An improved algorithm for computing Steiner minimal trees in Euclidean $d$-space

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The Euclidean Steiner Problem

A Feasible Solution
The Euclidean Steiner Problem

Determine:

- The number of Steiner points to be used
- The arcs of the tree
- Geometric position of the Steiner points
Steiner Tree/Topology

- A Steiner Tree (ST) is a tree that contains the N given terminals and k additional Steiner points, such that:
  - No two edges meet at a point with angle less than 120°.
  - Each terminal point has degree between 1 and 3.
  - Each Steiner point has degree equal to 3.
  - \( k \leq N-2 \).
- A Full Steiner Tree (FST) is an ST with the maximum N-2 Steiner points.
- A Steiner Topology (Full Steiner Topology) is a topology that meets the degree requirements of an ST (FST).
Exact Algorithms

ESP in the plane

• Extensive literature elucidating properties of SMTs in the plane that do not extend to $d>2$.

• 1961 Melzak
• 1985 Winter – GeoSteiner Algorithm
• 2001 Warme, Winter and Zacharisen - version 3.1 of the GeoSteiner (10000 terminals solved)
Exact Algorithms

GeoSteiner Algorithm

Figure 6: 532 cities in the United States
Exact Algorithms

General $d$-space: Gilbert and Pollak (1968)

- Find all Steiner topologies on the $N$ given terminals and $k$ Steiner points, with $k \leq N-2$.
- For each topology optimize the coordinates of the Steiner points.
- Output the shortest tree found.
Degenerate Steiner Topologies

• A topology is called a degeneracy of another if the former can be obtained from the latter by shrinking edges.

• Fact: each Steiner topology is either a full Steiner topology or a degeneracy of a full Steiner topology.
Exact Algorithms

- Find all Steiner topologies on the N given terminals and k Steiner points, with k=N-2.
- For each topology optimize the coordinates of the Steiner points.
- Output the shortest tree found.
Full Steiner Topologies

- The total number of full Steiner topologies for a graph with \( N \) terminals is given by

\[
f(N) = \frac{(2N-4)!}{2^{N-2}(N-2)!}
\]

\( f(2)=1, f(4)=3, f(6)=105, f(8)=10395, f(10)=2,027,025, f(12)=654,729,075 \)
Math Programming Formulation for ESTP
Fampa and Maculan (2004)

Given $a^1, a^2, \ldots, a^p \in \mathbb{R}^n$

Let

\[ P = \{1, \ldots, p\} \quad \text{and} \quad E_1 = \{[i, j] | i \in P, j \in S\} \]
\[ S = \{p + 1, \ldots, 2p - 2\} \quad \text{and} \quad E_2 = \{[i, j] | i \in S, j \in S\} \]

Define $G = (V, E)$, where

\[ V = P \cup S \quad \text{and} \quad E = E_1 \cup E_2 \]

Minimize $\Sigma_{(i,j) \in E} d_{ij}$

subject to:

\[
\begin{align*}
    d_{ij} &\geq ||a^i - x^j|| - M(1 - y_{ij}) \quad [i, j] \in E_1 \\
    d_{ij} &\geq ||x^i - x^j|| - M(1 - y_{ij}) \quad [i, j] \in E_2 \\
    d_{ij} &\geq 0 \quad [i, j] \in E \\
    \Sigma_{j \in S} y_{ij} &= 1 \quad i \in P \\
    \Sigma_{i<i',i \in S} y_{ij} &= 1 \quad j \in S - \{p+1\} \\
    y_{ij} &\in \{0, 1\} \quad [i, j] \in E \quad i \in S \\
    d_{ij} &\in \mathbb{R} \quad [i, j] \in E \\
    x^i &\in \mathbb{R}^n \quad i \in S
\end{align*}
\]

where $M = \max \{||a^i - a^j||, \ 1 \leq i < j \leq p\}$
Exact Algorithms

General $d$-space: Smith (1992)

- An implicit enumeration scheme to generate full Steiner topologies and a numerical algorithm to solve the ESP for a given topology.
- Computation of SMTs on vertices of regular polytopes led to disproof of Gilbert-Pollak conjecture on “Steiner ratio” in dimensions $d > 2$. 
Tree with $k$ Steiner points, $k+2$ terminals and $n$ edges ($n=2k+1$)

Tree with $k+1$ Steiner points, $k+3$ terminals and $n+2$ edges

Merging Operation
Enumeration Tree

- Nodes at level $k$ of tree enumerate full Steiner topologies with $k+3$ terminals, $k = 0, 1, \ldots, N-3$.
- Children of a given node are obtained by merging a new terminal node with each arc in current FST.
- **Good:** Merging operation cannot decrease minimum length of FST - allows pruning!
- **Bad:** No easy way to account for effect of missing terminal nodes.
- **Ugly:** Growth of tree is super-exponential with depth, and problems get larger at deeper levels.
Problem for a Given Topology

Topology T with k Steiner points, k+2 terminals and n edges (n=2k+1)

\[(P) \quad \text{Min} \quad \sum_{i=1}^{n} \| s_i \| \quad \text{s.t.} \quad A_i^T y + s_i = c_i, \quad i = 1, \ldots, n\]

\[(D) \quad \text{Max} \quad \sum_{i=1}^{n} c_i^T x_i \quad \text{s.t.} \quad \sum_{i=1}^{n} A_i x_i = 0 \quad \| x_i \| \leq 1, \quad i = 1, \ldots, n\]

where:

\[y = \begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix}\]

\[c_i = t_i \quad A_i^T = \begin{pmatrix} i_2 \\ \vdots \\ I_d \end{pmatrix}\]

Case 1:

\[c_i = 0_d \quad A_i^T = \begin{pmatrix} i_1 & i_2 \\ -I_d & I_d \end{pmatrix}\]
The Merging Operation

\[ \begin{align*}
(P) & \quad \text{Min} \quad \sum_{i=1}^{n} \|s_i\| \\
& \quad \text{s.t.} \quad A_i^T y + s_i = c_i, \quad i = 1, \ldots, n \\
(D) & \quad \text{Max} \quad \sum_{i=1}^{n} c_i^T x_i \\
& \quad \text{s.t.} \quad \sum_{i=1}^{n} A_i x_i = 0 \\
& \quad \quad \|x_i\| \leq 1, \quad i = 1, \ldots, n
\end{align*} \]

\[ \begin{align*}
(P^+) & \quad \text{Min} \quad \sum_{i=1}^{n+2} \|s_i\| \\
& \quad \text{s.t.} \quad A_i^{+T} y^+ + s_i = c_i^+, \quad i = 1, \ldots, n + 2 \\
(D^+) & \quad \text{Max} \quad \sum_{i=1}^{n+2} c_i^{+T} x_i \\
& \quad \text{s.t.} \quad \sum_{i=1}^{n+2} A_i^+ x_i = 0 \\
& \quad \quad \|x_i\| \leq 1, \quad i = 1, \ldots, n + 2
\end{align*} \]
Fixing Variables

Let:
\[ x_i = \bar{x}_i, \quad i \in \bar{E} \subset \{1, \ldots, n\} \]

\[ (\bar{D}^+) \quad \text{Max} \quad \bar{v} + \sum_{i \in E^+} c_i^T x_i \]
\[ \text{s.t.} \quad \sum_{i \in E^+} A_i^+ x_i = b^+ \]
\[ \|x_i\| \leq 1, \quad i \in E^+ \]

where:
\[ E^+ = \{1, \ldots, n + 2\} \setminus \bar{E}, \quad b = -\sum_{i \in \bar{E}} A_i^+ \bar{x}_i, \quad \bar{v} = \sum_{i \in \bar{E}} c_i^T \bar{x}_i \]

Theorem: Let $\bar{x}$ be an optimal solution of $(D)$. Then
\[ \text{SMT}(T) \leq \bar{D}^+ \leq \text{SMT}(T^+). \]
Topologies for the Subproblems

(a) (b) (c) (d) (e) (f) (g) (h) (i)
Smith versus Smith+

- In Smith+ use conic interior-point code (MOSEK) to obtain bounds on minimum length tree for given topology. Also use MOSEK to solve subproblems with fixed dual variables.
- Choose next terminal node to add so as to minimize number of children created/maximize sum of child bounds (*strong branching*). Note must extend Smith’s enumeration argument to allow for varying order in which terminals are added!
Computational Results
Instance from OR-Library with 12 terminals

<table>
<thead>
<tr>
<th>Level</th>
<th>Smith+ Nodes</th>
<th>Smith+ Fathom</th>
<th>Smith+ Elim</th>
<th>Smith Nodes</th>
<th>Smith Fathom</th>
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<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
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<tr>
<td>1</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>0</td>
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<td>2</td>
<td>9</td>
<td>0.40</td>
<td>0.68</td>
<td>15</td>
<td>0</td>
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<td>0.69</td>
<td>105</td>
<td>0</td>
</tr>
<tr>
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<td>385</td>
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<tr>
<td>5</td>
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<tr>
<td>6</td>
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<td>0.55</td>
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<tr>
<td>7</td>
<td>4</td>
<td>0.85</td>
<td>0.56</td>
<td>65</td>
<td>0.99</td>
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<td>8</td>
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<tr>
<td>9</td>
<td>20</td>
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<tr>
<td>Total</td>
<td>61</td>
<td></td>
<td></td>
<td>1566</td>
<td></td>
</tr>
</tbody>
</table>
Nodes on the B&B Tree

OR-Library

![Graph showing the relationship between terminal nodes and average B&B nodes for Smith and Smith+ over 6 to 18 terminal nodes. The graph includes a line for Smith and a line for Smith+. The y-axis represents average B&B nodes ranging from 1 to 1,000,000, and the x-axis represents terminal nodes ranging from 6 to 18.]
CPU Time (seconds)

OR-Library

Average CPU seconds

Terminal nodes

Smith

Smith+
## Effect of dimension $d$

<table>
<thead>
<tr>
<th>Dimension $d$</th>
<th>Average B&amp;B nodes</th>
<th>Average CPU seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Smith</td>
<td>Smith+</td>
</tr>
<tr>
<td>2</td>
<td>16,821.6</td>
<td>105.0</td>
</tr>
<tr>
<td>3</td>
<td>55,222.2</td>
<td>1,652.4</td>
</tr>
<tr>
<td>4</td>
<td>368,762.8</td>
<td>13,685.6</td>
</tr>
<tr>
<td>5</td>
<td>470,321.8</td>
<td>9,250.0</td>
</tr>
</tbody>
</table>

Average nodes/time for 5 randomly-generated instances with 10 terminals in $\mathbb{R}^d$ ($d=2,3,4$).
Conclusions

- Conic formulation provides rigorous bounds.
- Fixing dual variables allows for estimate of effect of next merge via solution of smaller problem.
- Novel setting for strong branching; effective in reducing size of the tree.
- More to do! Key problem with use of Smith’s enumeration scheme is approximating the effect of terminals that are not present in partial Steiner trees. May also be possible to use geometric conditions that are valid for $d>2$. 