

A Semidefinite Programming View on Spectral Properties of Graph Laplacians

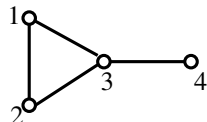
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TU Chemnitz

based on joint work with
Frank Göring, Susanna Reiss, Sebastian Richter,
Israel Rocha, Uwe Schwerdtfeger, Markus Wappler

Spectra of Graphs and Applications 2016
in honour of the 75th birthday of
Prof. Dragoš Cvetković

The Laplace matrix of a graph

- finite simple undirected Graph $G = (N, E)$,
 nodes $N = \{1, \dots, n\}$,
 edges $E \subseteq \{\{i, j\} : i, j \in N, i \neq j\}$ [$ij \in E$]

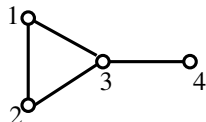


- Laplacian** $[L(G)]_{ij} = \begin{cases} \deg(i) & i = j \\ -1 & ij \in E \\ 0 & \text{otherwise} \end{cases}$

$$L = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

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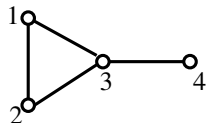
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- Properties: $L_w \succeq 0$ (sym., pos. semidef.)

$$u^T L_w u = \sum_{ij \in E} w_{ij} u^T E_{ij} u = \sum_{ij \in E} w_{ij} (u_i - u_j)^2 \geq 0$$

$$\lambda_1(L_w) = 0 \text{ with EV } \mathbf{1}, \quad \lambda_2(L_w) > 0 \text{ iff } G_w \text{ is connected}$$

The Laplacian is ubiquitous

- graph bisection [B1987,PR1995,FJ1998]
- maximum cut [DP1993,GW1995]
- TSP [CvCK1999]
- mixing rates of Markov chains/random walks [SBXD2006,W2000]
- expander graphs [HLW2006,L1994]
- maximum variance unfolding [WS2004]
- graph embeddings [LLR1995,BC2007]
- tensegrities and rigidity theory [C1999,C2005]
- the Colin de Verdière graph parameter [CdV1998,vdHLS1999]
- spectral graph theory [CDS1995,M1991,Ch1997,M2004,...]

Connections to mathematical physics via discrete Schrödinger operators, spin models, percolation ... (infinite graphs)

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More generally, . . .

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In particular

- minimizing the maximum eigenvalue and
- maximizing the second smallest eigenvalue (and further ones)

are convex problems solvable by Semidefinite Programming (SDP).

SDP duality offers a new view on eigenvectors.

LP \leftrightarrow SDP

$$\begin{array}{ll} \min & \langle c, x \rangle \\ \text{s.t.} & \langle a_i, x \rangle = b_i \\ & x \geq 0 \end{array}$$

$$\begin{array}{ll} \min & \langle C, X \rangle \\ \text{s.t.} & \langle A_i, X \rangle = b_i \\ & X \succeq 0 \end{array}$$

$x \in \mathbb{R}_+^n$ nonneg. orthant
(polyhedral)
 $\langle c, x \rangle = \sum_i c_i x_i$

$X \in \mathcal{S}_+^n$ pos. semidef. matrices
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$$\begin{array}{ll} \max & \langle b, y \rangle \\ \text{s.t.} & \sum_i a_i y_i + z = c \\ & z \geq 0 \end{array}$$

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primal and dual optima satisfy (if they exist)

without regularity condition
 $\langle c, x^* \rangle = \langle b, y^* \rangle$
 complementarity $\langle x^*, z^* \rangle = 0$

with strict feasibility on one side
 $\langle C, X^* \rangle = \langle b, y^* \rangle$
 complementarity $X^* Z^* = 0$

Example

$$\begin{array}{ll} \min & \langle C, X \rangle \\ \text{s.t.} & \langle I, X \rangle = 1 \\ & X \succeq 0 \end{array}$$

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set of primal optimal solutions

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columns of P form an orthonormal basis of the eigenspace of $\lambda_{\min}(C)$,

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columns of P form an orthonormal basis of the eigenspace of $\lambda_{\min}(C)$, each optimal $X = PUP^T$ satisfies complementarity $(\lambda_{\min}I - C)X = 0$.

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introduced by [Fiedler 1989]

(see also: fastest mixing Markov process on a graph [SBXD2006])

$$\max_{w \in \mathcal{W}} \lambda_2(L_w) \quad \mathcal{W} = \{w \in \mathbb{R}_+^E : \sum_{ij \in E} w_{ij} = 1\} \quad [= |E| \text{ orig.}]$$

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Optima have the form $X^* = PUP^T$ for an eigenspace basis P of $\lambda_2(L_{w^*})$. 

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idea based on vector labellings of [L1979], see also [LLR1995]

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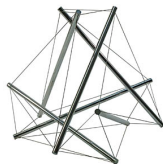
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 \langle \mathbf{1}\mathbf{1}^T, X \rangle &= \mathbf{1}^T V^T V \mathbf{1} = 0, \quad \text{thus} \quad V \mathbf{1} = \sum v_i = 0
 \end{aligned}$$

Spread out $v_i \in \mathbb{R}^n$ for $i \in N$ as far apart as possible with barycenter in the origin and distances at most 1 for $ij \in E$.

Tensegrities [Connelly1998]

Bars, cables or struts link vertices
under tension so as to form an integrity
→ graph with edges of fixed/max/min length



andydoro.com/tensegrity

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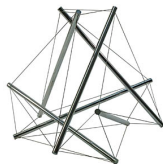
In equilibrium, all *tensions* w_{ij} (positive/negative) along the edges ij must cancel out in each vertex $v_i \in \mathbb{R}^n$ ($i \in N$),

$$\text{for } i \in N : \sum_{j:ij \in E} w_{ij}(v_i - v_j) = 0 \quad [\text{compl.}]$$

Such w_{ij} define an *equilibrium stress* and lead to *stress matrix* Ω with $\Omega_{ij} = -w_{ij}$ for $ij \in E$, $\Omega_{ii} = \sum_{ij \in E} w_{ij}$ and $= 0$ otherwise.

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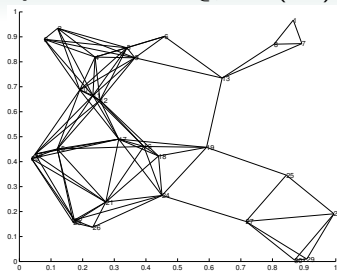
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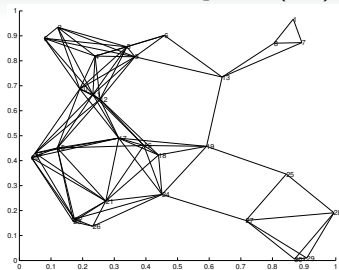
Note: $\Omega = L_w$ and the tensions w may be interpreted as Lagrange multipliers of a corresponding optimization problem.

Example for $\max_{W \in \mathcal{W}} \lambda_2(L_W)$:

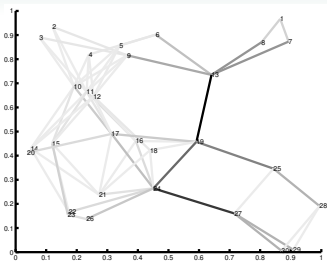


original graph (random)

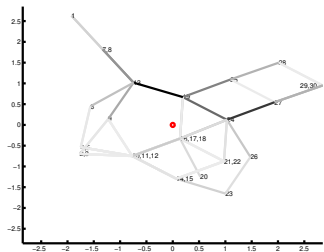
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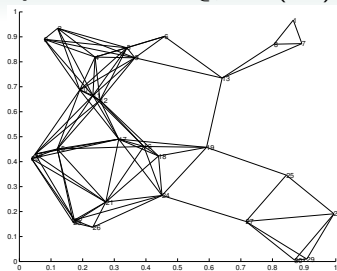


optimal weights for λ_2



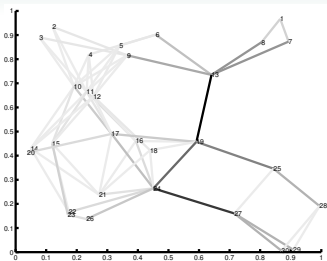
a rotational embedding (2D)

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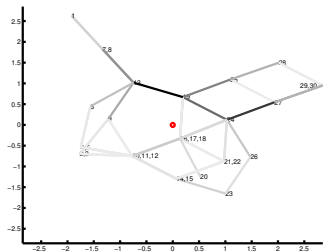


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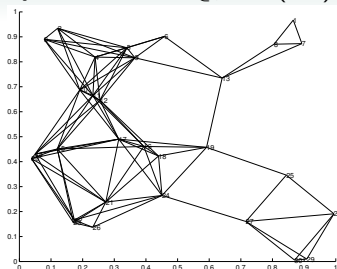


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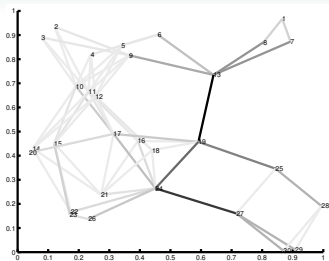
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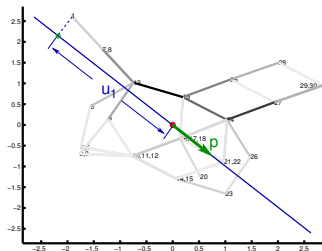


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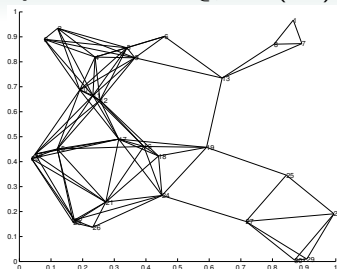


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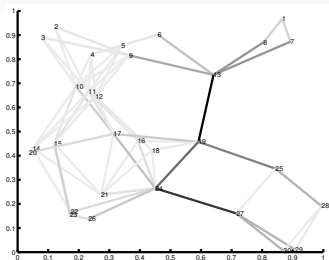
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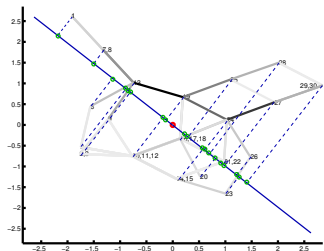


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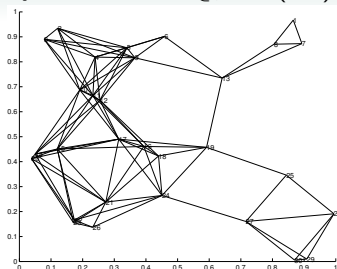


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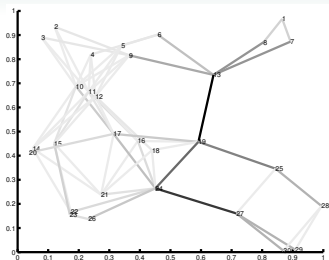
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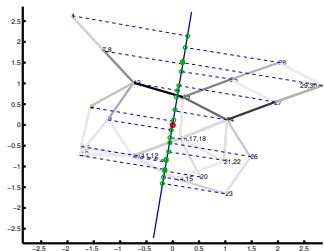


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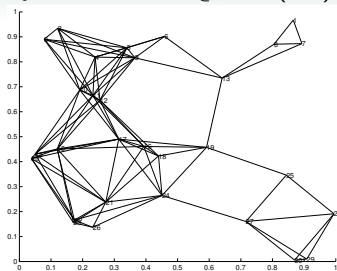


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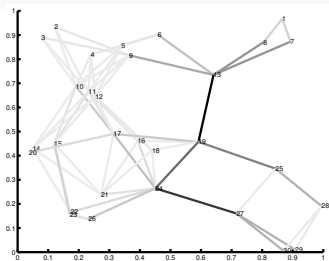
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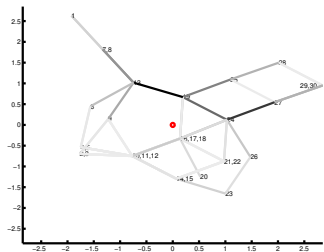


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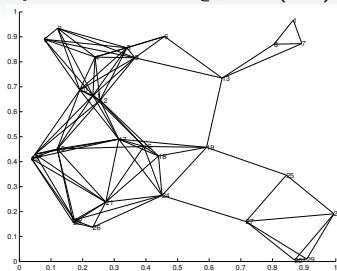


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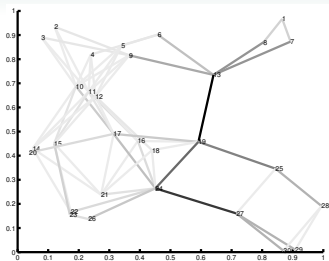
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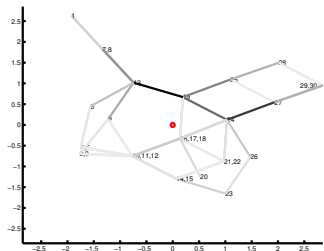


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- What about λ_{\max} ?



optimal weights for λ_2



a rotational embedding (2D)

Symmetric arguments lead to an embedding for λ_{\max} [GHR2012]

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

$$\min_{w \in \mathcal{W}} \lambda_{\max}(L_w)$$

as SDP:

$$\begin{aligned} \max \quad & \lambda \\ \text{s.t.} \quad & \sum_{ij \in E} w_{ij} E_{ij} + \mu \mathbf{1}\mathbf{1}^T \succeq \lambda I \\ & \mathbf{1}^T w = 1, w \geq 0 \end{aligned}$$

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divide by $\lambda_{\text{opt}} > 0$

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dualize

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

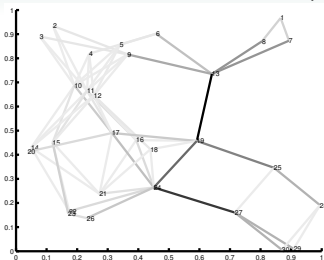
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embedding: set $X = V^T V$ with $V = [v_1, \dots, v_n]$

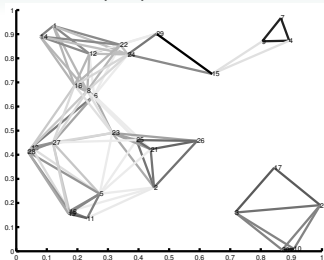
$$\begin{aligned} \max \quad & \sum \|v_i\|^2 \\ \text{s.t.} \quad & \|v_i - v_j\|^2 \leq 1, \quad ij \in E \\ & \sum v_i = 0, v_i \in \mathbb{R}^n \end{aligned}$$

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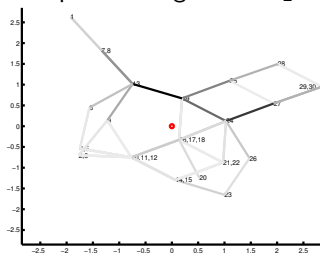
Example comparing $\max_w \lambda_2(L_w)$ to $\min_w \lambda_{\max}(L_w)$



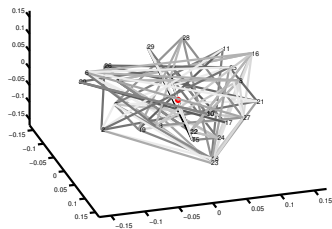
optimal weights for λ_2



optimal weights for λ_{\max}



an optimal λ_2 -embedding (2D!)
cables, G folds “outwards”



an optimal λ_{\max} -embedding (14D?)
struts, G folds “inwards”

What connections exist between eigenvectors of extremal eigenvalues and structural properties of the graph?

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

Connections to structural properties . . .

While extremal eigenvalues are related to cuts, the corresponding eigenvectors seem related to vertex separators.

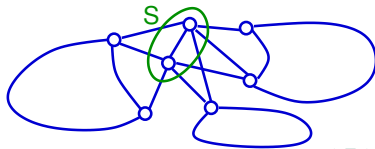
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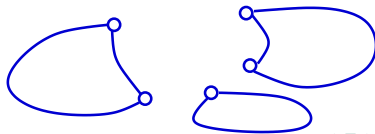
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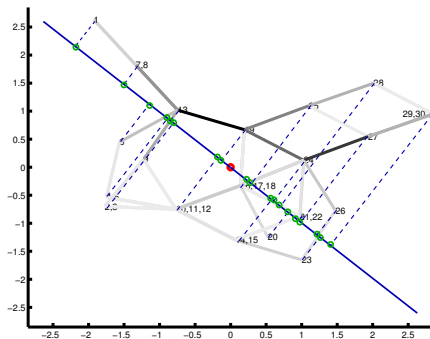
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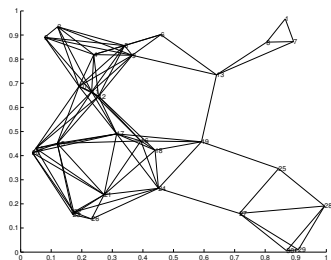
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Recall, projection onto any one-dimensional subspace yields an EV

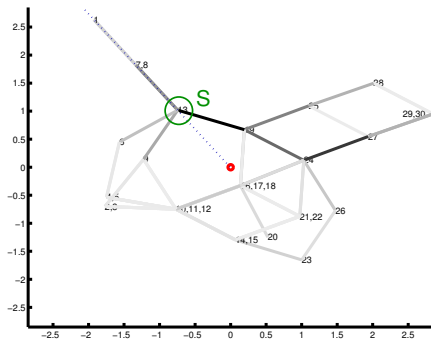


optimal weights for λ_2
G folds outwards

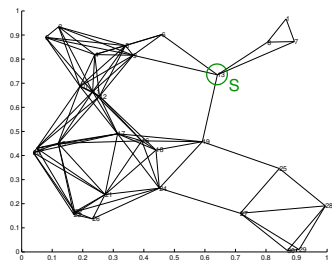


original graph

Rotational view: nodes are hinges, separated parts dangle outwards

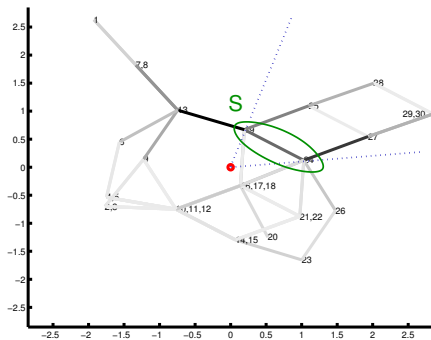


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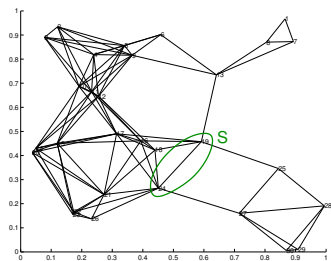


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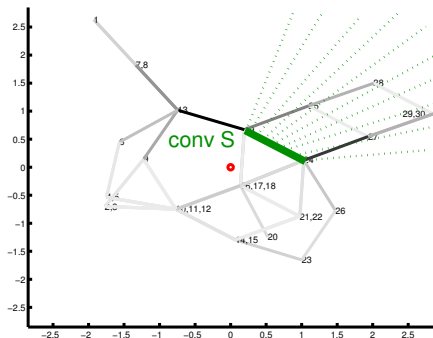


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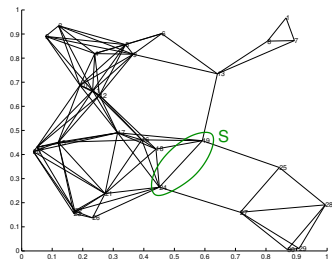


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optimal weights for λ_2
 G folds outwards



original graph

If the origin is the sun,
 the convex hull of the separator blocks the light for separated nodes,
 “separated parts lie in the shadow of the separator”.

Separators and Optimality of Embeddings [GHW08,GHR12]

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 $\mathcal{S} = \{v_i : i \in S\}$.

$$\lambda_2(L_w)$$

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

Separator-Shadow Th.

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

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

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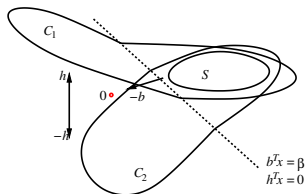
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geometric proof idea:



Sketch of Proof:

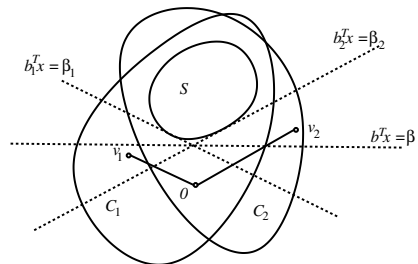
Assume, for contradiction, the theorem does not hold, then w.l.o.g.

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

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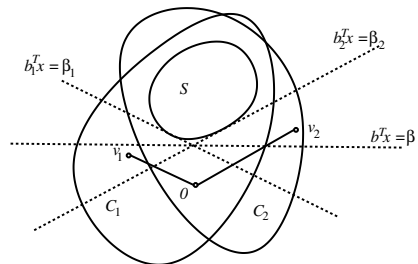
$b_i^T x < \beta_i$ separates $[0, v_i]$ from \mathcal{S}

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

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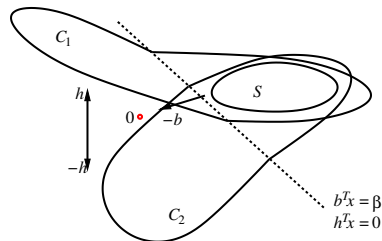
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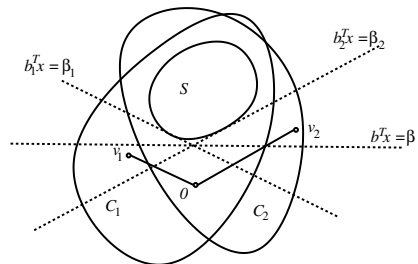
choose $\alpha \in [0, 1]$ so that both
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$\sum v_i = 0 \Rightarrow$ lin. dep., thus h exists

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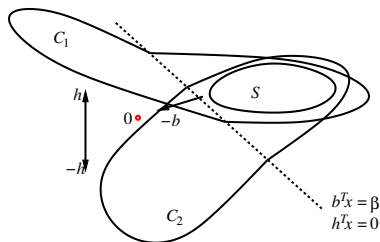
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Verify: epsilon movement improves solution \Rightarrow contradiction to optimality \square

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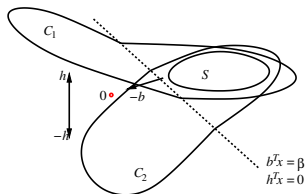
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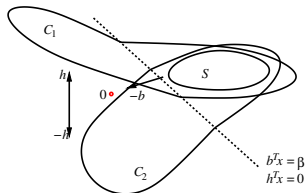
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$$[v_i, 0] \cap \text{conv } \mathcal{S} \neq \emptyset \quad \forall i \in C_j$$

geometric proof idea:



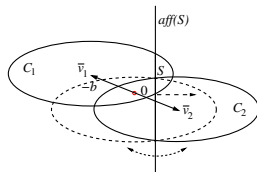
$$\lambda_{\max}(L_w)$$

Separator's Sunny Side Th.

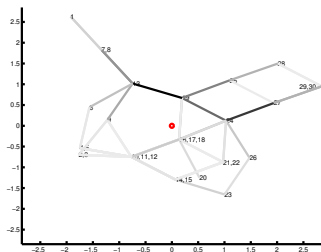
Let $\bar{v}_j = \frac{1}{|C_j|} \sum_{i \in C_j} v_i$, $j \in \{1, 2\}$, be the barycenter of C_j , then

$$\bar{v}_j \in \text{aff}(\mathcal{S}) - \text{cone}(\mathcal{S}) \text{ for } j \in \{1, 2\}$$

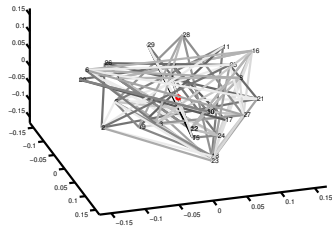
geometric proof idea:



When do there exist optimal embeddings of small dimension?



an optimal λ_2 -embedding
2D!



an optimal λ_{\max} -embedding
14D?

Tree-Width

[Halin1976(cf. Diestel2000),RS]

Given $G = (N, E)$,

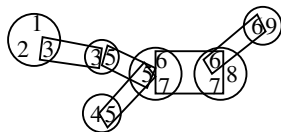
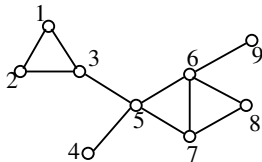
let $T = (\mathcal{N}, \mathcal{E})$ be a tree with $\mathcal{N} \subseteq 2^N$ and $\mathcal{E} \subseteq \binom{\mathcal{N}}{2}$ so that

- (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.



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

Existence of low dimensional solutions [GHW08,GHR12]

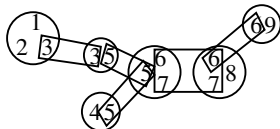
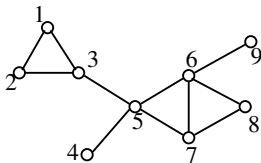
$$\lambda_2(L_w)$$

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

Tree-Width Bound

There exists an optimal embedding of dimension at most

$$tw(G) + 1$$



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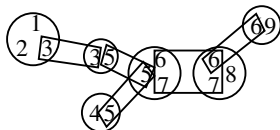
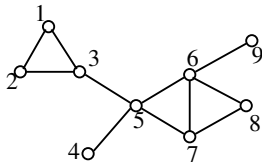
algorithmic proof idea:

given a tree decomposition,

start at a 0-node,

try to flatten all adjacent nodes

or move on to the next 0-node



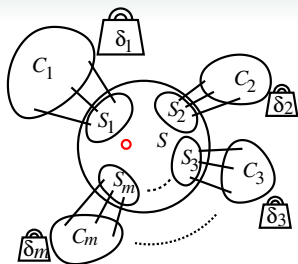
Theorem [Separators Containing the Origin]

[GHW08]

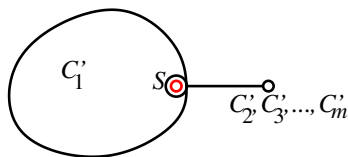
Let $v_i \in \mathbb{R}^n$ for $i \in N$ be an optimal solution of (EMB) for a connected graph $G = (N, E)$ and let $S \subset N$ with $0 \in \mathcal{S} = \text{conv}\{v_s : s \in S\}$ be a separator in G inducing a partition (S, C_1, \dots, C_m) of N so that no node in C_j is adjacent to a node in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

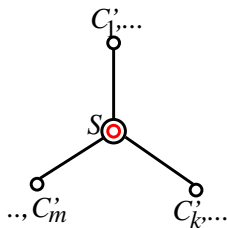
initial embedding



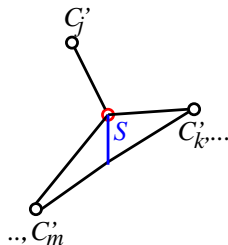
(i) $\delta_1 > \delta_2 + \dots + \delta_m$
 $\rightarrow \dim(S, C'_1)$



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



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



Existence of low dimensional solutions [GHW08,GHR12]

$\lambda_2(L_w)$

$\lambda_{\max}(L_w)$

Tree-Width Bound

There exists an optimal embedding of dimension at most

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needs separator shadow + involved result for separators with $0 \in \text{conv } S$

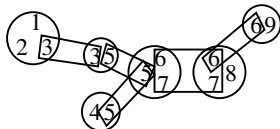
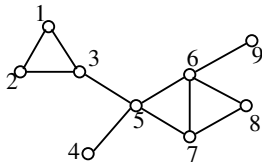
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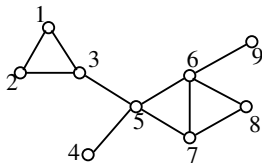
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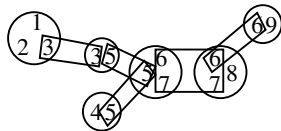
Obs.: in separated sets no forces interact outside separator space.

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

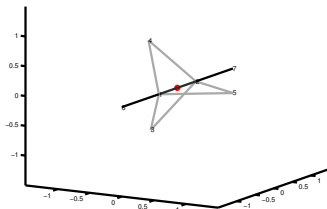
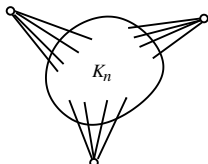


The Tree-Width bounds are sharp

[GHW08,GHR12]

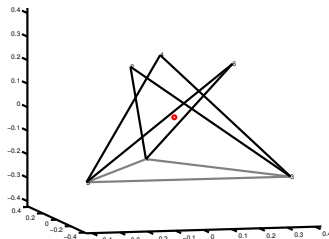
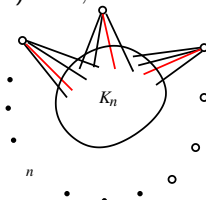
$$\lambda_2(L_W)$$

For $n \geq 4$, connect three vertices completely to K_n
 $tw(G) = n$, $\dim = n + 1$



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

Connect n vertices completely to K_n , delete a perfect matching
 $tw(G) = n$, $\dim = n + 1$



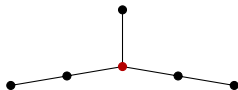
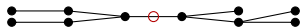
Computing Weights Combinatorially

$$\lambda_2(L_w)$$

separator shadow for trees

→ absolute center of gravity

[F1990,W2013]



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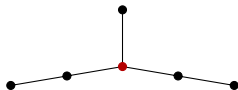
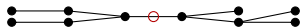
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explicit formulas for double brooms [RR2016]

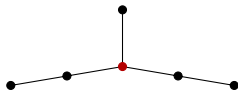
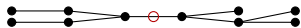


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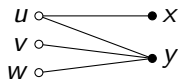


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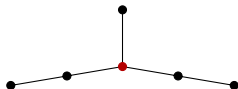
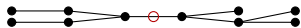
\exists 1-dim opt. emb. iff bipartite
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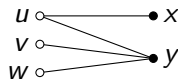


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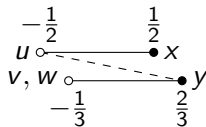


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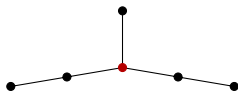
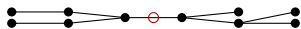
splits bipartite graphs into balanced
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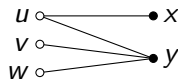


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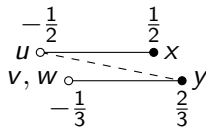


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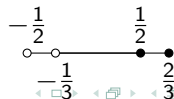
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comb. alg. for trees and bipartite
 graphs [HRS2015] (cmp. [P1995])



Rotational Dimension of a Graph [GHW2011]

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

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

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

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

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

- G connected: $\text{rotdim}(G) := \max\{\dim_G(s, l) : s \in \mathbb{Z}_+^N, l \in \mathbb{Z}_+^E\}$
- $G = (\emptyset, \emptyset)$ $\text{rotdim}(G) := -1$
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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

[GHW2011]

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 $\text{rotdim}(K_{3,3}) = 3$]

Conclusion and Outlook

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- For which graph classes is it possible to improve the tree-width bound on the existence of low-dimensional solutions?
- The rotational dimension (worst minimal λ_2 -dimension over all node-weights and edge-lengths) seems tightly related to the Colin de Verdière graph parameter μ (is $\text{rotdim} \leq \mu$?) and the Gram dimension of a graph [LV2014].
- What is the forbidden minor characterization for $\text{rotdim} \leq 3$?

Thank You for Your attention!

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Many happy returns!

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

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

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