An Interior Point Method for Multifacility Location Problems with Forbidden Regions

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Abstract

In this paper we consider generalizations of multifacility location problems in which as an additional constraint the new facilities are not allowed to be located in a prespecified region. We propose several different solution schemes for this non-convex optimization problem. These include a linear programming type approach, penalty approaches and barrier approaches. Moreover, structural results as well as illustrative examples showing the difficulties of this problem are presented.

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Introduction

In continuous multifacility location problems one has usually given a set of fixed facilities and is looking for locations of some new facilities. The quality of a set of new locations is evaluated by an objective function in which the exchange intensity between the new and the old facilities as well as between the new facilities is taken into account.

Many researchers have looked at this problem (see [28] for a recent survey and references therein) and a lot of results have been derived up to now.

However, when dealing with continuous location models as approximations to real-world problems, we have naturally the problem of taking geographically given settings into account. We may, for example, not be able to choose a specific location for a new facility because this location is in the middle of a lake, inside a protection area or because there is already a building.

This paper deals with an extension of classical multifacility problems: restricted multifacility problems, where forbidden regions in which no new facility can be placed have to be respected. For structural results on restricted single facility location problems as well as for efficient solution algorithms for specific distance measures (l_1,l_∞, l_2^2 and polyhedral gauges) the reader is referred to [14, 16, 23] and references therein.

In contrast to the single facility case only very specific instances of restricted multifacility location problems have been investigated up to now. In [24] a solution procedure for the two-facility case with a forbidden rectangle is discussed, while a linear programming approach for the ℓ_1-case is given in [15]. The aim of this paper is to provide general structural results as well as algorithms to find locally optimal solutions for a broad class of restricted multifacility location problems. Since our focus is on the theory of possible solution approaches, extensive numerical tests are beyond the scope of this paper and will be discussed in a forthcoming, more practically oriented article.

The rest of the paper is organized as follows. First we give a formal definition of the problem. Section 2 states fundamental properties of the problem and illustrates its difficulties. The next section discusses several possible approaches how forbidden regions can be included in optimization schemes and shows their drawbacks. Section 4 presents an alternative barrier approach which avoids a lot of these previously discussed drawbacks. The paper ends with some possible extensions and conclusions.

1 Formulation of the Problem

In what follows, we will denote by $\mathrm{int}(S)$, $\mathrm{cl}(S)$ and $\mathrm{bd}(S)$ the interior, the closure and the boundary of a given set S. Moreover, we will use the concept of gauges in the sense of Minkowski [20, pp. 131–135] to measure distances between pairs of points in $\mathbb{R}^d$. To be more specific, a *gauge* γ is defined by

$$\gamma(x) := \inf\{\lambda > 0 \mid x \in \lambda B\},$$

where $B \subset \mathbb{R}^d$ is a convex compact set with $0 \in \mathrm{int}(B)$, called the *unit ball* of γ. The distance between two points $x, y \in \mathbb{R}^d$ can now be computed by $\gamma(x - y)$. A

gauge is nonnegative, zero only at the origin, positively homogeneous, subadditive and in particular convex. Note that every norm is a gauge, but arbitrary gauges do not need to be symmetric. Therefore, gauges open up lots of possibilities to model nonsymmetric distances (see below).

Now let F be a nonempty, finite set of nodes, $\emptyset \neq E \subseteq F \times F$ and $G := (F, E)$ be a directed graph. The node set F represents a set of facilities, while the edge set E corresponds to interactions between these objects. If, for every facility $f \in F$, a *location* $x_f \in \mathbb{R}^d$ is known, one can calculate the total cost of these interactions by building the sum over all distances between locations for which the corresponding nodes are connected by an edge. Assume that the locations of some of the facilities are fixed in advance. The problem is to find locations for the other facilities such that the total cost of interactions is minimized. Moreover, it is quite natural to have different gauges to measure distances between different pairs of facilities. This leads to the following notation.

Let the node set F be partitioned into the nonempty sets A and V. For all $a \in A$ let a fixed vector $x_a \in \mathbb{R}^d$ be given, called the *known* or *old location* of the corresponding facility. The nodes $v \in V$ represent facilities for which the best location is still unknown. For every edge $e \in E$ let there be given a weight $\omega_e \neq 0$ and a gauge γ_e. The cost of the interaction between two nodes connected by an edge is measured by the corresponding gauge, while the weight serves as a proportionality factor. As it has already been done in the literature [27], we assume without loss of generality that G as well as the subgraph induced by G with node set V are connected. Otherwise, the problem decomposes into several independent ones, one for each connectivity component. Other assumptions which can be made without loss of generality can be found in [27, 7].

In this paper, we are mainly concerned with gauges γ_e derived from an affine-linear transformation and the subsequent use of an ℓ_p-norm. Gauges of this kind belong to the class of *skewed norms* introduced by Plastria [26]. More formally, for every edge $e \in E$ a matrix $\boldsymbol{B}_e \in \mathbb{R}^{d \times d}$ of full rank, a norm $\|\cdot\|_{p_e}$ with $p_e \in [1, \infty]$ and a vector $y_e \in \mathbb{R}^d$ with $\|\boldsymbol{B}_e^{-\top} y_e\|_{q_e} < 1$ should be given. Here, $\|\cdot\|_{q_e}$ denotes the dual norm to $\|\cdot\|_{p_e}$ with $1/p_e + 1/q_e = 1$. The gauge γ_e is then defined by

$$\gamma_e(x) := \|\boldsymbol{B}_e x\|_{p_e} + y_e^\top x.$$

Note that γ_e is differentiable for all $x \neq 0$ as long as $1 < p_e < \infty$. With gauges of this type, it is easy to cover applications like ships moving in a current, planes flying in a steady wind, or ground movement in an area with slopes [17].

The set of all families $X = (x_v)_{v \in V}$ with $x_v \in \mathbb{R}^d$ for all $v \in V$ will be denoted by $(\mathbb{R}^d)^V$. This set, equipped with the usual addition and scalar multiplication, is a real vectorspace. A location x_v for a node $v \in V$ is called *new location* of the corresponding facility.

Now, let in addition to the vectors $x_a \in \mathbb{R}^d$ $(a \in A)$ a family $(x_v)_{v \in V} \in (\mathbb{R}^d)^V$ be given. For any edge $e = (f, g) \in E$ set $x_e := x_f - x_g$.

As a last prerequisite before we state the problem, we have to describe how we model forbidden regions in this paper. Let $\boldsymbol{A} \in \mathbb{R}^n \times \mathbb{R}^d$ be a matrix and $b \in \mathbb{R}^n$ be a vector.

The *forbidden region* is then defined to be the set

$$\mathcal{R} := \{x \in \mathbb{R}^d \mid \boldsymbol{A}x < b\}. \tag{1}$$

Definition 1.1 (Multifacility Location Problem) *The* continuous minisum multifacility location problem with mixed gauges *is the following optimization problem:*

Find a minimum $(\hat{x}_v)_{v\in V} \in (\mathbb{R}^d)^V$ *of the function*

$$\begin{aligned} \Psi : (\mathbb{R}^d)^V &\longrightarrow \mathbb{R} \\ (x_v)_{v\in V} &\longmapsto \sum_{e\in E} \omega_e \gamma_e(x_e), \end{aligned} \tag{2}$$

with $(x_v)_{v\in V} \in \mathbb{R}^d$.

Definition 1.2 (Restricted Multifacility Location Problem) *The* restricted continuous minisum multifacility location problem with mixed gauges *is the following optimization problem:*

Find a minimum $(\hat{x}_v)_{v\in V} \in (\mathbb{R}^d)^V$ *of the function*

$$\begin{aligned} \Psi : (\mathbb{R}^d)^V &\longrightarrow \mathbb{R} \\ (x_v)_{v\in V} &\longmapsto \sum_{e\in E} \omega_e \gamma_e(x_e), \end{aligned} \tag{3}$$

subject to the constraints

$$x_v \notin \mathcal{R} \text{ for all } v \in V.$$

By "minimum" we mean not only global optima, but also arbitrary local minima. The set of feasible points for (3) is given by

$$\mathcal{F} := (\mathbb{R}^d \setminus \mathcal{R}) \times (\mathbb{R}^d \setminus \mathcal{R}) \times \cdots \times (\mathbb{R}^d \setminus \mathcal{R}) = (\mathbb{R}^d \setminus \mathcal{R})^V. \tag{4}$$

For $z \in \mathbb{R}$ define

$$z_+ := \max\{z, 0\}.$$

If f is a real-valued function, we will use the notation f_+ to denote the function defined by

$$f_+(x) := (f(x))_+ .$$

In what follows, we will also make use of the index set $I := \{1, \ldots, n\}$.

2 A Result about the Solution Set

The following result is a generalization of a theorem by Hamacher and Nickel [15], who considered only the single-facility case. The theorem below connects the unrestricted problem (2) with the restricted problem (3).

Theorem 2.1 *If there exists no solution of (2) which is also a solution of (3), then for every solution $(\hat{x}_v)_{v\in V}$ of (3) there exists at least one facility $w \in V$ such that the location $\hat{x}_w \in \mathbb{R}^d$ belongs to the boundary of $\mathcal{R}$.*

Proof: If every solution of (2) is not a solution of (3), it follows that for every solution $\hat{X} = (\hat{x}_v)_{v\in V} \in \mathcal{F}$ of (3) we have $\hat{X} \in \mathrm{bd}(\mathcal{F})$. This means that there exists a sequence $X_i = ((x_v^{(i)})_{v\in V})_{i\in\mathbb{N}}$ with $X_i \in (\mathbb{R}^d)^V \setminus \mathcal{F}$ for all $i \in \mathbb{N}$ and $\lim_{i\to\infty} x_v^{(i)} = \hat{x}_v$ for all $v \in V$. Therefore, for all $i \in \mathbb{N}$ there exists at least one $v_i \in V$ such that $x_{v_i}^{(i)} \in \mathcal{R}$. Because V is a finite set, we may choose an infinite subsequence $((x_v^{(i_j)})_{v\in V})_j$ with $w := v_{i_j}$ fixed. Then we have $x_w^{(i_j)} \in \mathcal{R}$ for all $j \in \mathbb{N}$ but $\lim_{j\to\infty} x_w^{(i_j)} = \hat{x}_w \notin \mathcal{R}$ and therefore $\hat{x}_w \in \mathrm{bd}(\mathcal{R})$. □

Remark 2.2 *The theorem above also holds if the costfunction Ψ is an arbitrary function and $\mathcal{R} \subseteq \mathbb{R}^d$ is an arbitrary set. Especially, it is allowed to use a finite union of forbidden regions.*

The following example shows that one can not expect to find all optimal new facility locations on the boundary of $\mathcal{R}$.

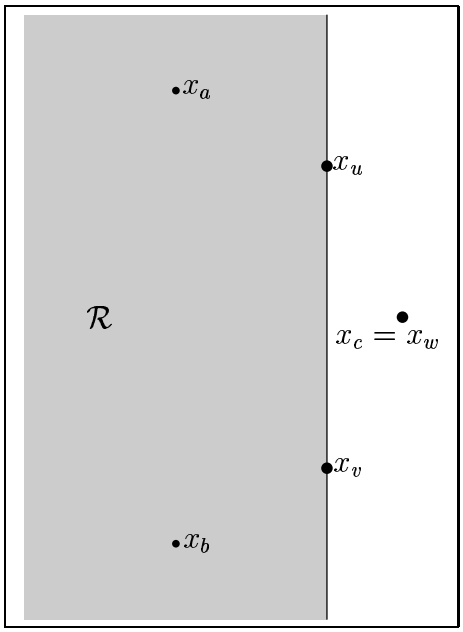

Figure 1: Illustration for Example 1. Not all locations of the optimal solution are on the boundary of $\mathcal{R}$.

Example 1 (based on [25]) *Let $d = 2$, $A = \{a, b, c\}$ and $V = \{u, v, w\}$. The coordinates of the given facilities are $x_a = (0, 3)^\top$, $x_b = (0, -3)^\top$ and $x_c = (3, 0)^\top$.*

All distances are measured with the Euclidean norm $\|\cdot\|_2$. *Let* $\omega_{(u,a)} = \omega_{(v,b)} = 2$, $\omega_{(w,c)} = \omega_{(u,w)} = \omega_{(v,w)} = 1$ *and all other weights be* 0. *The forbidden region is given by*

$$\mathcal{R} = \{x \in \mathbb{R}^2 \mid x_1 < 2\} .$$

The following table shows the optimal solutions for the unrestricted problem, the restricted problem and the best solution such that every new location is on the boundary of the forbidden region. All numbers are rounded to three decimal places.

type of problem	x_u	x_v	x_w	*obj. value*
unrestricted problem	$(0,2)^\top$	$(0,-2)^\top$	$(1.732,0)^\top$	8.196
restricted problem	$(2,2)^\top$	$(2,-2)^\top$	$(3,0)^\top$	13.416
best sol. on $\mathrm{bd}(\mathcal{R})$	$(2,1.845)^\top$	$(2,-1.845)^\top$	$(2,0)^\top$	13.928

We can see that the optimal solution for the restricted problem does not have all locations on the boundary of $\mathcal{R}$ *(cf. Figure 1). It should be noted that this counterexample works with all* ℓ_p*-norms.*

The last example in this section shows that we have to expect an exponential number of local or global optima.

Example 2 *Consider the following multifacility location problem on the real line: let* $d = 1$, $A = \{a\}$, $x_a = 0$, $E = V \times A$, $\omega_{(v,a)} = 1$ *for all* $v \in V$ *and define the forbidden region by* $\mathcal{R} =]-1,1[$. *With* $m = |V|$, *there are exactly* 2^m *different global optima, each one corresponding to a vertex of the* m*-dimensional hypercube* $[-1,1]^m$. *Small pertubations of* x_a *and* $\mathcal{R}$ *will lead to a problem with one global optimum and* $2^m - 1$ *local optima, the costfunction value of each of these differing from the optimal one by an arbitrary small amount.*

3 Getting Rid of the Forbidden Region

3.1 A Linear Programming Formulation

In this section we show how a solution method based on linear programming can be derived if we restrict ourselves to polyhedral gauges as distance measures, as it is the case with the classical ℓ_1- and ℓ_∞-norms. Although the main goal of this paper is to develop solution algorithms for the general situation, we have included this section because the following approach is easy to implement.

In the case of polyhedral gauges we have a convex polyhedron B_e as unit ball for a gauge γ_e ($e \in E$). The polar of B_e is denoted B_e^0 and the set of extreme points for B_e^0 is denoted $\mathrm{ext}(B_e^0)$. With this notation we can rewrite the unrestricted multifacility location problem in the case where all $\omega_e \geq 0$ as a linear program [29],

$$\text{minimize} \quad \sum_{e \in E} \omega_e z_e \tag{5}$$

$$\text{subject to} \quad x_e^\top b^e \leq z_e \;\; \forall\, e \in E,\; b^e \in \mathrm{ext}(B_e^0). \tag{6}$$

If we allow also $\omega_e < 0$ we have a d. c. problem instead of a linear program. For solution methods in this case see [18]. Now, denote the row vectors of the matrix $\boldsymbol{A}$ in definition (1) by a_i $(i \in I)$ and let Ω be the set of all $|V|$-tuples over I. Further, let $\Theta(k)$ denote the k-th component of a $|V|$-tuple $\Theta \in \Omega$. Then for any feasible solution $(x_v)_{v \in V}$ of the restricted multifacility problem (3) there exists a $\Theta \in \Omega$ such that the linear program (5)–(6) together with the constraints

$$x_v^\top a_{\Theta(v)} \geq b_{\Theta(v)} \quad \forall\, v \in V. \tag{7}$$

characterizes $(x_v)_{v \in V}$. The following algorithm is now straightforward.

1. For all $\Theta \in \Omega$ do

   Solve the linear program (5)–(6) with the corresponding additional set of constraints (7) for the actual Θ.

2. Output: the best solution found in Step 1.

As one easily recognizes, the time complexity of this algorithm is only polynomial if we fix the number of new facilities $|V|$. It should be noted that this approach is a generalization of the algorithm presented in [15]. Of course one may use sophisticated branch and bound procedures instead of a complete enumeration. However, this does not effect the worst case complexity.

3.2 A Penalty Approach

We have $\boldsymbol{A}x < b$ if and only if $\max_{i \in I}(a_i^\top x - b_i) < 0$. For a given $(x_v)_{v \in V} \in (\mathbb{R}^d)^V$, it follows that we have $\boldsymbol{A}x_v < b$ for at least one $v \in V$ if and only if

$$\min_{v \in V} \max_{i \in I}(a_i^\top x_v - b_i) < 0.$$

By defining

$$g_i(x) := ((b_i - a_i^\top x)_+)^2 \qquad (i \in I)$$

and

$$h(x) := \prod_{i \in I} g_i(x)$$

we get

$$p((x_v)_{v \in V}) := \sum_{v \in V} h(x_v),$$

a *regularized penalty function*. Here, we have $p(X) > 0$ if and only if $X \notin \mathcal{F}$ and $p(X) = 0$ if and only if $X \in \mathcal{F}$. It is also clear that p is continuously differentiable. The

same approach can be used if the forbidden region $\mathcal{R} \subseteq \mathbb{R}^d$ is defined as $\mathcal{R} := \{x \in \mathbb{R}^d \mid r(x) < 0\}$ with a differentiable function $r : \mathbb{R}^d \longrightarrow \mathbb{R}$.

Note that the objective function is not differentiable everywhere. This is a major hindrance, but it can be overcome by using, for example, a hyperboloid approximation [11, 10, 1] with parameter $\delta > 0$. If we denote the approximation of the objective function by Ψ_δ, we have $\Psi_\delta \in C^\infty$ [4, 19]. Note that this approach increases the ill-conditioning of the problem and slows down some optimization algorithms, such that certain safeguards and acceleration techniques should be employed [7, 8, 9]. By defining

$$\tilde{\Psi}_{\delta,\mu}(X) := \Psi_\delta(X) + \frac{1}{\mu} p(X),$$

we arrive at a sequence of parametrized unrestricted optimization problems with a differentiable objective function $\tilde{\Psi}_{\delta,\mu}$. A standard penalty approach then constructs a sequence of approximations to a local solution of (3). The approximation parameter $\delta > 0$ can also be changed in every iteration by choosing an appropriate sequence $(\delta_k)_{k \in \mathbb{N}}$ with $\delta_k > 0$ for all $k \in \mathbb{N}$ and $\lim_{k \to \infty} \delta_k = 0$. This leads to an even better approximation of the original problem.

However, it is well known that the unrestricted optimization problems derived above tend to get increasingly ill-conditioned when the parameter μ approaches 0. Up to now, this ill-conditioning can only be avoided under special assumptions [3]. Another possibility to overcome this hindrance consists in using notoriously robust (and notoriously slow) methods like Simulated Annealing. Such a method can also be used to generate a good feasible starting point near a global optimum for a nonlinear optimization method, which is able to find this optimum in a much more efficient way than the heuristic method.

3.3 Approximating the Forbidden Region

By defining the function

$$\varphi_\varepsilon(x) := -\sum_{i \in I} \left((a_i^\top x - b_i)_+ \right)^2 + \varepsilon,$$

which is differentiable in $\mathbb{R}^d$ for all $\varepsilon > 0$, we can use the functions

$$\varphi_{v,\varepsilon}((x_v)_{v \in V}) := \varphi_\varepsilon(x_v)$$

to describe outer approximations for the restrictions given by $\mathcal{R}$. If $\delta > 0$ is the parameter used to control the hyperbolic approximation of Ψ, we can opt for solving the problem

$$\begin{array}{rll} \text{minimize} & \Psi_\delta(X) & \\ \text{subject to} & \varphi_{v,\varepsilon}(X) \leq 0 & (v \in V). \end{array} \tag{8}$$

Since (8) contains the two parameters $\varepsilon > 0$ and $\delta > 0$, we will denote this problem $(P_{\delta,\varepsilon})$.

We will now show that the approach of this subsection may run into numerical difficulties when the parameter ε is reduced. For fixed $\delta > 0$ the point $(X^{(\varepsilon)}, (y_v^{(\varepsilon)})_{v\in V}) = ((x_v^{(\varepsilon)})_{v\in V}, (y_v^{(\varepsilon)})_{v\in V})$ is a Kuhn-Tucker point of $(P_{\delta,\varepsilon})$, if the following conditions hold:

$$\nabla_{x_w}\left(\Psi_\delta(X^{(\varepsilon)}) + \sum_{v\in V} y_v^{(\varepsilon)}\varphi_{v,\varepsilon}(X^{(\varepsilon)})\right) = 0 \qquad \forall\, w \in V, \tag{9}$$

$$\varphi_{w,\varepsilon}(X^{(\varepsilon)}) \le 0 \qquad \forall\, w \in V, \tag{10}$$

$$y_w^{(\varepsilon)} \ge 0 \qquad \forall\, w \in V, \tag{11}$$

$$\sum_{w\in V} y_w^{(\varepsilon)}\varphi_{w,\varepsilon}(X^{(\varepsilon)}) = 0. \tag{12}$$

It is easy to prove that

$$\nabla\varphi_\varepsilon(x_w^{(\varepsilon)}) = O(\sqrt{\varepsilon})$$

holds for those $x_w^{(\varepsilon)}$ with $\varphi_\varepsilon(x_w^{(\varepsilon)}) = 0$. Now let $(X^{(\varepsilon)})_\varepsilon$ have an accumulation point for $\varepsilon \searrow 0$. According to Theorem 2.1, the only interesting case to consider is the one in which no unrestricted minimum is a solution to the restricted problem. Then (9) shows that

$$y_w^{(\varepsilon)}\sqrt{\varepsilon} \not\longrightarrow 0$$

holds for at least one $w \in V$ if $\varepsilon \searrow 0$. Therefore, at least one Lagrange multiplier tends to infinity when working with φ_ε. This is usually an indication for ill-posed problems.

Note that for a Kuhn-Tucker point $(X^{(\varepsilon)}, (y_v^{(\varepsilon)})_{v\in V})$ the family $X^{(\varepsilon)}$ is not necessarily a local optimum of $(P_{\delta,\varepsilon})$, since this problem is nonconvex. On the other hand, it is easily seen that each feasible point in $(P_{\delta,\varepsilon})$ satisfies the usual constraint qualification [5, p. 19]. This means that at each minimum the Kuhn-Tucker conditions mentioned above hold.

Another drawback of this approach will be discussed in the following example. Let X be an accumulation point of a sequence of points $(X^{(\varepsilon)})_\varepsilon$, such that there exists no feasible descent direction at $X^{(\varepsilon)}$ in the problem $(P_{\delta,\varepsilon})$. This is an important necessary optimality condition. But it turns out that X is not necessarily a solution of the restricted problem with objective function Ψ_δ.

Example 3 *Let $d = 2$, $V = \{v\}$, $A = \{a\}$, $x_a := (0,0)^\top$, $\omega_{va} := 1$ and $\gamma_{va} := \|\cdot\|_2$. The forbidden region should be the set $\mathcal{R} :=]-1,1[\times]-1,0[$. The optimum of (2) is $(0,0)^\top$, while (3) has additionally another local optimum at $(0,-1)^\top$. The same is true if Ψ is approximated by Ψ_δ for sufficiently small values of $\delta > 0$. In $(P_{\delta,\varepsilon})$ we have local optima at $(0,\sqrt{\varepsilon})^\top$ and $(0,-1-\sqrt{\varepsilon})^\top$. Moreover, there exists no feasible descent direction at $(1+\sqrt{\varepsilon},0)^\top$ and $(-1-\sqrt{\varepsilon},0)^\top$. But these two points do not converge to a local optimum of Ψ_δ or Ψ for $\varepsilon \searrow 0$.*

Instead, we have only the following result.

Theorem 3.1 *Let $(\varepsilon_k)_{k\in\mathbb{N}}$ be a sequence of real numbers with $\varepsilon_k > 0$ for all $k \in \mathbb{N}$ and $\lim_{k\to\infty} \varepsilon_k = 0$. Let $(X_k)_{k\in\mathbb{N}}$ be a corresponding sequence of solutions of $(P_{\delta,\varepsilon_k})$. If $\omega_e > 0$ for all $e \in E$ it follows that at least one feasible accumulation point of this sequence exists. Furthermore, in the case of arbitrary weights, if every X_k is a global optimum to $(P_{\delta,\varepsilon_k})$, then every accumulation point of the sequence $(X_k)_{k\in\mathbb{N}}$ is in* $\arg\min\{\Psi_\delta(X) \mid X \in \mathcal{F}\}$.

Proof: For $\varepsilon > 0$, every solution to $(P_{\delta,\varepsilon})$ is feasible to (3). Since Ψ_δ is coercive for all $\delta > 0$, the sequence $(X_k)_{k\in\mathbb{N}}$ has at least one accumulation point $\hat{X}$. It is also clear that this point is feasible.

In the case of arbitrary weights, assume that every X_k is a global optimum to $(P_{\delta,\varepsilon_k})$, but that there exists a point $\overline{X} \in \mathcal{F}$ such that $\Psi_\delta(\overline{X}) < \Psi_\delta(\hat{X})$. We may also assume without loss of generality that $\lim_{k\to\infty} X_k = \hat{X}$. Otherwise we use a subsequence with this property. If we denote by $\mathcal{F}_k$ the set of feasible points of $(P_{\delta,\varepsilon_k})$, there exists a sequence $(\overline{X}_k)_{k\in\mathbb{N}}$ of points $\overline{X}_k \in \mathcal{F}_k$ with $\lim_{k\to\infty} \overline{X}_k = \overline{X}$. Then it follows that $\Psi_\delta(\overline{X}_k) < \Psi_\delta(X_k)$ for sufficiently large k, a contradiction. □

4 A Barrier Approach

By defining the function

$$\varphi(x) := \sum_{i\in I} \left((a_i^\top x - b_i)_+\right)^2,$$

which is differentiable on $\mathbb{R}^d$, we have $\varphi(x) = 0$ if and only if $x \in \mathrm{cl}(\mathcal{R})$ and $\varphi(x) > 0$ if and only if $x \notin \mathrm{cl}(\mathcal{R})$. Therefore, we can define the two barrier functions

$$B_1((x_v)_{v\in V}) := \sum_{v\in V} \frac{1}{\varphi(x_v)}$$

and

$$B_2((x_v)_{v\in V}) := -\sum_{v\in V} \ln(\varphi(x_v)).$$

Now we may search for minima of the sequence of functions

$$\tilde{\Psi}_{\delta,\mu}(X) := \Psi_\delta(X) + \mu B_j(X),$$

replacing μ by a sequence of parameters $(\mu_k)_{k\in\mathbb{N}}$ with $\mu_k > 0$ for all $k \in \mathbb{N}$ and $\lim_{k\to\infty} \mu_k = 0$.

However, similar arguments as the ones presented in the last section show that we may run into numerical difficulties when solving these problems.

To overcome the drawbacks of the previous approaches, we now propose a method based on a special barrier function. First, we define

$$\alpha(t) := \begin{cases} e^{-1/t} & : \quad t > 0 \\ 0 & : \quad t \le 0. \end{cases}$$

Then $\alpha'(t) = (e^{-1/t})/t^2$ for $t > 0$ and $\alpha'(0) = 0$, which means that α is differentiable on $\mathbb{R}$. Likewise, $\alpha^{(k)}(t) = \alpha(t)p_k(t)/t^{2^k}$ with a polynomial p_k for $t > 0$, but $\alpha^{(k)}(0) = 0$. Therefore, we have $\alpha \in C^\infty(\mathbb{R})$. Moreover, it is $\alpha(\mathbb{R}) \subseteq [0, 1[$. By defining $h_i(x) := a_i^\top x - b_i$ and $\beta_i(x) := (\alpha \circ h_i)(x)$ for all $i \in I$, we arrive at

$$\nu(x) := \sum_{i \in I} \beta_i(x) \begin{cases} > 0 & \text{if } x \notin \mathrm{cl}(\mathcal{R}) \\ = 0 & \text{else.} \end{cases}$$

Observe that $\nu \in C^\infty(\mathbb{R}^d)$. Now we can use the barrier function

$$B((x_v)_{v \in V}) := -\sum_{v \in V} \ln(\nu(x_v)),$$

which is in $C^\infty(\mathrm{int}(\mathcal{F}))$. Furthermore, we have for all feasible $(x_v)_{v \in V}$ and $w \in V$ that

$$\begin{aligned} \nabla_{x_w} B((x_v)_{v \in V}) &= -\frac{1}{\nu(x_w)} \nabla \nu(x_w) \\ &= -\frac{1}{\nu(x_w)} \sum_{i \in J_w} \alpha'(h_i(x_w)) \nabla h_i(x_w) \\ &= -\frac{1}{\nu(x_w)} \sum_{i \in J_w} \frac{\beta_i(x_w)}{h_i^2(x_w)} a_i, \end{aligned}$$

where $J_w := \{i \in I \mid a_i^\top x_w - b_i > 0\}$. With

$$\tilde{\Psi}_{\delta,\mu}(X) := \Psi_\delta(X) + \mu B(X)$$

we try to find a minimum of $\tilde{\Psi}_{\delta,\mu}$. For $\mu \searrow 0$ we know that every accumulation point of a sequence of global minima of $\tilde{\Psi}_{\delta,\mu}$ is a solution to (3), as it is also the case for penalty functions. Results concerning local convergence under quite weak assumptions can be found in [5, 30].

4.1 Searching for Minima I

When using Newton's method on $\tilde{\Psi}_{\delta,\mu}$ in order to compute a minimum, we need the gradient $\nabla\tilde{\Psi}_{\delta,\mu}$ and the Hessian $\nabla^2\tilde{\Psi}_{\delta,\mu} = \nabla^2\Psi_\delta + \mu\nabla^2 B$. With this matrix, a Newton step amounts to solving

$$(\nabla^2\tilde{\Psi}_{\delta,\mu}(X^{(k)}))\Delta X^{(k)} = -\nabla\tilde{\Psi}_{\delta,\mu}(X^{(k)})$$

for $\Delta X^{(k)}$ and then defining $X^{(k+1)} := X^{(k)} + \Delta X^{(k)}$.

For all $v, w \in V$ we have

$$\nabla^2_{x_v x_w} B((x_v)_{v \in V}) = 0$$

if $v \neq w$ and

$$\begin{aligned}
&\nabla^2_{x_w x_w} B((x_v)_{v\in V}) \\
&= -\sum_{j\in J_w} \frac{1}{\nu^2(x_w) h_j^4(x_w)} a_j \left(\nu(x_w)\beta_j(x_w) a_j^\top \right. \\
&\qquad \left. -\beta_j(x_w) \left(h_j^2(x_w) \sum_{k\in J_w} \frac{\beta_k(x_w)}{h_k^2(x_w)} a_k^\top + 2\nu(x_w) h_j(x_w) a_j^\top \right) \right) \\
&= -\sum_{j\in J_w} \frac{\beta_j(x_w)}{\nu^2(x_w) h_j^4(x_w)} a_j \left(\nu(x_w)(1-2h_j(x_w)) a_j^\top - h_j^2(x_w) \sum_{k\in J_w} \frac{\beta_k(x_w)}{h_k^2(x_w)} a_k^\top \right) \quad (13)
\end{aligned}$$

As the above calculation has shown, there will be no fill-in when using $\nabla^2 \tilde{\Psi}_{\delta,\mu}$ instead of $\nabla^2 \Psi_\delta$, because the only changes occur in the blocks $\nabla^2_{x_w x_w} \Psi_\delta$. But these blocks are nonzero, anyway. As a result, Newton's method used on restricted problems needs in every step the same computational effort as Newton's method used on unrestricted problems, provided that the evaluation of the Hessian is not too time consuming. To calculate this Hessian, we have to evaluate $\nabla^2 \Psi_\delta$ and B (and storing intermediate results like $\nu(x_v)$, $\beta_i(x_v)$ and $h_i(x_v)$ $(v \in V, i \in I)$, which costs $O(|V|nd)$ operations and the same amount of storage space). Then the vectors a_j $(j \in J_w, w \in V)$ are scaled according to (13) with $O(|V|nd)$ multiplications and divisions. The scaled vectors can be summed up with the same amount of additions and the corresponding dyadic products can be computed with $|V|d^2/2$ multiplications. Adding the appropriate blocks to $\nabla^2 \Psi_\delta$ costs another $|V|d^2/2$ additions. A subsequent Cholesky factorization on $\nabla^2 \tilde{\Psi}_{\delta,\mu}$ then needs $|V|^3 d^3/6$ operations. This factorization is the bottleneck of the computation as long as $n = o(|V|^2 d^2)$. It should be noted that the factorization cost can be significantly reduced by reordering the unknowns, i. e. applying a fill-in heuristic on $\nabla^2 \Psi_\delta$. Moreover, only one reordering is necessary for all Newton steps, and this reordering can be done on the graph G. Of course, this is helpful only if the graph G of interactions between the objects $f \in F$ is sufficiently sparse.

A truncated Newton Method [2, 22] is another solution approach for our nonlinear optimization problem. By using a CG-method for solving the linear system, it is not necessary to compute the dyadic products mentioned above. Instead, the particular structure of the algorithm makes it possible to transform those products into $|V|$ dot products between vectors in $\mathbb{R}^d$ and subsequent scalar multiplications of $|V|$ real numbers with other d-dimensional vectors. The main computational burden then results from matrix-vector multiplications with the matrix $\nabla^2 \Psi_\delta((x_v)_{v\in V})$.

It has to be noted that the Hessian $\nabla^2 \tilde{\Psi}_{\delta,\mu}$ does not need to be positive definite. This represents a difficulty which can be overcome by various techniques. For example, one can use the regularization technique of Levenberg and Marquardt (see, e. g. [6, 21, 13]) and a corresponding iterative procedure or the modified Cholesky-decomposition proposed by Gill and Murray [12]. Especially the last one is appealing here, because the sparsity structure of the linear system above remains the same for all iterations.

One of the main drawbacks of this approach is that the Hessians get increasingly ill-conditioned at minima of $\tilde{\Psi}_{\delta,\mu}$ for $\mu \searrow 0$. Therefore, we propose another method based on the function $\tilde{\Psi}_{\delta,\mu}$ in the next subsection.

4.2 Searching for Minima II

Now we try to compute minima of $\tilde{\Psi}_{\delta,\mu}$ by using the necessary conditions of first order, namely

$$\nabla_{x_w} \tilde{\Psi}_{\delta,\mu}((x_v)_{v\in V}) = \nabla_{x_w} \Psi_\delta((x_v)_{v\in V}) + \mu \nabla_{x_w} B((x_v)_{v\in V}) = 0 \quad \forall\, w \in V. \tag{14}$$

To this end, we define the additional variables

$$z_w^{(i)} := \frac{\beta_i(x_w)}{\nu(x_w) h_i^2(x_w)}$$

for $i \in I$ and $w \in V$. Then we then have

$$\nabla_{x_w} B((x_v)_{v\in V}) = -\sum_{j\in J_w} z_w^{(j)} a_j$$

for all $w \in V$. Hence, (14) is equivalent to the system

$$\nabla_{x_w} \Psi_\delta((x_v)_{v\in V}) - \mu \sum_{j\in J_w} z_w^{(j)} a_j \;=\; 0 \qquad \forall\, w \in V \tag{15}$$

$$z_w^{(i)} \nu(x_w) h_i^2(x_w) - \beta_i(x_w) \;=\; 0 \qquad \forall\, w \in V,\ i \in I \tag{16}$$

This is a system with the $|V|(d+n)$ unknowns x_v and $z_v^{(i)}$ $(v \in V,\, i \in I)$.

With $m := |V|$, we may assume without loss of generality that $V = \{1, \ldots, m\}$. This enables us to identify a family of locations $X := (x_v)_{v\in V} \in (\mathbb{R}^d)^V$ with the point $(x_1^\top, \ldots, x_m^\top)^\top$ in the vector space $\mathbb{R}^{dm}$. We index the d-dimensional subvectors x_v of X by $v \in V$. Likewise, we identify families $Z := (z_w^{(i)})_{(w,i)\in V\times I}$ of real numbers with points

$$(z_1^{(1)}, \ldots, z_1^{(n)}, \ldots, z_m^{(1)}, \ldots, z_m^{(n)})^\top$$

in the vector space $\mathbb{R}^{nm}$. Here, we index each component $z_w^{(i)}$ of Z by $(w,i) \in V \times I$. If we define the function

$$F : \mathbb{R}^{nm+dm} \longrightarrow \mathbb{R}^{nm+dm} \tag{17}$$

by

$$F_\ell(Z,X) := \begin{cases} z_w^{(i)} h_i^2(x_w)\nu(x_w) - \beta_i(x_w) & :\ \ell = (w,i) \in V \times I, \\ (\nabla_{x_w}\Psi_\delta)((x_v)_{v\in V}) - \mu \sum_{j\in J_w} z_w^{(j)} a_j & :\ \ell = w \in V, \end{cases}$$

we have to find a solution to the system

$$F(Z,X) = F((z_w^{(i)})_{(w,i)\in V\times I}, (x_v)_{v\in V}) = 0. \tag{18}$$

Note that we have only implicit restrictions on the variables X and Z.

For fixed $\mu > 0$, we will solve this system by Newton's method. After choosing a suitable starting vector $Y_0 = (Z_0, X_0)$, we have to solve the system

$$(F'(Y_k))\Delta Y_k = -F(Y_k), \tag{19}$$

in each step k of this iterative procedure. Here, $F'(Y_k)$ is the Jacobian of F at Y_k. After this, we set $Y_{k+1} := Y_k + \Delta Y_k$. The entries of the Jacobian are easy to compute:

1. $\ell = w \in V$: it is $F_\ell(Z, X) \in \mathbb{R}^d$. It follows that

$$\begin{aligned}
\frac{\partial F_\ell}{\partial x_v}(Z,X) &= \nabla^2_{x_w x_v}\Psi_\delta((x_v)_{v\in V}) \in \mathbb{R}^d \times \mathbb{R}^d \qquad \text{for all } v \in V,\\
\frac{\partial F_\ell}{\partial z_v^{(i)}}(Z,X) &= 0 \in \mathbb{R}^d \qquad \text{for all } v \in V \setminus \{w\} \text{ and } i \in I,\\
\frac{\partial F_\ell}{\partial z_w^{(j)}}(Z,X) &= -\mu a_j \in \mathbb{R}^d \qquad \text{for all } j \in J_w,\\
\frac{\partial F_\ell}{\partial z_w^{(i)}}(Z,X) &= 0 \in \mathbb{R}^d \qquad \text{for all } i \notin J_w.
\end{aligned}$$

2. $\ell = (w, i) \in V \times I$: we have $F_\ell(Z, X) \in \mathbb{R}$ and

$$\begin{aligned}
\frac{\partial F_\ell}{\partial x_w}(Z,X) &= z_w^{(i)}\left(2h_i(x_w)\nu(x_w)a_i^\top + h_i^2(x_w)\sum_{j\in J_w}\frac{\beta_j(x_w)}{h_j^2(x_w)}a_j^\top\right) - \frac{\beta_i(x_w)}{h_i^2(x_w)}a_i^\top\\
&= \left(2z_w^{(i)}h_i(x_w)\nu(x_w) - \frac{\beta_i(x_w)}{h_i^2(x_w)}\right)a_i^\top + z_w^{(i)}h_i^2(x_w)\sum_{j\in J_w}\frac{\beta_j(x_w)}{h_j^2(x_w)}a_j^\top\\
&\qquad \text{if } i \in J_w,\\
\frac{\partial F_\ell}{\partial x_w}(Z,X) &= z_w^{(i)}\left(2h_i(x_w)\nu(x_w)a_i^\top + h_i^2(x_w)\sum_{j\in J_w}\frac{\beta_j(x_w)}{h_j^2(x_w)}a_j^\top\right) \quad \text{if } i \notin J_w,\\
\frac{\partial F_\ell}{\partial x_v}(Z,X) &= (0,\ldots,0) \qquad \text{for all } v \in V \setminus \{w\},\\
\frac{\partial F_\ell}{\partial z_w^{(i)}}(Z,X) &= h_i^2(x_w)\nu(x_w) \in \mathbb{R},\\
\frac{\partial F_\ell}{\partial z_v^{(j)}}(Z,X) &= 0 \in \mathbb{R} \qquad \text{for } v \neq w \text{ or } j \neq i.
\end{aligned}$$

As it is easily seen, for all feasible $Y = (Z, X)$ the matrix $F'(Y)$ has the structure

$$F'(Y) = \begin{pmatrix} \boldsymbol{D} & \boldsymbol{C}_1 \\ \boldsymbol{C}_2 & \boldsymbol{H} \end{pmatrix}$$

with $\boldsymbol{H} = \nabla^2\Psi_\delta(X) \in \mathbb{R}^{dm} \times \mathbb{R}^{dm}$ symmetric, positive definite and possibly sparse,

$$\boldsymbol{D} = \operatorname{diag}(h_1^2(x_1)\nu(x_1), \ldots, h_n^2(x_1)\nu(x_1), \ldots, h_1^2(x_m)\nu(x_m), \ldots, h_n^2(x_m)\nu(x_m))$$

a diagonal matrix in $\mathbb{R}^{nm} \times \mathbb{R}^{nm}$,

$$\boldsymbol{C}_1 = \begin{pmatrix} \boldsymbol{F}_1 & & \boldsymbol{0} \\ & \ddots & \\ \boldsymbol{0} & & \boldsymbol{F}_m \end{pmatrix} \in \mathbb{R}^{nm} \times \mathbb{R}^{dm}$$

block diagonal with blocks

$$\boldsymbol{F}_w^\top := \left(\left(\frac{\partial F_{(w,1)}}{\partial x_w}(Y) \right)^\top, \ldots, \left(\frac{\partial F_{(w,n)}}{\partial x_w}(Y) \right)^\top \right) \in \mathbb{R}^d \times \mathbb{R}^n$$

$(w \in V)$ and

$$\boldsymbol{C}_2 = \begin{pmatrix} \hat{\boldsymbol{A}}_1 & & \boldsymbol{0} \\ & \ddots & \\ \boldsymbol{0} & & \hat{\boldsymbol{A}}_m \end{pmatrix} \in \mathbb{R}^{dm} \times \mathbb{R}^{nm}$$

block diagonal with blocks $\hat{\boldsymbol{A}}_v = -\mu(\delta_{1,v}a_1, \ldots, \delta_{n,v}a_n) \in \mathbb{R}^d \times \mathbb{R}^n$ $(v \in V)$, where $\delta_{j,w} = 1$ for $j \in J_w$ and $\delta_{j,w} = 0$ else. The matrix $\boldsymbol{C}_2$ will be sparse if $d \ll n$. If there exist a $w \in V$ and an $i \in I$ such that $h_i^2(x_w)\nu(x_w) = 0$, the matrix $\boldsymbol{D}$ is singular. However, the corresponding row and column in system (19) only contain zeroes, because we have $i \notin J_w$, $(\partial F_{(w,i)}/\partial x_w)(Y) = 0$ and $F_{(w,i)}(Y) = 0$. As a result, the system can be reduced and $\Delta z_w^{(i)}$ can be chosen arbitrary, e. g. $\Delta z_w^{(i)} = 0$. We may therefore assume without loss of generality that $\boldsymbol{D}^{-1}$ exists. The system (19)

$$\begin{pmatrix} \boldsymbol{D} & \boldsymbol{C}_1 \\ \boldsymbol{C}_2 & \boldsymbol{H} \end{pmatrix} \begin{pmatrix} \Delta Z \\ \Delta X \end{pmatrix} = - \begin{pmatrix} F_1(Z,X) \\ F_2(Z,X) \end{pmatrix}$$

can now be solved in two stages by eliminating ΔZ,

$$\Delta Z = -\boldsymbol{D}^{-1}(F_1(Z,X) + \boldsymbol{C}_1 \Delta X),$$

and solving the equation for the Schur complement,

$$(-\boldsymbol{C}_2\boldsymbol{D}^{-1}\boldsymbol{C}_1 + \boldsymbol{H})\Delta X = -F_2(Z,X) + \boldsymbol{C}_2\boldsymbol{D}^{-1}F_1(Z,X). \tag{20}$$

Note that $\boldsymbol{C}_2\boldsymbol{D}^{-1}\boldsymbol{C}_1 \in \mathbb{R}^{dm} \times \mathbb{R}^{dm}$ is a block diagonal matrix with blocks in $\mathbb{R}^d \times \mathbb{R}^d$. Since $\boldsymbol{H}$ has already the blocks $\nabla^2_{x_v x_v}\Psi_\delta$ on its diagonal, there will be no fill-in.

Unfortunately, the matrix in (20) is not symmetric. Therefore, it is natural to employ Gaussian elimination. Since this takes twice as much time as the Cholesky method for symmetric systems, it is not clear if the method proposed in this subsection is competitive with the method from Subsection 4.1.

5 Extensions and Conclusions

The approach decribed in Section 4 can also be used if every facility $v \in V$ has its own forbidden region $\mathcal{R}_v \subset \mathbb{R}^d$. Another easy extension is the case of a forbidden ellipsoid, paraboloid or hyperboloid. The interior of each of these sets can be represented as

$$\mathcal{R} := \{x \in \mathbb{R}^d \mid q(x) > 0\}$$

with a quadratic function $q(x) := x^\top \boldsymbol{M} x + c^\top x + \eta$. Here, $\boldsymbol{M} \in \mathbb{R}^{d \times d}$ is a symmetric matrix, $c \in \mathbb{R}^d$ and $\eta \in \mathbb{R}$. A barrier function with an even simpler structure than the ones described in Section 4 is now given by

$$B((x_v)_{v \in V}) := -\sum_{v \in V} \ln(q(x_v)).$$

With $\tilde{\Psi}_{\delta,\mu} := \Psi_\delta + \mu B$ we see that

$$\nabla_{x_w} \tilde{\Psi}_{\delta,\mu}((x_v)_{v \in V}) = \nabla_{x_w} \Psi_\delta((x_v)_{v \in V}) - \frac{\mu}{q(x_w)} \left(2\boldsymbol{M} x_w + c\right).$$

Therefore,

$$\nabla^2_{x_w x_v} \tilde{\Psi}_{\delta,\mu}((x_v)_{v \in V}) = \nabla^2_{x_w x_v} \Psi_\delta((x_v)_{v \in V})$$

if $v \neq w$ and

$$\begin{aligned} &\nabla^2_{x_w x_w} \tilde{\Psi}_{\delta,\mu}((x_v)_{v \in V}) \\ &= \nabla^2_{x_w x_w} \Psi_\delta((x_v)_{v \in V}) - \frac{\mu}{(q(x_w))^2} \left(2q(x_w)\boldsymbol{M} - (2\boldsymbol{M} x_w + c)(2\boldsymbol{M} x_w + c)^\top\right). \end{aligned}$$

As it is easily seen, the Hessian of this objective function shares many properties with the Hessian from Subsection 4.1. In fact, all the remarks made there about using Newton's method and solving the corresponding linear system hold here, too.

Extensions like other types of forbidden regions or specific feasible regions for the facilities $v \in V$ can also be handled by this kind of approach, provided that the corresponding barrier functions are at hand.

In this paper we have presented mainly improvement methods leading to a local optimum. It is therefore useful for implementations to combine the presented procedures with meta-heuristics like simulated annealing, tabu search or other local optima avoiding schemes. The successful application of these procedures highly depends on intensive numerical testing with various data instances. Such an elaborated discussion of the numerical aspects is, in our opinion, far beyond the scope of this paper. Our aim was to present a new problem, demonstrate its main difficulties and develop theoretical properties and solution techniques. However, implementations are under research and numerical tests will be contained in a forthcoming, more practical oriented paper.

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