Mathematical Optimization Models for the Euclidean Steiner Tree Problem in R^d

N. Maculan¹, Marcia Fampa¹, H. Ouzia², R. V. Pinto³

Universidade Federal do Rio de Janeiro, Brazil¹ Sorbonne Université, Paris, France² Universidade Federal Rural do Rio de Janeiro, Brazil³

¹maculan@cos.ufrj.br

1 fampa@cos.ufrj.br

2 hacene.ouzia@sorbonne.universite.fr

3 renanvp@ufrrj.br

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal July 21-26 2024** 1/50

The History

Challenge of Fermat in the 17th century

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal Campana Andrée 1986** - Montréal July 21-26 2024 2 / 50

The History

Challenge of Fermat in the 17th century

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Triangle: Three given points

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Triangle: Three given points

• Torricelli (1647) pointed out a solution when the triangle formed by the three given points does not have an angle $>$ 120.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Triangle: Three given points

- Torricelli (1647) pointed out a solution when the triangle formed by the three given points does not have an angle $> 120.$
- Heinen (1837) apparently is the first to prove that, for a triangle in which an angle is $>$ 120, the vertex associated with this angle is the minimizing point.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

$$
||\overrightarrow{XA}|| = \sqrt{(x_a - x)^2 + (y_a - y)^2}
$$

\n
$$
||\overrightarrow{XB}|| = \sqrt{(x_b - x)^2 + (y_b - y)^2}
$$

\n
$$
||\overrightarrow{XC}|| = \sqrt{(x_c - x)^2 + (y_c - y)^2}
$$

\n
$$
\nabla \mathcal{D} = \begin{pmatrix} \frac{\partial \mathcal{D}}{\partial x} \\ \frac{\partial \mathcal{D}}{\partial y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
$$

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Fermat's Challenge as an Optimization Problem

Three Forces in Equilibrium

 $\nabla \mathcal{D} = \vec{r} + \vec{s} + \vec{r} = \vec{0}$

Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.

Fermat's Challenge as an Optimization Problem

Pós-Graduação e Pesquisa de Fontobar

Steiner Minimal Tree Problem

Find a minimum tree that spans these points using or not extra points, which are called Steiner points.

Steiner Minimal Tree Problem

Find a minimum tree that spans these points using or not extra points, which are called Steiner points.

This is a very well known problem in combinatorial optimization.

Steiner Minimal Tree Problem

Find a minimum tree that spans these points using or not extra points, which are called Steiner points.

- This is a very well known problem in combinatorial optimization.
- This problem has been shown to be NP-Hard.

Steiner Minimal Tree Problem

Find a minimum tree that spans these points using or not extra points, which are called Steiner points.

- This is a very well known problem in combinatorial optimization.
- This problem has been shown to be NP-Hard.
- All distances are considered to be Euclidean.

Problem Definition

An example in \mathbb{R}^3 : Icosahedron

Pós-Graduação e Pesquisa de Engenharia

Number of Steiner Points

Given p points $x^i \in \mathbb{R}^n$, $i = 1, 2, ..., p$, the maximum number of Steiner points is $p - 2$.

Number of Steiner Points

Given p points $x^i \in \mathbb{R}^n$, $i = 1, 2, ..., p$, the maximum number of Steiner points is $p - 2$.

Degree of Steiner Points

A nondegenerated Steiner point has degree (valence) equal to 3.

Number of Steiner Points

Given p points $x^i \in \mathbb{R}^n$, $i = 1, 2, ..., p$, the maximum number of Steiner points is $p - 2$.

Degree of Steiner Points

A nondegenerated Steiner point has degree (valence) equal to 3.

Steiner Points Edges

The edges emanating from a nondegenerated Steiner point lie in a plane and have mutual angle equal to 120°.

Steiner Topology

It is a topology that satisfies all the Steiner Tree properties.

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal July 21-26 2024** 8 / 50

Steiner Topology

It is a topology that satisfies all the Steiner Tree properties.

Number of Topologies (Gilbert and Pollack)

The total number of different topologies with k Steiner points is

$$
C_{p,k+2}\frac{(p+k-2)!}{k!2^k},
$$

where p is the number of given points in \mathbb{R}^n .

Steiner Topology

It is a topology that satisfies all the Steiner Tree properties.

Number of Topologies (Gilbert and Pollack)

The total number of different topologies with k Steiner points is

$$
C_{p,k+2}\frac{(p+k-2)!}{k!2^k},
$$

where p is the number of given points in \mathbb{R}^n .

Full Steiner Topologies ($k = p - 2$)

The total number of different topologies with $k = p - 2$ Steiner points is

$$
1 \cdot 3 \cdot 5 \cdot 7 \ldots (2p-5) = (2p-5)!!.
$$

For example, if $p = 10$, the Number of Full Steiner Topologies is equal to

$$
15!!=2,027,025.
$$

Example of Local Optimization

Finding the best solution...

Minimize
$$
||x^3 - x^5|| + ||x^2 - x^5|| + ||x^5 - x^6|| + ||x^1 - x^6|| + ||x^4 - x^6||
$$

subject to x^5 and $x^6 \in \mathbb{R}^n$.

COPPE Instituto Alberto Luiz Coimbra de UFRJ

Given p different points in $Rⁿ$, the ESTP seeks to find a minimum tree that spans these points using or not extra points, which are called Steiner points. The length of each edge is the Euclidean distance between its ends.

We consider a special graph $G = (V, E)$ as follows:

Let $P = \{1, 2, ..., p-1, p\}$ be the set of indices associated with the given points in $R^n: x^1, x^2, ..., x^{p-1}, x^p$, and a set of indices $S = \{p+1, p+2, ..., 2p-3, 2p-2\}$ associated with the Steiner points also in $R^n: x^{p+1}, x^{p+2}, ..., x^{2p-3}, x^{2p-2}.$ We take $V = P \cup S$. We denote $[i, j]$ $i < j$, i and $j \in V$ an edge of G. Thus we define $E_1 = \{[i, j] \mid i \in P, j \in S\}$, $E_2 = \{[i, j] \mid i < j$, i and $j \in S\}$, and $E = E_1 \cup E_2$.

A tree which is an optimal solution for the ESTP is a sub-graph of $G = (V, E)$. We consider the following variables:

$$
x^i \in \mathbb{R}^n, \ i \in \mathcal{S}, \tag{1}
$$

$$
y_{ij} \in \{0, 1\}, \ \ [i, j] \in E. \tag{2}
$$

- 6 given points.
- 4 Steiner points.

- 6 given points.
- 4 Steiner points.
- All possible edges among Steiner points.

- 6 given points.
- 4 Steiner points.
- All possible edges among Steiner points.
- All possible connections between a given point and a Steiner point.

3

 $\overline{2}$

7 8

1

6

- 6 given points.
- 4 Steiner points.
- All possible edges among Steiner points.
- All possible connections between a given point and a Steiner point.
- All possible edges.

- 6 given points.
- 4 Steiner points.
- All possible edges among Steiner points.
- All possible connections between a given point and a Steiner point.
- All possible edges.
- An example of a set of possible edges.

Maculan-Michelon-Xavier (2000) [1]

$$
\text{(P1):} \quad \text{Minimize} \quad \sum_{[i,j] \in E} ||x^i - x^j|| \, y_{ij} \text{ subject to} \tag{3}
$$

$$
\sum_{j\in S}y_{ij} = 1, i\in P,
$$
\n(4)

$$
\sum_{i < j, i \in S} y_{kj} = 1, \ \ j \in S - \{p+1\},\tag{5}
$$

$$
\sum_{i\in P} y_{ij} + \sum_{kj, k\in S} y_{jk} = 3, \quad j\in S,
$$
 (6)

$$
x^{i} \in \mathbb{R}^{n}, i \in S,
$$

\n
$$
y_{ij} \in \{0, 1\}, [i, j] \in E,
$$

\n(8)

We consider $||x^i - x^j|| \approx \sqrt{\sum_{k=1}^n (x_k^i - x_k^j)^2 + \lambda^2}$

Instituto Alberto Luiz Coimbra de **UFRJ**
First Formulation: an example with $p = 6$

First Formulation: another example

If we don't considerer

$$
\sum_{k
$$

Second Formulation (First Property)

If $\bar{x}^j \in R^n, \ j \in S$ and $\bar{y}_{ij} \in \{0,1\}, \ [i,j] \in E$ is an optimal solution, then

$$
\bullet \quad d_{ij}=||a^i-\bar x^j||\geqslant 0 \text{ or } d_{ij}=0 \text{, for all } [i,j]\in E_{\textbf{1}} \text{ and }
$$

•
$$
d_{ij} = ||\bar{x}^i - \bar{x}^j|| \geq 0
$$
 or $d_{ij} = 0$, for all $[i, j] \in E_2$.

Second Formulation (Second Property)

 $y_{ii} \in \{0, 1\}, \; [i, j] \in E$ is associated with a full Steiner Topology if, and only if, the following equations are satisfied:

$$
\sum_{j\in S} y_{ij} = 1, \quad i \in P,
$$
\n
$$
\sum_{j\in S} y_{ij} = 1, \quad j \in S - \{p+1\},
$$
\n
$$
\sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S,
$$

Second Formulation (Third Property)

In a minimum Steiner tree with more than three terminal nodes, all Steiner points have no more than two connections with terminal nodes. So, if $p > 3$,

$$
\sum_{i\in P}y_{ij}\leqslant 2,\;j\in S.
$$

Note that...

When we consider

$$
||x^{i} - x^{i}|| \approx \sqrt{\sum_{i=1}^{n} (x_{i}^{i} - x_{i}^{i})^{2} + \lambda^{2}},
$$

error propagations may happen.

Note that...

When we consider

$$
||x^{i}-x^{j}|| \approx \sqrt{\sum_{i=1}^{n}(x_{i}^{i}-x_{i}^{j})^{2}+\lambda^{2}},
$$

error propagations may happen.

Note that...

When we consider

$$
||x^{i}-x^{j}|| \approx \sqrt{\sum_{i=1}^{n}(x_{i}^{i}-x_{i}^{j})^{2}+\lambda^{2}},
$$

error propagations may happen.

Ouzia-Maculan (2018) [4]

$$
\text{(P3):} \quad \text{Minimize} \quad \sum_{[i,j] \in \mathbf{E}} \sqrt{\sum_{k=1}^{n} d_{ijk}^2} \quad \text{subject to} \tag{18}
$$

$$
-y_{ij} \leq d_{ijk} \leq y_{ij}, [i,j] \in E, k = 1, 2, ..., n,
$$
 (19)

$$
-(1-y_{ij}) + (x_k^i - x_k^j) \le d_{ijk} \le (x_k^i - x_k^j) + (1-y_{ij}), \quad [i,j] \in E, \ k = 1,2,...,n,
$$
 (20)

$$
\sum_{j\in S} y_{ij} = 1, \quad i \in P,
$$
\n(21)

$$
\sum_{i < j, i \in S} y_{kj} = 1, \ \ j \in S - \{p+1\},\tag{22}
$$

$$
\sum_{i\in P} y_{ij} + \sum_{kj,k\in S} y_{jk} = 3, \quad j\in S,
$$
\n
$$
(23)
$$

$$
x^{i} \in \mathbb{R}^{n}, i \in S,
$$

\n
$$
y_{ij} \in \{0, 1\}, [i, j] \in E,
$$

\n
$$
d_{ijk} \in \mathbb{R}.
$$

\n(26)

$$
d_{ijk} \in \mathbb{R}.
$$

OPPE Instituto Alberto Luiz Coimbra de UFRJ

Ouzia-Maculan (2018) [4]

$$
\text{(P4):} \quad \text{Minimize} \quad \sum_{[i,j] \in \mathsf{E}} \sqrt{d_{ij}} \quad \text{subject to} \tag{27}
$$

$$
d_{ij} \geqslant \sum_{k=1}^{n} (x_k^j - x_k^j)^2 - (1 - y_{ij}), \ [i, j] \in E, \tag{28}
$$

$$
d_{ij} \geqslant 0, [i,j] \in E \tag{29}
$$

$$
\sum_{j \in S} y_{ij} = 1, \quad i \in P,
$$
\n(30)

$$
\sum_{i < j, i \in S} y_{kj} = 1, \ \ j \in S - \{p+1\},\tag{31}
$$

$$
\sum_{i\in P} y_{ij} + \sum_{kj, k\in S} y_{jk} = 3, \quad j\in S,
$$
\n(32)

$$
x^{i} \in \mathbb{R}^{n}, \ i \in S,
$$
\n
$$
(33)
$$

$$
y_{ij} \in \{0, 1\}, \quad [i, j] \in E,\tag{34}
$$

$$
d_{ij} \in \mathbb{R}.\tag{35}
$$

Maculan-Ouzia-Pinto (2020) [5]

$$
(P5): \quad \text{Minimize} \quad \sum_{[i,j] \in \mathsf{E}} d_{ij} \quad \text{subject to} \tag{36}
$$

$$
d_{ij}^2 \geq \sum_{k=1}^n t_{ijk}^2, \quad [i,j] \in E, \tag{37}
$$

$$
-y_{ij} \leq t_{ijk} \leq y_{ij}, \quad [i,j] \in E, \ k = 1,2,...,n,
$$
 (38)

$$
-(1-y_{ij})+(x_k^i-x_k^j)\leq t_{ijk} \leq (x_k^i-x_k^j)+(1-y_{ij}), \quad [i,j] \in E, \ k=1,2,...,n,
$$
 (39)

$$
\sum_{j\in S} y_{ij} = 1, \quad i \in P,\tag{40}
$$

$$
\sum_{i < j, i \in S} y_{kj} = 1, \ \ j \in S - \{p+1\},\tag{41}
$$

$$
\sum_{i\in P} y_{ij} + \sum_{kj, k\in S} y_{jk} = 3, \quad j\in S,
$$
 (42)

$$
x^i \in \mathbb{R}^n, \ i \in S,
$$
\n⁽⁴³⁾

$$
y_{ij} \in \{0,1\}, \ \ [i,j] \in E,\tag{44}
$$

$$
d_{ij} \geq 0, \quad [i,j] \in E. \tag{45}
$$

Instituto Alberto Luiz Coimbra de UFRJ

Maculan-Ouzia-Pinto (2020) [5]

We added to model (P5) many families of constraints to eliminate isomorphic trees, based on the idea presented by Smith in his paper [6].

The author presents a bijection between every possible full Steiner topology on p terminal points and vectors in $a \in \mathbb{N}^{p3}$, where $1 \le a_i \le 2i + 1$, $i = 1, ..., p3$.

The edges are labeled and each a_i indicates which edge the $(i + 1)$ -th Steiner point will be placed on.

We call the resulting model (P6).

To represent the Smith vector, we define the binary variables

$$
v_{ij} \in \{0, 1\},
$$
 $i = 1, ..., p - 3, j = 1, ..., 2i + 1,$

that assume value 1 if $a_i = j$. We must have

$$
\sum_{j=1}^{2i+1} v_{ij} = 1, \quad \forall i = 1, \ldots, p-3.
$$
 (46)

To control the edges labeling, we define the binary variables

$$
e_{ijkl} \in \{0,1\}, \qquad i=0,\ldots,p-3, \ j=1,\ldots,2i+3, \ k \in \{1,2\}, \ l=1,\ldots,2p-2.
$$

We will have $e_{iik} = 1$ if, in stage i of the construction of the tree, vertex k of edge j is l.

We must have

$$
\sum_{l=1}^{2p-2} e_{ijkl} = 1, \quad \forall i, j, k.
$$
 (47)

along with some initial conditions (corresponding to the null-vector or the 3-terminal topology):

$$
e_{0j1j}=1, \qquad j=1,2,3,\tag{48}
$$

$$
e_{0j2(p+1)} = 1, \qquad j = 1, 2, 3. \tag{49}
$$

In iteration $i > 0$, the new Steiner point will be placed in the middle of edge a_i , or, in our notation, in the middle of edge j, such that $v_{ij} = 1$. We write, for all $i = 1, \ldots, p - 3, j = 1, \ldots, 2i + 3, l = 1, \ldots, 2p - 2,$

$$
e_{ij1} = e_{(i-1)j1l}, \t\t(50)
$$

$$
-v_{ij} + e_{(i-1)/2} \le e_{ij2} \le e_{(i-1)/2} + v_{ij}, \qquad (51)
$$

$$
v_{ij} \leq e_{ij2(i+1+\rho)} \leq 2 - v_{ij}.
$$
\n
$$
(52)
$$

For the two new edges added at each iteration, we have, for all $i = 1, \ldots, p - 3, l = 1, \ldots, 2p - 2,$

$$
e_{i(2i+2)1(i+3)} = 1, \tag{53}
$$

$$
e_{i(2i+2)2(i+1+p)}=1,
$$
\n(54)

$$
e_{i(2i+3)1l} = \sum_{j=1}^{2i+1} v_{ij} \cdot e_{(i-1)j2l}, \qquad (55)
$$

$$
e_{i(2i+3)2(i+1+p)} = 1.
$$
 (56)

 \sim \sim

We can linearize the binary product in equation [\(55\)](#page-49-0) using the McCormick inequalities.

Finally, we relate variables e_{iikl} to the variables y_{ii} . For all $i = 1, \ldots, 2p - 2, j = p + 1, \ldots, 2p - 2, i < j, k = 1, \ldots, 2p - 3,$

$$
y_{ij} \ge e_{(p-3)k1i} + e_{(p-3)k2j} - 1.
$$
 (57)

The experiments were performed on a machine equipped with an Intel(R) Xeon(R) i7 8700 CPU @ 3.20GHz with 12 cores and 64GB DRAM of memory.

Models (P1) to (P4) were solved using BARON 21.1.7. Models (P5) and (P6) were solved using XPRESS 8.11.0.

Main idea: starting with the Fermat point, add one Steiner point at a time.

Before all Steiner points are added, there will be at least one Steiner point with degree greater than 3. Let s be one of these points. A new Steiner point will be added to the tree to reduce the degree of s.

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal July 21-26 2024** 34 / 50

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal July 21-26 2024** 34 / 50

Maculan, Fampa, Ouzia, Pinto **ISMP2024 - Montréal July 21-26 2024** 34 / 50

PPE

From the topology in the left, no choice for the new Steiner point location will result in the optimal Steiner tree (depicted in the right).

Two new heuristics for the Euclidean Steiner Tree Problem in \mathbb{R}^n [7]:

Heur1 : always choose minimum angle Heur2 : tests all angles and pick the smallest resulting tree

Heuristics - Computational complexity

Let
$$
D = \max_{i,j=1,...,p} ||a^{i} - a^{j}||
$$
.

Consider a fixed topology and let E be the set of edges of this tree. An interior-point algorithm^{*} can compute an ε -optimal solution in

$$
O\left(\sqrt{|E|}\left(\log\left(\frac{D}{\varepsilon}\right) + \log|E|\right)\right)
$$

iterations, where $|E|$ is the number of edges in the tree.

Using
$$
D = 1
$$
 and $\varepsilon = 10^{-16}$,
\n
$$
\sqrt{|E|} \left(\log_{10} \left(\frac{D}{\varepsilon} \right) + \log_{10} |E| \right) \le \sqrt{2p - 3} \left(16 + \log_{10} (2p - 3) \right).
$$

Therefore, the computational complexity has order of

$$
\sqrt{p}+\sqrt{p}\,\log(p)\,.
$$

[∗]G. Xue, Y. Ye. An efficient algorithm for minimizing a sum of Euclidean norms with applications. SIAM Journal on Optimization 4(7):1017–1036, 1997.

Heuristic 1 ($D = 1$ and $\varepsilon = 10^{-16}$):

The search for the minimum angle is most costly in the first iteration, when there are p edges connecting every terminal to the Fermat-Weber point.

There are $p(p-1)/2 = O(p^2)$ pair of edges to have their angles computed. Therefore, at each iteration, the quantity of operations has order of

$$
p^2 + \sqrt{p} + \sqrt{p} \, \log(p) \, .
$$

Then the total of computational operations performed by Heuristic 1, after $O(p)$ iterations, has order of

$$
p^3 + p\sqrt{p} + p\sqrt{p}\,\log(p)\,.
$$

Heuristic 2 ($D = 1$ and $\varepsilon = 10^{-16}$):

The model for a fixed topology has to be solved for each pair of consecutive edges. Then each iteration of Heuristic 2 has order of

$$
p^2(\sqrt{p}+\sqrt{p}\,\log(p)).
$$

As Heuristic 2 performs $p - 3$ iterations, the total of computational operations performed by Heuristic 2 has order of

$$
p^3(\sqrt{p}+\sqrt{p}\,\log(p)).
$$

Platonic solids:

* Best solution found after 30 days of execution of Smith's algorithm [6].

Hypercubes:

* Conjecture [6]: optimal solution value is $(2^{n-1}-1)\sqrt{3}+1$.

Numerical experiments

Hypercube in \mathbb{R}^7

∗ Instances from D.R. Dreyer and M.L. Overton. Two heuristics for the Euclidean Steiner tree problem. Journal of Global Optimization 13:95–106, 1998.

Instances from V. do Forte, F.M.T. Montenegro, J.A.M. Brito and N. Maculan. Iterated local search algorithms for the Euclidean Steiner tree problem in n dimensions. International Transactions in Operational Research (ITOR) 23(6):1185–1199, 2016.

Random instances:

Random instances:

[1] N. Maculan, Ph. Michelon and A.E. Xavier. The Euclidean Steiner tree problem in \mathbb{R}^n : a mathematical programming formulation. Annals of Operations Research, 96:209-220, 2000.

[2] M.H.C. Fampa and N. Maculan. A new relaxation in conic form for the Euclidean Steiner problem in \mathbb{R}^n . RAIRO - Operations Research, 35(4):283-394, 2001.

[3] M.H.C. Fampa and N. Maculan. Using a conic formulation for finding Steiner minimal trees. Numerical Algorithms, 35(4):315-330, 2004.

[4] H. Ouzia and N. Maculan. Mixed integer nonlinear optimization models for the Euclidean Steiner tree problem in \mathbb{R}^d , Journal of Global Optimization (JOGO), 83(1): 119-138, 2022.

[5] R.V. Pinto, H. Ouzia, N. Maculan. A new second-order conic optimization model for the $\check{\rm E}$ uclidean Steiner tree problem in \mathbb{R}^d . International Transactions in Operational Research, v. 1, p. 1, 2023.

[6] W. D. Smith. How to find Steiner minimal trees in Euclidean d-space. Algorithmica, 7:137–177, 1992.

[7] R.V. Pinto, N. Maculan. A new heuristic for the Euclidean Steiner Tree Problem in Rⁿ. TOP, v. 31, p. 391-413, 2023.

Remembering my professors and co-authors who left us: Jean Abadie Claude Berge Egon Balas Jacques Ferland Francesco Maffioli Clóvis Gonzaga Michel Minoux

Merci beaucoup Thank you Muchas gracias Muito obrigado Hartelijk dank

