the line passing through the $\lambda = 0$ location and the approximate location is not necessarily at the optimal location. Let (x_0, y_0) be the location for $\lambda = 0$, (x_A, y_A) be the approximate location found by (9), and (x^*, y^*) the optimal location. It can be easily shown that the point on the line passing through the $\lambda = 0$ location and the approximate location, which is closest to the optimal location, is at $(x_0 + \theta(x_A - x_0), y_0 + \theta(y_A - y_0))$, where:

$$\theta = \frac{(x_A - x_0)(x^* - x_0) + (y_A - y_0)(y^* - y_0)}{(x_A - x_0)^2 + (y_A - y_0)^2}$$

The value of θ cannot be calculated if the optimal location is not available. We propose to estimate it by simulating the 100 problems from Section 3.1.2 and propose a value for θ that will yield a better approximation in most cases.

We obtained 100 values of θ for the 100 problems. 61 of them are between 1 and 2. The average of all 100 values was 1.66, and the median was 1.56. We minimized the sum of squares of distances from the optimal location as a function of θ and the minimum was obtained for $\theta = 1.57$. We therefore recommend to apply $\theta = 1.57$. The improved approximation is

$$(\hat{x}, \hat{y}) = (1.57x_A - 0.57x_0, 1.57y_A - 0.57y_0)\,.$$

The sum of squares from the optimal solution is 0.1121 for the $\lambda = 0$ location, 0.0284 for the approximate solution, and drops to 0.0157 for the improved approximate solution. The improved approximate solution performed best for these 100 instances.

Such an improved approximate starting solution is similar to a proposed improvement to the Weiszfeld algorithm (Drezner, 1992; Ostresh, 1978). If (x_0, y_0) is the current iteration, and (x', y') is the next Weiszfeld iteration calculated by equation (10), the suggestion is to use a multiplier θ and apply for the next iteration $x'' = x_0 + \theta(x' - x_0)$, and similarly for y. Ostresh (1978) proved convergence for $1 \leq \theta \leq 2$. Drezner (1992) found by simulation that $\theta = 1.8$ performed best. In our improved approximation we proposed, based on simulation, to apply $\theta = 1.57$.

4. The Single Facility Competitive Location Model

Competitive location models can be traced back to Hotelling (1929) who assumed that customers patronize the closest facility. This rule implicitly assumes that all facilities are equally attractive. Reilly (1931) suggested the gravity model assuming that customers who live between two cities will patronize stores in each city proportionally to the city's size and inversely proportional to the square of the distance to the city. This rule imitates the physics law of gravity. In the geographical literature it is referred to as central place theory (Christaller, 1966; Clark & Rushton, 1970). The theory asserts that settlements function as central places providing services to surrounding areas.

Huff (1964, 1966) suggested that the probability that customers patronize a retail facility is proportional to its attractiveness (Huff suggested floor area as a measure of attractiveness) and to a distance decay function $f(d) = \frac{1}{d^\lambda}$ where λ is a parameter that may depend on the retail category. It was optimally solved in Drezner & Drezner (2004).

Wilson (1976) suggested an exponential decay function $f(d) = e^{-\lambda d}$ which was used in many subsequent papers (Aboolian *et al.*, 2007a,b, 2009; Drezner & Drezner, 2008; Fernández *et al.*, 2007; Sáiz *et al.*, 2009). Drezner (2006) compared power and exponential decay on a real data set and showed that exponential decay fits the data better. Therefore, we apply the exponential distance decay function. Other competitive location models include: the utility or random utility models (Drezner & Drezner, 1996; Leonardi & Tadei, 1984), cover based models (Drezner *et al.*, 2011, 2012), the flow interception model (Berman & Krass, 1998). For recent reviews see Drezner (2019, 2022); Eiselt *et al.* (2015).

4.1 *Notation*

n	Number of demand points
p	Number of existing facilities
$0 \le q \le p$	Number of existing facilities in your own chain numbered $1, \dots, q$
d_{ij}	Distance between demand point i and existing facility j
λ	Decay parameter
A_j	Attractiveness of existing facility j
$A_j e^{-\lambda d_{ij}}$	Utility of existing facility j as observed by demand point i
$X = (x, y)$	Unknown location of the new facility
$d_i(X)$	Distance between demand point i and location X
A	Attractiveness of the new facility
$Ae^{-\lambda d_i(X)}$	Utility of the new facility as observed by demand point i
B_i	Available buying power at demand point i

4.2 *Formulation*

The market share $M(X(\lambda))$ captured by the chain when adding a new facility located at $X = (x, y)$ is by the gravity (Huff) model:

$$M(X(\lambda)) = \sum_{i=1}^{n} B_i \frac{\sum_{j=1}^{q} A_j e^{-\lambda d_{ij}} + Ae^{-\lambda d_i(X)}}{\sum_{j=1}^{p} A_j e^{-\lambda d_{ij}} + Ae^{-\lambda d_i(X)}} = \sum_{i=1}^{n} B_i - \sum_{i=1}^{n} B_i \frac{\sum_{j=q+1}^{p} A_j e^{-\lambda d_{ij}}}{\sum_{j=1}^{p} A_j e^{-\lambda d_{ij}} + Ae^{-\lambda d_i(X)}} \tag{11}$$

The objective is to maximize $M(X(\lambda))$ for a given λ by finding the best location X for the new facility. Drezner *et al.* (2018) assumed that the attractiveness levels are normally distributed rather than all the customers residing at a demand point have the same perception of attractiveness. Drezner *et al.* (2020) refined the model by defining different λ's for different facilities. More attractive facilities have a shallower decline in attractiveness for larger distances than less attractive facilities. Drezner *et al.* (2022) further refined the model by adding a constant distance to the d_{ij} distances.

We solve the original gravity model (11). Define:

$$\alpha_i(q, \lambda) = \sum_{j=q+1}^{p} A_j e^{-\lambda d_{ij}}; \;\; \beta_i(\lambda, X) = Ae^{-\lambda d_i(X)} \tag{12}$$

$$M(X(\lambda)) = \sum_{i=1}^{n} B_i - \sum_{i=1}^{n} B_i \frac{\alpha_i(q, \lambda)}{\alpha_i(0, \lambda) + \beta_i(\lambda, X)} \tag{13}$$

$$\frac{\partial \alpha_i(q,\lambda)}{\partial \lambda} = -\sum_{j=q+1}^{p} A_j d_{ij} e^{-\lambda d_{ij}}; \quad \frac{\partial \beta_i(\lambda, X)}{\partial \lambda} = -d_i(X)\beta_i(\lambda, X); \quad \frac{\partial \beta_i(\lambda, X)}{\partial d_i(X)} = -\lambda \beta_i(\lambda, X) \tag{14}$$

4.3 *The Case* $\lambda = 0$

The case $\lambda = 0$, which was not analyzed in previous papers, is used as the starting point of the trajectory. We show how to obtain the optimal location for $\lambda = 0$. For $\lambda = 0$ the market share is constant and every point leads to the same market share.

$$M(X,0) = \frac{\sum_{j=1}^{q} A_j + A}{\sum_{j=1}^{p} A_j + A} \sum_{i=1}^{n} B_i$$

Lemma 1. : For a very small λ the maximum point can be found by maximizing the derivative by λ at $\lambda \to 0$.

Proof: For any λ there exists, by the mean value theorem, $0 \le \bar{\lambda} \le \lambda$ such that

$$M(X(\lambda)) = M(X,0) + \lambda \left.\frac{\partial M(X(\lambda))}{\partial \lambda}\right|_{\lambda=\bar{\lambda}}$$

Since $M(X,0)$ is constant in X, maximizing $M(X(\lambda))$ for an infinitesimal λ is the same as maximizing $\left.\frac{\partial M(X(\lambda))}{\partial \lambda}\right|_{\lambda \to 0}$. □

Theorem 1. : For $\lambda \to 0$, the solution point to maximizing $M(X(\lambda))$ (13) is the solution point to minimizing

$$F(X) = \sum_{i=1}^{n} B_i d_i(X) \tag{15}$$

Proof: By (14):

$$\frac{\partial M(X(\lambda))}{\partial \lambda} = \sum_{i=1}^{n} B_i \frac{-\frac{\partial \alpha_i(q,\lambda)}{\partial \lambda}\left[\alpha_i(0,\lambda) + \beta_i(\lambda,X)\right] + \left[\frac{\partial \alpha_i(0,\lambda)}{\partial \lambda} + \frac{\partial \beta_i(\lambda,X)}{\partial \lambda}\right]\alpha_i(q,\lambda)}{\left[\alpha_i(0,\lambda) + \beta_i(\lambda,X)\right]^2}.$$

For $\lambda = 0$:

$$\frac{\partial M(X(\lambda))}{\partial \lambda}\bigg|_{\lambda=0} = \sum_{i=1}^{n} B_i \frac{\sum_{j=q+1}^{p} A_j d_{ij} \left[\sum_{j=1}^{p} A_j + A\right] - \left[\sum_{j=1}^{p} A_j d_{ij} + A d_i(X)\right] \sum_{j=q+1}^{p} A_j}{\left[\sum_{j=1}^{p} A_j + A\right]^2} \tag{16}$$

By Lemma 1 the solution to maximizing $M(X(\lambda))$ as $\lambda \to 0$ is the solution to maximizing (16). Eliminating all constants, the maximum point minimizes $F(X) = \sum_{i=1}^{n} B_i d_i(X)$ □

4.4 *Solution by the trajectory approach*

By Theorem 1 the solution to $\lambda = 0$ is the solution to a Weber problem (Weber, 1909), and can be easily found by, for example, Drezner (1992); Weiszfeld (1937), and the trajectory method described in Section 3. The trajectory connecting $\lambda = 0$ to the given λ can be constructed. The problem is finding $X(\lambda) = (x(\lambda), y(\lambda))$ that minimizes by (13):

$$F(x, y, \lambda) = \sum_{i=1}^{n} B_i \frac{\alpha_i(q, \lambda)}{\alpha_i(0, \lambda) + \beta_i(\lambda, x, y)} \equiv \sum_{i=1}^{n} B_i f_i(x, y, \lambda) \tag{17}$$

For simplicity in the next derivations we assume that X is the optimal value $X(\lambda)$ for a given λ.

$$\frac{\partial f_i}{\partial x} = \frac{-\alpha_i(q, \lambda)\frac{\partial \beta_i(\lambda, x, y)}{\partial x}}{\left[\alpha_i(0, \lambda) + \beta_i(\lambda, X)\right]^2} = \lambda \frac{x - x_i}{d_i(X)} \frac{\alpha_i(q, \lambda)\beta_i(\lambda, X)}{\left[\alpha_i(0, \lambda) + \beta_i(\lambda, X)\right]^2}$$

Define

$$\gamma_i(\lambda, X) = \frac{\beta_i(\lambda, X)\alpha_i(q, \lambda)}{\left[\alpha_i(0, \lambda) + \beta_i(\lambda, X)\right]^2}$$

Since the derivative of $F(x(\lambda), y(\lambda), \lambda)$ by x and y are zero, and removing the λ,

$$\sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \frac{x - x_i}{d_i(X)} = \sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \frac{y - y_i}{d_i(X)} = 0\,. \tag{18}$$

In addition:

$$\frac{\partial \gamma_i(\lambda, X)}{\partial \lambda} = \frac{\frac{\partial \beta_i(\lambda, X)}{\partial \lambda}\alpha_i(q, \lambda) + \beta_i(\lambda, X)\frac{\partial \alpha_i(q, \lambda)}{\partial \lambda}}{\left[\alpha_i(0, \lambda) + \beta_i(\lambda, X)\right]^2} - 2\frac{\beta_i(\lambda, X)\alpha_i(q, \lambda)\left[\frac{\partial \alpha_i(0, \lambda)}{\partial \lambda} + \frac{\partial \beta_i(\lambda, X)}{\partial \lambda}\right]}{\left[\alpha_i(0, \lambda) + \beta_i(\lambda, X)\right]^3}$$

By (14) $\frac{\partial \alpha_i(q,\lambda)}{\partial \lambda} = -\sum_{j=q+1}^{p} A_j d_{ij} e^{-\lambda d_{ij}}$, $\frac{\partial \beta_i(\lambda,X)}{\partial \lambda} = -d_i(X)\beta_i(\lambda,X)$. leading to:

$$\frac{\partial \gamma_i(\lambda,X)}{\partial \lambda} = -\beta_i(\lambda,X)\left\{\frac{d_i(X)\alpha_i(q,\lambda) + \sum_{j=q+1}^{p} A_j d_{ij} e^{-\lambda d_{ij}}}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^2} - 2\frac{\alpha_i(q,\lambda)\left[\sum_{j=1}^{p} A_j d_{ij} e^{-\lambda d_{ij}} + d_i(X)\beta_i(\lambda,X)\right]}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^3}\right\} \tag{19}$$

$$\begin{aligned}\frac{\partial \gamma_i(\lambda,X)}{\partial x} &= \alpha_i(q,\lambda)\frac{\partial \beta_i(\lambda,X)}{\partial x}\frac{\alpha_i(0,\lambda)-\beta_i(\lambda,X)}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^3} \\ &= -\lambda\alpha_i(q,\lambda)\beta_i(\lambda,X)\frac{\alpha_i(0,\lambda)-\beta_i(\lambda,X)}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^3}\times\frac{x-x_i}{d_i(X)} \end{aligned} \tag{20}$$

$$\frac{\partial \gamma_i(\lambda,X)}{\partial y} = -\lambda\alpha_i(q,\lambda)\beta_i(\lambda,X)\frac{\alpha_i(0,\lambda)-\beta_i(\lambda,X)}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^3}\times\frac{y-y_i}{d_i(X)} \tag{21}$$

Define

$$\delta_i(\lambda,X) = -\lambda\alpha_i(q,\lambda)\beta_i(\lambda,X)\frac{\alpha_i(0,\lambda)-\beta_i(\lambda,X)}{\left[\alpha_i(0,\lambda)+\beta_i(\lambda,X)\right]^3} \tag{22}$$

then

$$\frac{\partial \gamma_i(\lambda,X)}{\partial x} = \delta_i(\lambda,X)\frac{x-x_i}{d_i(X)};\ \ \frac{\partial \gamma_i(\lambda,X)}{\partial y} = \delta_i(\lambda,X)\frac{y-y_i}{d_i(X)} \tag{23}$$

$$\frac{d}{dx}\left(\frac{x-x_i}{d_i(X)}\right) = \frac{(y-y_i)^2}{d_i^3(X)};\ \ \frac{d}{dy}\left(\frac{x-x_i}{d_i(X)}\right) = -\frac{(x-x_i)(y-y_i)}{d_i^3(X)} \tag{24}$$

and similarly for the derivatives of $\frac{y-y_i}{d_i(X)}$.

Applying (14)–(24) yields the following expressions required for the calculation of $\frac{dx}{d\lambda}$ and $\frac{dy}{d\lambda}$ in equation (3):

$$\frac{\partial F(x,y,\lambda)}{\partial x} = \lambda \sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{x-x_i}{d_i(X)} = 0 \tag{25}$$

$$\frac{\partial F(x,y,\lambda)}{\partial y} = \lambda \sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{y-y_i}{d_i(X)} = 0 \tag{26}$$

$$\frac{\partial^2 F(x,y,\lambda)}{\partial x \partial \lambda} = \sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{x-x_i}{d_i(X)} + \lambda \sum_{i=1}^{n} B_i \frac{\partial \gamma_i(\lambda, X)}{\partial \lambda} \times \frac{x-x_i}{d_i(X)} \tag{27}$$

$$\frac{\partial^2 F(x,y,\lambda)}{\partial y \partial \lambda} = \sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{y-y_i}{d_i(X)} + \lambda \sum_{i=1}^{n} B_i \frac{\partial \gamma_i(\lambda, X)}{\partial \lambda} \times \frac{y-y_i}{d_i(X)} \tag{28}$$

$$\frac{\partial^2 F(x,y,\lambda)}{\partial^2 x} = \lambda \sum_{i=1}^{n} B_i \left\{ \delta_i(\lambda, X) \times \frac{(x-x_i)^2}{d_i^2(X)} + \gamma_i(\lambda, X) \times \frac{(y-y_i)^2}{d_i^3(X)} \right\} \tag{29}$$

$$\frac{\partial^2 F(x,y,\lambda)}{\partial^2 y} = \lambda \sum_{i=1}^{n} B_i \left\{ \delta_i(\lambda, X) \times \frac{(y-y_i)^2}{d_i^2(X)} + \gamma_i(\lambda, X) \times \frac{(x-x_i)^2}{d_i^3(X)} \right\} \tag{30}$$

$$\frac{\partial^2 F(x,y,\lambda)}{\partial x \partial y} = \lambda \sum_{i=1}^{n} B_i \left\{ \delta_i(\lambda, X) \times \frac{(x-x_i)(y-y_i)}{d_i^2(X)} - \gamma_i(\lambda, X) \times \frac{(x-x_i)(y-y_i)}{d_i^3(X)} \right\} \tag{31}$$

The first term in (27) and (28) is equal to zero by (18). Equations (27) to (31) are problematic for $\lambda = 0$ because all derivatives are zero. To address this issue we prove the following lemma:

LEMMA 2. : $\lim_{\lambda \to 0} \frac{\sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{x-x_i}{d_i(X)}}{\lambda} = \sum_{i=1}^{n} B_i \frac{\partial \gamma_i(\lambda, X)}{\partial \lambda} \times \frac{x-x_i}{d_i(X)}$.

Proof: By (18) $\sum_{i=1}^{n} B_i \gamma_i(\lambda, X) \times \frac{x-x_i}{d_i(X)} = 0$. Therefore, the lemma follows by L'Hopital rule. □

We can remove the multiplier λ from all equations when substituting into (3), and replace the first term in (27) and (28) with its ratio by λ. By Lemma 2, for the special case $\lambda = 0$, equation (27) after removing the λ multiplier is $\frac{\partial^2 F(x,y,\lambda)}{\partial x \partial \lambda} = 2 \sum_{i=1}^{n} B_i \frac{\partial \gamma_i(\lambda, X)}{\partial \lambda} \times \frac{x-x_i}{d_i(X)}$, and similarly for (28).

4.5 *Computational experiments*

We solved the competitive location model locating a facility in Orange County, California. The data were presented in Drezner (2006), and are also available in Drezner *et al.* (2020). There are seven existing malls in Orange County and 3,112 customers residing at 81 zip codes were intercepted at these malls. The seven malls sorted by their attractiveness level are listed in Table 2.

TABLE 2 *Shopping malls and their attractiveness (A_j)*

j	Shopping mall	Zip code	A_j
1	Orange mall	92865	0.177
2	Laguna Hills mall	92653	0.595
3	Westminster mall	92683	1.011
4	Main place	92701	1.154
5	Brea mall	92821	1.529
6	Fashion island	92660	2.367
7	South Coast plaza	92626	2.484

A new mall is planed to be built in the area. We found the best location of a new mall, which is not part of a chain, for seven instances. Each instance had a different attractiveness level. We selected the seven attractiveness levels of the existing malls depicted in Table 2. Different attractiveness levels result in different locations for the new mall.

We solved the seven instances in Mathematica (Wolfram, 2021) by Nelder-Mead and our proposed trajectory method. The Nelder–Mead method (Aloise *et al.*, 2018; Nelder & Baker, 1972; Nelder & Mead, 1965) is one of the direct search methods for global optimization available in Wolfram's Mathematica 13 (Wolfram, 2021) with the default settings. We find the location that yields the maximum market share calculated by (11). We report for each instance the results obtained by one run of Nelder-Mead, and the best results obtained by solving each instance 25 times. The trajectory approach has no random component and was implemented only once. The trajectories were determined using Mathematica's implementation of the classic Runge–Kutta method (the first set, RK4, in Table 1). First, the initial solution was found by minimizing (15). Next, the second derivatives (27)–(31) were used to determine the set of ordinary differential equations (3), which were numerically solved with RK4, starting from the initial solution.

The results by Nelder-Mead are compared with the results obtained by the trajectory method and depicted in Table 3. If a solution by a certain method is the best known solution, it is marked in boldface. The trajectory method found the best known solution in six of the seven instances, and in the seventh one found a very close market share. Decreasing the step size h in RK4 will converge to the best known value. Nelder-Mead, applied once, found the best known solution in three instances and in four cases the market share was significantly lower in a different region of Orange County. When the number of runs of Nelder-Mead was increased to 25, staring each run from a randomly generated starting solution, all seven instances yielded the best known solution at least once.

The seven trajectories are depicted in Figure 4. On the left is the whole area of Orange County with the Pacific Ocean on the bottom left. On the right, the area of interest that includes the seven trajectories is zoomed in. In the figure:

- The 81 zip codes are marked in grey disks whose area is proportional to the population count.
- The seven existing malls are marked with circles with the mall number next to them.
- The seven trajectories all start at $\lambda = 0$.
- The locations of the facilities at the end of their respective trajectory are marked with empty circles with the attractiveness level depicted next to each location.

TABLE 3 *Calculated locations and percent market shares*

	Best	Nelder-Mead (One Run)			Nelder-Mead (25 Runs)			Trajectory		
A	known	x	y	M	x	y	M	x	y	M
0.177	**3.098%**	20.172	10.682	2.139%	5.369	25.025	**3.098%**	5.343	25.024	3.094%
0.595	**9.087%**	19.380	10.846	5.651%	7.004	24.495	**9.087%**	7.004	24.495	**9.087%**
1.011	**13.917%**	18.742	11.452	8.163%	7.288	24.157	**13.917%**	7.288	24.157	**13.917%**
1.154	**15.388%**	18.557	11.638	8.899%	7.286	23.988	**15.388%**	7.286	23.988	**15.388%**
1.529	**18.918%**	7.314	23.127	**18.918%**	7.314	23.127	**18.918%**	7.314	23.127	**18.918%**
2.367	**25.473%**	7.458	22.839	**25.473%**	7.458	22.839	**25.473%**	7.458	22.839	**25.473%**
2.484	**26.271%**	7.511	22.789	**26.271%**	7.511	22.789	**26.271%**	7.511	22.789	**26.271%**

The bold values are the best known results obtained for each row.

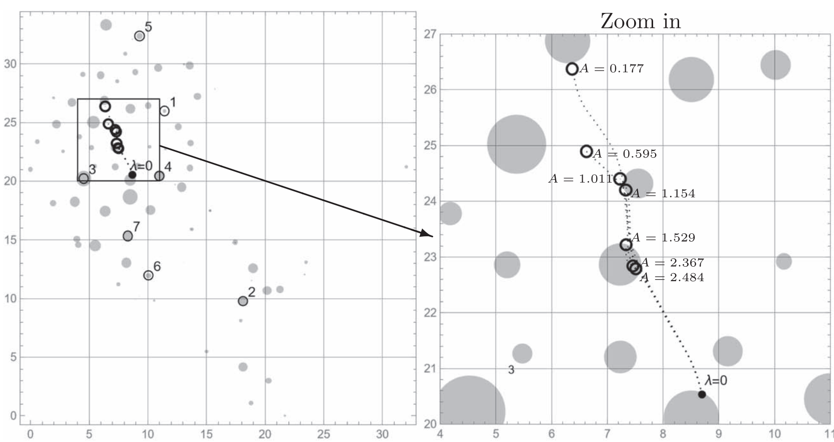

FIG. 4. The trajectories of solving locations for seven facilities.

The seven trajectories almost coincide for small values of λ and look like one trajectory. The trajectories are shorter for larger values of the attractiveness A. The location of the new facility is closer to the $\lambda = 0$ location for larger values of A. All seven locations of the new facility are in the same region of the county in the square on the left figure which is zoomed in on the right. The one-run Nelder-Mead locations (not depicted) are in a different region for the four less attractive facilities (see Table 3). They are all near existing facility 2.

5. Conclusions

We proposed solving non-constrained optimization problems by a trajectory method. A parameter λ is introduced into the optimization problem. For a particular value $\lambda = \lambda_0$, the optimal solution is easily obtained. The original optimization problem is defined for another value $\lambda = \lambda_1$. A trajectory connects the easily obtained solution for λ_0, to the desired solution for λ_1. We trace the trajectory and the desired solution for λ_1 is at the end of the trajectory. See, for example, the first paragraph in Section 3.

The contribution of the paper is showing that the trajectory method is not limited to the three examples solved in Drezner & Wesolowsky (1978a,b, 1982). Many examples that can benefit from this method are presented and two of them are solved in this paper.

For future research we propose to apply the trajectory approach to a variety of unconstrained optimization problems such as those listed in Section 1.1. It is especially convenient to apply it for solving location problems.

Data availability

Hosted on the Open Science Framework: https://osf.io/j8dh7/?view_only=80103deb1971410cb39aca3effa3c937

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RESEARCH

Extensions to Competitive Facility Location with Multi-purpose Trips

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Abstract
Existing location models considering multi-purpose shopping behavior limit the number of stops a customer makes to two. We introduce the multi-purpose (MP) competitive facility location model with more than two stops. We locate one or more facilities in a competitive environment, assuming a shopper may stop multiple times during one trip to purchase different complementary goods or services. We show that when some or all trips are multi-purpose, our model captures at least as much market share as the MP models with fewer purposes. Our extensive simulation experiments show that the MP models work best when multiple new facilities are added. As the number of facilities increases, however, the returns diminish due to cannibalization. Also, with significant increases in complexity for each additional stop added, expanding the model beyond three purposes may not be practical.

Keywords Facility location · Competitive facility location · Multi-purpose shopping · Market share

1 Introduction

Competitive facility location models focus on locating one or more new facilities in an area where other competing facilities already exist. The goal is for the added facilities to capture the maximum possible market share. Customers select a facility to patron according to various criteria, such as distance and facility attractiveness. These two factors are traditionally used to measure the market share captured by a new facility.

One of the extensions of classic competitive facility location is the introduction of multi-purpose (MP), multi-stop shopping. The idea comes from the observation

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that when running errands, customers sometimes combine multiple purposes into a single trip. This behavior, sometimes called "trip-chaining", has been studied quite extensively in other fields, such as transportation, marketing and economics (see for example: O'Kelly (1981), Eaton and Lipsey (1982), Ghosh and McLafferty (1984), McLafferty and Ghosh (1986), Thill and Thomas (1987), Oppewal and Holyoake (2004), Arentze et al. (2005)). While consumers have incentives to engage in multi-purpose shopping, firms are able to increase their market share when they set up their location in proximity to other retailers, either providing easier access to complementary goods or facilitating comparison shopping. This relationship is at the core of the theory of central places, dating back to 1950 s (Eaton and Lipsey 1982).

In the context of competitive location, when considering customers shopping for complementary goods, the problem can be described as follows. There are multiple locations selling a variety of complementary goods on the market. Our chain's competitors are also present on the market. Customers can make separate shopping trips to purchase each good (single purpose) or combine purchases of different goods into a single trip (multi-purpose). Considering the possibility of such multi-purpose customer behavior, the question is how to locate a new facility or facilities so that our chain captures the maximum market share.

As an example, consider a shopper in the suburban USA who sets out from home by car to visit a store. The shopper decides to also get coffee and stop at a gas station during the same trip. As a chain of coffee shops competing against other coffee shops in the area, we wish to open a new location to attract the available demand. We will try to choose the location that is "on the way" for customers running other errands. Consider another shopper in a European city who walks to a nearby grocery store. During the same outing, the shopper chooses to stop at a nearby pharmacy and a vegetable stand, which constitutes a three-purpose trip. A shopper can, of course, choose to make one stop only (single-purpose) or choose two out of three destinations (two-purpose). Being a chain of vegetable stands, we need to consider that a customer may not always walk with a single purpose in mind but rather visit multiple destinations along the way. This may influence our chain's decision on where to locate a new vegetable stand in order to increase the chance of attracting demand.

In this paper, we propose a model that incorporates multi-purpose trips with more than two stops. The motivation comes from the fact that the existing models, both discrete and continuous, involve only two-purpose trips (Drezner et al. 2023a, b; Kalczynski et al. 2024; Marianov et al. 2018; Méndez-Vogel et al. 2023; Lüer-Villagra et al. 2022). According to various sources however (Federal Highway Administration 2017; O'Kelly 1981; Leszczyc et al. 2004; Méndez-Vogel et al. 2023), customers sometimes choose to run more than two errands during a single trip. We demonstrate to what extent this additional knowledge about customer behavior improves the chain's ability of capturing more of the available market share. Our focus is solely on shopping for complementary goods. Comparison shopping, although an important type of multi-purpose behavior, is not a subject of this work.

Considering a model with multiple stops requires determining the order in which different locations are visited. A number of studies in cognitive psychology have shown that people are able to solve small instances of the Traveling Salesman Problem (TSP) nearly optimally and practically effortlessly (MacGregor and Ormerod

1996; Vickers et al. 2001; Dry et al. 2006). See MacGregor and Chu (2011) for a comprehensive review. Moreover, in their empirical study, O'Kelly and Miller (1984) have shown that in many cases, shoppers tend to intuitively choose the shortest path, especially for those multi-purpose trips for which the difference between the shortest and the longest path is prominent. Therefore, although our model works for any order of stops, in our experiments we incorporate a shortest path algorithm. Sometimes customers may prefer a certain order of visited locations, for example visiting a facility that offers perishable goods at the end (Drezner et al. 2023a), or choosing the closest location as the first or the last stop (O'Kelly and Miller 1984), which can result in longer tour for three or more stops.

In the subject literature, sometimes the term "multi-purpose" is utilized in reference to shopping for multiple products, which does not necessarily entail multiple stops (Mulligan 1983; Ghosh and McLafferty 1984; Thill 1992). This paper follows the terminology adopted in most of the recent competitive location papers, where multi-purpose trips are multi-stop or multi-store (Drezner et al. 2023a; Marianov et al. 2018).

The paper is organized as follows. In Section 2 we discuss the literature relevant to the multi-purpose behavior in competitive facility location. In Section 3 we provide the formulation of the single-facility multi-purpose model and its extension to multi-facility problem, as well as the details of the solution techniques. In Section 4 we discuss the criteria for a fair comparison of the models and present the results of extensive computational experiments. We discuss the results in Section 5, which is followed by the conclusion and future research avenues in Section 6.

2 Literature Review

2.1 Competitive Facility Location

Since the competitive location model was first introduced by Hotelling (1929), competitive location has been a popular area of research. See Drezner and Eiselt (2024) for the most recent comprehensive review of competitive facility location research. Hotelling proposed that a customer selects a facility to patronize based on price and transportation cost. When competitors charge the same price, customers choose to patronize the closest facility. This premise became known as the proximity rule. Another approach was suggested by Reilly (1931), who introduced a gravity model. According to the gravity model, customers patronize the facilities in the nearby cities proportionally to each city's size and inversely-proportionally to to the square of distance. This notion of distance decay became a key element of the competitive location models. There are two most commonly used decay functions: power decay and exponential decay. The power decay function, $f(d) = d^{-\lambda}$, where d is the distance and $\lambda > 0$ is the decay parameter, was proposed by Huff (1964, 1966). In Huff's model, the probability that customers will patronize a facility is proportional to its attractiveness and to the distance decay function. Huff also noticed that the distance decay varies depending on the retail category. Drezner and Drezner (2004) provided an optimal solution to this model in a single-facility scenario. Wilson (1974) proposed a different decay function, $f(d) = e^{-\lambda d}$, in which the probability of patronizing a facility declines exponentially. Drezner (2006) and later Drezner and Zerom (2024) tested both decay models in the study of shopping malls in Orange County, California, and showed a better fit of the exponential decay model. Based on these findings, we chose to use exponential decay in our model. Also, our focus is strictly on distance. Readers interested in an in-depth discussion on attractiveness are referred to Drezner and Zerom (2024).

2.2 Multi-purpose, Multi-stop Trips in Facility Location

The original location models assumed a single-purpose (1P) consumer behavior. In a 1P model, a customer visits only one location to purchase a good or service, and then returns to the point of origin. However, these models do not fully reflect the way people shop (O'Kelly 1981; Thill and Thomas 1987; Eaton and Lipsey 1982; McLafferty and Ghosh 1986). In reality, customers often shop for multiple products at the same time. Moreover, they frequently tend to visit multiple locations during a single trip. Leszczyc et al. (2004) showed that 34% of grocery shopping trips were multi-purpose, while Méndez-Vogel et al. (2023) cited between 30% and even 74%, and O'Kelly (1981) reported 58%. The results of the 2017 National Household Travel Survey (NHTS), reported in Table 1, showed that close to 26% trips were multi-purpose (Federal Highway Administration 2017), with 20.8% two-purpose (2P), 4.5% three-purpose (3P), and 1.5% four-purpose trips (4P). Trips with more than four stops accounted for the remaining 0.7%.

Early work in multi-purpose facility location was focused on minimizing travel cost. Suzuki and Hodgson (2005) presented a discrete model with two types of facilities. They showed that when multi-purpose behavior exists, the services tend to cluster in joint facilities. Berman and Huang (2007) studied the problem on the network while Araghi et al. (2014) considered it on a tree. Li and Tong (2017) concentrated on accessibility in the context of the p-median problem.

When aiming at capturing the maximum market share, the focus has been either on substitute products (Marianov and Méndez-Vogel 2023; Méndez-Vogel et al. 2024) or complementary products (Drezner et al. 2023a, b; Lüer-Villagra et al. 2022; Marianov et al. 2018; Méndez-Vogel et al. 2023; Kalczynski et al. 2024), which resulted in different research avenues.

Two-purpose trips with customers shopping for non-essential, complementary products were considered by Marianov et al. (2018), Drezner et al. (2023a, b), Méndez-Vogel et al. (2023) and Lüer-Villagra et al. (2022). Drezner et al. (2023a) located a single facility, assuming that a certain proportion of trips was two-purpose (2P). They showed that the extension of a classic competitive single-purpose model allows for capturing more market share. They also noted that for non-zero proportions of 2P trips, the optimal location of the new facility shifts towards clusters of facilities offering different

Table 1 Percentage of multi-purpose trips. Source: NHTS Survey (Federal Highway Administration 2017)

Year	1P	2P	3P	4P	more
2005	72.5%	20.8%	4.5%	1.5%	0.7%
2017	74.1%	19.2%	4.5%	0.5%	0.3%

product types. Kalczynski et al. (2024) expanded the 2P model by locating multiple facilities of a chain that sell the same product. They addressed the potential issue of cannibalization (competition among chain facilities) and demonstrated how the combination of multiple facilities and 2P trips increased captured market share. Drezner et al. (2023b) replaced a given proportion of 2P trips with a stochastic one. They considered five known decision analysis rules and found optimal locations for each of these rules.

Marianov et al. (2018) introduced a discrete duopoly follower's problem which includes 2P trips. They showed that the inclusion of 2P trips increases the tendency of the facilities to locate close to each other or co-locate. Lüer-Villagra et al. (2022) extended on this model by considering decisions made by a leader who has knowledge about a follower who enters the market offering a different product. Méndez-Vogel et al. (2023) extended the follower problem from (Marianov et al. 2018) by introducing random utility customer choice rules.

Other research focuses on comparison shopping, where the products are substitutes and the customer visits multiple stores in a single trip before making a purchase (Marianov and Méndez-Vogel 2023; Méndez-Vogel et al. 2024). Such models assume that a customer may return to a previously visited location to conduct a purchase there. Comparison shopping is beyond the scope of this paper, which focuses strictly on shopping for non-competitive products.

3 Formulations

3.1 Continuous Single-Facility Multi-purpose Model

A single retail facility, such as a coffee shop, is located with the objective of attracting the maximum possible market share. Other competing coffee shops are present in the area. There is a proportion of customers who combine purchasing a product at this facility with a visit to multiple other facilities selling other products or services, such as groceries or gas. These other facilities do not compete with our chain or one another because they sell complementary products. They are often located close together and create retail-rich areas. Drezner et al. (2023a) refer to these facilities as "clusters" to indicate locations with multiple types of facilities such as plazas or shopping malls. In this paper we use the term "non-competing facilities (NCFs)" and their types can be grocery stores, gas stations, etc. Note that multiple NCFs of each type can be located in the area.

Consider an area with n demand points, each with a buying power b_i for $i = 1, 2, \ldots, n$, dedicated to our product. During a single trip, a customer residing at a demand point i chooses to visit up to q NCFs of different types (one per each type) in addition to visiting a coffee shop (either our chain's or the competitors'). The total distance is established as a tour (e.g., the shortest) between the demand point i and the facilities visited during the multi-purpose trip.

Let:

- n be the number of demand points
- b_i be the buying power dedicated to our product

- $\hat{p}$ be the number of competing facilities
- q be the number of types of NCFs visited in a single multi-purpose trip
- $p_1, p_2, \ldots, p_q$ be the number of NCFs of each type
- A be the attractiveness level of the new facility
- X be the location of the new facility
- $\hat{X}_j$ for $j = 1, 2, \ldots, \hat{p}$ be the locations of competing facilities
- $\hat{A}_j$ for $j = 1, 2, \ldots, \hat{p}$ be the attractiveness levels of competing facilities
- $Y_{k,m}$ for $k = 1, 2, \ldots, q$ and $m = 1, 2, \ldots, p_q$ be the locations of NCFs of type k
- $A'_{k,m}$ for $k = 1, 2, \ldots, q$ and $m = 1, 2, \ldots, p_q$ be the attractiveness levels of NCFs of type k
- $d(X, Y)$ be the distance between facilities X and Y
- $d_i(X)$ be the distance from the demand point i to facility X
- $h_i(\{X, Y, \ldots\})$ be a tour among the demand point i and points $X, Y, \ldots$ (for the shortest tour and symmetric distances, $h_i(\{X\}) = 2d_i(X)$ and $h_i(\{X, Y\}) = d_i(X) + d(X, Y) + d_i(Y)$, but the shortest tour algorithm has to be used for more intermediate points (Miklas-Kalczynska and Kalczynski 2021).

The objective function of the original competitive facility location gravity model (i.e., relative increase in market share captured by our chain's facility) can be written with this notation as a "1P trip", i.e., a trip to our or competitor's facility without visiting any cluster facilities:

$$M_0(X) = \sum_{i=1}^{n} b_i \frac{Af(h_i(\{X\}))}{Af(h_i(\{X\})) + \sum_{j=1}^{\hat{p}} \hat{A}_j f(h_i(\{\hat{X}_j\}))}. \tag{1}$$

In addition, the second summand of the denominator does not depend on X and can be represented as a vector of n scalars:

$$\hat{V}_i = \sum_{j=1}^{\hat{p}} \hat{A}_j f(h_i(\{\hat{X}_j\})). \tag{2}$$

This leads to a simplified version of (1):

$$M_0(X) = \sum_{i=1}^{n} b_i \frac{Af(h_i(\{X\}))}{Af(h_i(\{X\})) + \hat{V}_i}. \tag{3}$$

Let $\mathbb{S}$ be the superset of all **non-empty** subsets of q NCF type indices $\{1, 2, \ldots, q\}$. There are $2^q - 1$ such sets in the superset $\mathbb{S}$. For example, if $q = 3$, then $\mathbb{S} = \{\{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}\}$.

Denote by S an element of $\mathbb{S}$. For each $S \in \mathbb{S}$, we define a corresponding Cartesian of NCF indices in the following manner: $C_S = \{1, 2, \ldots, p_1\} \times \{1, 2, \ldots, p_2\} \times \cdots \times \{1, 2, \ldots, p_q\}$ (this is for the largest subset). Because we use a Cartesian, we need to fix the order of all sets in $\mathbb{S}$.

We allow indexing the sets of NCF locations and their attractiveness levels with sets of indices. All index sets must have equal sizes and corresponding ordering.

Such indexing results in a subset of elements of the same size as the indexing sets. Therefore, $Y_{\{2,3\},\{6,7\}} = \{Y_{2,6}, Y_{3,7}\}$.

For each subset $S \in \mathbb{S}$, the market share captured by facility X in an "MP trip", in which q NCFs of different types are visited in addition to one of the competing facilities, is:

$$M_S(X) = \sum_{i=1}^{n} b_i \frac{A \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X\} \cup Y_{S,C}))}{A \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X\} \cup Y_{S,C})) + \sum_{j=1}^{\hat{p}} \hat{A}_j \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{\hat{X}_j\} \cup Y_{S,C}))}. \quad (4)$$

The second summand in the denominator does not depend on X, so it can be represented as a vector of n scalars:

$$\hat{W}_i = \sum_{j=1}^{\hat{p}} \hat{A}_j \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{\hat{X}_j\} \cup Y_{S,C})). \quad (5)$$

Incorporating (5) in (4) results in a simplified formula:

$$M_S(X) = \sum_{i=1}^{n} b_i \frac{A \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X\} \cup Y_{S,C}))}{A \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X\} \cup Y_{S,C})) + \hat{W}_i}. \quad (6)$$

Suppose that π_S is the proportion of MP trips made to the subset S of NCF type indices. Then, the total market share attracted by the new facility X is:

$$M(X) = (1 - \sum_{S \in \mathbb{S}} \pi_S) M_0(X) + \sum_{S \in \mathbb{S}} \pi_S M_S(X), \quad (7)$$

where $0 \le \sum_{S \in \mathbb{S}} \pi_S \le 1$ and $0 \le \pi_S \le 1$ for $S \in \mathbb{S}$.

Note that in the 3P model, not all trips are three-purpose (and the same is true for any MP model). Instead, the model also includes some proportion of 1P trips, as well as two different options of 2P trips because there are two types of NCFs a customer can choose from. Assigning proportions to those different options of 2P trips is not straightforward. One can assume an equal split or consider various combinations of these proportions. We expand on this issue in Section 5.

When $q = 1$, $\mathbb{S} = \{\{1\}\}$, $C_S = \{\{1\}, \{2\}, \ldots, \{p_1\}\}$ and Eq. (7) reduces to the 2P model presented by Drezner et al. (2023a). When $q = 0$, Eq. (7) reduces to the 1P competitive location model, i.e., Eq. (1).

3.2 Continuous Multi-facility Multi-purpose Model

We now provide an MP extension of the 2P model by Kalczynski et al. (2024). Our model increases the number of purposes beyond just two, while locating multiple chain facilities.

Consider locating p facilities, each offering the same product, with the objective of maximizing the market share captured by our chain. A customer residing at a demand point i, in addition to visiting one of our chain's facilities X_j (or a competing one), may choose to visit up to q NCFs of different types during a single trip. We assume that only one facility of each type can be visited during the same MP trip.

Let:

- p be the number of our chain's new facilities to locate,
- X_j be the location of the j^{th} new facility, $j = 1, \ldots, p$,
- $\mathbf{X} = \{X_j, j = 1, \ldots, p\}$ be the vector of facility locations,
- A_j be the attractiveness level of the jth new facility, $j = 1, \ldots, p$.

Incorporating (2) and (5), we rewrite (1), (4), and (7) as:

$$M'_0(\mathbf{X}) = \sum_{i=1}^{n} b_i \frac{\sum_{j=1}^{p} A_j f(h_i(\{X_j\}))}{\sum_{j=1}^{p} A_j f(h_i(\{X_j\})) + \hat{V}_i}, \tag{8}$$

$$M'_S(\mathbf{X}) = \sum_{i=1}^{n} b_i \frac{\sum_{j=1}^{p} A_j \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X_j\} \cup Y_{S,C}))}{\sum_{j=1}^{p} A_j \sum_{C \in C_S} (\prod A'_{S,C}) f(h_i(\{X_j\} \cup Y_{S,C})) + \hat{W}_i}, \tag{9}$$

and

$$M'(\mathbf{X}) = (1 - \sum_{S \in \mathbb{S}} \pi_S) M_0(\mathbf{X}) + \sum_{S \in \mathbb{S}} \pi_S M'_S(\mathbf{X}) \tag{10}$$

When increasing the number of our chain facilities, we need to consider that some level of cannibalization of the market share will occur because of the fact that these facilities compete for a fixed demand. However, the market share gains resulting from establishing better locations should help reduce losses due to cannibalization (Plastria 2005; Drezner et al. 2011; Drezner and Eiselt 2024).

3.3 Solution Techniques

The continuous problem is non-linear and non-convex. Figure 1 demonstrates the market share solution surfaces for 1P, 2P, 3P and 4P single-facility models with 100 demand points. The graphs show that for each type of problem, there are relatively few local maxima. Moreover, the surface areas are rather smooth. However, the complexity of the first derivative of the objective function poses a serious issue for existing non-linear gradient-based solvers. In addition, the only constraints in the model are basic boxing constraints on the variables, so classical techniques, such as the Lagrangian relaxation (O'Kelly 1987), would not result in a simpler problem. Based on these observations, we chose to use SNOPT (Gill et al. 2005) as the solution technique, which is a local solver with multi-start that does not guarantee optimality. SNOPT's unique way of handling non-linear constraints separately from the linear ones, as well as its ability to efficiently approximate the first derivatives, makes it suitable for our problem.

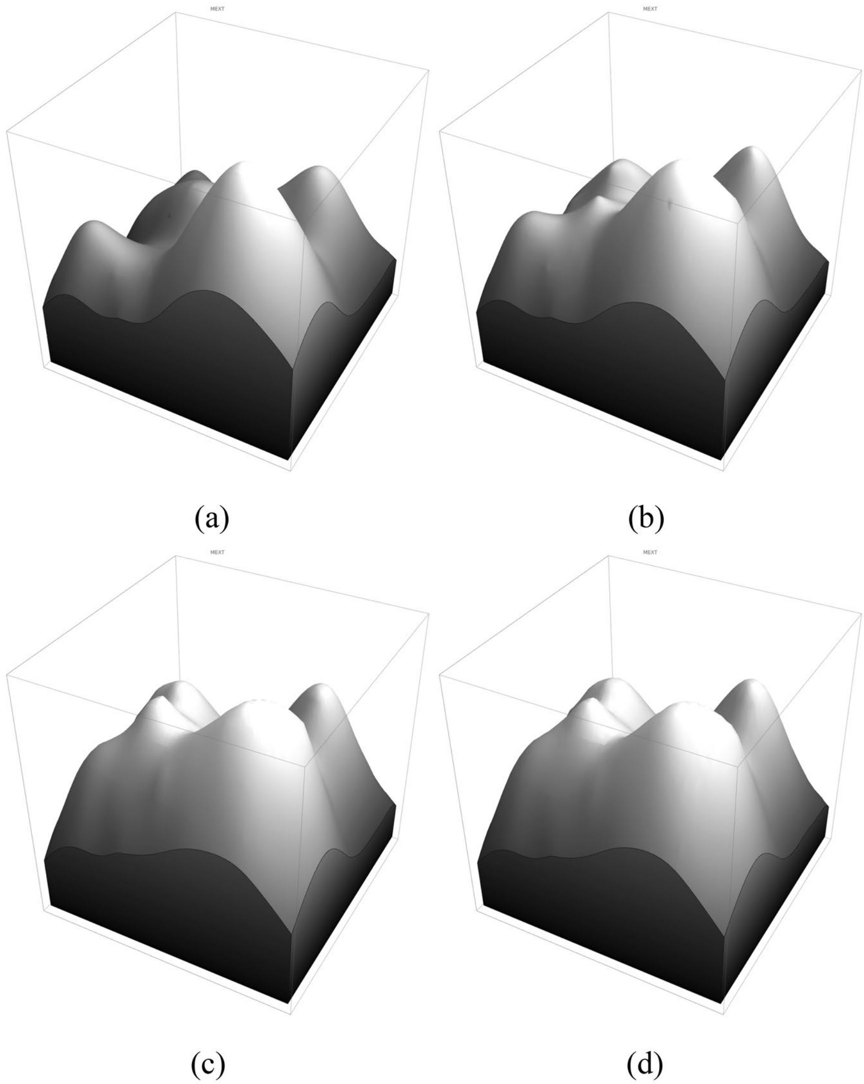

Fig. 1 Solution surfaces for a single-facility problem with $n = 100$; **a** 1P, **b** 2P, **c** 3P, **d** 4P

4 Computational Experiments

In this section, we first discuss valid comparison criteria for the models. Next, we present the results of the computational experiments and compare the models using the introduced criteria.

4.1 Comparison Criteria

It is expected that an MP model will allow the chain to capture more market share than a traditional 1P model, provided that the proportions of MP trips are estimated correctly. Note that in order to make valid comparisons between the 1P and the MP models, it is not sufficient to compare the optimal values of their objective function. Instead, the optimal *locations* obtained by the 1P model need to be applied to the MP objective.

In our model, an MP *instance* comprises a set of demand points with corresponding weights, locations of competing facilities, locations and types of NCFs, all attractiveness levels, and the proportions of MP trips. For example, a single instance may include two types of NCFs (grocery stores and gas stations), and four coffee shops that compete with our chain's coffee shop.

When using the 1P model's optimal locations to calculate the market share captured by the MP model on a given MP instance, the market share computed for the 1P locations will be no greater than the market share captured by the optimal solution to the MP model on that instance. This is because when the value of the objective function of a maximization problem is calculated for feasible arguments, it cannot be greater that the optimal objective value for this problem.

Note that in practice, even if only one proportion of MP trips is positive, the probability of obtaining an optimal solution to the MP instance using the optimal locations from the 1P model is virtually zero. We illustrate this in the *Discussion* section.

In our comparison criteria above, we consider comparing an MP model to the 1P model, which means that there is no need to transform NCF types and proportions when applying Eq. (10) to 1P locations. Before conducting the comparisons between two MP models, we must first formally define an MP model. Recall that q denotes the number of NCF types. A multi-purpose model is a $(q+1)$-purpose model if, and only if, each NCF type is visited in at least one trip. Otherwise, the ignored NCF type or types must be eliminated, and the model becomes a lower-purpose model. Formally, in a $(q+1)$-purpose model: $\bigcup_{S\in\mathbb{S}:\pi_S>0} = \{1, 2, \dots, q\}$.

Let q_1 and q_0 denote the numbers of types of NCFs for two models to be compared, such that $q_1 > q_0$, and the model with q_0 NCF types is the *baseline*.

The above comparison criteria can be extended by comparing two different MP models. The market share captured by a model with lower number of NCF types (q_0) will be no greater than the market share captured by a model with more NCF types (q_1), when using the instance of the higher-purpose model.

Comparing any $q_1 > 0$ (MP) model to a baseline model with $q_0 = 0$ (1P) only requires the locations determined by the 1P model. No transformations of proportions are necessary.

Let us now consider comparing an MP model with $q_1 > 1$ NCF types to the 2P model ($q_0 = 1$). The total number of NCFs ($p_1 + p_2 + \cdots + p_{q_1}$), their locations from the MP model, all attractiveness levels, as well as the proportion of 1P trips $(1-\pi)$ enter the 2P model unchanged. However, to ensure a fair comparison, the proportions of all MP trips in the MP model must add up to the proportion of 2P trips in the 2P model, i.e., $\pi = \sum_{S\in\mathbb{S}_{q_1}} \pi_S$.

Finally, let us consider comparing an MP model with q_1 NCF types to another MP model with q_0 NCF types, where $1 < q_0 < q_1$, i.e, using a 3P or higher purpose model as a baseline. Again, the total number and locations of NCFs will not change, although $q_1 - q_0$ types of NCFs will not be distinguished in the baseline model. The proportion of 1P trips in the models with q_1 and q_0 NCF types will be the same and equal to $1 - \sum_{S \in \mathbb{S}_{q_1}} \pi_S$. However, without additional information about the market with q_0 NCF types there is no way of determining either the assignment of NCFs to types or the proportions involving trips to q_0 NCF types, except when the proportion of trips to all q_1 NCF types is exactly 100%. In other words, although viable for $q_0 = 0$ or $q_0 = 1$, it is impossible to "reduce" the model with q_1 NCF types to the model with $q_0 > 1$ NCF types based solely on the information about the higher-purpose model, unless all higher-purpose trips include stops at all NCF types.

For example, when comparing a 4P model ($q_1 = 3$) to a 3P model ($q_0 = 2$), with $p_1 + p_2 + p_3$ NCFs, the following are the possible alternatives of MP trips (involving also a visit to a facility):

- one 4P trip to all NCF types,
- three options of 3P trips to each possible pair of NCF types,
- and three options of 2P trips to each of the NCF types.

When comparing with a 3P model, the number of NCFs remains the same ($p_1 + p_2 + p_3$), however we only consider two types ($q_0 = 2$). As a result, the possible alternatives of the MP trips are as follows:

- one 3P trip to all new NCF types,
- two options of 2P trips to each of the new NCF types.

The proportion of 1P trips for both the 4P and 3P models is the same: $(1 - \sum_{S \in \mathbb{S}_{q_1}} \pi_S)$, but in order to conduct the comparisons, we need to know the new NCF type assignment and the new proportions of the 2P and 3P trips in the 3P model, unless the proportion of 4P trips is exactly 100% and it will be used as the proportion of 3P trips in the 3P model.

Note that for the same reason we cannot compare 2P models with 1P models on the 3P instance. The instance used to compare the models must match the model with q_1 NCF types, and each of these types must be visited by customers.

Based on the discussion above, in the following section we compare a 3P model to a 1P model on multiple instances of different sizes using proportions based on the National Household Transportation Survey (Federal Highway Administration 2017). More detailed comparisons involving comparing our 3P model to 2P and 1P for multiple combinations of proportions of MP trips are presented in the Section 5.

4.2 Comparison Results

The experiments were conducted on instances incorporating 100 to 5,000 demand points and up to 15 facilities. They were run on virtualized Linux Ubuntu 20.04

LTS with 32 vCPUs and 384GB of vRAM. We used a VxRail V570F as a physical server, with Intel Xeon Gold 6248 @ 2.5GHz (2 125 socket, 20 cores per processor, 80 logical processors), 748GB RAM, and VMware vSAN storage. Although SNOPT does not support parallelization, available technology was utilized to run multiple instances of the solver simultaneously.

The instances were generated randomly, with the use of a pseudo-random number generator proposed by Law and Kelton (1991). All instances utilized in this paper are available at https://osf.io/n53rt/. We employed the exponential decay model with $\lambda = 1$, and we assumed all attractiveness levels to be the same (equal to 1) throughout. Utilizing the results from Federal Highway Administration (2017), we assumed the proportions of trips as follows: 75% of 1P, 20% of 2P, and 5% of 3P trips. The 2P component of the 3P model was split evenly between the two trip options, with 10% each.

The SNOPT solver with 100 random starts was used for each instance. Table 2 shows total run times in hours for the instances with different numbers of demand points and chain facilities being located. As expected, the run times increase significantly when more demand points and more facilities are added. It took nearly 4900 h of CPU time (combined for all CPUs used) to obtain these results (117 h on average for a combination of n and p). The range of processing times to find the best solution out of 100 starts was from 5.5 min to nearly 1700 h. The experiments were run in parallel on 24 CPUs, so the "wall clock" times were only about 4.2% of those reported. Also, SNOPT was run each time with 100 random starts. However, the post-hoc analysis showed that the average number of random starts needed to obtain the best-known solution was 5.09, with the maximum of 26.

Figure 2 shows a sample 3P model instance with $n = 100$ demand points, $\hat{p} = 10$ competing facilities, and two NCF types with $p_1 = p_2 = 10$ facilities each. Gray circles represent the demand points, empty circles represent competing facilities, while triangles and squares represent two different NCF types, each with ten locations. The weight of each demand point is represented by the size of the corresponding gray circle.

Table 3 shows the results of the comparisons of the 3P model to the 1P model for the instances of up to 5000 demand points and up to 15 new facilities. Even though the assumed proportions of MP trips were relatively small (5% of 3P trips and 10% of each option of 2P trips), the results show increases in the market shares captured by the chain when locating facilities according to the 3P model.

Table 2 Total run times (for all CPUs) in hours for the 3P model with $\pi_1 = \pi_2 = 0.1$ and $\pi_3 = 0.05$

	p						
n	1	2	3	4	5	10	15
100	0.09	0.27	0.60	1.41	1.80	9.30	39.96
200	0.08	0.74	1.62	2.23	4.48	24.15	65.15
500	0.42	2.11	3.63	9.40	18.50	80.43	203.26
1000	1.19	2.00	4.35	9.11	25.71	145.18	395.18
2000	0.90	4.20	10.11	23.70	45.22	251.40	798.31
5000	2.31	10.18	45.15	96.60	127.17	750.40	1668.34

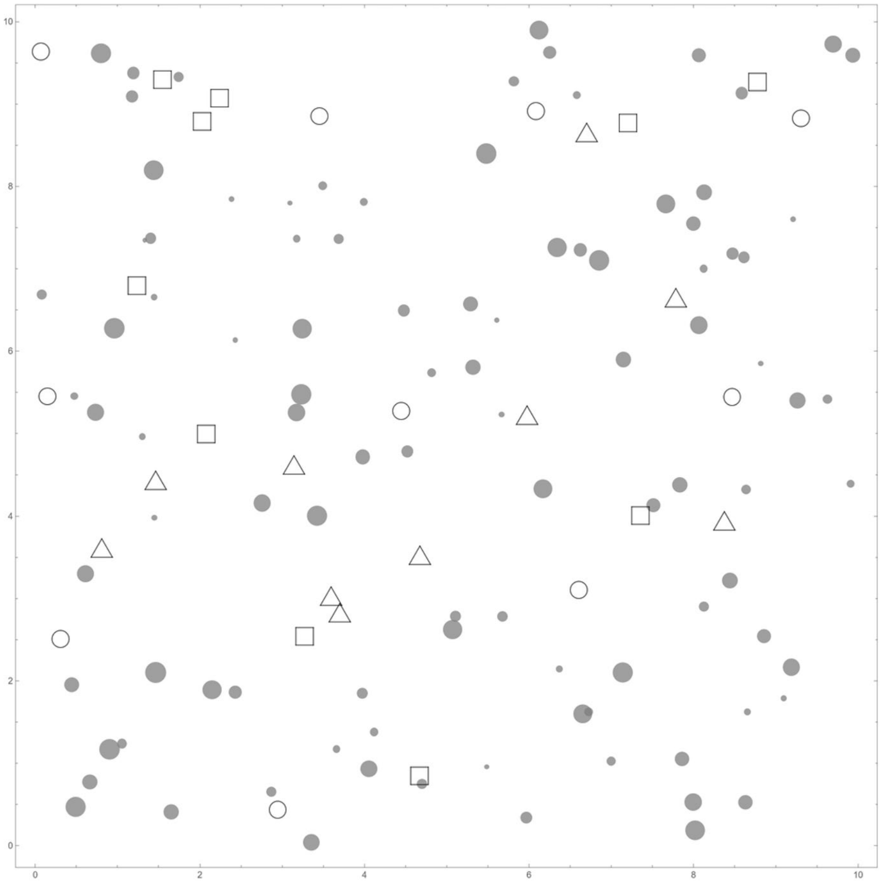

Fig. 2 3P instance with $n = 100$ demand points, $\hat{p} = 10$ competing facilities, $q = 2$ NCF types, and $p_1 = p_2 = 10$ facilities belonging to one of the two NCF types

Initially, as the number of chain facilities raises, the increases become more prominent. They peak generally between 3 to 5 added facilities, depending on the number of demand points. At some point however, growing number of added facilities starts to produce lesser effects. One explanation may be that increased density of chain locations can cannibalize part of the market share. The market share increases from the 3P model for the assumed proportions of MP trips are modest. The maximum relative improvement is 3.93% for $n = 200$ and $p = 4$. For $n = 100$, the maximum improvement is 3.23% for $p = 3$. In the Section 5 below, we will show that, for a different set of proportions, the improvements are much higher, up to 180.8% for $n = 100$.

Table 3 Market shares and relative improvements of the 3P model with $\pi_1 = \pi_2 = 0.1$ and $\pi_3 = 0.05$ over the 1P model for various combinations of the numbers of the demand points and the facilities located

$n = 100$				$n = 200$				$n = 500$			
p	1P	3P	3P/1P	p	1P	3P	3P/1P	p	1P	3P	3P/1P
1	0.1335	0.1337	0.17%	1	0.1283	0.1288	0.38%	1	0.1343	0.1365	1.69%
2	0.2353	0.2355	0.08%	2	0.2243	0.2326	3.70%	2	0.2360	0.2450	3.83%
3	0.3203	0.3307	3.23%	3	0.3244	0.3289	1.39%	3	0.3229	0.3308	2.46%
4	0.4082	0.4108	0.65%	4	0.3804	0.3954	3.93%	4	0.3909	0.3995	2.21%
5	0.4571	0.4634	1.39%	5	0.4391	0.4443	1.19%	5	0.4393	0.4486	2.12%
10	0.6492	0.6518	0.41%	10	0.6157	0.6244	1.41%	10	0.6053	0.6163	1.82%
15	0.7434	0.7456	0.30%	15	0.7107	0.7152	0.63%	15	0.7031	0.7088	0.81%
$n = 1000$				$n = 2000$				$n = 5000$			
p	1P	3P	3P/1P	p	1P	3P	3P/1P	p	1P	3P	3P/1P
1	0.1301	0.1321	1.59%	1	0.1263	0.1295	2.59%	1	0.1201	0.1235	2.77%
2	0.2344	0.2394	2.13%	2	0.2364	0.2411	1.98%	2	0.2270	0.2338	3.00%
3	0.3062	0.3163	3.29%	3	0.3128	0.3201	2.35%	3	0.3015	0.3093	2.56%
4	0.3805	0.3902	2.53%	4	0.3803	0.3893	2.38%	4	0.3660	0.3792	3.62%
5	0.4260	0.4385	2.93%	5	0.4241	0.4390	3.51%	5	0.4124	0.4285	3.89%
10	0.5988	0.6064	1.26%	10	0.6015	0.6084	1.15%	10	0.5923	0.5999	1.28%
15	0.6953	0.7008	0.79%	15	0.6996	0.7034	0.54%	15	0.6922	0.6988	0.96%

5 Discussion

Table 4 presents the results of the comparisons between the 1P, 2P and 3P models conducted on the instance displayed in Fig. 2. The solutions used to calculate each MP model market share were the best-known solutions to the model instances with 100% trips being MP. According to Drezner et al. (2023a), when 2P trips are considered, market share sometimes more than doubles compared to the 1P model. For our instances, the improvement reaches 178.99%. A similar pattern is observed for the 3P model, which improves the 1P model result for a single facility by 180.8%. The improvements become less prominent as the number of facilities increases. Although the single-facility 3P model is only slightly better than the 2P model, the improvements are more prominent when more facilities are added. When locating four facilities, the 3P model improves the 2P model by 17.46%. It took nearly 99 h of CPU time to obtain all these results (14 hrs average for each p). The range of processing times to find the best solution out of 100 random starts was from 8 min for $p = 1$ to 66 h for $p = 15$.

An extension of Table 4 containing the comparisons for different combinations of proportions and for multiple facilities ($p = 2$, $p = 3$, $p = 4$ and $p = 5$) is provided in the Appendix. Following Drezner et al. (2023a) and Kalczynski et al. (2024), we used 0.2 increments of the proportions of MP trips. While there are only

Table 4 Model comparisons for n=100 demand points assuming 100% MP trips in the 2P and 3P models

	n = 100, 3P obj. based on			Relative impr. in obj.		
p	1P	2P	3P	2P/1P	3P/1P	3P/2P
1	0.0934	0.2606	0.2623	178.99%	180.83%	0.66%
2	0.1938	0.4064	0.4110	109.69%	112.04%	1.12%
3	0.2784	0.5187	0.5367	86.32%	92.79%	3.48%
4	0.3993	0.5474	0.6430	37.10%	61.03%	17.46%
5	0.4121	0.6543	0.6810	58.77%	65.26%	4.09%
10	0.6404	0.7264	0.8086	13.43%	26.27%	11.32%
15	0.6970	0.8064	0.8633	15.70%	23.86%	7.06%

6 proportions to consider in the 2P model (0, 0.2, 0.4, 0.6, 0.8, 1), for the 3P model there are 56 combinations of proportions. Only 45 of them, however, are valid. 11 combinations, such that $\{\pi_1 \geq 0, \pi_2 = 0, \pi_3 = 0\}$ or $\{\pi_1 = 0, \pi_2 \geq 0, \pi_3 = 0\}$, were removed for the reasons mentioned in Section 4. The results of these extensive experiments show the maximum improvement of the 3P model over the 1P model of 180.83%, 112.04%, 92.79%, 64.23%, and 65.26% for $p = 1, 2, 3, 4$, and 5 respectively. The maximum improvements of the 3P model over the 2P model were 15.6%, 16.24%, 26.49%, 25.27%, and 20.93% for the same values of p. It took nearly 645 h of CPU time (2 hrs per instance on the average) to get these results with times to find the best solution out of 100 random starts ranging from 2.5 min for $p = 1$ up to 64.5 h for $p = 5$.

Our results suggest that higher-purpose models provide more value for multi-facility problems, but cannibalization effects diminish these returns for larger numbers of facilities. Also, the additional increase in the objective value from the 3P model is much smaller than the one from the 2P model. In particular, based on Table 4 and its extension in the Appendix, the improvements of the 3P model over the 2P model did not exceed 30%, compared to over 180% improvements gained by the 2P model over the 1P model. Based on Table 5, the average improvement from the 2P model was 42.99% and the average additional improvement from the 3P model was only 6.87%. What is more, Figs. 3 and 4 show that the changes of locations of facilities for different proportions of MP trips are relatively small. We, therefore, believe that this trend of diminishing returns from additional purposes will continue and - given that trips with four purposes and more are very rare (see Table 1) - the 3P model is sufficient for most practical applications.

We used the best-known solutions from Table 5 to check whether visiting the nearest facility first or last would change the results (O'Kelly and Miller 1984), but in all cases, the shortest tour obtained by the traveling salesman algorithm had the nearest facility as either the first or the last. However, a test on 1 million randomly generated 3P trips revealed that the two strategies are consistent only 90.03% of the time. It appears that the differences between these two approaches do not affect the multip-urpose model.

Figure 3 shows the locations of the solutions to the single-facility 1P, 2P and 3P models for different sets of proportions of MP trips on the instance from Section 4. Two areas of the image are magnified and several notable 3P locations, which yielded the largest increase in market share captured over 2P and 1P models, are labeled. The notation 3P:$\pi_S = \{0, 0, 1\}$ denotes the 3P model with $\pi_1 = 0\%$ of 2P trips of the first type, $\pi_2 = 0\%$ of 2P trips of the second type, and $\pi_3 = 100\%$ of 3P trips. 2P:$\pi = 0.2$ denotes the 2P model with the proportion of 2P trips equal to 0.2. Consistent with the results obtained by Drezner et al. (2023a), at $\pi = 0.6$ the optimal location for the 2P model "jumps" and locates close to an NCF. The 2P

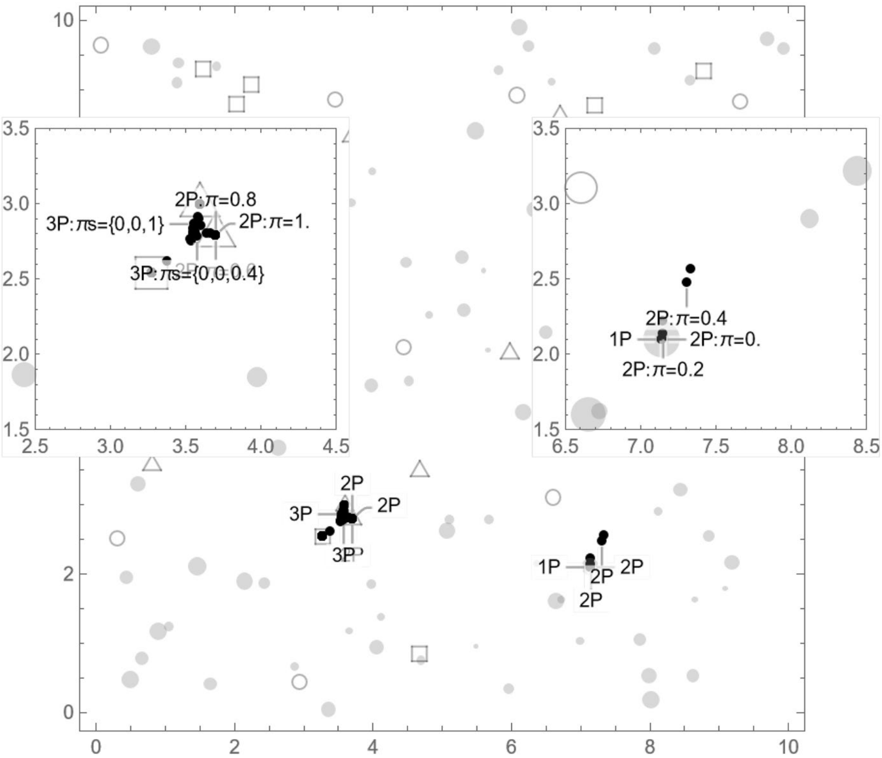

Fig. 3 Locations of the solutions to 1P, 2P, and 3P models on the instance presented in Fig. 2 with different proportions of MP trips and $p = 1$

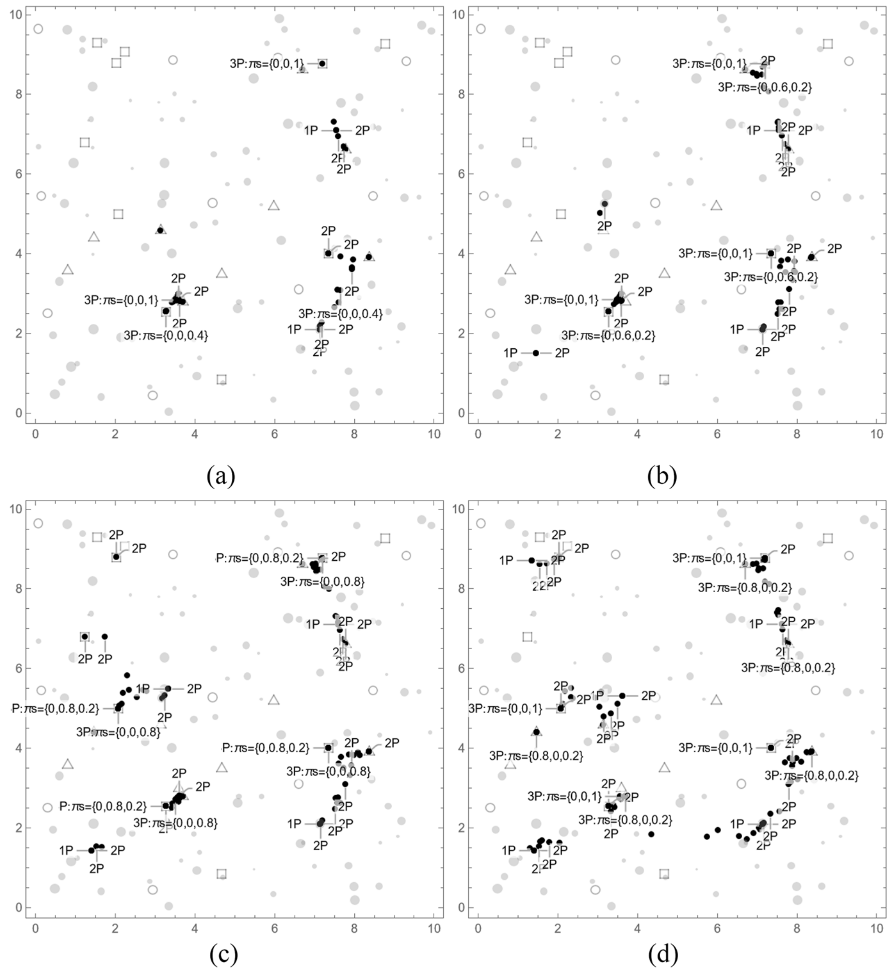

Fig. 4 Locations of solutions to 1P, 2P, 3P models for **a** $p = 2$, **b** $p = 3$, **c** $p = 4$, **d** $p = 5$, and multiple proportions

model location remains in that vicinity as π increases to 1 (100% of MP trips). The 3P model with 100% 3P trips is also located in that area. Figure 3 does not show evidence of significant re-locations or shifts. The relative proximity of the locations resulting from different models suggests the existence of certain "core" locations, which is consistent with earlier findings (Drezner et al. 2023a) and may help with determining efficient heuristic solutions to the problem.

6 Conclusions

Proximity to non-competing facilities (NCFs) offering products in different retail categories, can influence the customer's decision whether or not to patronize our chain's facility.

While earlier work in the area of competitive facility location studies multi-purpose shopping, the number of stops various authors considered did not go beyond two. In this paper, we look to locate chain facilities in a competitive scenario, while introducing the possibility of more than two stops made by customers shopping for complementary goods. We formulate both single- and multi-facility, multi-purpose continuous location models, assuming certain proportions of single-purpose and multi-purpose trips. In addition, we provide an appropriate method for comparing the models and we demonstrate that MP models with more stops will capture at least as much market share as models with fewer stops.

The results of our experiments show that expanding the 2P model to 3P produces substantial improvements (up to 26.5%) for some combinations of proportions of MP trips when multiple facilities are being located. However, when too many facilities are added, the gains from using a 3P model diminish. Also, it appears that expanding the model beyond three purposes may not be justifiable from a practical standpoint. A mix of 1P, 2P, and 3P trips in the 3P model seems to reflect reality adequately.

Our MP model requires establishing proportions for trips with different numbers of stops, including proportions for various combinations of stops in the case of all lower-purpose trips. One future research avenue might focus on incorporating approximate proportions instead. Such a model would treat all or some of the proportions as variables with corresponding constraints, e.g., that they are within 5% of the assumed proportions.

Another future research avenue might consider shopping for substitute products and comparison-shopping (Marianov et al. 2020). A customer travels to multiple stores that sell substitute products before deciding on a purchase. In such models, a customer may return to a previously-visited facility during the same trip.

Appendix

Figure 4 shows the best-known locations of the solutions to 1P, 2P and 3P models for different numbers of added facilities ($p = 2$, $p = 3$, $p = 4$ and $p = 5$) and different combinations of proportions. The results show clustering of locations similar to that observed by Kalczynski et al. (2024) with only a few outliers. Only those 3P locations were annotated, for which the 3P model yielded the largest increases in market share over 1P and 2P.

Table 5 presents the comparisons of the relative market share improvements for different combinations of proportions and for different numbers of added facilities ($p = 2$, $p = 3$, $p = 4$ and $p = 5$). Each is the best result of SNOPT optimization with 100 random starts. They provide strong support for our conclusions.

Table 5 Comparisons for different combinations of proportions and different numbers of added facilities ($p = 2$, $p = 3$, $p = 4$ and $p = 5$), $n = 100$

{0., 0., 0.2}			{0.2, 0.2, 0.}			{0.2, 0., 0.2}			{0., 0.2, 0.2}			{0., 0., 0.4}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	0.16	0.08	1	1.19	0.04	1	7.96	6.23	1	5.82	4.13	1	18.05	15.60
2	0.21	0.54	2	2.87	3.70	2	6.70	6.53	2	12.62	15.29	2	14.72	16.24
3	3.91	0.51	3	7.75	0.78	3	11.44	1.21	3	13.51	3.43	3	16.02	2.71
4	0.75	0.41	4	2.02	1.61	4	3.42	3.09	4	6.20	3.34	4	7.13	4.39
5	2.08	1.68	5	3.63	2.38	5	6.48	4.15	5	7.46	6.41	5	9.83	7.66
{0.4, 0.2, 0.}			{0.4, 0., 0.2}			{0.2, 0.4, 0.}			{0.2, 0.2, 0.2}			{0.2, 0., 0.4}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	20.81	0.00	1	39.70	0.00	1	19.20	5.66	1	31.87	0.34	1	50.69	0.00
2	15.09	0.06	2	22.54	1.67	2	24.62	5.80	2	25.79	1.86	2	29.80	0.58
3	18.00	0.49	3	25.11	1.81	3	22.54	8.05	3	25.03	5.02	3	29.82	4.22
4	9.15	3.47	4	12.49	6.94	4	13.37	4.65	4	14.40	5.96	4	16.51	8.28
5	10.40	2.40	5	16.38	5.96	5	11.96	4.79	5	14.89	5.53	5	19.01	7.30
{0., 0.4, 0.2}			{0., 0.2, 0.4}			{0., 0., 0.6}			{0.6, 0.2, 0.}			{0.6, 0., 0.2}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	34.64	9.21	1	47.31	3.56	1	62.46	0.35	1	55.69	0.00	1	77.45	0.33
2	40.29	10.69	2	41.28	6.62	2	42.53	3.20	2	32.47	3.72	2	41.17	7.26
3	33.77	16.29	3	35.16	11.95	3	36.95	8.43	3	35.87	2.69	3	44.27	4.63
4	21.68	9.71	4	21.88	10.33	4	22.22	11.05	4	21.57	10.96	4	26.69	16.20

Table 5 (continued)

{0., 0.4, 0.2}			{0., 0.2, 0.4}			{0., 0., 0.6}			{0.6, 0.2, 0.}			{0.6, 0., 0.2}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
5	19.33	10.60	5	22.06	11.01	5	25.03	11.62	5	23.81	6.19	5	31.59	11.17
{0.4, 0.4, 0.}			{0.4, 0.2, 0.2}			{0.4, 0., 0.4}			{0.2, 0.6, 0.}			{0.2, 0.4, 0.2}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	47.68	0.63	1	67.60	0.02	1	89.64	0.23	1	50.86	9.36	1	64.67	3.93
2	38.71	1.13	2	41.32	0.16	2	50.13	3.59	2	54.31	4.61	2	55.13	2.41
3	36.92	6.57	3	41.41	5.33	3	49.13	6.61	3	46.85	18.00	3	48.15	13.59
4	24.18	11.43	4	25.99	13.67	4	30.22	18.09	4	32.56	16.85	4	32.48	17.48
5	21.54	3.36	5	26.61	6.06	5	33.55	10.23	5	28.87	8.67	5	29.28	7.38
{0.2, 0.2, 0.4}			{0.2, 0., 0.6}			{0., 0.6, 0.2}			{0., 0.4, 0.4}			{0., 0.2, 0.6}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	80.49	0.44	1	102.21	0.21	1	67.77	12.25	1	82.04	6.85	1	96.86	2.49
2	55.93	0.38	2	61.50	1.51	2	72.10	5.64	2	72.68	3.53	2	73.24	1.58
3	49.86	9.99	3	54.41	8.79	3	59.86	26.49	3	60.99	21.58	3	62.10	17.21
4	32.57	18.22	4	34.35	20.46	4	42.20	23.83	4	41.88	24.32	4	41.57	24.79
5	31.35	7.49	5	36.38	9.98	5	37.62	13.33	5	38.03	11.99	5	39.76	11.75

Table 5 (continued)

{0., 0., 0.8}			{0.8, 0.2, 0.}			{0.8, 0., 0.2}			{0.6, 0.4, 0.}			{0.6, 0.2, 0.2}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	115.76	0.52	1	97.03	0.03	1	122.37	0.63	1	86.95	0.06	1	110.42	0.00
2	74.57	0.21	2	51.83	5.53	2	60.52	8.69	2	54.26	0.07	2	60.67	1.70
3	63.65	13.61	3	55.99	0.27	3	64.34	0.58	3	54.13	0.77	3	61.21	0.12
4	41.30	25.27	4	36.30	13.69	4	41.76	18.14	4	36.25	9.72	4	39.86	12.62
5	42.89	12.61	5	39.80	14.13	5	48.60	20.93	5	35.18	3.33	5	41.73	8.00
{0.6, 0., 0.4}			{0.4, 0.6, 0.}			{0.4, 0.4, 0.2}			{0.4, 0.2, 0.4}			{0.4, 0., 0.6}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	136.23	0.53	1	84.46	4.28	1	101.16	0.56	1	124.56	0.18	1	150.41	0.44
2	71.62	6.13	2	69.93	2.72	2	70.53	0.74	2	73.19	0.10	2	83.73	4.00
3	69.60	0.43	3	62.14	7.95	3	64.05	3.49	3	68.07	0.87	3	75.02	0.28
4	44.71	16.53	4	43.69	11.59	4	43.55	11.59	4	44.66	12.55	4	48.24	15.43
5	50.51	14.34	5	39.29	0.00	5	40.80	0.79	5	45.42	3.79	5	53.10	8.94
{0.2, 0.8, 0.}			{0.2, 0.6, 0.2}			{0.2, 0.4, 0.4}			{0.2, 0.2, 0.6}			{0.2, 0., 0.8}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	87.60	12.25	1	103.28	7.06	1	119.60	2.83	1	139.56	0.56	1	165.06	0.41
2	88.27	5.84	2	88.62	3.79	2	88.95	1.88	2	89.62	0.27	2	96.83	2.19
3	74.68	18.60	3	75.67	12.70	3	76.63	7.54	3	78.07	3.29	3	82.66	1.29

Table 5 (continued)

{0.2, 0.8, 0.}			{0.2, 0.6, 0.2}			{0.2, 0.4, 0.4}			{0.2, 0.2, 0.6}			{0.2, 0., 0.8}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
4	54.07	15.27	4	53.42	14.99	4	52.80	14.74	4	52.22	14.49	4	53.47	15.62
5	47.85	0.00	5	48.28	0.00	5	49.36	0.44	5	52.56	2.30	5	57.80	5.50
{0., 0.8, 0.2}			{0., 0.6, 0.4}			{0., 0.4, 0.6}			{0., 0.2, 0.8}			{0., 0., 1.}		
	Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.			Rel. % of Imp.	
p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P	p	3P/1P	3P/2P
1	106.28	14.68	1	122.51	9.54	1	139.43	5.30	1	157.06	1.75	1	180.83	0.66
2	108.64	6.71	2	108.67	4.74	2	108.71	2.90	2	108.74	1.18	2	112.04	1.12
3	88.85	23.37	3	89.66	17.28	3	90.45	11.94	3	91.22	7.23	3	92.79	3.48
4	64.23	18.56	4	63.30	18.22	4	62.42	17.90	4	61.59	17.59	4	61.03	17.46
5	56.99	0.00	5	57.43	0.00	5	58.30	0.27	5	61.53	2.03	5	65.26	4.09

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Declarations

Competing Interests The authors declare no competing interests.

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