

Graph Realizations Corresponding to Optimized Extremal Eigenvalues of the Laplacian

Christoph Helmberg

joint work with

Frank Göring

Susanna Reiß (Dienelt)

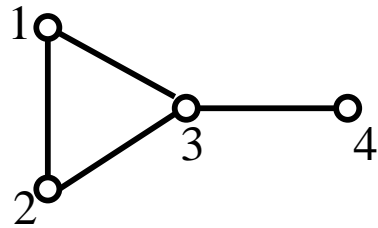
Markus Wappler

TU Chemnitz

- Introduction: Laplacian and Algebraic Connectivity
- Eigenvalue Optimization and Embedding Problems
- Separators and Optimal Embeddings
- Tree-Width Bound on Minimal Dimensions
- Sharpness of the Bounds
- Rotational Dimension of a Graph

Introduction

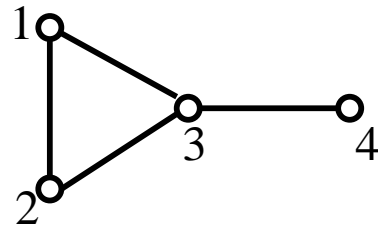
- simple undirected Graph $G = (N, E)$, $N = \{1, \dots, n\}$, $E \subseteq \{ij : i, j \in N, i \neq j\}$
- Laplacian $L(G) = \text{Diag}(Ae) - A$ A ... adjacency matrix, $e = [1, 1, \dots, 1]^T$



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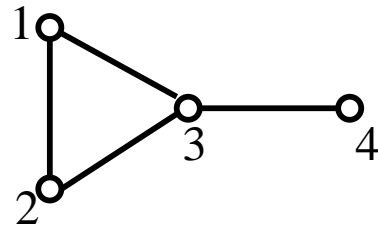


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- weighted Laplacian for $w \geq 0$: $L_w(G) = \sum_{ij \in E} w_{ij} E_{ij}$ $E_{ij} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{matrix} i \\ j \end{matrix}$

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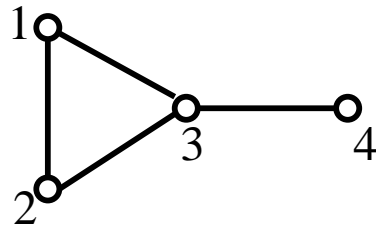


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- [\[Fiedler 1973, 1989, 1993\]](#) $\lambda_2(L(G)) > 0$ iff G is connected
proved close ties to edge and node connectivity, “algebraic connectivity”
- EV to $\lambda_2(L)$ used in many partitioning heuristics, “Fiedler vector”
- Laplacian Spectrum in Graph Theory, see e.g. [\[Mohar 1991, 2004\]](#)

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[Fiedler 1989] did this for λ_2

$$\max_{w \in \mathcal{W}} \lambda_2(L_w) \quad \mathcal{W} = \{w \in \mathbb{R}_+^E : \sum_{ij \in E} w_{ij} = w^T e \leq 1\}$$

→ *Absolute Algebraic Connectivity*

[Fiedler 1990] exhibits formula for optimal weights in trees.

From Eigenvalues to Embeddings in the Eigenspace

$$\max_{w \in \mathcal{W}} \lambda_2(L_w)$$

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dualize

$$\begin{aligned} \max \quad & \langle I, X \rangle \\ \text{s.t.} \quad & \langle E_{ij}, X \rangle \leq 1, \quad ij \in E \\ & \langle e e^T, X \rangle = 0 \\ & X \succeq 0 \end{aligned}$$

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embedding: set $X = V^T V$ with $V = [v_1, \dots, v_n]$

$$\begin{aligned} \max \quad & \sum \|v_i\|^2 \\ \text{s.t.} \quad & \|v_i - v_j\|^2 \leq 1, \quad ij \in E \\ & \sum v_i = 0 \\ & v_i \in \mathbb{R}^n \end{aligned}$$

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($\sum v_i = 0$ holds, as well)

The embedding problem

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 λ_{\max} : nodes are pressed inwards and edges are struts of length 1
 w_{ij} is the force acting on the cable/strut $ij \in E$
- For any $u \in \mathbb{R}^n$ the projection $V^T u$ yields an eigenvector to λ_{opt} .
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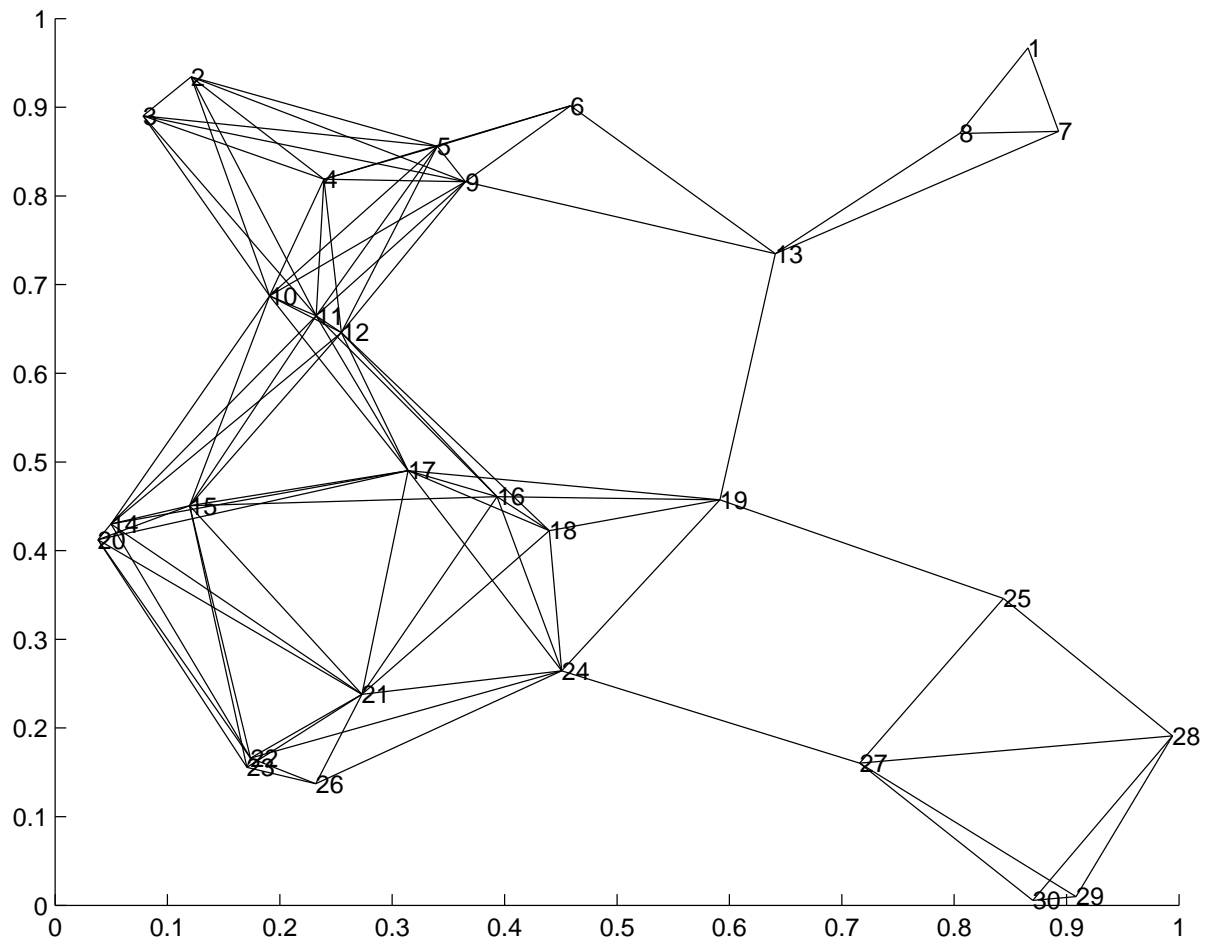
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- Replace the origin by the barycenter $\bar{v} = \frac{1}{n} \sum v_i$

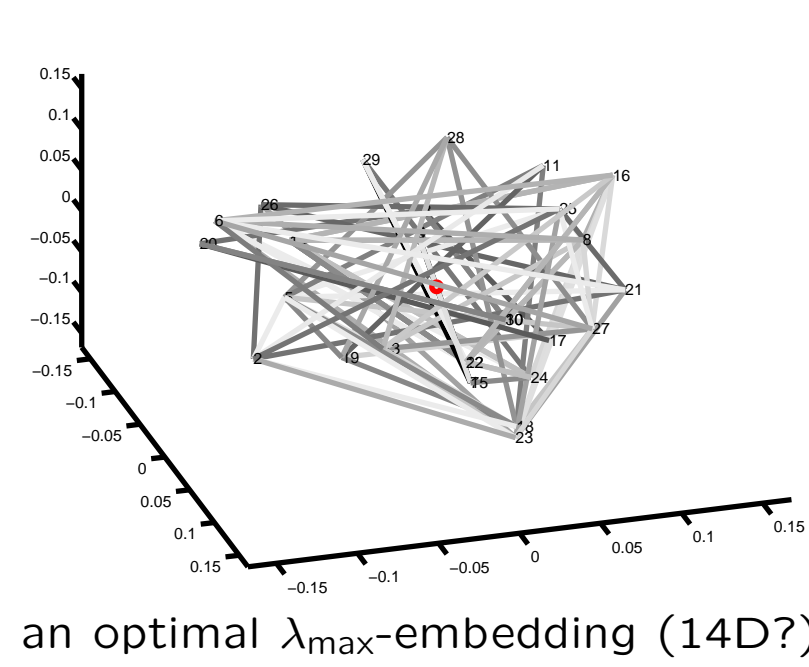
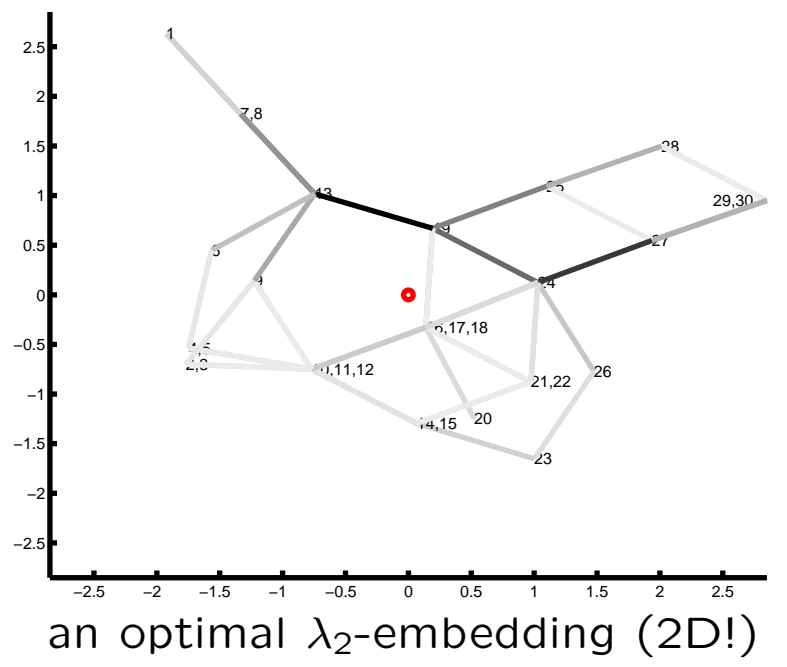
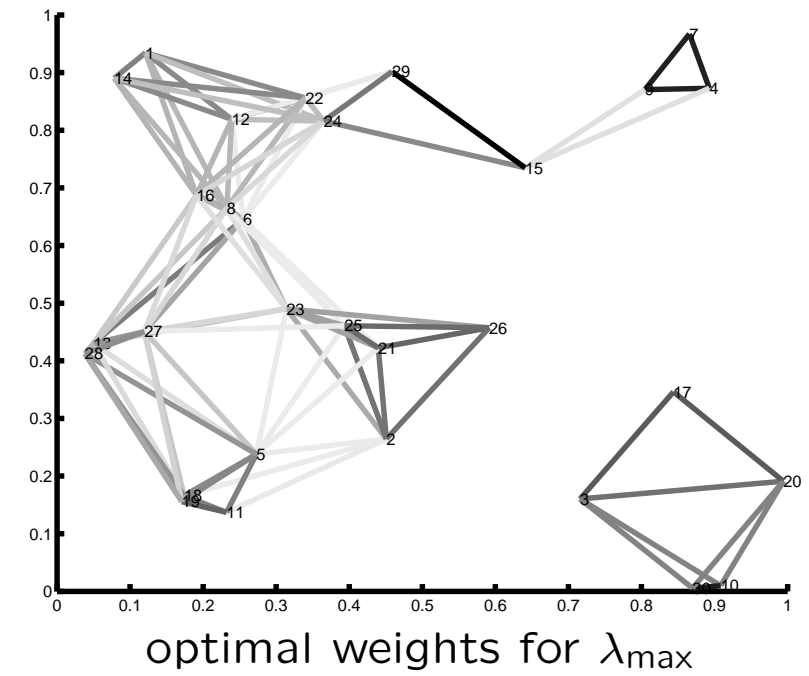
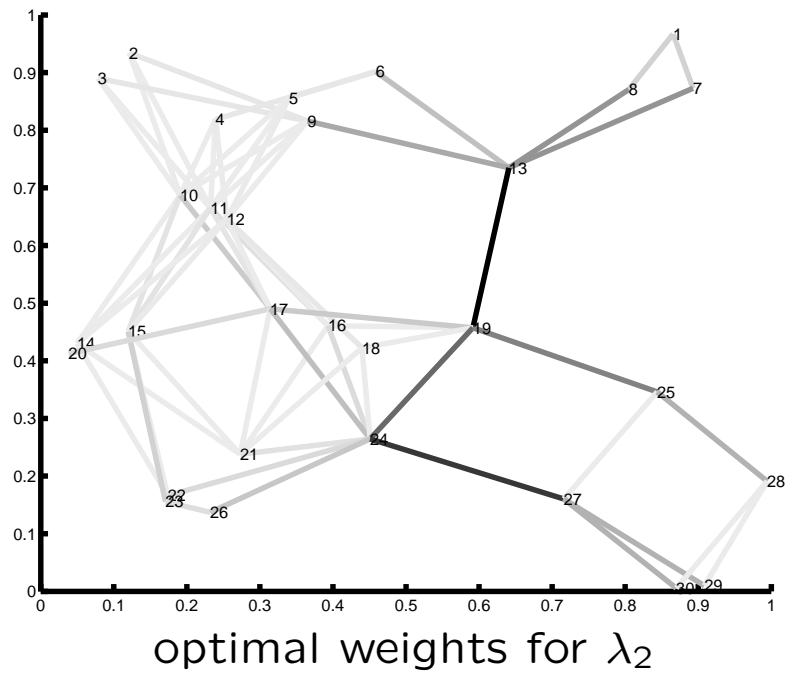
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then $\sum \|v_i - \bar{v}\|^2 = \frac{1}{n} \sum_{i,j} \|v_i - v_j\|^2$ is the *variance*.

Equivalent/Related Problems

- λ_2 : Fastest Mixing Markov Processes [\[SunBoydXiaoDiaconis2006\]](#)
 λ_2 is the rate of convergence to the stationary distribution
also give an interpretation as maximizing conductance
- Maximum Variance Unfolding (visualization in data mining) [\[WeinbergerSaul2004\]](#)
- Tensegrity Theory [\[Connelly1999\]](#)
the variance corresponds to the potential and L_w to the stress matrix
- Graph Realizations [\[BelkConnelly2007\]](#)
- low dimensional embeddings [\[LinialLondonRabinovich1995\]](#)
- Expanders [\[HooryLinialWigderson2006\]](#)
- Colin de Verdière and related graph parameters [\[CdV98,vdHolst03\]](#)





Connections to the (node-)separator structure

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Tree-Width

Given $G = (N, E)$, let $T = (\mathcal{N}, \mathcal{E})$ be a tree with $\mathcal{N} \subseteq 2^N$ and $\mathcal{E} \subseteq \binom{\mathcal{N}}{2}$ so that

(i) $N = \bigcup_{U \in \mathcal{N}} U$.

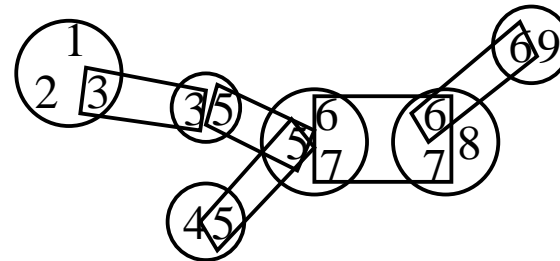
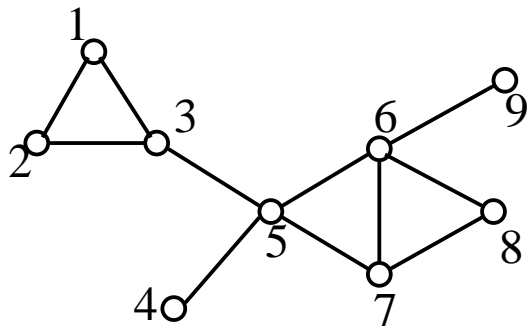
(ii) For every $e \in E$ there is a $U \in \mathcal{N}$ with $e \subseteq U$.

(iii) If $U_1, U_2, U_3 \in \mathcal{N}$ with U_2 on the T -path from U_1 to U_3 , then $U_1 \cap U_3 \subseteq U_2$.

Then T is called a *tree-decomposition* of G .

The *width* of T is the number $\max\{|U| - 1 : U \in \mathcal{N}\}$.

The *tree-width* $tw(G)$ is the least width of any tree-decomposition of G .



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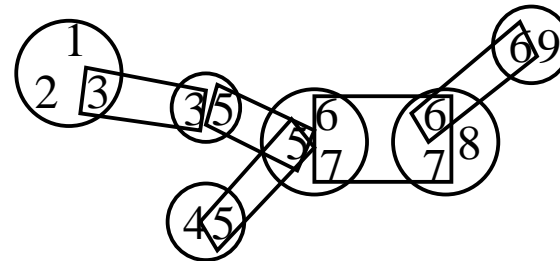
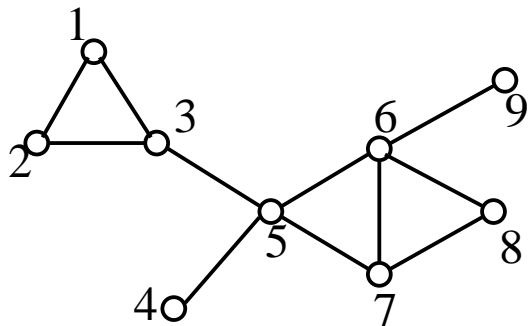
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Any $U \in \mathcal{N}$ and any $U \cap U'$ with $\{U, U'\} \in \mathcal{E}$ is a separator of G .

Main Result 1: Separators and Optimality of Embeddings

Given optimal $v_i \in \mathbb{R}^n$, $i \in N$, of a connected graph $G = (N, E)$ and a separator $S \subset N$ separating G into node sets C_1, C_2 so that no edges run between C_1 and C_2 , let $\mathcal{S} = \{v_i : i \in S\}$.

$$\lambda_2(L_w)$$

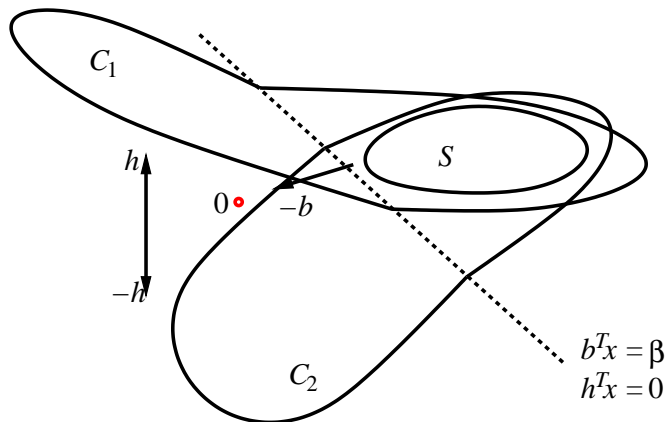
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Separator-Shadow Th.

For at least one $j \in \{1, 2\}$

$$[v_i, 0] \cap \text{conv } \mathcal{S} \neq \emptyset \quad \forall i \in C_j$$

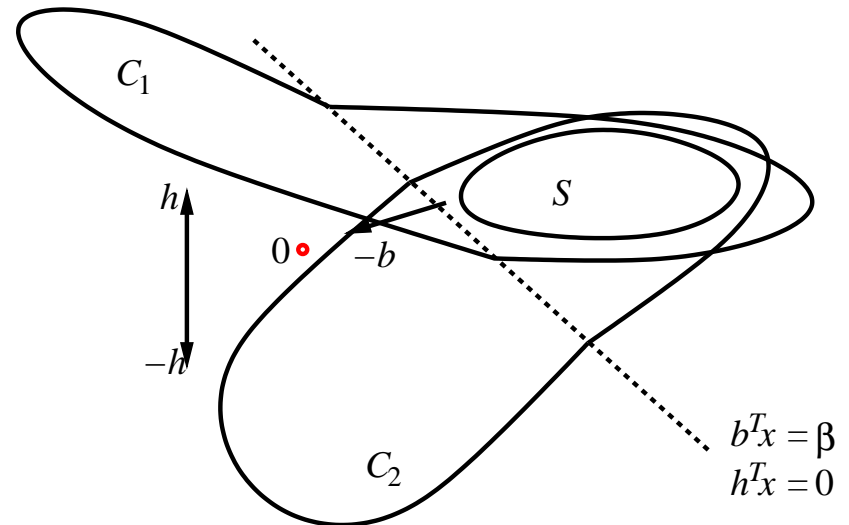
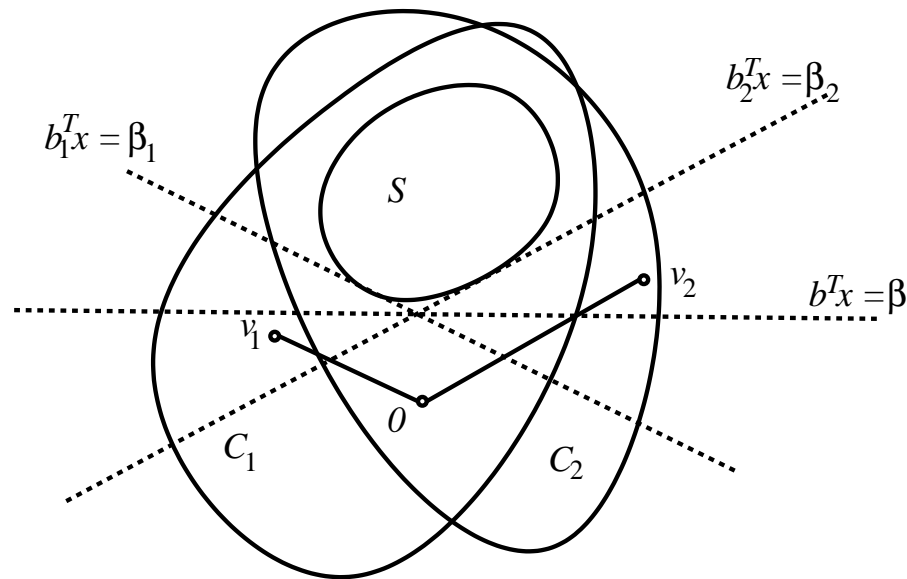
geometric proof idea:



Sketch of Proof: by contradiction

Assume the Theorem does not hold, then w.l.o.g.

there are points v_1, v_2 with $1 \in C_1, 2 \in C_2$ and $[0, v_1] \cap S = [0, v_2] \cap S = \emptyset$.



$b_i^T x < \beta_i$ separates $[0, v_i]$ from S

$$\begin{bmatrix} b \\ \beta \end{bmatrix} = \alpha \begin{bmatrix} b_1 \\ \beta_1 \end{bmatrix} + (1 - \alpha) \begin{bmatrix} b_2 \\ \beta_2 \end{bmatrix}$$

choose $\alpha \in [0, 1]$ so that both $C_i \cap \{x : b^T x < \beta\} \neq \emptyset$

$\sum v_i = 0 \Rightarrow$ lin. dep., thus h exists

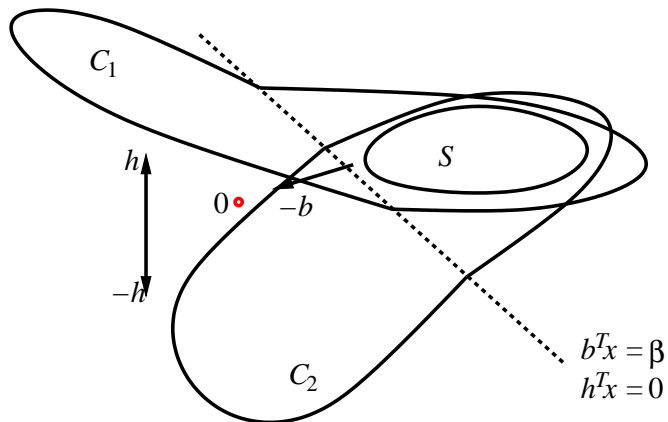
Verify: epsilon movement improves solution \Rightarrow contradiction to optimality \square

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$\lambda_2(L_w)$	$\lambda_{\max}(L_w)$
<p>Separator-Shadow Th. For at least one $j \in \{1, 2\}$ $[v_i, 0] \cap \text{conv } \mathcal{S} \neq \emptyset \quad \forall i \in C_j$</p>	<p>Separator's Sunny Side Th. Let $\bar{v}_j = \frac{1}{ C_j } \sum_{i \in C_j} v_i$, $j \in \{1, 2\}$, be the barycenter of C_j, then $\bar{v}_j \in \text{aff}(\mathcal{S}) - \text{cone}(\mathcal{S})$ for $j \in \{1, 2\}$</p>

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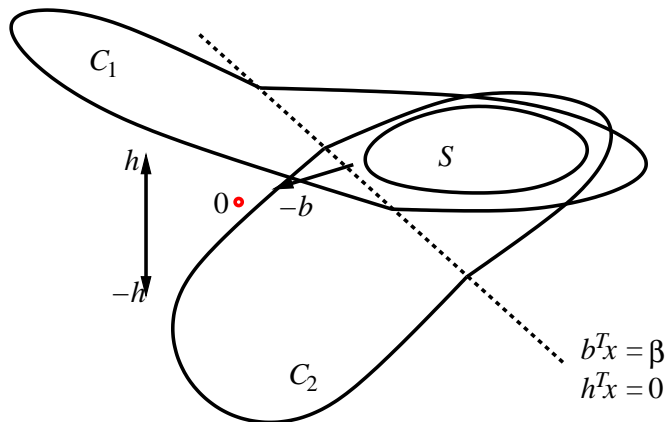
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Separator's Sunny Side Th.

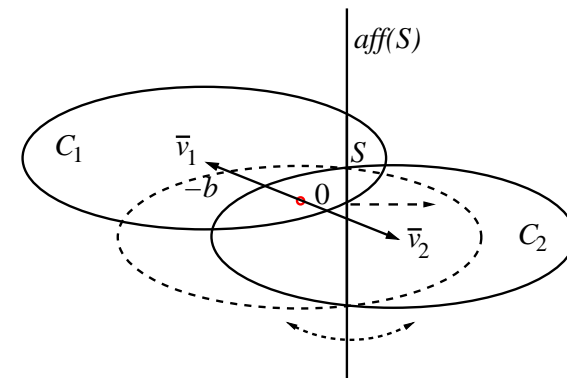
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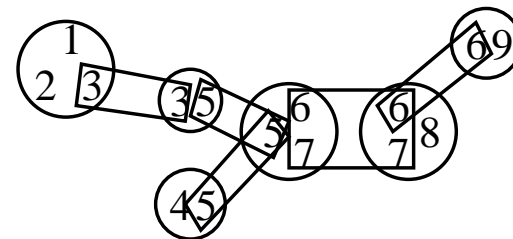
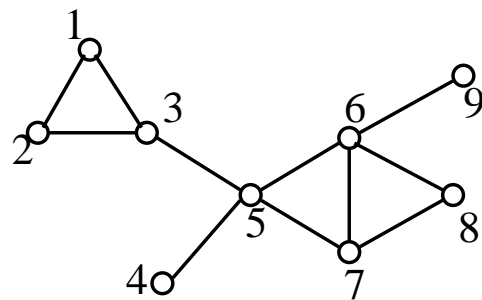


geometric proof idea:



Main Result 2:
Structural bounds on the existence of low dimensional solutions

$\lambda_2(L_w)$	$\lambda_{\max}(L_w)$
<p>Tree-Width Bound</p> <p>There exists an optimal embedding of dimension at most</p> $tw(G) + 1$	
<p>needs separator shadow + involved result for separators with $0 \in \text{conv } S$</p> <p>algorithmic proof idea: given a tree decomposition, start at a 0-node, try to flatten all adjacent nodes or move on to the next 0-node</p>	

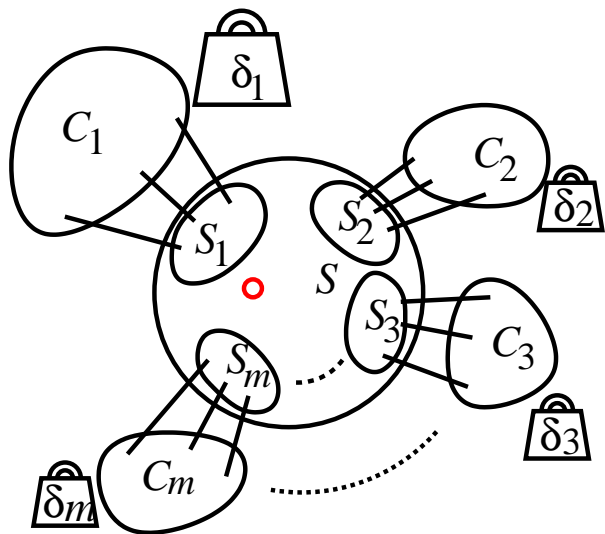


Theorem [Separators Containing the Origin]

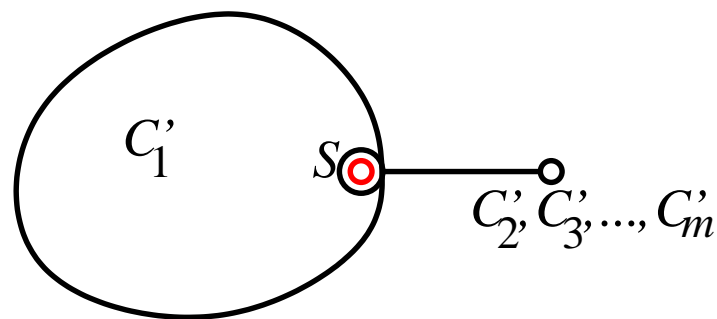
Let $v_i \in \mathbb{R}^n$ for $i \in N$ be an optimal solution of (EMB) for a connected graph $G = (N, E)$ and let $S \subset N$ with $0 \in \mathcal{S} = \text{conv}\{v_s : s \in S\}$ be a separator in G inducing a partition (S, C_1, \dots, C_m) of N so that no node in C_j is adjacent to a node in C_h for $j \neq h$, $j, h \in M = \{1, \dots, m\}$. Set $\mathcal{L} = \text{span } \mathcal{S}$ and, for $j \in M$, $\delta_j = \sum_{i \in C_j} \|p_{\mathcal{L}^\perp}(v_i)\|$.

- (i) If $\delta_{\hat{j}} > \sum_{j \in M \setminus \{\hat{j}\}} \delta_j$ for one $\hat{j} \in M$ then there exist $h \in \mathcal{L}^\perp$ and an optimal embedding $v'_i \in \mathbb{R}^n$ of (EMB) with $v'_i = v_i$ for $i \in S$, $v'_i \in \mathcal{L} + \text{span}\{h, v_i : i \in C_{\hat{j}}\}$ for $i \in C_{\hat{j}}$ and $v'_i \in \mathcal{L} + \{\delta \sum_{i \in C_j} v'_i : \delta \geq 0\}$ for $i \in \bigcup_{j \in M \setminus \{\hat{j}\}} C_j$. If, in addition, there exists $\bar{b} \in \text{span}\{v_i : i \in C_{\hat{j}}\}$, $\|\bar{b}\| = 1$ so that $\langle \bar{b}, v_i \rangle \geq 0$ for all $i \in C_{\hat{j}}$, then such an embedding exists with $h = 0$.
- (ii) If $\delta_{\hat{j}} \leq \sum_{j \in M \setminus \{\hat{j}\}} \delta_j$ for all $\hat{j} \in M$ then there exist vectors $d_1, d_2, d_3 \in \mathcal{L}^\perp$, $\|d_1\| = \|d_2\| = \|d_3\| = 1$ with $\dim \text{span}\{d_1, d_2, d_3\} \leq 2$, $b_j \in \{d_1, d_2, d_3\}$, $j \in M$, and an optimal embedding $v'_i \in \mathbb{R}^n$, $i \in N$, of (EMB) with $v'_i = v_i$ for $i \in S$ so that for each $j \in M$ we have $v'_i \in \mathcal{L} + \{\delta b_j : \delta \geq 0\}$ for all $i \in C_j$. One may assume $b_j = d_1$ for at most one $j \in M$.
- (iii) If, in case (ii), the index $\hat{j} \in M$ is the only $j \in M$ satisfying $b_j = d_1$ and at most $|S| - 1$ nodes of S are adjacent to nodes in $C_{\hat{j}}$, then there is an optimal embedding of dimension at most $|S|$.

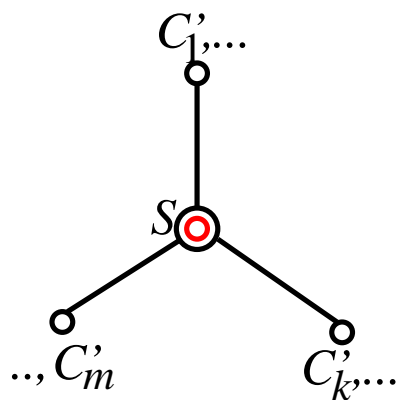
initial embedding



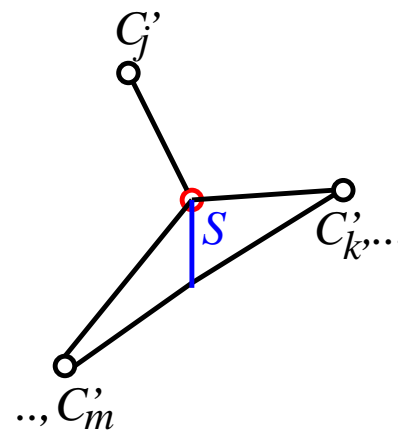
(i) $\delta_1 > \delta_2 + \dots + \delta_m \rightarrow \dim(S, C'_1)$



(ii) $\delta_1 \leq \delta_2 + \dots + \delta_m \rightarrow \dim(S) + 2$

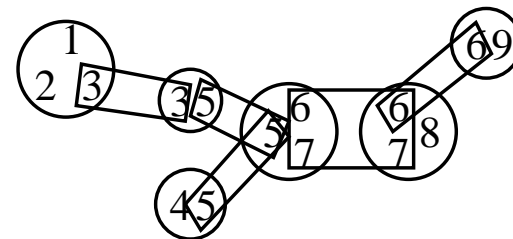
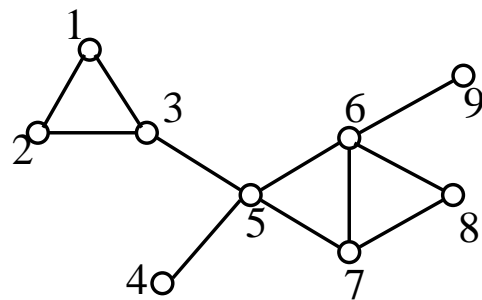


(iii) if (ii) $\wedge j$ single $\wedge |S_j| < |S| \rightarrow \dim(S) + 1$



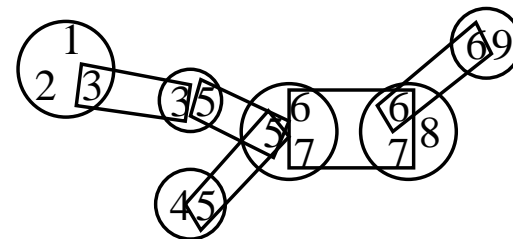
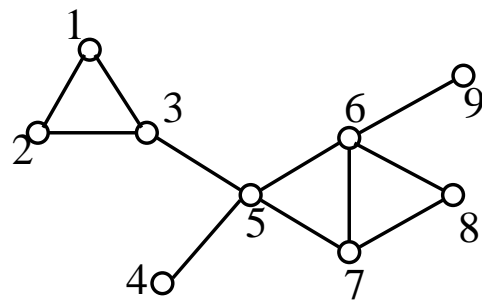
Main Result 2:
Structural bounds on the existence of low dimensional solutions

$\lambda_2(L_w)$	$\lambda_{\max}(L_w)$
<p>Tree-Width Bound</p> <p>There exists an optimal embedding of dimension at most</p> $tw(G) + 1$	
<p>needs separator shadow + involved result for separators with $0 \in \text{conv } S$</p> <p>algorithmic proof idea: given a tree decomposition, start at a 0-node, try to flatten all adjacent nodes or move on to the next 0-node</p>	



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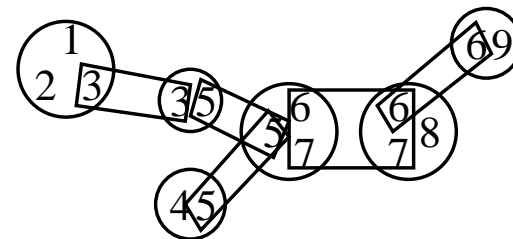
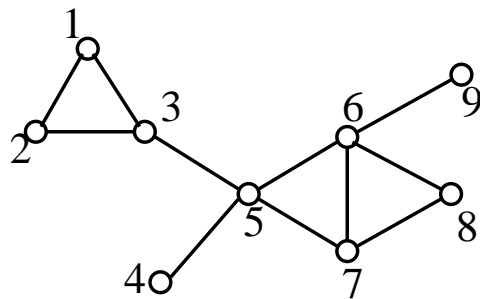
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Structural bounds on the existence of low dimensional solutions

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<p>needs separator shadow + involved result for separators with $0 \in \text{conv } S$</p> <p>algorithmic proof idea: given a tree decomposition, start at a 0-node, try to flatten all adjacent nodes or move on to the next 0-node</p>	<p>Obs.: in separated sets no forces interact outside separator space.</p> <p>algorithmic proof idea: given a tree decomposition, find a node S with maximal $\dim(\text{lin}(S))$. For adjacent nodes U, rotate basis of U outside $\text{lin}(S \cap U)$ into $\text{lin}(S)$, continue recursively</p>

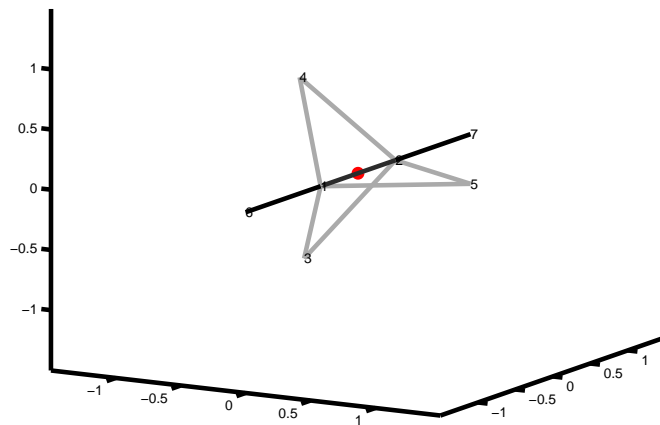
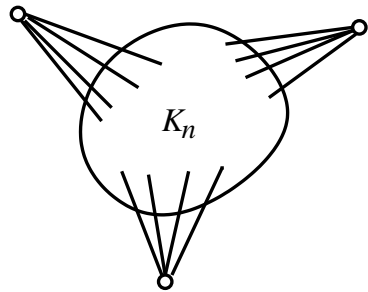


Result 3: Sharpness of Tree-Width Dimension Bounds

$$\lambda_2(L_w)$$

For $n \geq 4$, connect three vertices completely to K_n

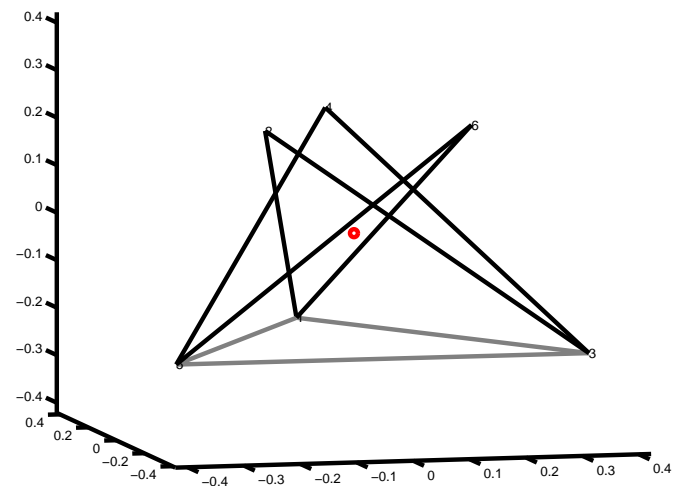
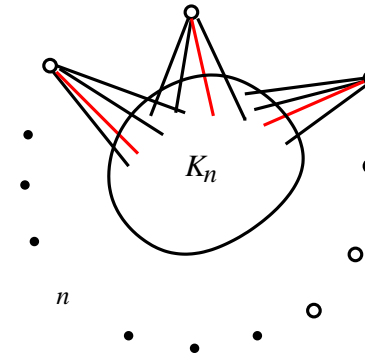
$$tw(G) = n, \quad \dim = n + 1$$



$$\lambda_{\max}(L_w)$$

Connect n vertices completely to K_n , delete a perfect matching

$$tw(G) = n, \quad \dim = n + 1$$



Result 4: A Graph Realization for Fiedler Vectors

Fiedler vectors: eigenvectors to $\lambda_2(L(G))$

starting point of spectral graph partitioning heuristics

Idea: Try to spread out the vertices even further by redistributing the edge lengths $\rightarrow l_{ij}$ for $ij \in E$

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To obtain an SDP: bound the edge lengths by $\sum l_{ij}^2 \leq |E|$

$$(F) \quad \begin{array}{ll} \max & \sum_{i \in N} \|v_i\|^2 \\ \text{s.t.} & \|v_i - v_j\| \leq l_{ij} \quad \text{for } ij \in E, \\ & \sum_{i \in N} v_i = 0, \\ & \sum_{ij \in E} l_{ij}^2 \leq |E|, \\ & l \in \mathbb{R}^E, v_i \in \mathbb{R}^n \text{ for } i \in N \end{array}$$

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Theorem. For $G = (N, E)$ connected and $V = [v_1, \dots, v_n]$ optimal for (F), $\sum_{i \in N} \|v_i\|^2 = \frac{|E|}{\lambda_2(L(G))}$ and $V^\top u$ is an eigenvector of $\lambda_2(L(G))$ for $u \in \mathbb{R}^n$.

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Theorem. $G = (N, E)$ connected, $u \in \mathbb{R}^n$, $\|u\| = 1$ eigenvector to $\lambda_2(L(G))$, then $X = \frac{|E|}{\lambda_2(L(G))} uu^\top$ and $l_{ij}^2 = \frac{|E|}{\lambda_2(L(G))} (u_i - u_j)^2$, $ij \in E$ is optimal for (F).

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\Rightarrow Maximum rank optimal solution gives a map of the eigenspace of $\lambda_2(L(G))$.

The same works out for λ_{\max} , as well.

Generalized λ_2 -Problem \rightarrow Rotational Dimension of a Graph

Given connected $G = (N, E)$, node weights $s_i \geq 0$, edge lengths $l_{ij} \geq 0$,

$$\begin{aligned} \text{EMB}(s, l) \quad & \max \sum_{i \in N} s_i \|v_i\|^2 \\ & \text{s.t.} \quad \sum_{i \in N} s_i v_i = 0 \\ & \quad \|v_i - v_j\|^2 \leq l_{ij} \quad ij \in E \\ & \quad v_i \in \mathbb{R}^n \text{ for } i \in N. \end{aligned}$$

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Minimal dimension of an optimal solution for weights s and length l

$$\dim_G(s, l) = \min\{\dim \text{span} \{v_i : i \in N\} : v_i \text{ optimal for EMB}(s, l)\}$$

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Rotational Dimension of $G = (N, E)$:

- G connected: $\text{rotdim}(G) := \max\{\dim_G(s, l) : s \in \mathbb{Z}_+^N, l \in \mathbb{Z}_+^E\}$
- $G = (\emptyset, \emptyset)$ $\text{rotdim}(G) := -1$
- G not connected: $\text{rotdim}(G) := \max\{\text{rotdim}(C) : C \text{ is a component of } G\}$

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One can prove (for connected G):

$$\begin{aligned} \text{rotdim}(G) &= \max\{\dim_G(s, l) : s \in \mathbb{R}_+^N, l \in \mathbb{R}_+^E\} \\ &= \max\{\dim_G(s, l) : s \in \mathbb{R}_{++}^N, l \in \mathbb{R}_{++}^E\} \end{aligned}$$

Observation The rotational dimension is a minor monotone graph parameter.

Results for the Rotational Dimension

Theorem [Separator-Shadow]

Let $v_i \in \mathbb{R}^n$, $i \in N$, be optimal for $\text{EMB}(s, l)$ for a connected $G = (N, E)$, let $C_1 \dot{\cup} S \dot{\cup} C_2$ partition N so that no node in C_1 is adjacent to a node in C_2 . Then, for at least one $j \in \{1, 2\}$, for every $i \in C_j$ the straight line segment $[0, v_i]$ intersects the convex hull of the points in S .

Theorem [Tree-Width]

Given a connected graph $G = (N, E)$ with node weights $s \in \mathbb{R}_+^N$ and edge lengths $l \in \mathbb{R}_+^E$, there exists an optimal solution of $\text{EMB}(s, l)$ having dimension at most tree-width of G plus one.

Forbidden Minor Characterizations

- $\text{rotdim}(G) \leq 0 \Leftrightarrow$ all components are nodes (forbidden K_2)
- $\text{rotdim}(G) \leq 1 \Leftrightarrow$ all components are paths (forbidden $K_3, K_{1,3}$)
- $\text{rotdim}(G) \leq 2 \Leftrightarrow$ all components are outerplanar (forbidden $K_4, K_{2,3}$)

Open: $\text{rotdim}(G) \leq 3?$ [forbidden K_5 , but $\text{rotdim}(K_{3,3}) = 3$]

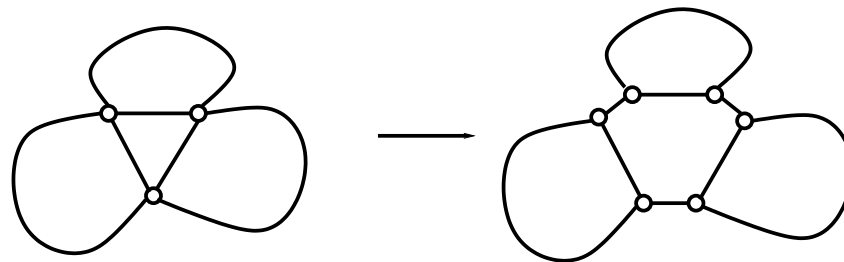
$\text{rotdim}(G) \leq 2 \Leftrightarrow$ **all components of G are outerplanar**

Outerplanar graphs are characterized by forbidden minors K_4 and $K_{2,3}$

- $\text{rotdim}(K_4) = 3$: regular 3-dim simplex,
 - $\text{rotdim}(K_{2,3}) = 3$: Let $N = \{1, 2\} \cup \{3, 4, 5\}$ and choose $l_{1i} = 1$ and $l_{2i} = 2$ for $i \in \{3, 4, 5\}$.
-

Main idea of $\text{rotdim}(\text{outerplanar}) \leq 2$:

Take a connected outerplanar graph G' and enlarge it to a connected outerplanar graph G having maximum degree ≤ 3 :



The former is a minor of the latter, so $\text{rotdim}(G') \leq \text{rotdim}(G)$.

Given an optimal embedding v_i of G for $s > 0$ and $l > 0$, we show $\dim \text{span} \{v_i : i \in N\} \leq 2$ by case distinction w.r.t. the position of the origin.

Concluding Remarks

- Results show a clear connection between separator structure and structural properties of the extremal eigenvectors
- For many classes of graphs the tree-width bounds are far from optimal:
Theorem for λ_{\max} :
Any bipartite graph has a 1-dim optimal embedding
- Conjecture for λ_2 : planar graphs have 3-dim optimal embeddings
- Relation of Rotational Dimension to the Colin de Verdière number?
(certainly not equal, but maybe $\text{rot dim} \leq \mu$)