

# The Euclidean Steiner Tree Problem in n-Space

## *Mixed-Integer Nonlinear Optimization Models*

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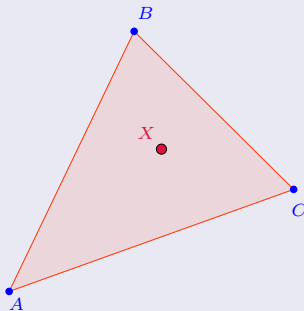
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- 2 Properties
- 3 First Formulation
- 4 Second Formulation
- 5 Second Formulation: Experiments on Platonic Solids

# 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

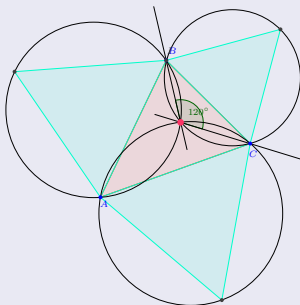


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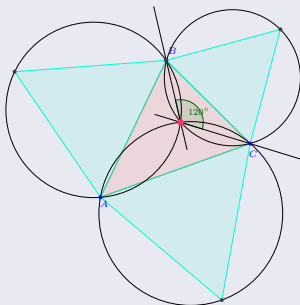


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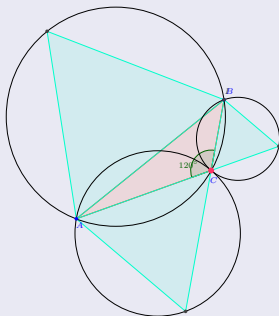
- **Torricelli** (1647) pointed out a solution when the triangle formed by the three given points does not have an angle  $\geq 120^\circ$ .

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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  $\geq 120$ , the vertex associated with this angle is the minimizing point.

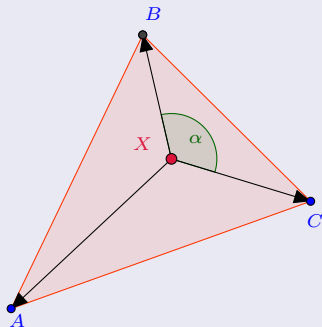


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*Given three points in the plane, find a fourth point such that the sum of its distance to the three given points is minimum.*

## Fermat's Challenge as an Optimization Problem



$$\text{Minimize } \mathcal{D} = ||\vec{XA}|| + ||\vec{XB}|| + ||\vec{XC}||$$

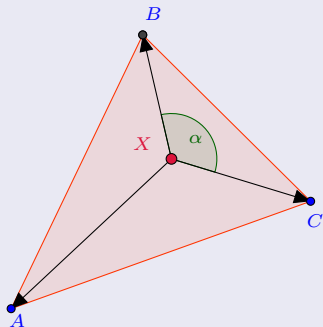


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$$\text{Minimize } \mathcal{D} = ||\vec{XA}|| + ||\vec{XB}|| + ||\vec{XC}||$$

The solution is given when

$$\nabla \mathcal{D} = 0.$$





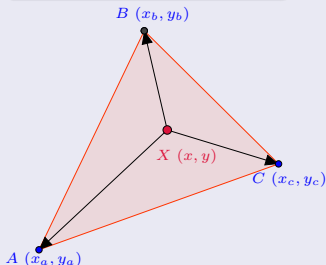
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$$\text{Min } \mathcal{D} = ||\vec{XA}|| + ||\vec{XB}|| + ||\vec{XC}||$$



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

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

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

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



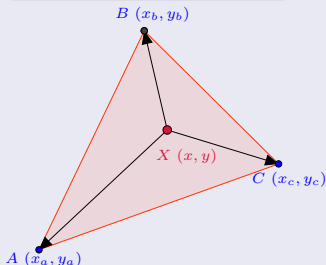
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$$\frac{\partial \mathcal{D}}{\partial y} = \frac{y_a - y}{||\vec{XA}||} + \frac{y_b - y}{||\vec{XB}||} + \frac{y_c - y}{||\vec{XC}||} = 0$$



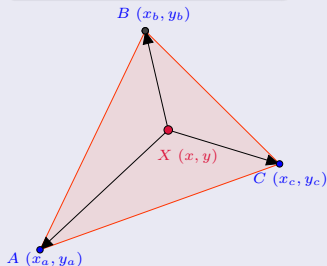
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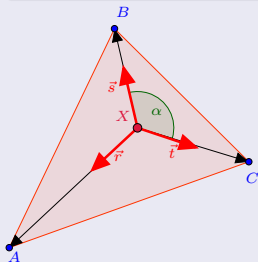
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Three Forces in Equilibrium

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

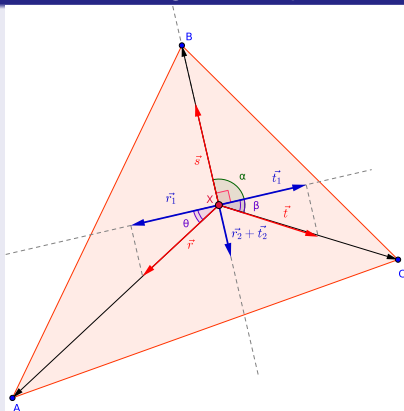


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## Fermat's Challenge as an Optimization Problem



Three Forces in Equilibrium  
( $0^\circ < \theta, \beta < 90^\circ$ )

$$\begin{aligned} \|\vec{r}_1\| &= \|\vec{t}_1\| \Rightarrow \cos(\theta) = \cos(\beta) \\ &\Rightarrow \theta = \beta \end{aligned}$$

$$\begin{aligned} \|\vec{r}_2 + \vec{t}_2\| &= \|\vec{s}\| \Rightarrow \sin(\theta) + \sin(\beta) = 1 \\ &\Rightarrow \sin(\theta) = \sin(\beta) = \frac{1}{2} \\ &\Rightarrow \theta = \beta = 30^\circ \end{aligned}$$

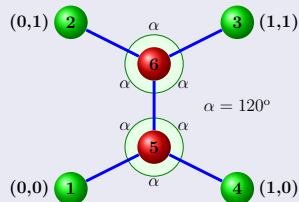
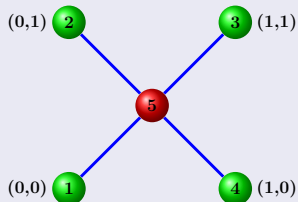
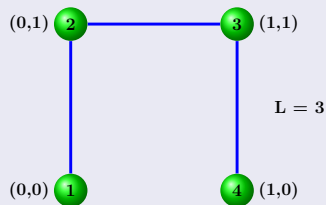
$$\alpha = 90^\circ + \beta \Rightarrow \alpha = 120^\circ.$$

# The History

An example with four points in the plane...

(0,1) 2                      3 (1,1)

(0,0) 1                      4 (1,0)



Now, consider  $p$  given points in  $\mathbb{R}^n$ .

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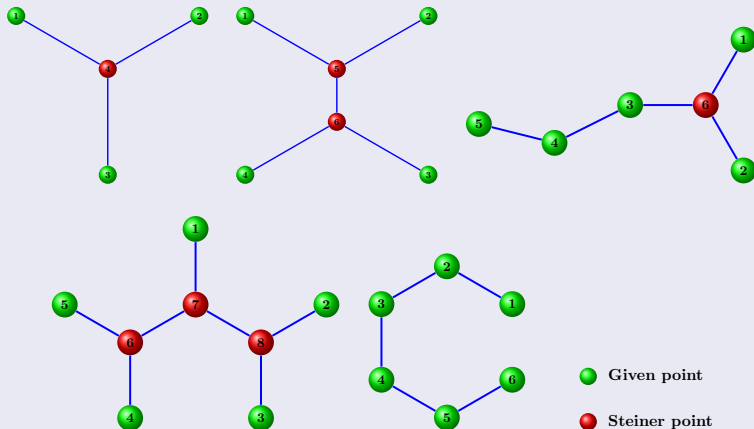
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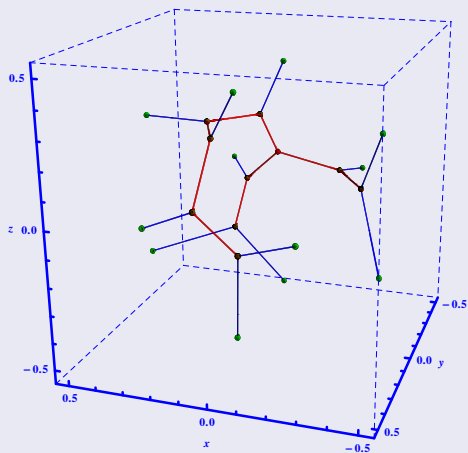
*Find a minimum tree that spans these points using or not extra points, which are called Steiner points.*

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- This problem has been shown to be NP-Hard.
- All distances are considered to be Euclidean.

## Some examples of Steiner points in $\mathbb{R}^2$



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



## Number of Steiner Points

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

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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  $120^\circ$* .

## Steiner Topology

It is a topology that satisfy 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

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

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

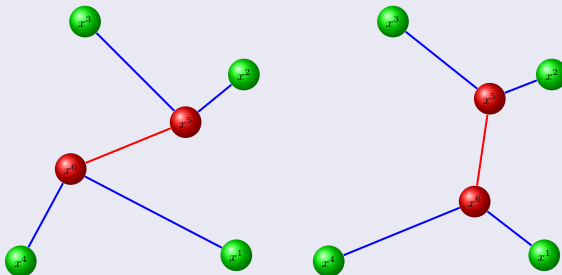
The total number of different topologies with  $k = p - 2$  Steiner points is

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

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

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

## Example of Local Optimization

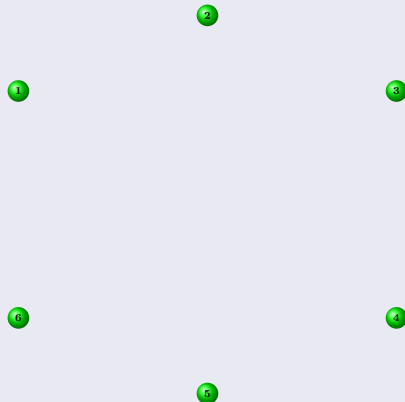


## Finding the best solution...

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

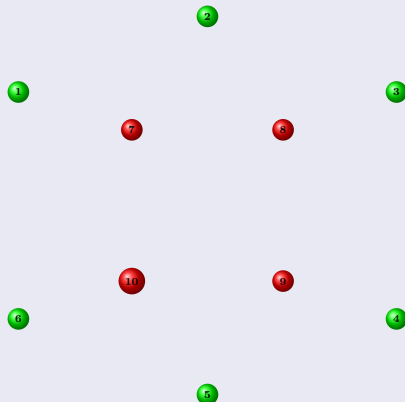
## First Formulation: an example with $p = 6$

- 6 given points.



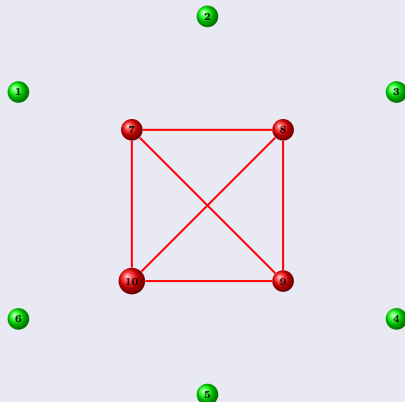
## First Formulation: an example with $p = 6$

- 6 given points.
- 4 Steiner points.



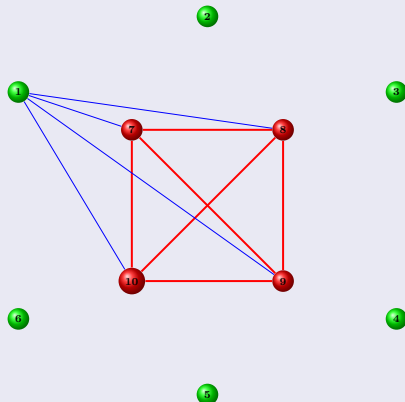
## First Formulation: an example with $p = 6$

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



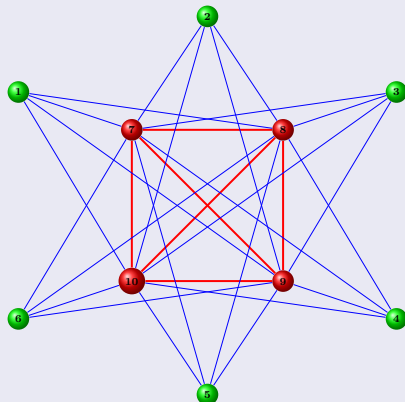
## First Formulation: an example with $p = 6$

- 6 given points.
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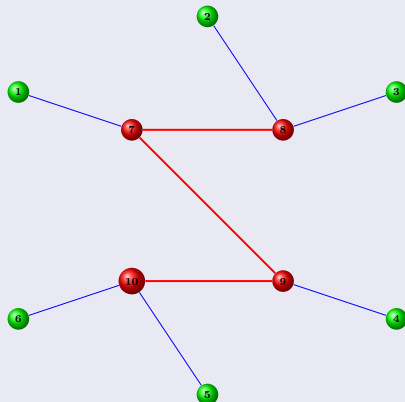
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## First Formulation: an example with $p = 6$

- 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.
- An example of a set of possible edges.



Given  $p$  points in  $\mathbb{R}^n$ , we define a especial graph  $G = (V, E)$ .

## First Formulation

Let's consider...

- $P = \{1, 2, \dots, p\}$  as the set of vertices indices which are related to the given points.
- $S = \{p + 1, p + 2, \dots, 2p - 2\}$  as the set of vertices indices which are related to the Steiner points.
- $x^i$  as the coordinates of vertex  $i \in P \cup S$ .
- $y_{ij}$  as the binary variable associated with the edge  $\{i, j\} \in E$ , such as:

$$y_{ij} = \begin{cases} 0, & \text{if there is no edge } \{i, j\} \in E \text{ in the solution;} \\ 1, & \text{otherwise.} \end{cases}$$

Given  $p$  points in  $\mathbb{R}^n$ , we define a especial graph  $G = (V, E)$ .

## First Formulation

$$(P) : \text{Minimize } \sum_{[i,j] \in E} \|x^i - x^j\| y_{ij} \text{ subject to} \quad (1)$$

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P = \{1, 2, \dots, p\}, \quad (2)$$

$$\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S - \{p+1\}, \quad (3)$$

$$x^i \in \mathbb{R}^n, \quad i \in S, \quad (4)$$

$$y_{ij} \in \{0, 1\}, \quad [i, j] \in E, \quad (5)$$

where  $\|x^i - x^j\| = \sqrt{\sum_{l=1}^n (x_l^i - x_l^j)^2}$  is the Euclidean distance between  $x^i$  and  $x^j$ .

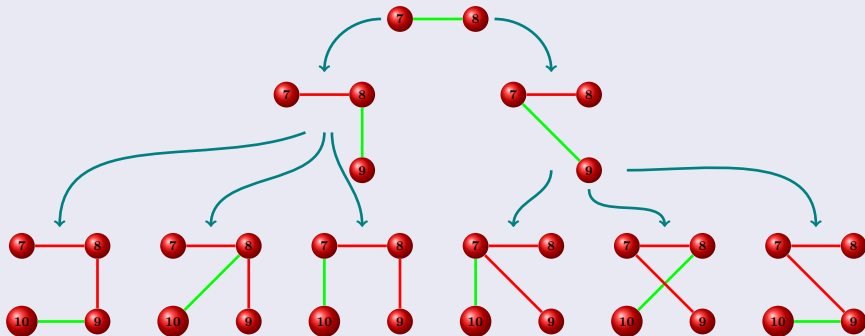
## First Formulation: an example with $p = 6$

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

$$y_{7,8} = 1$$

$$y_{7,9} + y_{8,9} = 1$$

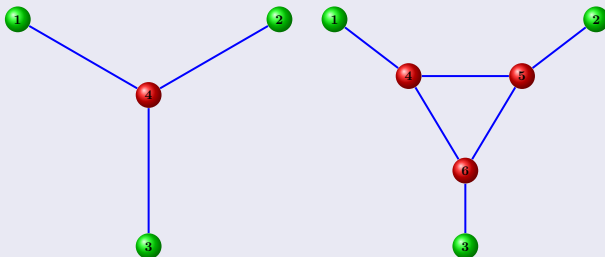
$$y_{7,10} + y_{8,10} + y_{9,10} = 1$$



## First Formulation: another example

If we don't consider

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



## First Formulation (another way to write)

$$(P) : \text{Minimize } \sum_{[i,j] \in E} (t_{ij}^2 - u_{ij}^2) \text{ subject to} \quad (6)$$

$$\|x^i - x^j\| - (t_{ij} + u_{ij}) \leq 0, \quad [i,j] \in E, \quad (7)$$

$$y_{ij} - (t_{ij} - u_{ij}) = 0, \quad [i,j] \in E, \quad (8)$$

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P = \{1, 2, \dots, p\}, \quad (9)$$

$$\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S = \{p+1, \dots, 2p-2\}, \quad (10)$$

$$\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S - \{p+1\}, \quad (11)$$

$$x^i \in \mathbb{R}^n, \quad i \in S, \quad (12)$$

$$y_{ij} \in \{0, 1\}, \quad [i,j] \in E. \quad (13)$$

## First Formulation: Lagrangian Relaxation

$$\begin{aligned}\mathcal{L}(x, y, t, u, \alpha, \beta) &= \sum_{[i,j] \in E} (t_{ij}^2 - u_{ij}^2) + \sum_{[i,j] \in E} [||x^i - x^j|| - (t_{ij} + u_{ij})]\alpha_{ij} + \\ &+ \sum_{[i,j] \in E} [y_{ij} - (t_{ij} - u_{ij})]\beta_{ij}\end{aligned}$$

or

$$\begin{aligned}\mathcal{L}(x, y, t, u, \alpha, \beta) &= \sum_{[i,j] \in E} [t_{ij}^2 - u_{ij}^2 - (\alpha_{ij} + \beta_{ij})t_{ij} - (\alpha_{ij} - \beta_{ij})u_{ij}] + \\ &+ \sum_{[i,j] \in E} \alpha_{ij}||x^i - x^j|| + \sum_{[i,j] \in E} \beta_{ij}y_{ij},\end{aligned}$$

where

- $\alpha_{ij} \geq 0$  is the dual variable associated to constraint (7).
- $\beta_{ij} \in \mathbb{R}$  is the dual variable associated to constraint (8).

## First Formulation: Lagrangian Relaxation and The Dual Program

$$\mathcal{D}(\alpha, \beta) = \text{minimum } \{\mathcal{L}(x, y, t, u, \alpha, \beta) \text{ subject to (15) – (20)}\} \quad (14)$$

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P, \quad (15)$$

$$\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S, \quad (16)$$

$$\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S - \{p+1\}, \quad (17)$$

$$y_{ij} \in \{0, 1\}, \quad [i, j] \in E, \quad (18)$$

$$0 \leq t_{ij} + u_{ij} \leq M, \quad (19)$$

$$x^i \in R^n, \quad i \in S \quad (20)$$

where  $M = \text{maximum } \{\|x^i - x^j\| \text{ for } 1 \leq i \leq j \leq p\}$ .





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We define

$$\mathcal{D}_1(t, u, \alpha, \beta) = \text{minimum } \left\{ \sum_{[i,j] \in E} [t_{ij}^2 - u_{ij}^2 - (\alpha_{ij} + \beta_{ij})t_{ij} - (\alpha_{ij} - \beta_{ij})u_{ij}] \mid \text{s.t. (19)} \right\},$$

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We define

$$\mathcal{D}_2(x, \alpha) = \text{minimum } \left\{ \sum_{[i,j] \in E} \alpha_{ij} \|x^i - x^j\| \mid \text{s.t. (20)} \right\},$$

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where  $M = \text{maximum } \{\|x^i - x^j\| \text{ for } 1 \leq i \leq j \leq p\}$ .

We define

$$\mathcal{D}_3(y, \beta) = \text{minimum } \left\{ \sum_{[i,j] \in E} \beta_{ij} y_{ij} \mid \text{s.t. (15) - (18)} \right\},$$

## First Formulation: Lagrangian Relaxation and The Dual Program

$$\mathcal{D}(\alpha, \beta) = \text{minimum } \{\mathcal{L}(x, y, t, u, \alpha, \beta) \text{ subject to (15) – (20)}\} \quad (14)$$

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P, \quad (15)$$

$$\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S, \quad (16)$$

$$\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S - \{p+1\}, \quad (17)$$

$$y_{ij} \in \{0, 1\}, \quad [i, j] \in E, \quad (18)$$

$$0 \leq t_{ij} + u_{ij} \leq M, \quad (19)$$

$$x^i \in R^n, \quad i \in S \quad (20)$$

where  $M = \text{maximum } \{\|x^i - x^j\| \text{ for } 1 \leq i \leq j \leq p\}$ .

Thus we can write

$$\mathcal{D}(\alpha, \beta) = \mathcal{D}_1(t, u, \alpha, \beta) + \mathcal{D}_2(x, \alpha) + \mathcal{D}_3(y, \beta).$$

## First Formulation: Lagrangian Relaxation and The Dual Program

$$\mathcal{D}(\alpha, \beta) = \text{minimum } \{\mathcal{L}(x, y, t, u, \alpha, \beta) \text{ subject to (15) – (20)}\} \quad (14)$$

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$$x^i \in R^n, \quad i \in S \quad (20)$$

where  $M = \text{maximum } \{\|x^i - x^j\| \text{ for } 1 \leq i \leq j \leq p\}$ .

The Dual Problem will be

$$\text{Maximize } \mathcal{D}(\alpha, \beta) \text{ subject to} \quad (21)$$

$$\alpha \geq 0, \quad [i, j] \in E, \quad (22)$$

$$\beta \in R, \quad [i, j] \in E. \quad (23)$$

## First Formulation: Lagrangian Relaxation and The Dual Program

The Lagrangian Relaxation and The Dual Program were proposed by

*N. Maculan, P. Michelon and A. E. Xavier, in*

*The Euclidean Steiner problem in  $\mathbb{R}^n$  : A mathematical programming formulation, Annals of Operations Research, vol. 96, pp. 209-220, 2000.*

## The Idea

To improve the enumeration scheme presented by Smith<sup>a</sup>, by the inclusion of **lower bounds** which are obtained from the Dual Problem Solution.

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<sup>a</sup>W. D. Smith, *How to find Steiner minimal trees in Euclidean d-space*, Algorithmica, vol. 7, pp. 137-177, 1992.



## First Formulation: more improvements were proposed in...

C. D'Ambrosio, M. Fampa, J. Lee, and S. Vigerske. *On a nonconvex MINLP formulation of the Euclidean Steiner tree problems in  $n$ -space*, LNCS (SEA 2015), vol. 9125, pp. 122-133, 2015.

## The Idea

In this paper, C. D'Ambrosio (École Polytechnique), M. Fampa (UFRJ), J. Lee (University of Michigan), and S. Vigerske (GAMS) address some of the relevant issues:

- non-differentiability of  $\| \cdot \|$
- tightness of the N. Maculan, P. Michelon and A. E. Xavier formulation
- using geometry for nonlinear tightening



## Second Formulation

$$(P) : \text{Minimize } \sum_{[i,j] \in E} d_{ij} \text{ subject to} \quad (24)$$

$$d_{ij} \geq \|a^i - x^j\| - M(1 - y_{ij}), \quad [i,j] \in E_1, \quad (25)$$

$$d_{ij} \geq \|x^i - x^j\| - M(1 - y_{ij}), \quad [i,j] \in E_2, \quad (26)$$

$$d_{ij} \geq 0, \quad [i,j] \in E \quad (27)$$

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P, \quad (28)$$

$$\sum_{i < j, i \in S} y_{kj} = 1, \quad j \in S - \{p+1\}, \quad (29)$$

$$\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S, \quad (30)$$

$$x^i \in \mathbb{R}^n, \quad i \in S, \quad (31)$$

$$y_{ij} \in \{0, 1\}, \quad [i,j] \in E, \quad (32)$$

$$d_{ij} \in \mathbb{R}. \quad (33)$$

We consider  $\begin{cases} \|x^i - x^j\| \approx \sqrt{\sum_{l=1}^n (x_l^i - x_l^j)^2 + \lambda^2} \\ M = \text{maximum}\{\|a^i - a^j\| \text{ for } 1 \leq i \leq j \leq p\} \text{ in general,} \\ E_1 = \{[i,j] | i \in P, j \in S\}, E_2 = \{[i,j] | i \in S, j \in S\} \text{ e } E = E_1 \cup E_2 \end{cases}$



## Second Formulation (First Property)

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

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

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

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

## 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  $p > 3$ ,

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

## 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.

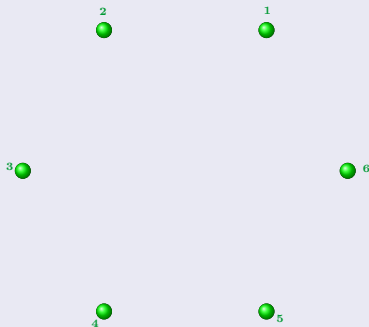
## Note that...

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.

## Example: Regular Hexagon



- 6 given points.
- Each given point is in a vertex of a Regular Hexagon.
- Each side of the Hexagon is equal to 1.

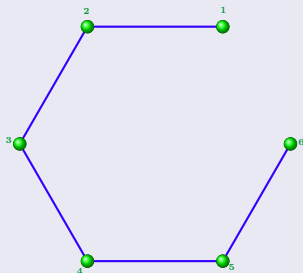
## Note that...

When we consider

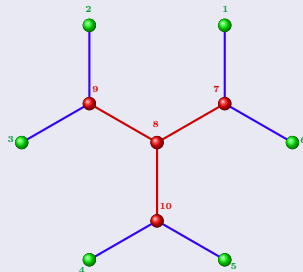
$$||x^i - x^j|| \approx \sqrt{\sum_{l=1}^n (x_l^i - x_l^j)^2 + \lambda^2},$$

error propagations may happen.

## Example: Regular Hexagon



- Objective Function: 5
- $\lambda^2 = 10^{-8}$



- Objective Function:  $5.196 = 3\sqrt{3}$
- $\lambda^2 = 10^{-6}$

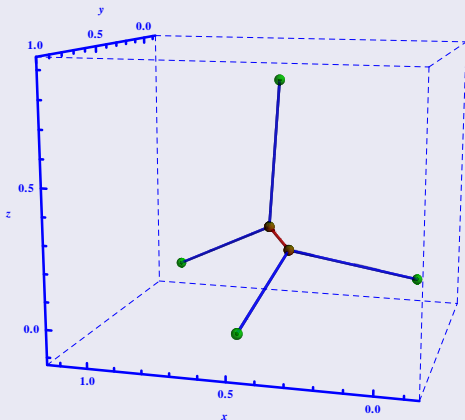
## Second Formulation: Experiments on Platonic Solids

**Tabela:** The Second Formulation (SF) applied to three Platonic solids.

Platonic Solids	Tetrahedron		Octahedron		Cube	
	SF <sub>1</sub>	SF <sub>2</sub>	SF <sub>1</sub>	SF <sub>2</sub>	SF <sub>1</sub>	SF <sub>2</sub>
$D_{MST}$	2,43911	2,43911	2,86801	2,86801	3,57735	3,57735
Execution Time (s)	3,27	3,51	133,43	205,80	25.052,6	10.804
Iterations	2257	160	52.279	83.345	9.355.941	4.356.522
Nodes	10	10	202	940	79.718	35.944

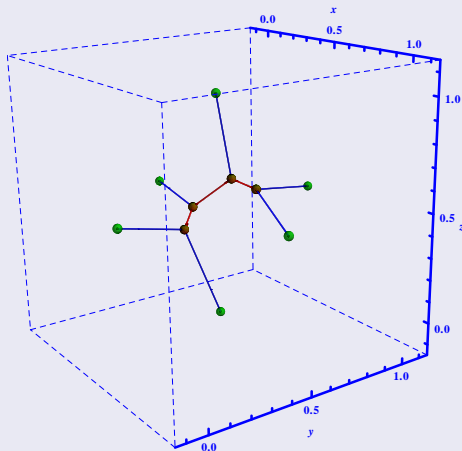
- SF<sub>1</sub> is the model without the constraint of the third property.
- SF<sub>2</sub> is the model with this constraint.
- $D_{MST}$  is the length of the minimum Steiner tree obtained.
- BONMIN package from COIN-OR Library and AMPL are used.
- $\lambda^2$  is used in order to allow the problem to be differentiable.
- In this case, we set the input data, so that the param  $M$  in constraints (26)-(27), could be considered equal to 1.

## Second Formulation: One Solution for a Tetrahedron



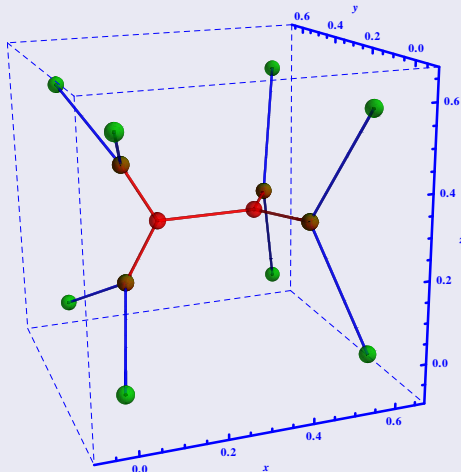
- Number of Points (Green): 4
- Number of Steiner Points (Red): 2
- Objective Function: 2.43911
- Execution Time: 3.27 s

### Second Formulation: One Solution for an Octahedron



- Number of Points (Green): 6
- Number of Steiner Points (Red): 4
- Objective Function: 2.86801
- Execution Time: 2.22 min

## Second Formulation: One Solution for a Cube

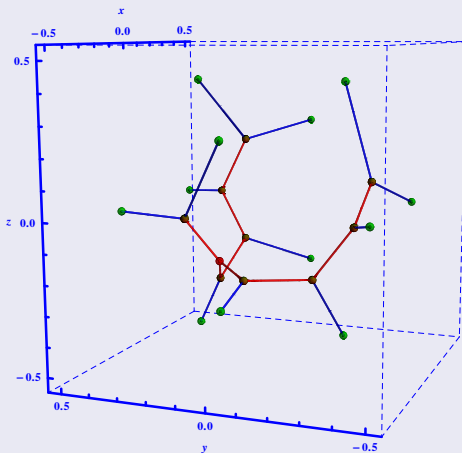


- Number of Points (Green): 8
- Number of Steiner Points (Red): 6
- Objective Function: 3.57735
- Execution Time: 3 h



# Second Formulation: Experiments on Platonic Solids

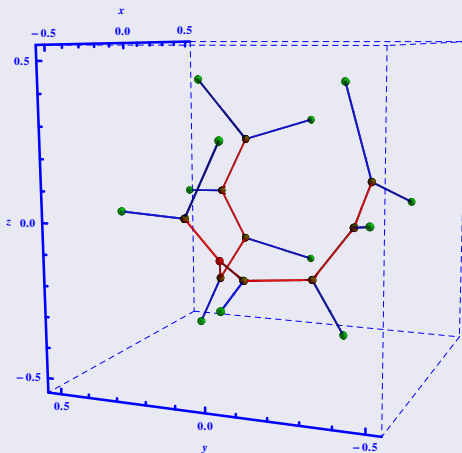
## Second Formulation: One Solution for an Icosahedron



- Number of Points (Green): 12
- Number of Steiner Points (Red): 10
- Objective Function: 4.90531
- Execution Time: 48 h (not finished).

# Second Formulation: Experiments on Platonic Solids

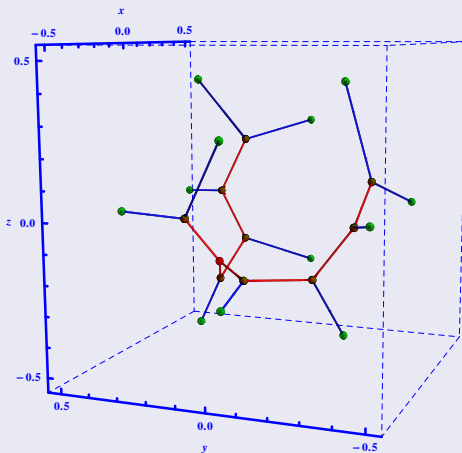
## Second Formulation: One Solution for an Icosahedron



- Number of Points (Green): 12
- Number of Steiner Points (Red): 10
- Objective Function: 4.90531
- Execution Time: 48 h (not finished).
- It is important to note that the value of the objective function corresponds to 18,312620163, when the icosahedron has edges equal to 2.

# Second Formulation: Experiments on Platonic Solids

## Second Formulation: One Solution for an Icosahedron



- Number of Points (Green): 12
  - Number of Steiner Points (Red): 10
  - Objective Function: 4.90531
  - Execution Time: 48 h (not finished).
- 
- It is important to note that the value of the objective function corresponds to 18,312620163, when the icosahedron has edges equal to 2.
  - The best solution presented in literature for the icosahedron with edges equal to 2 was 18,5529.

## Second Formulation: More improvements...

### Second Formulation: more improvements were proposed in...

M. Fampa, J. Lee, and W. Melo. *A specialized branch-and-bound algorithm for the Euclidean Steiner tree problem in  $n$ -space*, Computational Optimization and Applications, vol. 63(2) DOI 10.1007/s10589-016-9835-z, 2016.

### The Idea

M. Fampa (UFRJ), J. Lee (University of Michigan), and W. Melo (UFU) address some of the relevant issues:

- Isomorphic subproblems.
- Tightness of the Second Formulation

# Thank you!