A Hyperbolic Smoothing Approach to the Fermat-Weber Location Problem

Vinicius Layter Xavier[1]
Felipe Maia Galvão França[1]
Adilson Elias Xavier[1]
Priscila Machado Vieira Lima[2]
[1]Dept. of Systems Engineering and Computer Science
Graduate School of Engineering (COPPE)
Federal University of Rio de Janeiro - BRAZIL
P.O. Box 68511
Rio de Janeiro,RJ 21941-972, BRAZIL
e-mail: {vinicius, felipe, adilson}@cos.ufrj.br
[2]MMC,DEMAT, Rural Federal University of Rio de Janeiro
e-mail: priscilamvl@ufrrj.br

Abstract

The Fermat-Weber Location Problem, also known as the continuous p-median problem, is considered here. A particular case of Fermat-Weber problem corresponds to the minimum sum-of-distances clustering problem. The mathematical modeling of this problem leads to a $min - sum - min$ formulation which, in addition to its intrinsic bi-level nature, is strongly nondifferentiable. In order to overcome these difficulties, the so called Hyperbolic Smoothing methodology, which follows a smoothing strategy using a special C^∞ differentiable class function, is adopted. The final solution is obtained by solving a sequence of low dimension differentiable unconstrained optimization subproblems which gradually approach the original problem. For the purpose of illustrating both the reliability and the efficiency of the method, a set of computational experiments was performed, making use of traditional test problems described in the literature.

Keywords: Fermat-Weber Problem, Min-Sum-Distances Clustering Problem, Nondifferentiable Programming

1 Introduction

The Fermat-Weber problem, or the location-allocation problem, has different names, as discussed by Wesolowski (1993). It is both a nondifferentiable and a nonconvex mathematical problem, with a large number of local minimizers, as presented by Rubinov (2006). So, it is a global optimization problem.

The core focus of this paper is the smoothing of the $min-sum-min$ problem engendered by the modeling of the Fermat-Weber problem. The process whereby this is achieved is an extension of a smoothing scheme, called Hyperbolic Smoothing, applied in Santos (1997) for nondifferentiable problems in general, used in Chaves (1997) for the $min-max$ problem and, more recently, adopted in Xavier and Oliveira (2004) for the covering of plane domains by circles. This technique was developed through an adaptation of the hyperbolic penalty method originally introduced by Xavier (1982).

By smoothing we mean the substitution of an intrinsically nondifferentiable two-level problem by a C^∞ differentiable single-level alternative. This is achieved through the solution of a sequence of differentiable subproblems which gradually approaches the original problem. In the present application, each subproblem, by using the Implicit Function Theorem, can be transformed into a low dimension unconstrained one. Due to the fact that the function has an infinite number of derivatives, it can be comfortably solved by using the most powerful and efficient algorithms, such as conjugate gradient, quasi-Newton or Newton methods.

Although this paper considers the particular Fermat-Weber problem, it must be emphasized that the proposed methodology, Hyperbolic Smoothing, can be used in exactly the same way for solving different $min-sum-min$ problems, e.g. clustering problems. The $min-sum$ location problems originated in the 17th century, when Fermat posed the question of, given three points in a plane, find a median point in the plane such that the sum of the distances from each of the points to the median point is minimized. Alfred Weber, a century ago, presented the same problem for a general number of points, also adding weights on each point to consider customer demand. The Weber problem locates facilities (medians) at *continuous* locations in the Euclidian plane, as presented by Koopmans and Beckmann (1957).

The remainder of this work is organized in the following way. A step-by-step definition of the Fermat-Weber problem, followed by the original hyperbolic smoothing approach and the derived algorithm are presented in the next section. Computational results are presented in section 3. Brief conclusions are drawn in section 4.

2 The Fermat-Weber Problem Formulation

Let $S = \{s_1, \ldots, s_m\}$ denote a set of m cities or locations in an Euclidean planar space $\mathbb{R}^2$, with a corresponding set of demands $W = \{w_1, \ldots, w_m\}$, to be attended by q, a given number of facilities. To formulate the Fermat-Weber problem as a $min - sum - min$ problem, we proceed as follows. Let $x_i, i = 1, \ldots, q$ be the locations of facilities or centroids, $x_i \in \mathbb{R}^2$. The set of these centroid coordinates will be represented by $X \in \mathbb{R}^{2q}$. Given a point $s_j \in S$, we initially calculate the Euclidian distance from s_j to the nearest centroid:

$$z_j = \min_{i=1,\ldots,q} \|s_j - x_i\|_2. \tag{1}$$

The Fermat-Weber problem consists in the location of q facilities in order to minimize the total transportation cost:

$$\begin{aligned} & minimize \sum_{j=1}^{m} w_j \, z_j && (2) \\ \text{subject to} \quad & z_j = \min_{i=1,\ldots,q} \|s_j - x_i\|_2, \quad j = 1, \ldots, m. \end{aligned}$$

In order to obtain a completely differentiable formulation we perform a series of transformations. First let us perform a relaxation of the equality constraints:

$$\begin{aligned} & minimize \sum_{j=1}^{m} w_j \, z_j && (3) \\ \text{subject to} \quad & z_j - \|s_j - x_i\|_2 \le 0, \quad j = 1, \ldots, m, \ \ i = 1, \ldots, q. \end{aligned}$$

Since z_j variables are not bounded from below, in the intrinsic minimization procedure, $z_j \to 0_+$, $j = 1, \dots, m$. In order to obtain the desired equivalence, we must, therefore, modify problem (3). We do so by first letting $\varphi(y)$ denote $max\{0, y\}$ and then observing that, from the set of inequalities in (3), it follows that

$$\sum_{i=1}^{q} \varphi(z_j - \|s_j - x_i\|_2) = 0, \quad j = 1, \dots, m. \tag{4}$$

Using (4) in place of the set of inequality constraints in (3), we would obtain an equivalent problem maintaining the undesirable property that $z_j, j = 1, \dots, m$; which still has no lower bound. Considering, however, that the objective function of problem (3) will force each $z_j, j = 1, \dots, m$, downward, we can think of bounding the latter variables from below by including a perturbation ε in (4). So, the following modified problem is obtained:

$$minimize \sum_{j=1}^{m} w_j z_j \tag{5}$$

$$\text{subject to} \quad \sum_{i=1}^{q} \varphi(z_j - \|s_j - x_i\|_2) \geq \varepsilon , \quad j = 1, \dots, m$$

for $\varepsilon > 0$. Since the feasible set of problem (2) is the limit of that of (5) when $\varepsilon \to 0_+$, we can then consider solving (2) by solving a sequence of problems like (5) for a sequence of decreasing values for ε that approaches zero.

Analyzing problem (5), the definition of function φ endows it with an extremely rigid nondifferentiable structure, which makes its computational solution very hard. In view of this, the numerical method we adopt for solving problem (1), takes a smoothing approach. From this perspective, let us define the function: $\phi(y, \tau) = \left(y + \sqrt{y^2 + \tau^2} \right) /2$, for $y \in \mathbb{R}$ and

$\tau > 0$. By using function ϕ in the place of function φ, the problem

$$
\begin{aligned}
&\textit{minimize} \quad \sum_{j=1}^{m} w_j \, z_j & (6)\\
&\text{subject to} \quad \sum_{i=1}^{q} \phi(z_j - \|s_j - x_i\|_2, \tau) \geq \varepsilon, \quad j = 1, \ldots, m.
\end{aligned}
$$

is produced.

Now, the Euclidean distance $\|s_j - x_i\|_2$ is the single nondifferentible component on problem (6). So, to obtain a completely differentiable problem, it is still necessary to smooth it. For this purpose, let us define the function $\theta(s_j, x_i, \gamma) = \sqrt{\sum_{l=1}^{n} (s_j^l - x_i^l)^2 + \gamma^2}$ for $\gamma > 0$. By using function θ in place of the distance $\|s_j - x_i\|_2$, the following completely differentiable problem is now obtained:

$$
\begin{aligned}
&\textit{minimize} \quad \sum_{j=1}^{m} w_j \, z_j & (7)\\
&\text{subject to} \quad \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) \geq \varepsilon, \quad j = 1, \ldots, m.
\end{aligned}
$$

So, the properties of functions ϕ and θ allow us to seek a solution to problem (5) by solving a sequence of subproblems like problem (7), produced by the decreasing of the parameters $\gamma \to 0$, $\tau \to 0$, and $\varepsilon \to 0$.

First, the objective function minimization process of problem (7) will work for reducing the values $z_j \geq 0, j = 1, \ldots, m$, to the utmost. On the other hand, given any set of centroids $x_i, i = 1, \ldots, q$, each constraint is a monotonically increasing function in z_j. So, these constraints will certainly be active and problem (7) will finally be equivalent to the following problem:

$$
\begin{aligned}
&\textit{minimize} \quad \sum_{j=1}^{m} w_j \, z_j & (8)\\
&\text{subject to} \quad h_j(z_j, x) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \quad j = 1, \ldots, m.
\end{aligned}
$$

The dimension of the variable domain space of problem (8) is $(2q+m)$. As, in general, the value of the parameter m, i.e., the cardinality of the set S of observations s_j, is large, problem (8) has a large number of variables. However, it has a separable structure, because each variable z_j appears only in one equality constraint. Therefore, as the partial derivative of $h(z_j, x)$ with respect to $z_j,\ j = 1, \ldots, m$ is not equal to zero, it is possible to use the Implicit Function Theorem to calculate each component $z_j,\ j = 1, \ldots, m$ as a function of the centroid variables $x_i,\ i = 1, \ldots, q$. In this way, the unconstrained problem

$$minimize\ f(x) = \sum_{j=1}^{m} w_j\, z_j(x) \tag{9}$$

is obtained, where each $z_j(x)$ results from the calculation of the single zero of each equation below, since each term ϕ above strictly increases together with variable z_j.

$$h_j(z_j, x) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \quad j = 1, \ldots, m. \tag{10}$$

Again, due to the Implicit Function Theorem, the functions $z_j(x)$ have all derivatives with respect to the variables $x_i,\ i = 1, \ldots, q$, and therefore it is possible to calculate the gradient of the objective function of problem (9),

$$\nabla f(x) = \sum_{j=1}^{m} w_j\, \nabla z_j(x) \tag{11}$$

where

$$\nabla z_j(x) = -\nabla h_j(z_j, x)\ /\ \frac{\partial h_j(z_j, x)}{\partial z_j}. \tag{12}$$

In this way, it is easy to solve problem (9) by making use of any method based on first order derivative information. Finally, it must be emphasized that problem (9) is defined on a $(2q)-$dimensional space, so it is a small problem, since the number of facilities, q, is, in general, very small for real applications.

The solution of the original location problem can be obtained by using an algorithm which solves an infinite sequence of optimization problems, where the parameters ε, τ and γ are gradually reduced to zero, just as in other smoothing methods.

Simplified HSFW Algorithm

Initialization Step: Choose initial values: x^0, γ^1 , τ^1 , ε^1.

Choose values $0 < \rho_1 < 1$, $0 < \rho_2 < 1$, $0 < \rho_3 < 1$; let $k = 1$.

Main Step: Repeat until a stopping rule is attained

Solve problem (9) with $\gamma = \gamma^k$, $\tau = \tau^k$ and $\varepsilon = \varepsilon^k$, starting at the initial point x^{k-1} and let x^k be the solution obtained.

Let $\gamma^{k+1} = \rho_1 \, \gamma^k$, $\tau^{k+1} = \rho_2 \, \tau^k$, $\varepsilon^{k+1} = \rho_3 \, \varepsilon^k$, $k := k + 1$. ■

Notice that when the algorithm causes τ and γ to approach 0, the constraints of the subproblems, as given in (7), tend to those of (5). In addition, the algorithm causes ε to approach 0, so, in a simultaneous movement, solving problem (5) gradually approaches the original location problem (2).

3 Computational Results

The computational results presented below were obtained from a preliminary implementation of the HSFW algorithm. Numerical experiments have been carried out on a PC Intel Celeron with 2.7GHz CPU and 512MB RAM; programs were coded using Compac Visual FORTRAN, Version 6.1. The unconstrained minimization tasks were carried out by means of a Quasi-Newton algorithm employing the BFGS updating formula from the Harwell Library, available in: (http://www.cse.scitech.ac.uk/nag/hsl/).

In order to show the performance of the proposed algorithm, results obtained by solving five standard test problems from the literature are presented:

1 - The 287 customer ambulances problem from Bongartz et al. (1994);

q	$f_{optimal}$	$f_{HSFW_{Best}}$	E_{Best}	$Occur.$	E_{Mean}	$Time_{Mean}$
2	14427,59	14427,60	0,00	88	0.05	0.12
3	12095,44	12095,50	0,00	100	0.00	0.17
4	10661,48	10661,60	0,00	27	3.39	0.20
5	9715,63	9733,54	0,18	48	3.42	0.25
6	8787,56	8787,70	0,00	7	5.09	0.32
7	8160,32	8160,44	0,00	6	4.40	0.39
8	7564,29	7564,41	0,00	1	5.32	0.46
9	7088,13	7088,26	0,00	11	4.31	0.54
10	6705,04	6705,16	0,00	2	2.66	0.63
11	6351,59	6361,53	0,16	10	2.02	0.79
12	6033,05	6041,18	0,13	1	1.31	0.96
13	5725,19	5744,88	0,34	4	1.44	1.07
14	5469,65	5481,66	0,22	3	1.21	1.18
15	5224,70	5230,96	0,12	2	1.36	1.32
16	4981,96	4989,91	0,16	4	1.55	1.51
17	4755,19	4761,50	0,13	2	2.03	1.83
18	4547,37	4554,41	0,15	2	2.05	2.02
19	4342,06	4361,22	0,44	2	2.33	2.19
20	4148,84	4155,76	0,17	2	2.47	2.36
25	3348,71	3350,69	0,06	1	3.00	3.60
30	2716,91	2720,66	0,14	1	4.51	5.55
35	2238,18	2246,82	0,39	1	4.77	7.94
40	1900,84	1914,50	0,72	1	3.80	9.94
45	1630,31	1654,84	1,50	1	3.38	13.70
50	1402,58	1448,67	3,29	1	4.45	19.04

Table 1: Results for the bon287 Instance

2 - P654, U1060, D15112 and Pla85900, which uses points in the plane from the TSPLIB collection of challenge problems of Reinelt (1991), where the demands assume unitary values, $w_j = 1$, $j = 1, \ldots, m$.

The last four data sets are available in the site: http://www.iwr.uni-heidelberg.de/groups/comopt/software/TSPLIB95/

Tables 1–3 contain: the number of facilities q; the optimal solution value $f_{optimal}$, or the putative global solution value $f_{putative}$, i.e., the best known solution for the instance, taken in Plastino et al. (2012) or in Brimberg et al. (2000); the best objective function value produced by the HSFW algorithm $f_{HSFW_{Best}}$ by using one hundred random starting points; the perceptual deviation value of the best HSFW value related to the optimal or putative

q	$f_{putative}$	$f_{HSFW_{Best}}$	E_{Best}	$Occur.$	E_{Mean}	$Time_{Mean}$
2	815313.0	815313.0	0.00	100	0.00	0.07
3	551063.0	551063.0	0.00	64	0.07	0.13
4	288191.0	288191.0	0.00	81	14.12	0.20
5	209069.0	209069.0	0.00	71	12.40	0.27
6	180488.0	180488.0	0.00	29	5.73	0.39
7	163704.0	163704.0	0.00	13	5.64	0.55
8	147051.0	147051.0	0.00	11	4.83	0.73
9	130936.0	130936.0	0.00	11	5.91	0.89
10	115339.0	115339.0	0.00	20	7.61	1.13
11	100133.0	100133.0	0.00	14	13.87	1.37
12	94152.05	94152.1	0.00	12	11.03	1.58
13	89454.76	89454.8	0.00	6	8.82	1.96
14	84807.69	84807.7	0.00	3	7.56	2.26
15	80177.04	80198.0	0.03	9	7.41	2.65
20	63389.02	63640.9	0.40	3	9.04	5.97

Table 2: Results for the P654 Instance

global value E_{Best}; the number of occurrences of the best solution $Occur.$; the perceptual deviation value E_{Mean} of the 100 solutions related to the best HSFW value and the mean CPU time given in seconds $Time_{Mean}$. Tables 4–5 do not contain any value associated to the putative global or best solution value because it was impossible to find any previous solution for these instances.

First, the results presented in Tables 1-5 show a consistent performance of the HSFW Algorithm, since columns E_{Mean} present small values. Columns $Occur.$ present expressive values, particularly for small number of facilities when the number of local minima points is smaller, indicates again a a consistent performance of the algorithm. Columns $Time_{Mean}$ illustrate the efficiency of the proposed algorithm. The comparison with results obtained by other algorithms, presented in first three tables, by column E_{Best}, show the robustness of the proposed methodology. It was impossible to find any previous record of solutions for the last two instances.

q	$f_{putative}$	$f_{HSFW_{Best}}$	E_{Best}	$Occur.$	E_{Mean}	$Time_{Mean}$
5	1851880	1852610	0.04	98	0.01	1.35
10	1249565	1250450	0.07	44	0.21	3.01
15	980132	980617	0.05	9	1.11	6.23
20	828802	829249	0.05	1	1.55	11.39
25	722061	721850	-0.03	4	2.09	18.12
30	638263	638686	0.07	1	2.60	26.89
35	577527	579280	0.30	1	2.89	37.58
40	529866	531706	0.35	1	2.91	52.40
45	489650	492658	0.61	1	2.57	78.72
50	453164	458641	1.21	1	2.47	83.41
55	422770	428909	1.45	1	2.68	104.34
60	397784	405151	1.85	1	2.57	124.67
65	376760	381491	1.26	1	2.60	150.06
70	357385	361719	1.21	1	2.97	176.02
75	340242	346522	1.85	1	2.74	208.66
80	326053	333114	2.17	1	2.61	250.60
85	313738	318698	1.58	1	3.07	279.82
90	302837	310766	2.62	1	2.43	324.98
95	292875	297720	1.65	1	3.16	386.20
100	283113	287294	1.48	1	2.70	423.36

Table 3: Results for the U1060 Instance

4 Conclusions

In this paper, a new method for the solution of the Fermat-Weber problem is proposed. Computational experimental results presented in this paper were obtained by using a particular and simple set of criteria for all specifications. However, the HSFW algorithm is a general framework that can support different implementations.

The most relevant computational task associated with the HSFW algorithm consists on the determination of the zeros of m equations (10), one equation for each observation point, for the calculation of each objective function value of problem (9). However, since these calculations are completely independent, they can be easily parallelized.

Finally, it must be noticed that the Fermat-Weber problem is a global optimization problem with several local minima, so that the proposed algorithm can only produce local minima.

q	$f_{HSFW_{Best}}$	$Occur.$	E_{Mean}	$Time_{Mean}$
2	0.688513D8	100	0.00	2.02
3	0.549316D8	100	0.00	4.23
4	0.459830D8	73	1.51	6.12
5	0.401359D8	96	0.31	8.79
6	0.366573D8	64	0.80	11.72
7	0.339779D8	70	0.75	15.83
8	0.317781D8	74	0.73	20.79
9	0.300421D8	32	0.69	24.83
10	0.285082D8	48	0.82	31.40

Table 4: Results for the D15112 Instance

q	$f_{HSFW_{Best}}$	$Occur.$	E_{Mean}	$Time_{Mean}$
2	0.746571D10	100	0.00	19.81
3	0.542509D10	100	0.00	37.80
4	0.435943D10	99	0.00	57.66
5	0.375564D10	99	0.00	86.54
6	0.333836D10	99	0.00	124.19
7	0.305697D10	99	0.00	166.04
8	0.286268D10	99	0.00	227.56
9	0.270703D10	98	0.00	274.68
10	0.258860D10	97	0.00	367.22

Table 5: Results for the Pla85900 Instance

References

BONGARTZ, I., CALAMAI, P.H. and CONN, A.R. (1994). "A Projection Method for l_p Norm Location-Allocation Problems", Mathematical Programming 66, pp. 283-312.

BRIMBERG, J.; HANSEN, P.; MLADENOVIC, N. and TAILLARD, E. D. (2000), "Improvements and Comparison of Heuristics for Solving the Multisource Weber Problem", Operations Research, v. 48, p. 129-135.

CHAVES, A.M.V. (1997) " Resolução do Problema Minimax Via Suavização", M.Sc. Thesis - COPPE - UFRJ, Rio de Janeiro. (in Portuguese)

KOOPMANS, T.C. and BECKMANN, M. (1957) "Assignment Problems and the Location of Economic Activities", *Econometrica*, Vol. 25, N. 1, pp. 53-76.

PLASTINO, A.; FUCHSHUBER, R.; MARTINS, S.L.; FREITAS, A.A. and SALHI, S. (2011) "A Hybrid Data Mining Metaheuristic for the $p-$Median Problem", Statistical Analysis and Data Mining, Vol. 4, pp. 313-335.

REINELT, G. (1991) "TSP-LIB: A Traveling Salesman Library", ORSA J. Comput. pp.

376-384.

RUBINOV, A. (2006) "Methods for Global Optimization of Nonsmooth Functions with Applications", *Applied and Computational Mathematics*, 5, no. 1, pp. 3-15.

SANTOS, A.B.A. (1997) "Problemas de Programação Não- Diferenciável: Uma Metodologia de Suavização", M.Sc. thesis - COPPE - UFRJ, Rio de Janeiro. (in Portuguese)

WESOLOWSKY, G. O. (1993) "The Weber Problem: History and Perspectives", Location Sciences, n.1 ,p. 5-23.

XAVIER, A.E. (1982) "Penalização Hiperbólica: Um Novo Método para Resolução de Problemas de Otimização", M.Sc. Thesis - COPPE - UFRJ, Rio de Janeiro. (in Portuguese)

XAVIER, A.E. (2010) "The Hyperbolic Smoothing Clustering Method", Pattern Recognition, Vol 43, pp. 731-737.

XAVIER, A.E. and XAVIER, V.L. (2011) "Solving the Minimum Sum-of-Squares Clustering Problem by Hyperbolic Smoothing and Partition into Boundary and Gravitational Regions", Pattern Recognition, Vol 44 pp 70-77

XAVIER, V.L. (2012) "Resolução do Problema de Agrupamento segundo o Critério de Minimização da Soma de Distâncias", M.Sc. thesis - COPPE - UFRJ, Rio de Janeiro. (in Portuguese)