Geometric Spanning Trees Minimizing the Wiener Index

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Outline

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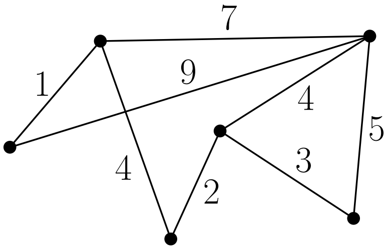
Wiener Index in Graphs

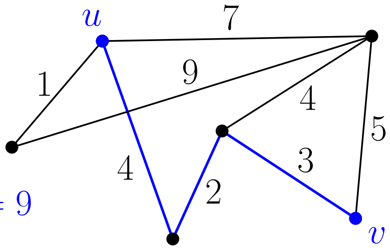
- Let $G = (V, E)$ be a wieghted undirected graph.



Wiener Index in Graphs

- Let $G = (V, E)$ be a wieghted undirected graph.
- Let $\delta_G(u, v)$ denote the **shortest (minimum-wieght) path** between the vertices u and v in G.

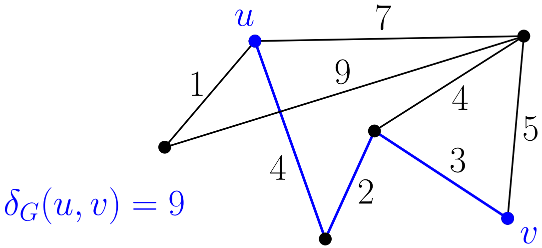
$$\delta_G(u, v) = 9$$



Wiener Index in Graphs

- Let $G = (V, E)$ be a wieghted undirected graph.
- Let $\delta_G(u, v)$ denote the **shortest (minimum-wieght) path** between the vertices u and v in G.
- The **Wiener index** of G, $W(G)$, is defined as the sum of the shortest paths between every pair of vertices in G, i.e.,

$$W(G) = \sum_{u,v \in V} \delta_G(u, v)$$



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Motivation and Related Works

In Chemistry:

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Most of works related to Wiener index focus on computing and bounding the Wiener index of specific graphs or classes of graphs.

Motivation and Related Works

In Network Design: Given an undirected graph $G = (V, E)$ and a (non-negative) weight function (representing the delay on each edge), the **routing cost** $c(T)$ of a spanning tree T of G is

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- **MRCST** is NP-complete, even if all edge weights are 1 [Johnson et al. 1978].
- There exists a PTAS for **MRCST** [Wu et al. 2000].

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Problem: Given a set P of n points in the plane, compute a spanning tree on P that minimizes the Wiener index (the edge weights are their Euclidean lengths).

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Optimal Tree is Planar

Let P be a set of n points in the plane and let T be a tree that minimizes the Wiener index.

Lemma 1

T is planar.

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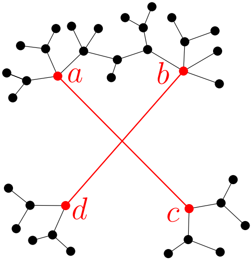
Proof:

- Assume towards a contradiction that there are two crossing edges (a, c) and (b, d) in T.



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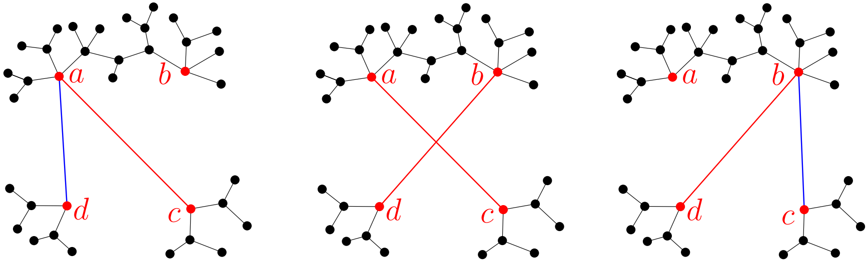
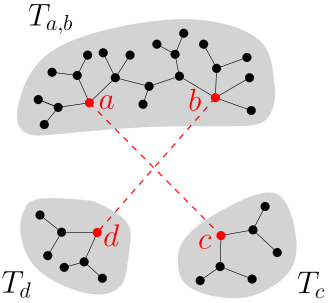


Optimal Tree is Planar (Proof of Lemma 1)

- Let T_{ab}, T_c, and T_d be the sub-trees obtained by removing the edges (a, c) and (b, d) from T.



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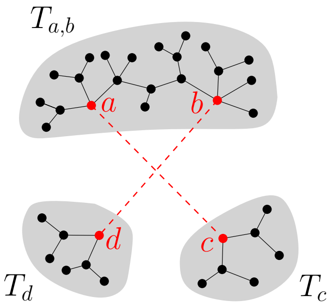

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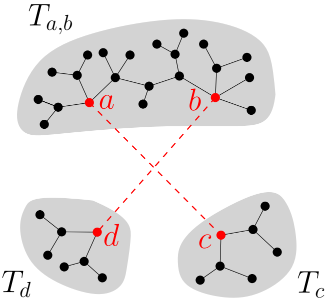
- Let $\delta_a(T_{ab}) = \sum_{p \in T_{ab}} \delta_T(a, p)$ denote the total weight of the paths from a to every point in T_{ab}



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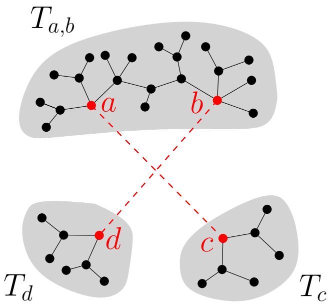
- Let $\delta_a(T_{ab}) = \sum_{p \in T_{ab}} \delta_T(a, p)$ denote the total weight of the paths from a to every point in T_{ab} (Similarly, $\delta_b(T_{ab})$, $\delta_c(T_c)$, $\delta_d(T_d)$).



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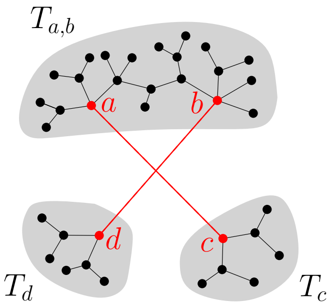
$$W(T) = W(T_{ab}) + n_c \cdot \delta_a(T_{ab}) + n_d \cdot \delta_b(T_{ab})$$



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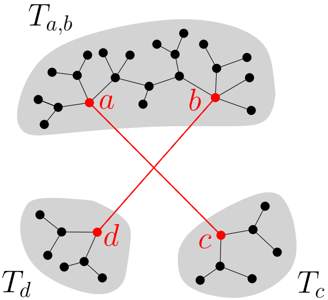

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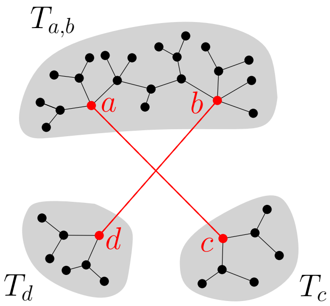

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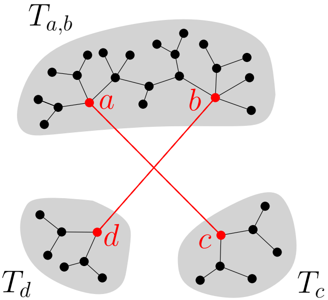

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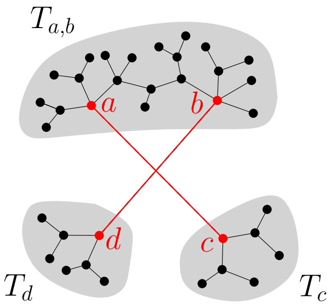

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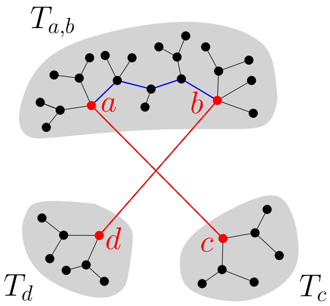
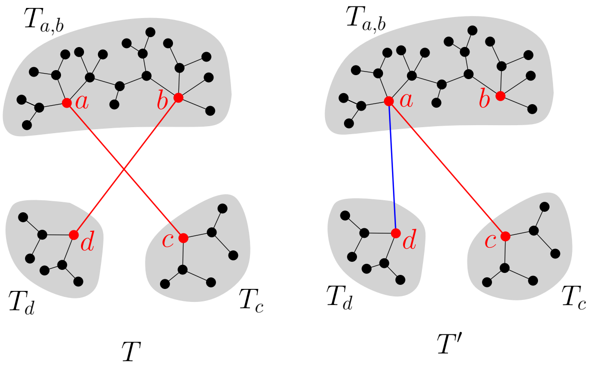


Optimal Tree is Planar (Proof of Lemma 1)

- Let T' be the spanning tree of P obtained from T by replacing the edge (b, d) by the edge (a, d).



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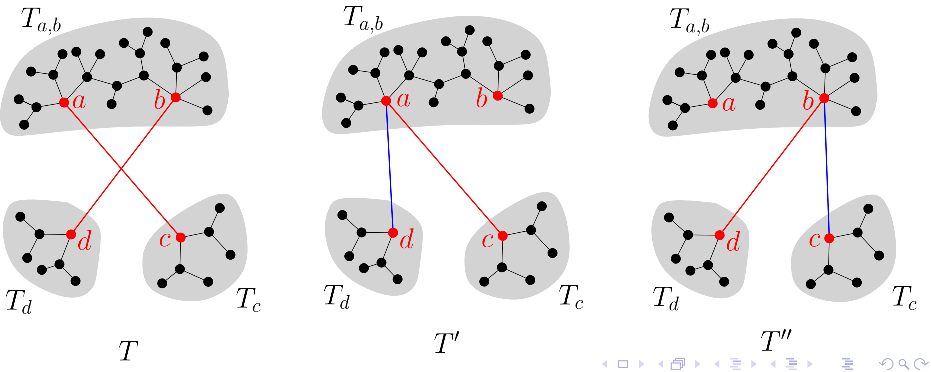
- Let T' be the spanning tree of P obtained from T by replacing the edge (b, d) by the edge (a, d).
- Let T'' be the spanning tree of P obtained from T by replacing the edge (a, c) by the edge (b, c).



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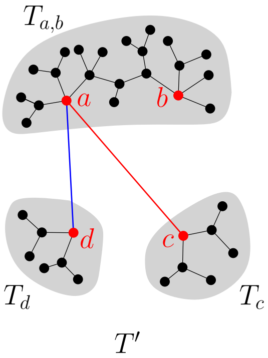
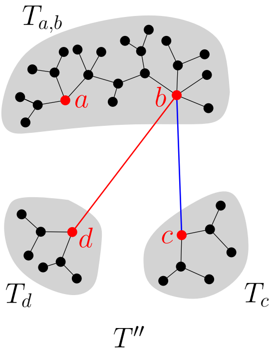


Optimal Tree is Planar (Proof of Lemma 1)

and

$$\begin{aligned} W(T'') = {} & W(T_{ab}) + (n_c + n_d) \cdot \delta_b(T_{ab}) \\ & + W(T_c) + (n_{ab} + n_d) \cdot \delta_c(T_c) + n_c(n_{ab} + n_d) \cdot |bc| \\ & + W(T_d) + (n_{ab} + n_c) \cdot \delta_d(T_d) + n_d(n_{ab} + n_c) \cdot |bd| \end{aligned}$$



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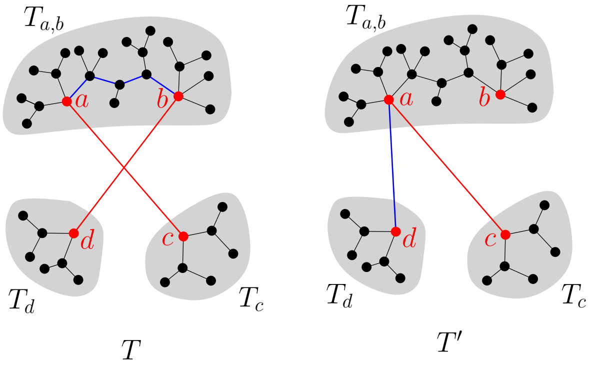
$$W(T) - W(T') = n_d\big(\delta_b(T_{ab}) - \delta_a(T_{ab})\big) + n_d(n_{ab} + n_c)\big(|bd| - |ad|\big) + n_c \cdot n_d \cdot \delta_T(a, b)$$



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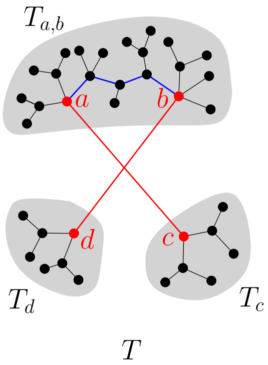

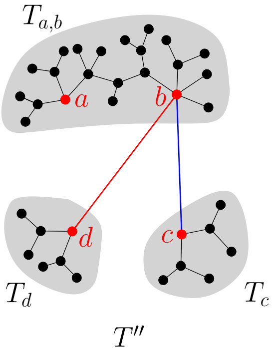

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- Since $n_c > 0$ and $n_d > 0$, we have

$$\delta_b(T_{ab}) - \delta_a(T_{ab}) + (n_{ab} + n_c)\big(|bd| - |ad|\big) + n_c \cdot \delta_T(a, b) \leq 0$$

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$$(n_{ab}+n_c)\big(|bd|-|ad|\big)+(n_{ab}+n_d)\big(|ac|-|bc|\big)+(n_c+n_d)\cdot\delta_T(a,b) \le 0$$

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- That is,

$$n_{ab}\big(|bd| + |ac| - |ad| - |bc|\big) + n_c\big(|bd| + \delta_T(a,b) - |ad|\big) + n_d\big(|ac| + \delta_T(a,b) - |bc|\big) \leq 0$$

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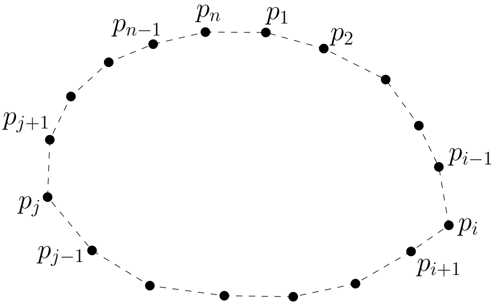
- Since $n_{ab}, n_c, n_d > 0$, and, by the triangle inequality, $|bd| + |ac| - |ad| - |bc| > 0$, $|bd| + \delta_T(a,b) - |ad| > 0$, and $|ac| + \delta_T(a,b) - |bc| > 0$, this is a contradiction. ■

Outline

Optimal Tree of Points in Convex Position

Let $P = \{p_1, p_2, \ldots, p_n\}$ be a set of n points in convex position:



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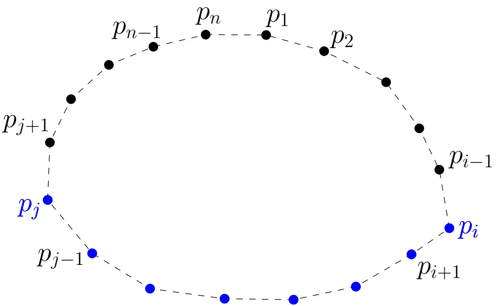
- For each $1 \leq i \leq j \leq n$, let $P[i, j] \subseteq P$ be the set $\{p_i, p_{i+1}, \ldots, p_j\}$.



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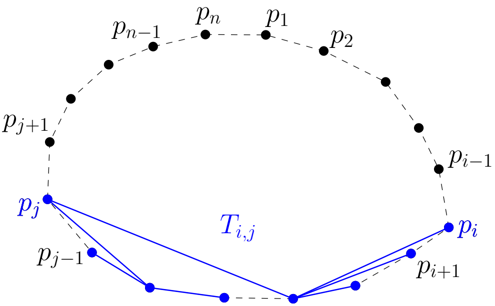

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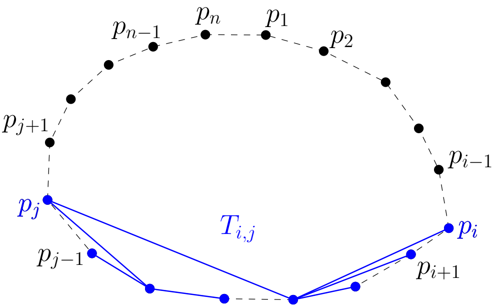
- Let $\delta_i(T_{i,j})$ be the total weight of the paths from p_i to every point of $P[i,j]$ in $T_{i,j}$ (Similarly, $\delta_j(T_{i,j})$).



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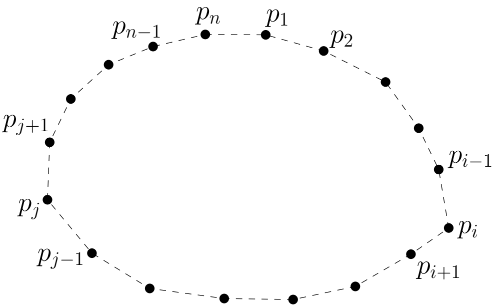

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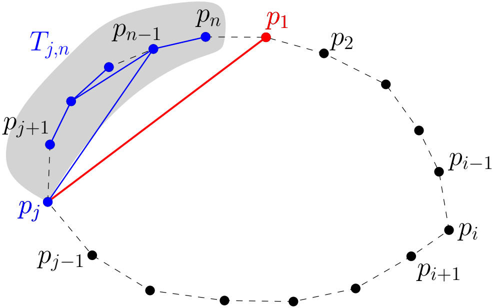
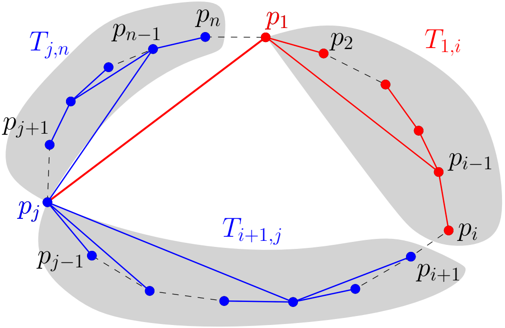


Optimal Tree of Points in Convex Position

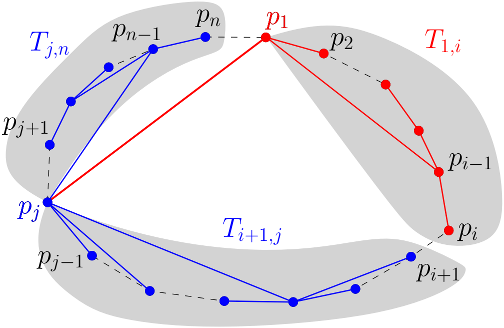
- Let T be a (planar) minimum Wiener index spanning tree of P and let $W^* = W(T)$.
- Let p_j be the point with maximum j that is connected to p_1 in T.
- Moreover, there exists an index $1 \le i < j$ such that all the points in $P[1, i]$ are closer to p_1 than to p_j in T, and all the points in $P[i + 1, j]$ are closer to p_j than to p_1 in T.



Optimal Tree of Points in Convex Position

Hence,

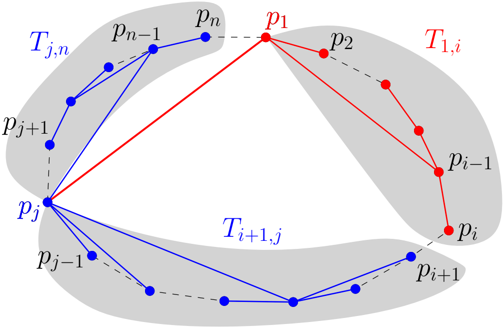
$$W^* = W(T_{1,i}) + (n-i) \cdot \delta_1(T_{1,i})$$



Optimal Tree of Points in Convex Position

Hence,

$$W^* = W(T_{1,i}) + (n-i) \cdot \delta_1(T_{1,i}) + W(T_{i+1,j}) + (n-j+i) \cdot \delta_j(T_{i+1,j})$$



Optimal Tree of Points in Convex Position

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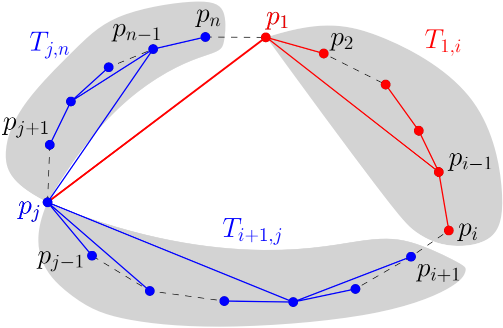

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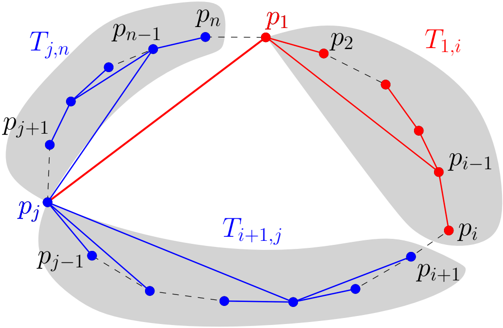
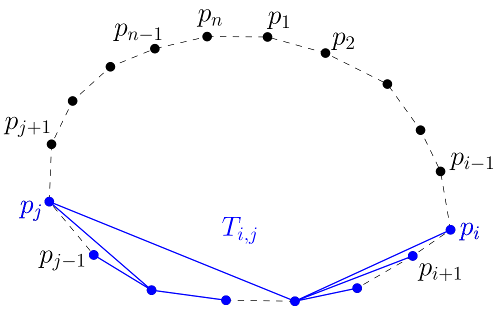


Optimal Tree of Points in Convex Position

- Let $W_j[i,j] = W(T_{i,j}) + (n-j+i-1) \cdot \delta_j(T_{i,j})$ be the minimum value obtained by a spanning tree $T_{i,j}$ of $P[i,j]$ rooted at p_j.



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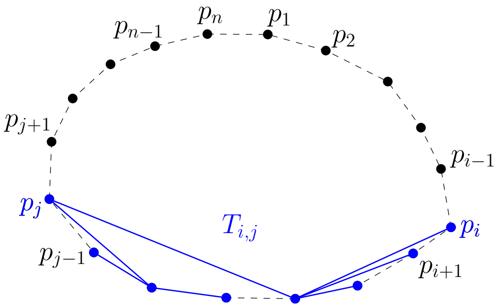

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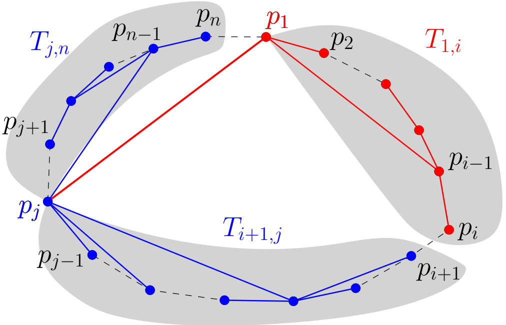
- Thus, we can write W^* as

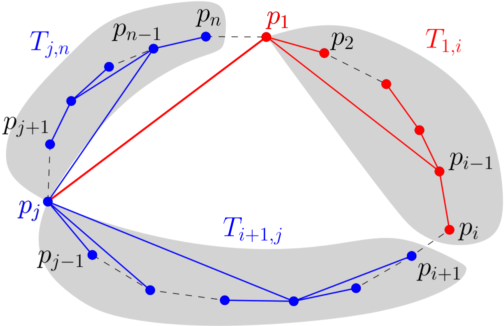
$$W^* = W_1[1,n] = W_1[1,i] + W_j[i+1,j] + W_j[j,n] + i(n-i) \cdot |p_1 p_j|$$



Optimal Tree of Points in Convex Position

Therefore, $W_1[1,n]$ can be recursively computed using

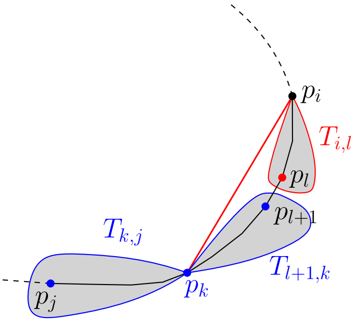
$$W_1[1,n] = \min_{\substack{1<j\leq n \\ 1\leq i<j}} \left\{ W_1[1,i] + W_j[i+1,j] + W_j[j,n] + i(n-i)\cdot|p_1p_j| \right\}$$



Optimal Tree of Points in Convex Position

Sub-problems: For every $1 \leq i < j \leq n$, we recursively compute:

$$W_i[i,j] = \min_{\substack{i<k\leq j \\ i\leq l<k}} \left\{ W_i[i,l] + W_k[l+1,k] + W_k[k,j] + (j-l)(n-j+l)\cdot|p_i p_k| \right\}$$



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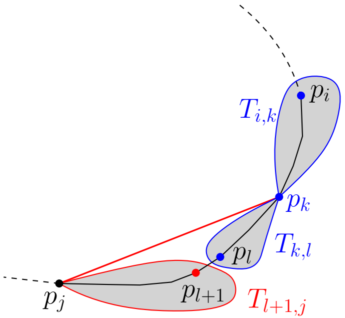

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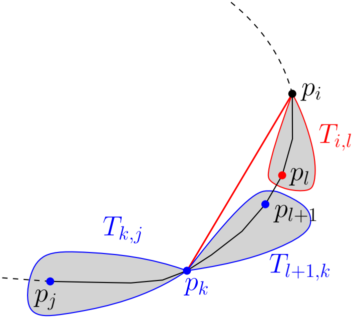

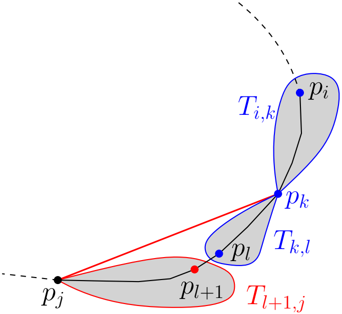

Optimal Tree of Points in Convex Position

Dynamic peogramming algorithm: We maintain two tables $\overleftarrow{M}$ and $\overrightarrow{M}$ each of size $n \times n$, such that $\overleftarrow{M}[i, j] = W_i[i, j]$ and $\overrightarrow{M}[i, j] = W_j[i, j]$, for each $1 \leq i < j \leq n$.

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Algorithm 2 *ComputeOptimal*(P)

1: **for** each $i \leftarrow 1$ to n **do**

  $\overleftarrow{M}[i,i] \leftarrow 0 \quad , \quad \overrightarrow{M}[i,i] \leftarrow 0$

2: **for** each $i \leftarrow n$ to 1 **do**

  for each $j \leftarrow i$ to n **do**

$$\overleftarrow{M}[i,j] \leftarrow \min_{\substack{i<k\leq j \\ i\leq l<k}} \left\{ \overleftarrow{M}[i,l] + \overrightarrow{M}[l+1,k] + \overleftarrow{M}[k,j] + (j-l)(n-j+l) \cdot |p_i p_k| \right\}$$

$$\overrightarrow{M}[i,j] \leftarrow \min_{\substack{i\leq k<j \\ k\leq l<j}} \left\{ \overrightarrow{M}[i,k] + \overleftarrow{M}[k,l] + \overrightarrow{M}[l+1,j] + (l-i+1)(n-l+i-1) \cdot |p_k p_j| \right\}$$

3: **return** $\overleftarrow{M}[1,n]$

Optimal Tree of Points in Convex Position

Theorem 2

Let P be a set of n points in convex position. Then, a spanning tree of P of minimum Wiener index can be computed in $O(n^4)$ time.

Hardness Proof

Euclidean Wiener Index Tree Problem: Given a set P of points in the plane, a cost W, and a budget B, decide whether there exists a spanning tree T of P, such that

$$W(T) = \sum_{p,q \in P} \delta_T(p,q) \leq W \text{ (the Wiener index of } T\text{), and}$$

$$wt(T) = \sum_{(p,q) \in T} |pq| \leq B \text{ (the weight of } T\text{).}$$

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Theorem 2

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Proof (sketch): We reduce from the Partition problem.

Partition: Given a set $X = \{x_1, x_2, \ldots, x_n\}$ of n positive integers with even $R = \sum_{i=1}^{n} x_i$, decide whether there is a subset $S \subseteq X$, such that $\sum_{x_i \in S} x_i = R/2$.

Hardness Proof

- Given an instance $X = \{x_1, x_2, \ldots, x_n\}$ of Partition, we construct a set P of $m = n^3 + 3n$ points as follows:

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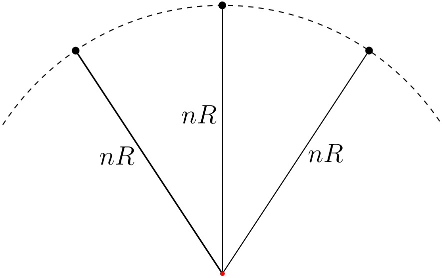

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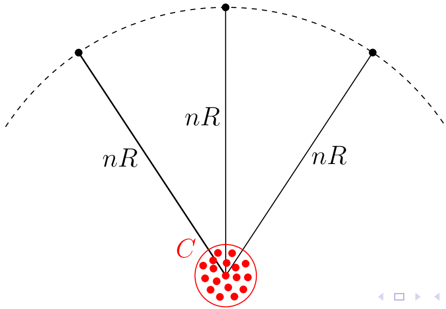

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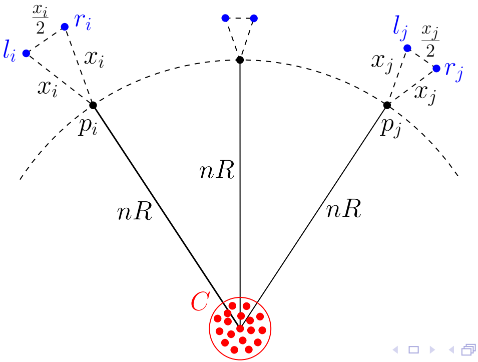

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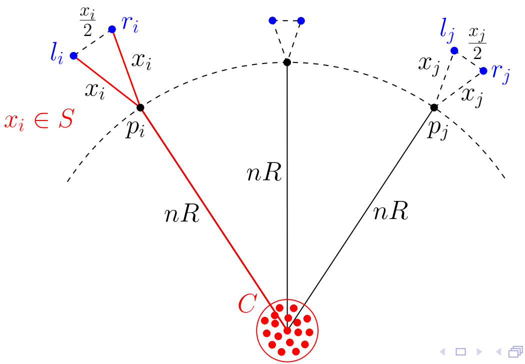

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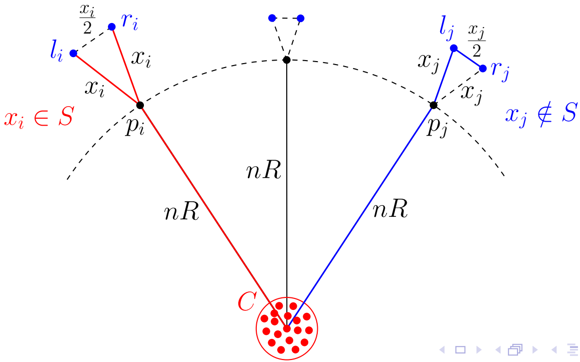
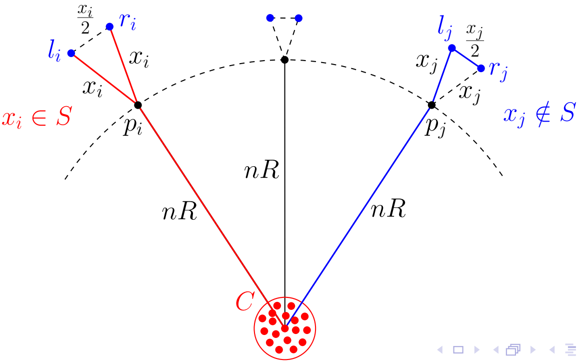


Hardness Proof

Finally, set $$B = n^2R + R + \frac{3}{4}R = \left(n^2 + \frac{7}{4}\right)R, \text{ and}$$

$$\begin{aligned} W &= 3n^2(m-3)R + \left(\frac{9}{4}m - \frac{13}{4}\right)R \\ &= 3n^5R + \frac{45}{4}n^3R - 9n^2R + \frac{27}{4}nR - \frac{13}{4}R \end{aligned}$$



Wiener Index Paths

Let P be a set of n points.

Theorem 4

The path that minimizes the Wiener index among all Hamiltonian paths of P is not necessarily planar.

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Proof: Consider the set P of $n = 2m + 2$ points located as follows.

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- Since the points in P_l are arbitrarily close to the origin $(0,0)$, any path connecting these points has a Wiener index zero (Similarly for the points in P_r).

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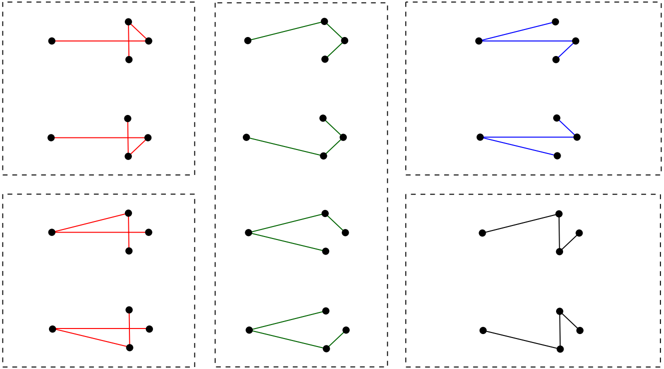

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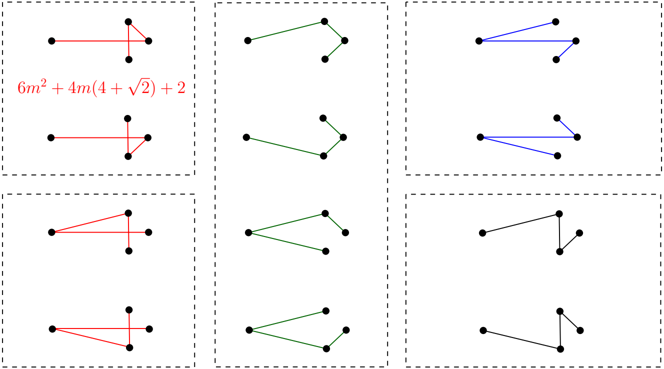

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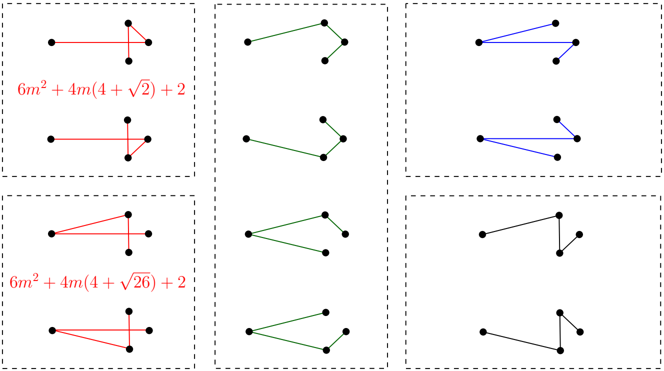

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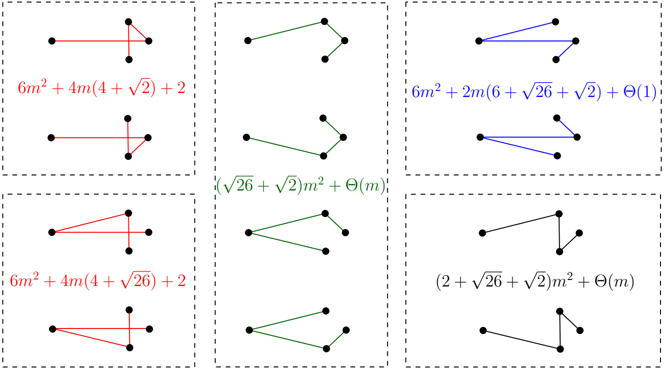

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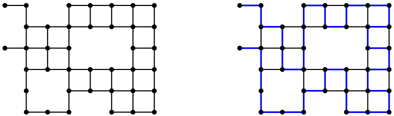

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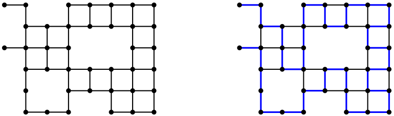

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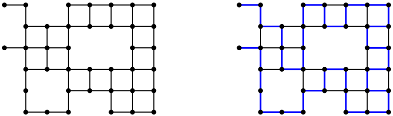
- It is well known that the Wiener index of a Hamiltonian path of n points, where each edge is of length one, is $\binom{n+1}{3}$.
- Thus, it is easy to see that a grid graph $G = (P, E)$ has a Hamiltonian path if and only if there exists a Hamiltonian path in the complete graph over P of Wiener index $\binom{n+1}{3}$. ∎



Summary

Given a set P of points in the plane, we showed that

1. The spanning tree of P that minimizes the Wiener index is planar.
2. One can solve the problem in polynomial time when the points of P are in convex position.
3. Given a cost W and a budget B, computing a spanning tree of P whose Wiener index is at most W and its weight is at most B is (weakly) NP-hard.
4. The Hamiltonian path of P that minimizes the Wiener index is not necessarily planar.
5. Computing a Hamiltonian path of P that minimizes the Wiener index is NP-hard.

Thank you

Questions?