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

Mathematical Models

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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.*

Triangle: Three given points
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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 $\geq 120^\circ$. 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 $D = ||\overrightarrow{XA}|| + ||\overrightarrow{XB}|| + ||\overrightarrow{XC}||$
The History

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Fermat’s Challenge as an Optimization Problem

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

The solution is given when $\nabla D = 0$. 
The History

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Fermat’s Challenge as an Optimization Problem

Min \( D = ||\overrightarrow{XA}|| + ||\overrightarrow{XB}|| + ||\overrightarrow{XC}|| \)

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

\( \nabla D = \begin{pmatrix} \frac{\partial D}{\partial x} \\ \frac{\partial D}{\partial y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \)
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Fermat’s Challenge as an Optimization Problem

Min \( D = \|\overrightarrow{XA}\| + \|\overrightarrow{XB}\| + \|\overrightarrow{XC}\| \)

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

\[
\frac{\partial D}{\partial y} = \frac{y_a - y}{\|\overrightarrow{XA}\|} + \frac{y_b - y}{\|\overrightarrow{XB}\|} + \frac{y_c - y}{\|\overrightarrow{XC}\|} = 0
\]
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Fermat’s Challenge as an Optimization Problem

Min \( D = ||\vec{XA}|| + ||\vec{XB}|| + ||\vec{XC}|| \)

\[
\begin{pmatrix}
\frac{\partial D}{\partial x} \\
\frac{\partial D}{\partial y}
\end{pmatrix}
= \begin{pmatrix}
\frac{x_a - x}{||\vec{XA}||} \\
\frac{y_a - y}{||\vec{XA}||}
\end{pmatrix}
+ \begin{pmatrix}
\frac{x_b - x}{||\vec{XB}||} \\
\frac{y_b - y}{||\vec{XB}||}
\end{pmatrix}
+ \begin{pmatrix}
\frac{x_c - x}{||\vec{XC}||} \\
\frac{y_c - y}{||\vec{XC}||}
\end{pmatrix}
= \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]

Unitary Vectors Sum
The History

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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

Min $D = ||XA|| + ||XB|| + ||XC||$

Three Forces in Equilibrium

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

Fermat’s Challenge as an Optimization Problem

Three Forces in Equilibrium

\[(0^\circ < \theta, \beta < 90^\circ)\]

\[||\vec{r}_1|| = ||\vec{t}_1|| \Rightarrow \cos(\theta) = \cos(\beta)\]
\[\Rightarrow \theta = \beta\]

\[||\vec{r}_2 + \vec{t}_2|| = ||\vec{s}|| \Rightarrow \sin(\theta) + \sin(\beta) = 1\]
\[\Rightarrow \sin(\theta) = \sin(\beta) = \frac{1}{2}\]
\[\Rightarrow \theta = \beta = 30^\circ\]

\[\alpha = 90^\circ + \beta \Rightarrow \alpha = 120^\circ.\]
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.*
Problem Definition

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This is a very well known problem in combinatorial optimization.
Problem Definition

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

**Steiner Minimal Tree Problem**

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

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

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

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

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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Given $p$ points $x^i \in \mathbb{R}^n$, $i = 1, 2, \ldots, p$, 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 $x^i \in \mathbb{R}^n$, $i = 1, 2, \ldots, p$, 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 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 $\mathbb{R}^n$. 
Steiner Topology

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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 \( \mathbb{R}^n \).

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

The total number of different topologies with \( k = p - 2 \) Steiner points is

\[
1 \cdot 3 \cdot 5 \cdot 7 \ldots (2p - 5) = (2p - 5)!!.
\]
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 $x^6 \in \mathbb{R}^n$. 
First Formulation: an example with $p = 6$

6 given points.
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- 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.

4 Steiner points.

All possible edges among Steiner points.

All possible connections between a given point and a Steiner point.
First Formulation: an example with $p = 6$

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

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

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

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

\[ x^i \in \mathbb{R}^n, \quad i \in S, \]

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

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

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First Formulation: an example with \( p = 6 \)

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

\[
y_{7,8} = 1
\]

\[
y_{7,9} + y_{8,9} = 1
\]

\[
y_{7,10} + y_{8,10} + y_{9,10} = 1
\]
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)

\[(P) : \text{Minimize } \sum_{[i,j] \in E} (t^2_{ij} - u^2_{ij}) \text{ subject to} \]

\[\|x^i - x^j\| - (t_{ij} + u_{ij}) \leq 0, \ [i,j] \in E, \]  
\[y_{ij} - (t_{ij} - u_{ij}) = 0, \ [i,j] \in E, \]  
\[\sum_{j \in S} y_{ij} = 1, \ i \in P = \{1, 2, \ldots, p\}, \]  
\[\sum_{i \in P} y_{ij} + \sum_{k<j, k \in S} y_{kj} + \sum_{k>j, k \in S} y_{jk} = 3, \ j \in S = \{p + 1, \ldots, 2p - 2\}, \]  
\[\sum_{k<j, k \in S} y_{kj} = 1, \ j \in S - \{p + 1\}, \]

\[x^i \in \mathbb{R}^n, \ i \in S, \]
\[y_{ij} \in \{0, 1\}, \ [i,j] \in E.\]
MINLP: Formulations for the Euclidean Steiner Problem

First Formulation: Lagrangian Relaxation

\[ \mathcal{L}(x, y, t, u, \alpha, \beta) = \sum_{[i,j] \in E} (t^2_{ij} - u^2_{ij}) + \sum_{[i,j] \in E} [||x^i - x^j|| - (t_{ij} + u_{ij})] \alpha_{ij} + \]

\[ + \sum_{[i,j] \in E} [y_{ij} - (t_{ij} - u_{ij})] \beta_{ij} \]

or

\[ \mathcal{L}(x, y, t, u, \alpha, \beta) = \sum_{[i,j] \in E} [t^2_{ij} - u^2_{ij} - (\alpha_{ij} + \beta_{ij})t_{ij} - (\alpha_{ij} - \beta_{ij})u_{ij}] + \]

\[ + \sum_{[i,j] \in E} \alpha_{ij}||x^i - x^j|| + \sum_{[i,j] \in E} \beta_{ij}y_{ij}, \]

where

\( \alpha_{ij} \geq 0 \) 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

\[
\mathcal{D}(\alpha, \beta) = \text{minimum} \ \{ L(x, y, t, u, \alpha, \beta) \ \text{subject to} \ (15) - (20) \} 
\]

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

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

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

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

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

\[
x^i \in \mathbb{R}^n, \ i \in S \quad (20)
\]

where \( M = \text{maximum} \ \{ ||x^i - x^j|| \ \text{for} \ 1 \leq i \leq j \leq p \} \).
First Formulation: Lagrangian Relaxation and The Dual Program

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

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

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

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

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

\[ 0 \leq t_{ij} + u_{ij} \leq M, \] (19)

\[ x^i \in \mathbb{R}^n, \ i \in S \] (20)

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

We define

\[ D_1(t, u, \alpha, \beta) = \text{minimum} \ \left\{ \sum_{[i,j] \in E} [t_{ij}^2 - u_{ij}^2 - (\alpha_{ij} + \beta_{ij})t_{ij} - (\alpha_{ij} - \beta_{ij})u_{ij}] \mid \text{s.t. (19)} \right\}, \]
First Formulation: Lagrangian Relaxation and The Dual Program

\[ D(\alpha, \beta) = \text{minimum} \ \{ L(x, y, t, u, \alpha, \beta) \ \text{subject to} \ (15) - (20) \} \]  

(14)

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

(15)

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

(16)

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

(17)

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

(18)

\[ 0 \leq t_{ij} + u_{ij} \leq M, \]  

(19)

\[ x^i \in \mathbb{R}^n, \quad i \in S \]  

(20)

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

We define

\[ D_2(x, \alpha) = \text{minimum} \ \left\{ \sum_{[i,j] \in E} \alpha_{ij} \|x^i - x^j\| \mid \text{s.t.} \ (20) \right\}, \]  

\[-10pt\]
MINLP: Formulations for the Euclidean Steiner Problem

First Formulation: Lagrangian Relaxation and The Dual Program

\[
D(\alpha, \beta) = \text{minimum } \{L(x, y, t, u, \alpha, \beta) \text{ subject to (15) – (20)}\} \tag{14}
\]

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

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

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

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

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

\[
x^i \in \mathbb{R}^n, \quad i \in S \tag{20}
\]

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

We define

\[
D_3(y, \beta) = \text{minimum } \left\{ \sum_{[i,j] \in E} \beta_{ij} y_{ij} \mid \text{s.t. (15) – (18)} \right\},
\]
MINLP: Formulations for the Euclidean Steiner Problem

First Formulation: Lagrangian Relaxation and The Dual Program

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

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

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

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

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

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

\[ x^i \in \mathbb{R}^n, \quad i \in S \quad (20) \]

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

Thus we can write

\[ D(\alpha, \beta) = D_1(t, u, \alpha, \beta) + D_2(x, \alpha) + D_3(y, \beta). \]
First Formulation: Lagrangian Relaxation and The Dual Program

\[ D(\alpha, \beta) = \text{minimum} \ \{ \mathcal{L}(x, y, t, u, \alpha, \beta) \text{ subject to } (15) - (20) \} \]  

\[ \sum_{j \in S} y_{ij} = 1, \ i \in P, \]  

\[ \sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \ j \in S, \]  

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

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

\[ 0 \leq t_{ij} + u_{ij} \leq M, \]  

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

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

The Dual Problem will be

\[ \text{Maximize } D(\alpha, \beta) \text{ subject to } \]

\[ \alpha \geq 0, \ [i, j] \in E, \]  

\[ \beta \in \mathbb{R}, \ [i, j] \in E. \]
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,

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.

MINLP: Formulations for the Euclidean Steiner Problem

Second Formulation

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

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

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

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

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

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

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

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

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

\[d_{ij} \in \mathbb{R} \quad (33)\]

We consider

\[
||x^i - x^j|| \approx \sqrt{\sum_{l=1}^{n} (x_{il}^i - x_{jl}^j)^2 + \lambda^2} \]

\[M = \text{maximum} \{||a^i - a^j|| \text{ for } 1 \leq i \leq j \leq p\}, \]

\[E_1 = \{[i, j] | i \in P, \ j \in S\}, \ E_2 = \{[i, j] | i \in S, \ j \in S\} \text{ e } E = E_1 \cup E_2 \]
MINLP: Formulations for the Euclidean Steiner Problem

Second Formulation (First Property)

If $\bar{x}^j \in \mathbb{R}^n$, $j \in S$ 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:

\[
\sum_{j \in S} y_{ij} = 1, \quad i \in P,
\]
\[
\sum_{k < j, k \in S} y_{kj} = 1, \quad j \in S \setminus \{p + 1\},
\]
\[
\sum_{i \in P} y_{ij} + \sum_{k < j, k \in S} y_{kj} + \sum_{k > j, k \in S} y_{jk} = 3, \quad j \in S,
\]
When we consider

\[ ||x^i - x^j|| \approx \sqrt{\sum_{l=1}^{n} (x^i_l - x^j_l)^2 + \lambda^2}, \]

error propagations may happen.
Note that...

When we consider

\[ ||x^i - x^j|| \approx \sqrt{\sum_{l=1}^{n} (x^i_l - x^j_l)^2 + \lambda^2}, \]

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

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

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: Experiments on Platonic Solids

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!