

Elements of simulated annealing in Pareto front search

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Abstract—Determination of the Pareto front of location problem solutions represents one of the very complex and computational time demanding tasks, when solved by exact means of mathematical programming. This paper is motivated by possible application of the metaheuristic simulated annealing to the process of obtaining a close approximation of the Pareto front by a set of non-dominated solutions of the p -location problem. Contrary to the other approaches, the suggested method is based on minimization of non-dominated solution set area, which directly describes quality of the approximation. Elements of the simulated annealing method are used for random breaking some limits imposed on local characteristics of the improving process. The presented results of the numerical experiments give an insight to relations among the simulated annealing parameters and optimization process efficiency.

Keywords—discrete location problems, bi-criteria decision-making, Pareto front, simulated annealing

I. INTRODUCTION

Establishing a new service system, optimization of existing one or any other form of public service system design problem is a matter of searching for the optimal deployment of service centers, stations or facilities, which are equipped with necessary material, people or other resources for demands satisfaction. Obviously, the combinatorial character of mentioned problems implies using different means of mathematical modelling, knowledge of software development or other advanced skills. Thus, the Operations Research experts cannot be neglected, when the strategic decisions are to be made. Thanks to the huge and rapid progress in almost all involved fields, we are capable of obtaining good results of large problem instances in a short time [1, 6, 7, 8, 9, 11, 21].

When talking about service system designing, it must be noted that we do not study private service systems here, because they are mostly aimed at making the biggest possible profit regardless the number of covered system users or the level of fairness in service accessibility. Thus, we concentrate only on public service systems, the existence of which is usually given by law. The purpose of public service systems is to guarantee the provision of service to all residents of a given area, regardless of economic profit or loss [14]. From the scientific point of view, the public service system design problem belongs to the family of discrete network location problems, which have been studied and effectively solved by many authors [3, 7, 8, 9, 11, 23, 27, 28]. As far as a concrete form of the problem is concerned, one of the most commonly used modelling concepts follows the weighted p -median problem [3, 4, 14, 17, 18, 19, 20, 21].

The solvability of public service system design problem depends mainly on the specific form of used objective

function and the model itself. Recently, there have been developed plenty of exact and approximate approaches, which can efficiently deal with a large problem size and/or extreme computations resources demands [1, 4, 6, 7, 8, 9, 20, 21, 27].

One of possible big disadvantages of common mathematical models consists in the restriction, that only one objective function can be optimized. Large service systems represent complex systems with many contradictory demands raised by different groups of people involved in the decision-making process and not all of them are suitable for being abstracted. Therefore, the main attention is paid to multi-objective service system optimization. For simplicity, only two contradictory objectives will be taken in consideration.

The main scientific goal of the paper consists of introducing a heuristic method based on simulated annealing principles, which should be able to produce a small set of solutions for further decision-making. The presented results of numerical experiments will give an insight to relations between the simulated annealing parameters and optimization process efficiency.

II. PUBLIC SERVICE SYSTEM WITH TWO CONFLICTING OBJECTIVES

The public service system design problem with two conflicting objectives can be formulated by means of mathematical programming after introducing necessary notations.

The goal is to choose exactly p service centers (p is a positive integer value) from given set of candidates (the set of candidates will be denoted by I and the cardinality of I will be denoted by m) so that the given objective functions take their optimal values. Basic mathematical models of such location problems follow the idea of equality of centers from the point of capacity restrictions or establishing costs. Furthermore, let J denote the set of possible users' locations. Obviously, the sets I and J may contain the same elements. The number of individual users located at $j \in J$ will be denoted as b_j . This integer non-negative coefficient may have many other interpretations, i.e. the number of expected demands for service during some period. Anyway, one can understand it as a general weight of the location j . The distance of a user located at j from the possible center location i will be denoted as non-negative d_{ij} . It can also express the time for service delivery [3, 11, 17, 19]. In addition, it is assumed that r nearest located centers participate in the provision of the service for users and q_k stands for probability of the case that the k -th nearest center is the closest one, which is available. Finally, let the function \min_k return the k -th smallest element from the list in the parameter of the function.

The basic decision of the weighted p -median problem concerns locating service centers at exactly p elements from the set I so that the given objective takes its minimal/maximal value. To model this decision, we introduce a zero-one variable $y_i \in \{0, 1\}$, which takes the value of one, if a center should be located at i , and it takes the value of zero otherwise.

After these preliminaries, the public service system design problem with two objective functions can be formulated in the form of (1).

$$\min \left\{ f_1(\mathbf{y}), f_2(\mathbf{y}) : \mathbf{y} \in \{0, 1\}^m, \sum_{i=1}^m y_i = p \right\} \quad (1)$$

Within this study, we will restrict ourselves on two objective functions $f_1(\mathbf{y})$ and $f_2(\mathbf{y})$, which will be denoted as so-called system and fair criteria respectively.

The system criterion $f_1(\mathbf{y})$ expressed by (2) takes into account all users and it is used to optimize the average distance from the system users to the nearest available service center.

$$f_1(\mathbf{y}) = \sum_{j \in J} b_j \sum_{k=1}^r q_k \min_k \{ d_{ij} : i \in I; y_i = 1 \} \quad (2)$$

The fair objective function value $f_2(\mathbf{y})$ formulated by (3) expresses the number of users, whose time distance from the nearest located service facility exceeds given limit D . This objective follows the request of certain level of fairness in access to the provided service [5, 18, 22, 23].

$$f_2(\mathbf{y}) = \sum_{j \in J} b_j \max \left\{ 0, \text{sign} \left(\min \{ d_{ij} : i \in I; y_i = 1 \} - D \right) \right\} \quad (3)$$

Without any doubts, mentioned system and fair criteria (2) and (3) are in a direct conflict. It means that improving one of them is not possible without worsening the value of the other one. If we optimized only the average accessibility of service for system users by minimizing $f_1(\mathbf{y})$, there would certainly be a group of people too far from the nearest source of provided service. On the other hand, if we minimized only the number of those who are disadvantaged by their location, we would worsen the value of $f_1(\mathbf{y})$.

Such a conflict of different quality criteria can be solved by producing so-called Pareto front of solutions or at least by its approximation. The main idea is that instead of one optimal solution of the problem, a specific small set of solutions is provided for further final decision.

III. NON-DOMINATED SOLUTION SET MANAGEMENT

Let us concentrate on the set of all feasible solutions of the original location problem (1) with any kind of used objective functions. A vector of location variables y_i for $i \in I$ can describe each feasible solution. Since each solution \mathbf{y} can be evaluated by two objectives $f_1(\mathbf{y})$ and $f_2(\mathbf{y})$, each element of the feasible solutions set can be visually reported by one point of two-dimensional Euclidean space. Obviously, the cardinality of the set of candidates for service center locating may take several hundreds or thousands. This fact implies that the set of all feasible solutions is extremely large and it cannot be processed completely. Thus, a suitable output of any multi-criteria optimization consists in so-called Pareto front [2, 10, 12, 13, 14, 15, 24, 25, 26].

Pareto front can be created as a small set of solutions holding the non-dominance property for each pair of its members. Let us note that in the bi-criteria optimization, each feasible solution P can be evaluated by two criteria $f_1(P)$ and $f_2(P)$ no matter what form they take. The non-dominance can be explained in the following way: A solution P is called a non-dominated solution if every other solution R for which $[f_1(P), f_2(P)] \neq [f_1(R), f_2(R)]$ satisfies the following inequality $f_1(P) < f_1(R)$ or $f_2(P) < f_2(R)$. The explanation of Pareto front can be easily understood from Fig. 1.

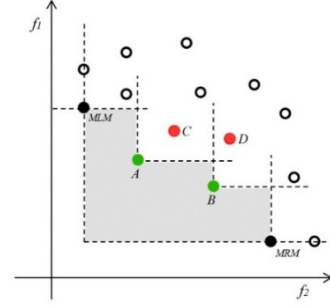


Fig. 1. Pareto front of non-dominated solutions.

If we look at Fig. 1, we can see that the green solutions A and B are members of the Pareto front, because they are not dominated by any other solution. Simply said, none of the Pareto front members is equally good or better in both quality criteria. On the contrary, the red solutions C and D can not belong to the Pareto front. The particle A dominates solution C and the solution D is dominated by both particles A and B . Based on the notion of Pareto front, the set of non-dominated solution is in order smaller than the original feasible solutions set and thus, it may be used as a suitable output for further decision-making. For completeness, let us note that MLM and MRM represent the bordering members of the Pareto front. While MLM denotes the most left member, symbol MRM is used to denote the most right one. The bordering members can be obtained by optimizing only one of given criteria.

Construction of the Pareto front is based on the following algorithm. Let us have an initial non-empty finite set of non-dominated solutions ordered according to the increasing value of f_2 . Furthermore, let us have a new candidate solution C to be inspected from the point of possible inclusion. The solution C is characterized by the values of associated objective functions $(f_1(C), f_2(C))$. The inspection is based on the task to find its position between predecessor P and successor S in the current set of non-dominated solutions so that $f_2(P) < f_2(C) \leq f_2(S)$. If $f_1(P) \leq f_1(C)$, then the candidate C is dominated by the predecessor P and it is abandoned. Otherwise, if the candidate solution C is not dominated by the successor S , the candidate becomes a new member of the updated set. Extension of the Pareto front by any new member may lead to its check. The following members of the sequence starting with the successor S are compared to C and if C dominates them, they are excluded from the updated set. If we look at Fig. 1 again, we can see that adding the solution A to the Pareto front may lead to excluding C and D (if they were added before) due to being dominated by A .

Comparison of two Pareto fronts can be realized via so-called area, which represents the size of the polygon defined by all members of the non-dominated solution set, as it is clearly shown in Fig. 1.

IV. NDSS GRADUAL REFINEMENT WITH SA ELEMENTS

The classical scheme of the gradual refinement consists of establishing an initial non-dominated solution set (*NDSS*) consisted of the most-left and right bordering solutions. The current *NDSS* solutions are processed in the order of increasing values of the objective f_2 . The solution y^k is used as a starting solution of the best-admissible neighborhood search, which tests the solutions differing from the current one only in one center location. The inspected solution is compared to the other solutions of the current *NDSS* and if it is non-dominated by any of them, it is inserted to the *NDSS*. This updating is accompanied by decrease of the *NDSS*-Area.

If the decrease exceeds a given threshold *MinDecrem*, then the neighborhood search is interrupted and the inspected solution is declared to be a new current solution. The processing of y^k terminates, when no move to a new current solution has been performed. Then, the k -th solution of current *NDSS* is compared to the original y^k and if the solutions differ, the new solution standing at the k -th position is processed. In the opposite case, *NDSS* processing continues with the $k+1$ st member of the *NDSS*. If the given time limit is not exhausted, the refinement process is repeated.

Based on the above classical gradual refinement process of the Pareto front approximation, we suggested a generalized version of the refinement process and added some elements of the simulated annealing approach into the refinement process.

First, we randomized the condition imposed on the move from the current solution to the new one. The original condition was met, when the *NDSS*-Area decrease (*Decrem*) was greater than or equal to the threshold *MinDecrem*. The randomized condition allows the move if either $Decrem \geq MinDecrem$ or a random trial issues the move permission with probability, which decreases with increasing value of the difference $MinDecrem - Decrem$. Probability P of the move permission is computed according to formula (4).

$$P(MinDecrem, Decrem, T) = e^{-(MinDecrem - Decrem)/T} \quad (4)$$

The parameter T being set at a small value near to zero causes that probability of the move permission is very low for any case $Decrem < MinDecrem$. Contrary to the classical simulated annealing approach, when the temperature T is gradually reduced to prohibit moves to a worse solution, in our case, we start with respecting the threshold *MinDecrem* in the first refinement process run and we allow random breaking the condition in the next runs. The parameter is gradually incremented in the suggested process.

As this version of refinement process is randomized, each start of it from the same initial *NDSS* may bring a different result. That is why, we repeat the refinement process several times and merge the obtained non-dominated solution sets.

Furthermore, we embedded the randomized refinement process into a cycle, where the number *Moves* of moves accepted during one run of the cycle is compared to a threshold *MinMoves* and the cycle is repeated subject to condition $Moves \geq MinMoves$.

The following steps can describe the complete process.

0. Initialize the starting *ccNDSS* by the non-dominated solution set consisted of two bordering solutions. Set up parameters *MinDecrem*, *MinMoves*, the starting temperature T and *maxTime*.

1. If $CPU\text{-time} > maxTime$ terminate, otherwise initialize working structure *NDSS* by *ccNDSS*, set up the number of performed moves (*Moves*) at zero and continue with step 2.
2. Perform the basic refinement process with the structure *NDSS* processing step-by-step the solutions $y^1, \dots, y^{noNDSS-1}$ and update the number *Moves* by adding the number of moves preformed during the basic refinement process.
3. Update the temperature T according to $T = a * T$.

If $Moves > MinMoves$, go to step 2. Otherwise update *ccNDSS* by merging *NDSS* and *cNDSS* and continue by step 1.

V. COMPUTATIONAL STUDY

The main goal of this computational study is to verify the described approach to obtaining a good approximation of Pareto front of the public service system designs. As the suggested metaheuristic depends on parameters of random trials, the next study is focused on the heating scheme, which influences performance of the metaheuristic. In this study, we performed series of experiments for various values of the base a used in the step 3 to update the temperature T . It is assumed that the parameter must be greater than or equal to 1 to ensure the proposed heating, but determination of a scope of this parameter values is matter of this research. The preliminary experiments were performed for the values 1, 1.5, 1.7, 1.8, 1.9 and 2, where the first values mean that the temperature stays constant and no heating is performed in the case. The starting values of initial T and the minimal decrement *MinDecrem* were determined as $T = 1000$ and $MinDecrem = 0.1$ percent of the initial *ccNDSS*-area.

The computational study was performed using the benchmarks derived from the Slovak self-governing regions. Individual instances of the benchmarks are denoted by the following names: Bratislava (BA), Banská Bystrica (BB), Košice (KE), Nitra (NR), Prešov (PO), Trenčín (TN), Trnava (TT) and Žilina (ZA). The sizes of the individual benchmarks are determined by integers m and p . The number m gives the cardinality of the set I and p gives the number of facilities to be located. The system criterion $f_1(y)$ expressed by (2) was computed for $r = 3$. The coefficients q_k for $k=1 \dots r$ were obtained from statistics presented in [16, 24, 25] and their values are: $q_1 = 77.063$, $q_2 = 16.476$ and $q_3 = 100 - q_1 - q_2$. The parameter D in the criterion (3) was set to 10.

All numerical experiments were run on a PC equipped with the 11th Gen Intel® Core™ i7 11700KF processor with the parameters: 3,6 GHz and 16 GB RAM. The algorithms were implemented in the Java language and run in the IntelliJ Idea environment. Since the benchmarks used in this computational study were used also in our previous research, the complete Pareto fronts are available and the corresponding values of *Area* are known. Here, *Area* denotes the absolute size of the polygon formed by members of Pareto front (see Fig. 1). The basic characteristics of the exact Pareto fronts are summarized in Table 1. Each row of the table corresponds to one studied benchmark characteristic. The columns of the table correspond to the individual problem instances. The row denoted by *NoS* gives the number of Pareto front solutions. In the row denoted by *Area* we provide the readers with the size of the polygon formed by all members of the set of non-dominated solutions.

TABLE I. BENCHMARKS CHARACTERISTICS AND THE EXACT PARETO FRONTS DESCRIPTIONS

	BA	BB	KE	NR
m	87	515	460	350
p	14	36	32	27
NoS	34	229	262	106
$Area$	569039	1002681	1295594	736846
	PO	TN	TT	ZA
m	664	276	249	315
p	32	21	18	29
NoS	271	98	64	97
$Area$	956103	829155	814351	407293

An individual experiment was organized in the following way. The suggested algorithm was run 10 times and the average values of studied characteristic were computed. To make the algorithm accuracy evaluation easier, it would be more sufficient to compare the relative gaps instead of absolute values of areas. The relative difference in percentage expressed by gap can be defined in the following way. Let A_{approx} denote the area of the resulting set of non-dominated solutions. Analogically, let A_{PF} denote the area of the complete Pareto front. Then the value of gap can be computed in percentage by (5).

$$gap = 100 * \frac{|A_{approx} - A_{PF}|}{A_{PF}} \quad (5)$$

The following Table 2 summarizes the obtained $gaps$ for $MinDecrem$ equal to one percent of the initial two-member $NDSS$ area.

TABLE II. GAPS OBTAINED BY HEURISTICS FOR $MINDECUREMENT = 1$

Base α	BA	BB	KE	NR	PO	TN	TT	ZA
1.0	3.5	7.8	6.5	8.5	5.3	4.5	9.6	8.8
1.5	1.8	1.5	3.0	0.5	5.2	0.7	0.4	0.1
1.7	2.0	0.9	1.8	0.5	3.8	0.7	0.5	0.1
1.8	1.9	0.9	1.8	1.0	3.3	0.7	0.4	0.1
1.9	2.0	0.9	2.3	0.5	2.2	0.7	0.5	0.1
2.0	2.0	0.7	1.7	1.1	2.1	0.7	0.5	0.1

Table 3 contains the average $gaps$ for $MinDecrement = 0.1$ percent and Table 4 is used for the results obtained for $MinDecrement = 0.01$ percent.

TABLE III. GAPS OBTAINED BY HEURISTICS FOR $MINDECUREMENT = 0.1$

Base α	BA	BB	KE	NR	PO	TN	TT	ZA
1.0	1.3	1.3	0.8	1.0	1.3	0.7	0.1	0.1
1.5	1.9	0.6	0.4	0.4	1.5	0.7	0.3	0.1
1.7	2.0	0.7	0.5	1.2	0.8	0.7	0.5	0.1
1.8	2.1	0.6	0.6	0.5	1.4	0.7	0.5	0.1
1.9	2.1	0.6	0.7	0.6	1.8	0.7	0.6	0.1
2.0	2.1	0.5	0.8	0.7	1.1	0.7	0.5	0.1

TABLE IV. GAPS OBTAINED BY HEURISTICS FOR $MINDECUREMENT = 0.01$

Base α	BA	BB	KE	NR	PO	TN	TT	ZA
1.0	0.2	0.4	1.2	0.4	1.4	0.7	0.1	0.0
1.5	2.2	0.4	1.2	0.4	0.6	0.7	0.6	0.1
1.7	2.2	0.5	1.1	0.7	0.8	0.7	0.6	0.1
1.8	2.1	0.5	1.4	0.7	1.8	0.7	0.7	0.2
1.9	2.7	0.5	1.2	0.8	1.0	0.7	0.6	0.1
2.0	3.1	0.4	1.1	1.1	0.3	0.7	0.5	0.1

VI. CONCLUSIONS

This paper was focused on public service system design problem. If there is only one objective function to be minimized, the problem is well solvable by available exact or heuristic approaches developed for different mathematical models. The solvability becomes a challenge if there are more conflicting criteria. In such situation, a Pareto front of non-dominated solutions can be produced as a suitable output of the computational process. The scientific goal of this paper consisted in introducing a heuristic approach based on simulated annealing bases. Its core task was to approximate the original Pareto front, which is hard to get in a short time.

The results of numerical experiments reported in presented computational study have shown that almost all results brought excellent results under two percent far from the exact value of area. The differences for given $MinDecrement$ values are minimal for various base values. As concerns the $MinDecrement$ value, the value 0.01 was the competition.

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