The Euclidean Steiner Tree Problem in $\mathbb{R}^n$
Mathematical Models

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UFRJ

Summary of talk

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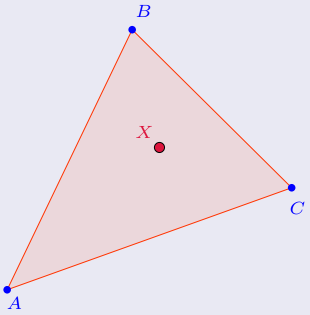
Challenge of Fermat in the 17th century

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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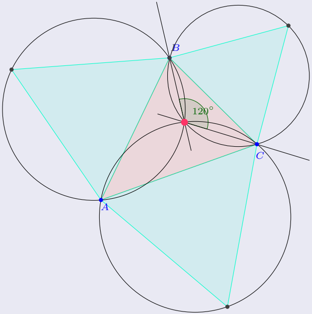

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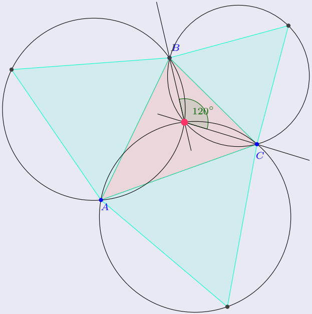

Torricelli (1647) pointed out a solution when the triangle formed by the three given points does not have an angle $\geq 120^{\circ}$.

The History

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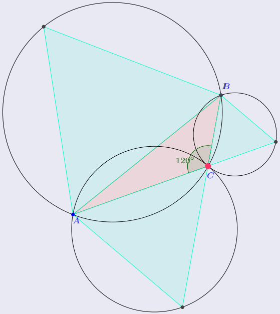

Torricelli (1647) pointed out a solution when the triangle formed by the three given points does not have an angle $\geq 120^\circ$.

Heinen (1837) apparently is the first to prove that, for a triangle in which an angle is $\geq 120^\circ$, the vertex associated with this angle is the minimizing point.

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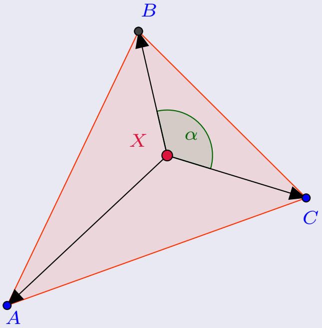
Fermat's Challenge as an Optimization Problem



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

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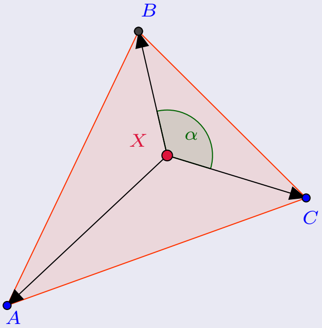

Minimize $\mathcal{D} = ||\overrightarrow{XA}|| + ||\overrightarrow{XB}|| + ||\overrightarrow{XC}||$

The solution is given when

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

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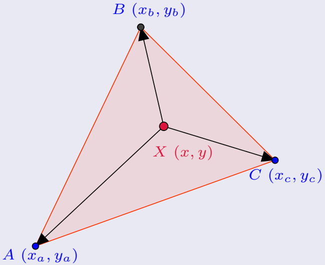

$$\begin{aligned}
||\overrightarrow{XA}|| &= \sqrt{(x_a - x)^2 + (y_a - y)^2} \\
||\overrightarrow{XB}|| &= \sqrt{(x_b - x)^2 + (y_b - y)^2} \\
||\overrightarrow{XC}|| &= \sqrt{(x_c - x)^2 + (y_c - y)^2}
\end{aligned}$$

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

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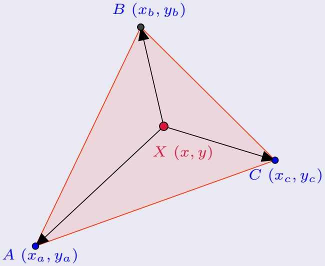

$$\frac{\partial \mathcal{D}}{\partial x} = \frac{x_a - x}{||\overrightarrow{XA}||} + \frac{x_b - x}{||\overrightarrow{XB}||} + \frac{x_c - x}{||\overrightarrow{XC}||} = 0$$

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

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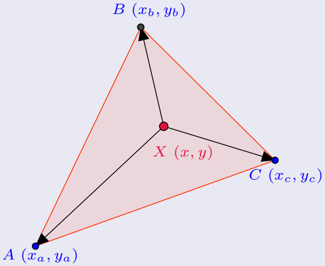

$$\begin{pmatrix} \dfrac{\partial \mathcal{D}}{\partial x} \\[2ex] \dfrac{\partial \mathcal{D}}{\partial y} \end{pmatrix} = \underbrace{\begin{pmatrix} \dfrac{x_a - x}{||\overrightarrow{XA}||} \\[2ex] \dfrac{y_a - y}{||\overrightarrow{XA}||} \end{pmatrix} + \begin{pmatrix} \dfrac{x_b - x}{||\overrightarrow{XB}||} \\[2ex] \dfrac{y_b - y}{||\overrightarrow{XB}||} \end{pmatrix} + \begin{pmatrix} \dfrac{x_c - x}{||\overrightarrow{XC}||} \\[2ex] \dfrac{y_c - y}{||\overrightarrow{XC}||} \end{pmatrix}}_{\text{Unitary Vectors Sum}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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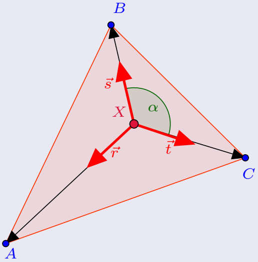

Three Forces in Equilibrium

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

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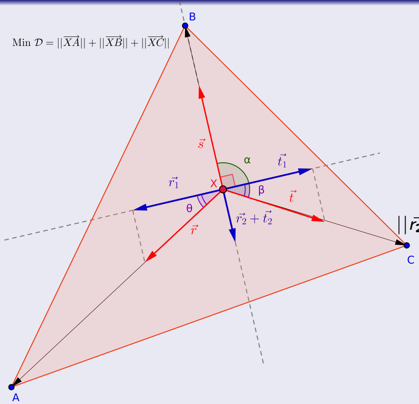

Three Forces in Equilibrium
$(0^\circ < \theta, \beta < 90^\circ)$

$$||\vec{r_1}|| = ||\vec{t_1}|| \quad \Rightarrow \quad \cos(\theta) = \cos(\beta)$$
$$\Rightarrow \quad \theta = \beta$$

$$||\vec{r_2} + \vec{t_2}|| = ||\vec{s}|| \quad \Rightarrow \quad \sin(\theta) + \sin(\beta) = 1$$
$$\Rightarrow \quad \sin(\theta) = \sin(\beta) = \frac{1}{2}$$
$$\Rightarrow \quad \theta = \beta = 30^\circ$$

$$\alpha = 90^\circ + \beta \quad \Rightarrow \quad \alpha = \mathbf{120}^\circ.$$

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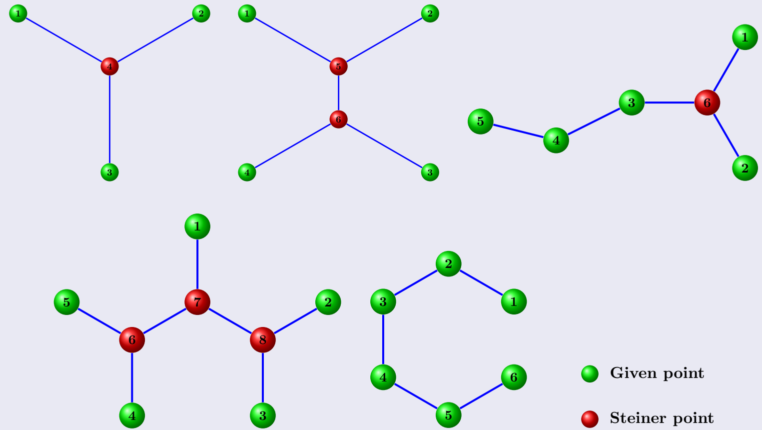
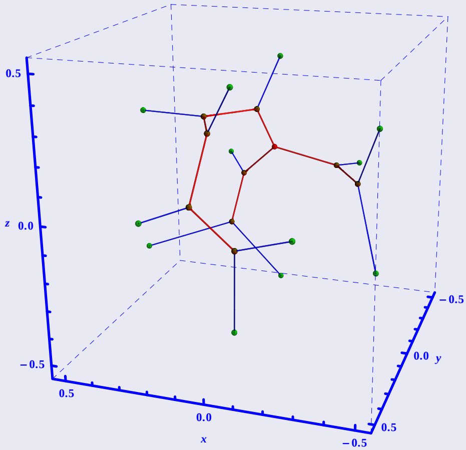
- This is a very well known problem in combinatorial optimization.
- This problem has been shown to be NP-Hard.
- All distances are considered to be Euclidean.

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



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



Number of Steiner Points

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

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

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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°*.

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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

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

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

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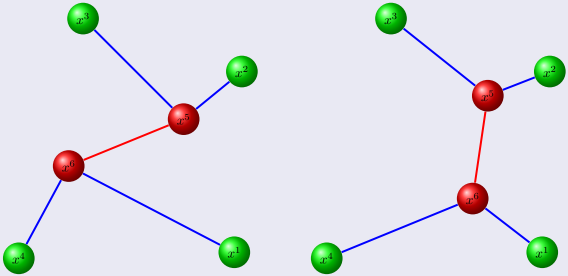
Full Steiner Topologies ($k = p - 2$)

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

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

Example of Local Optimization



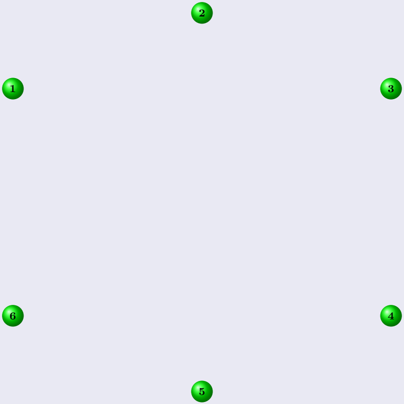
Finding the best solution...

$$\text{Minimize } ||x^3 - x^5|| + ||x^2 - x^5|| + ||x^5 - x^6|| + ||x^1 - x^6|| + ||x^4 - x^6||$$

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

First Formulation: an example with $p = 6$

6 given points.



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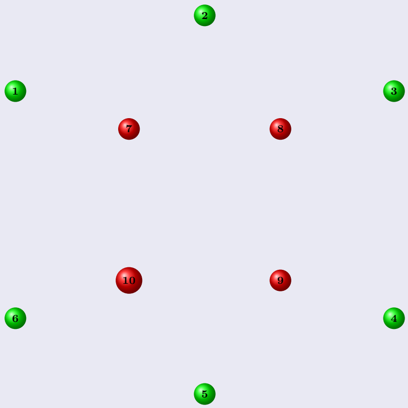
4 Steiner points.



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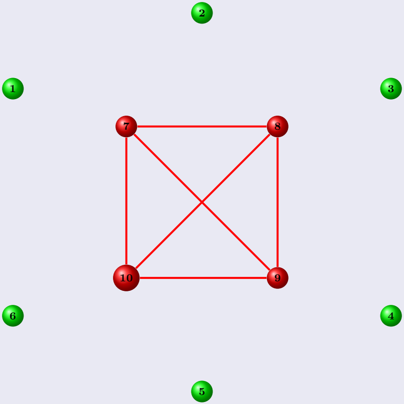
All possible edges among Steiner points.



First Formulation: an example with $p = 6$

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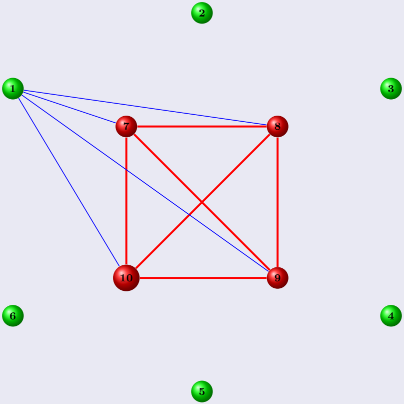
All possible edges among Steiner points.

All possible connections between a given point and a Steiner point.



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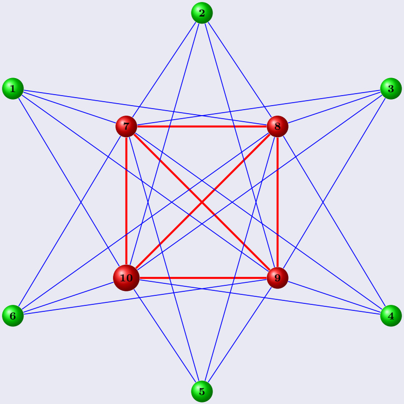

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First Formulation: an example with $p = 6$

6 given points.

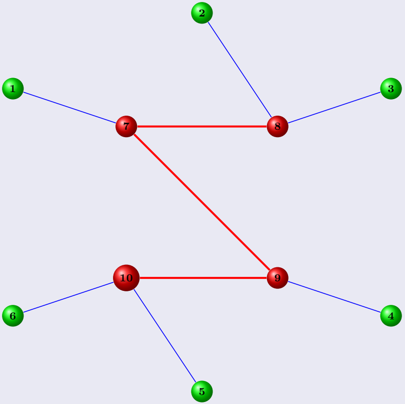
4 Steiner points.

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

$$(\mathbf{P}): \quad \textbf{Minimize} \sum_{[\mathbf{i},\mathbf{j}]\in \mathbf{E}} ||\mathbf{x}^{\mathbf{i}} - \mathbf{x}^{\mathbf{j}}||\mathbf{y}_{\mathbf{ij}} \ \textbf{subject to} \tag{1}$$

$$\sum_{j\in S} y_{ij} = 1, \quad i \in P = \{1, 2, \ldots, p\}, \tag{2}$$

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

$$x^i \in \mathbb{R}^n, \ i \in S, \tag{4}$$

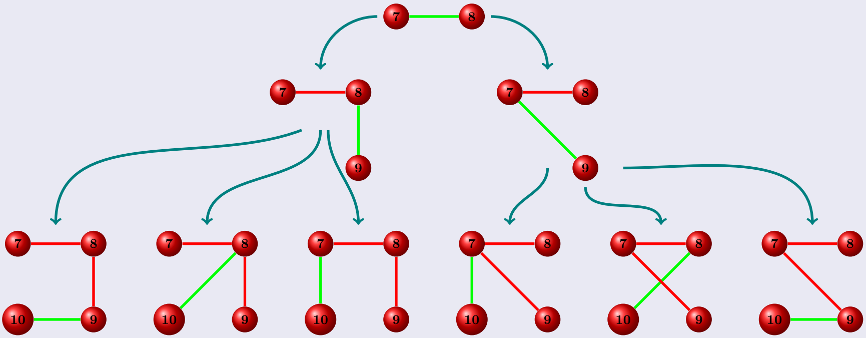
$$y_{ij} \in \{0, 1\}, \quad [i, j] \in E, \tag{5}$$

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 $p = 6$

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

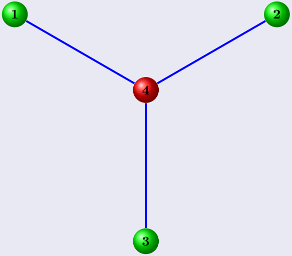
$$\begin{aligned} y_{7,8} &= 1 \\ y_{7,9} + y_{8,9} &= 1 \\ y_{7,10} + y_{8,10} + y_{9,10} &= 1 \end{aligned}$$

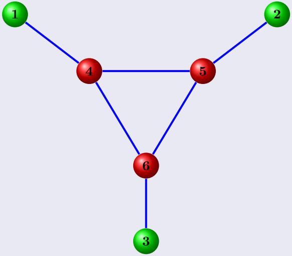


First Formulation: another example

If we don't considerer

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





First Formulation (another way to write)

$$\textbf{(P)}: \quad \textbf{Minimize} \sum_{[\mathbf{i},\mathbf{j}]\in \mathbf{E}} (\mathbf{t}_{\mathbf{ij}}^2 - \mathbf{u}_{\mathbf{ij}}^2) \ \textbf{subject to} \tag{6}$$

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

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

$$\sum_{j \in S} y_{ij} = 1, \quad i \in P = \{1, 2, \ldots, p\}, \tag{9}$$

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

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

$$x^i \in \mathbb{R}^n, \ i \in S, \tag{12}$$

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

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

$\alpha_{ij} \geqslant 0$ is the dual variable associated to constraint (7).

$\beta_{ij} \in R$ is the dual variable associated to constraint (8).

First Formulation: Lagrangian Relaxation and The Dual Program

$$\mathcal{D}(\alpha, \beta) = \textbf{ minimum } \{\mathcal{L}(x, y, t, u, \alpha, \beta) \textbf{ subject to } \mathbf{(15)} - \mathbf{(20)}\} \tag{14}$$

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

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

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

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

$$0 \leq t_{ij} + u_{ij} \leq M, \tag{19}$$

$$x^i \in R^n, \; i \in S \tag{20}$$

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

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We define

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

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

We define

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

First Formulation: Lagrangian Relaxation and The Dual Program

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

We define

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

First Formulation: Lagrangian Relaxation and The Dual Program

$$\mathcal{D}(\alpha,\beta) = \textbf{ minimum } \{\mathcal{L}(x,y,t,u,\alpha,\beta) \textbf{ subject to (15)} - \textbf{(20)}\} \tag{14}$$

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

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

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

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

$$0 \leq t_{ij} + u_{ij} \leq M, \tag{19}$$

$$x^i \in R^n, \quad i \in S \tag{20}$$

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

Thus we can write

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

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First Formulation: Lagrangian Relaxation and The Dual Program

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

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

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

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

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

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

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

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

The Dual Problem will be

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

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

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

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[a], by the inclusion of **lower bounds** which are obtained from the Dual Problem Solution.

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

Second Formulation

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

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

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

$$d_{ij} \geqslant 0, \; [i,j] \in E \tag{27}$$

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

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

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

$$x^i \in \mathbb{R}^n, \; i \in S, \tag{31}$$

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

$$d_{ij} \in \mathbb{R}. \tag{33}$$

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

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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

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

$d_{ij} = ||\bar{x}^i - \bar{x}^j|| \geqslant 0$ 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:

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

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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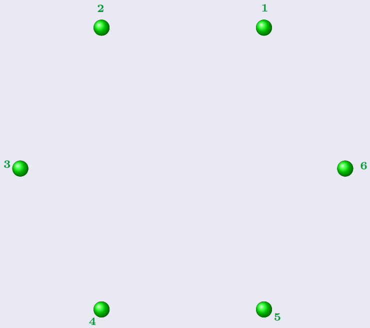
Note that...

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.

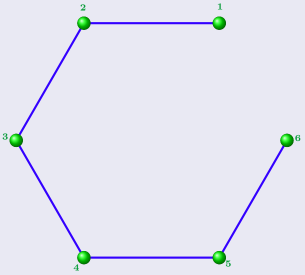
Note that...

When we consider

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

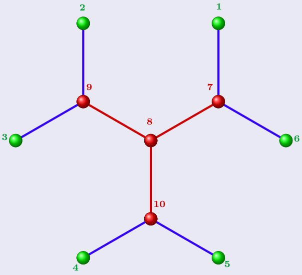
error propagations may happen.

Example: Regular Hexagon



Objective Function: 5

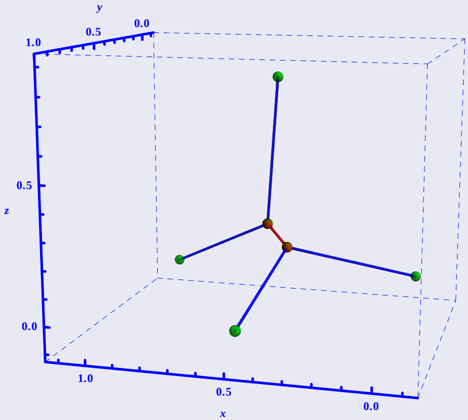
$\lambda^2 = 10^{-8}$



Objective Function: $5.196 = 3\sqrt{3}$

$\lambda^2 = 10^{-6}$

Second Formulation: One Solution for a Tetrahedron



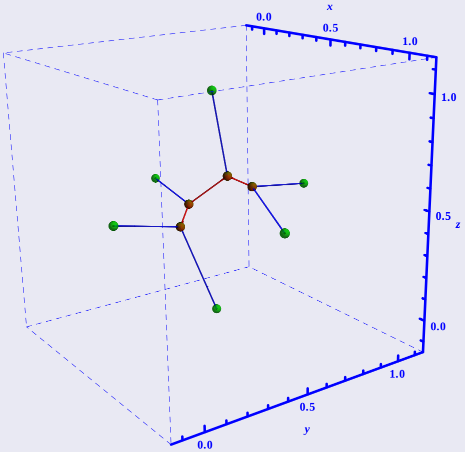
Number of Points (Green): 4

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

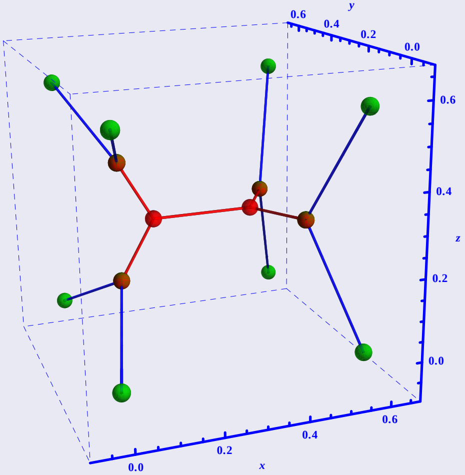
Number of Steiner Points (Red): 4

Objective Function: 2.86801

Execution Time: 2.22 min

Second Formulation: Experiments on Platonic Solids

Second Formulation: One Solution for a Cube



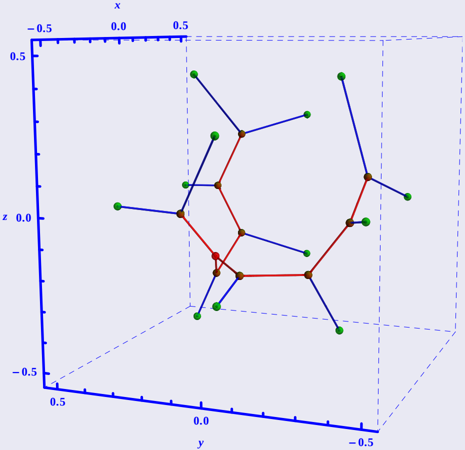
Number of Points (Green): 8

Number of Steiner Points (Red): 6

Objective Function: 3.57735

Execution Time: 3 h

Second Formulation: 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).

Thank you!

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