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

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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.





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



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Triangle: Three given points



- Torricelli (1647) pointed out a solution when the triangle formed by the three given points does not have an angle \geq 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.



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Fermat's Challenge as an Optimization Problem





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Fermat's Challenge as an Optimization Problem



$$\begin{aligned} \overrightarrow{\mathsf{KA}} &|| &= \sqrt{(x_a - x)^2 + (y_a - y)^2} \\ \overrightarrow{\mathsf{KB}} &|| &= \sqrt{(x_b - x)^2 + (y_b - y)^2} \\ \overrightarrow{\mathsf{KC}} &|| &= \sqrt{(x_c - x)^2 + (y_c - y)^2} \\ \nabla \mathcal{D} &= \begin{pmatrix} \frac{\partial \mathcal{D}}{\partial x} \\ \frac{\partial \mathcal{D}}{\partial y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{aligned}$$

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Three Forces in Equilibrium

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



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Steiner Minimal Tree Problem

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



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- 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



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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.



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Degree of Steiner Points

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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.



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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 .



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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

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

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

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

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Example of Local Optimization



Finding the best solution...

$$\begin{split} \text{Minimize } ||x^3 - x^5|| + ||x^2 - x^5|| + ||x^5 - x^6|| + ||x^1 - x^6|| + ||x^4 - x^6|| \\ \text{subject to } x^5 \text{ and } x^6 \in \mathbb{R}^n. \end{split}$$

Instituto Alberto Luiz Combra de Des-Graduação e Perspuisa de Engenharia Given p different points in R^n , 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 $E_1 = \{[i, j] \mid i \in P, j \in S\}, E_2 = \{[i, j] \mid i < j, i \text{ and } j \in S\}$, 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:

$$x^i \in \mathbb{R}^n, \ i \in S,$$
 (1)

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



First Formulation: an example with p = 6• 6 given points. 2 1 3 6 5 Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- 6 given points.
- 4 Steiner points.



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- 6 given points.
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- All possible edges.
- An example of a set of possible edges.



Maculan-Michelon-Xavier (2000) [1]

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

$$\sum_{j\in S} y_{ij} = 1, \quad i \in P, \tag{4}$$

$$\sum_{\langle j, i \in S} y_{kj} = 1, \ j \in S - \{p+1\},$$
(5)

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

$$x^{i} \in \mathbb{R}^{n}, i \in S,$$
(7)
$$y_{ii} \in \{0, 1\}, [i, j] \in E.$$
(8)

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





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First Formulation: an example with p = 6



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First Formulation: another example

If we don't considerer

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



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Fampa-Maculan (2001,2004) [2,3]	
$(P2): Minimize \ \sum_{[i,j] \in E} d_{ij} \ subject \ to$	(9)
$d_{ij} \hspace{0.2cm} \geqslant \hspace{0.2cm} x^{i}-x^{j} - M(1-$	$-y_{ij}), \ [i,j] \in E, \tag{10}$
$d_{ij} \hspace{0.2cm} \geqslant \hspace{0.2cm} 0, \hspace{0.2cm} [i,j] \in E$	(11)
$\sum_{j\in \mathcal{S}} y_{ij} \hspace{0.1 in} = \hspace{0.1 in} 1, \hspace{0.1 in} i \in \mathcal{P},$	(12)
$\sum_{i < j, i \in S} y_{kj} \hspace{0.5cm} = \hspace{0.5cm} 1, \hspace{0.5cm} j \in S - \{p+1\}$	}, (13)
$\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \ j \in S,$	(14)
$x^i\in \mathbb{R}^n,\;i\in \mathcal{S},$	(15)
$y_{ij} \in \{0,1\}, \ \ [i,j] \in E,$	(16)
$d_{ij}\in\mathbb{R}.$	(17)
We consider $\begin{cases} x^{i} - x^{j} \approx \sqrt{\sum_{k=1}^{n} (x_{k}^{i} - x_{k}^{j})^{2} + \lambda^{2}} \\ M = maximum\{ x^{i} - x^{j} \text{ for } 1 \leqslant i \leqslant j \leqslant p\} \text{ in general}, \end{cases}$	Сорре

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

- $d_{ij} = ||a^i \bar{x}^j|| \ge 0$ or $d_{ij} = 0$, for all $[i, j] \in E_1$ and
- $d_{ij} = ||\bar{x}^i \bar{x}^j|| \ge 0$ or $d_{ij} = 0$, for all $[i, j] \in E_2$.

Second Formulation (Second Property)

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

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

$$\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S - \{p+1\}$$

$$\sum_{e \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S,$$

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,

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

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Note that...

When we consider

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

error propagations may happen.



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Ouzia-Maculan (2018) [4]

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

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

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

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

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

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

$$x^{i} \in \mathbb{R}^{n}, i \in S,$$
 (24)
 $y_{ij} \in \{0,1\}, [i,j] \in E,$ (25)

$$I_{iik} \in \mathbb{R}$$
.

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(26)

Ouzia-Maculan (2018) [4]

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

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

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

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

$$\sum_{\langle j,i \in S} y_{kj} = 1, \ j \in S - \{p+1\},$$
(31)

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

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

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

$$d_{ij} \in \mathbb{R}.$$
 (35)

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Maculan-Ouzia-Pinto (2020) [5]

$$(P5): \mbox{ Minimize } \sum_{[i,j]\in {\sf E}} d_{ij} \mbox{ subject to } \eqno(36)$$

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

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

$$\sum_{\langle j,j \in S} y_{kj} = 1, \ j \in S - \{p+1\},$$
(41)

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

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

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

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

(45)

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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 $a \in \mathbb{N}^{p^3}$, 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

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

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

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



To control the edges labeling, we define the binary variables

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

We will have $e_{ijkl} = 1$ 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):

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

$$e_{0j2(p+1)} = 1, \qquad j = 1, 2, 3.$$
 (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, ..., p - 3, j = 1, ..., 2i + 3, l = 1, ..., 2p - 2,

 $e_{ij1l} = e_{(i-1)j1l},$ (50)

$$-v_{ij} + e_{(i-1)j2l} \le e_{ij2l} \le e_{(i-1)j2l} + v_{ij},$$
(51)

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

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

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

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

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

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

We can linearize the binary product in equation (55) using the McCormick inequalities.

Finally, we relate variables e_{ijkl} to the variables y_{ij} . 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.

	•	Tetrahedro	n
	obj	time (s)	nodes
P1	0.813	9	839
P2	0.813	0.5	11
P3	0.955	0.09	5
P4	0.813	300	60493
P5	0.813	0.01	11
P6	0.813	0.01	5



	Octahedron			
	obj	time (s)	nodes	gap
P1	0.9560	10800^{*}	160633	95.9
P2	0.9560	277	1803	0
P3	1.2075	38	1517	0
P4	0.9562	10800^{*}	418903	82.7
P5	0.9560	1	1797	0
P6	0.9560	0.01	209	0



	Cube				
	obj	time (s)	nodes	gap	
P1	1.1924	10800*	79513	99.9	
P2	1.1924	10800^{*}	30291	99.9	
P3	1.3458	10800^{*}	128019	79.8	
P4	1.2003	10800^{*}	151437	99.9	
P5	1.1924	634	1043859	0	
P6	1.1924	16	20869	0	



	Icosahedron			
	obj	time (s)	nodes	gap
P1	1.6571	10800*	877	99.9
P2	1.6649	10800^{*}	1025	99.9
P3	1.98	10800^{*}	1616	99.8
P4	1.7953	10800^{*}	4253	99.9
P5	1.6319	10800^{*}	11153041	94.2
P6	1.6256	10800^{*}	5192564	89.2



	Dodecahedron				
	obj	time (s)	nodes	gap	
P1	2.2617	10800*	936	99.9	
P2	2.5618	10800^{*}	14	99.9	
P3	3.182	10800^{*}	222	99.7	
P4	2.602	10800^{*}	38	99.9	
P5	2.3516	10800^{*}	3888898	99.9	
P6	2.6449	10800^{*}	98170	99.9	



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.











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PE







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

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

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 COPP 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:

Instance	р	n	Exact	Heur1	Heur2	t1(s)	t2(s)
Tetrahedron	4	3	2.439	2.439	2.439	0.1	0.3
Octahedron	6	3	2.868	2.868	2.868	0.3	2
Cube	8	3	6.196	6.196	6.196	0.5	4.5
Icosahedron	12	3	18.553	18.553	18.664	0.9	18
Dodecahedron	20	3	22.911*	23.125	23.003	2	76

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


Hypercubes:

р	n	$Conjecture^*$	Heur1	Heur2	t1(s)	t2(s)
16	4	13.124	13.124	13.124	1.4	38
32	5	26.981	26.981	26.981	5.5	247
64	6	54.694	54.694	54.694	24	1810
128	7	110.1192	110.286	110.2189	147	15000
256	8	220.9704	221.21	221.17	1060	150000

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



Numerical experiments

Hypercube in \mathbb{R}^7



Έ

Instance*	р	n	Exact	Heur1	Heur2	t1(s)	t2(s)
3-triangles	9	2	20.526	20.626	20.526	0.3	4
Ladder	10	2	8.3451	8.4641	8.3451	0.3	4.8



Instance*	р	n	Exact	Heur1	Heur2	t1(s)	t2(s)
3-triangles	9	2	20.526	20.626	20.526	0.3	4
Ladder	10	2	8.3451	8.4641	8.3451	0.3	4.8



* 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.



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р	n	Heur2	tie	ILS	avg ρ	std
8	3	242	417	341	0.95074	0.022992
9	3	233	344	423	0.95124	0.021056
10	3	187	289	524	0.95260	0.021165
11	3	167	247	586	0.95427	0.021401
10	4	147	240	613	0.93231	0.020701
10	5	151	231	618	0.91502	0.019970

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:

			Heur1		Heur2			
р	n	opt	gap	time	opt	gap	time	
5	2	98%	0.01%	0.07	100%	0%	0.48	
5	3	96%	0.03%	0.06	99%	0.002%	0.38	
5	4	97%	0.005%	0.06	99%	0.004%	0.36	
5	5	98%	0.01%	0.06	100%	0%	0.38	
10	2	66%	0.7%	0.3	74%	0.5%	5	
10	3	53%	0.6%	0.3	52%	0.5%	5	
10	4	56%	0.5%	0.3	48%	0.5%	4.3	
10	5	59%	0.2%	0.3	55%	0.3%	4.4	



Random instances:

_			Heur1		Heur2	_
р	n	n ga	ap tii	me g	ap tim	ıe
15	5 2	2 2	% 0	.6 1	.% 14	ł
50) 2	2 8	%	9 2	.% 45	9
10	0 2	2 14	6%	50 3	% 453	30



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



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