¿Cross-Connections?

Metric Embeddings, Graph Laplacians, Rank Minimization,

Christoph Helmberg (TU Chemnitz)

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Minimum Distortion Embeddings of Finite Metric Spaces

Further Embedding Problems

Generalized Laplacians and Nodal Domains

Low Rank Approaches

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Distance, Semimetric, Metric [DL97,LLR95]

Given a (finite) set N, a distance $d: N \times N \rightarrow \mathbb{R}_+$ satisfies

- symmetry: d(i,j) = d(j,i) for $i,j \in N$
- and d(i, i) = 0 for $i \in N$

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• the riangle-inequalities hold: $d(i,j) \le d(i,k) + d(k,j)$ for $i,j,k \in N$

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Depending on d, the pair (N, d) forms a distance/semimetric/metric space.

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Example: Given a connected graph G = (N, E), let d(i, j) denote the length of a shortest path between *i* and *j*, then (N, d) is a metric space.

Further examples:

MET_n in DL97: Symmetric nonnegative matrices of order n with diagonal 0 that satisfy all △-inequs, describe all semimetrics on n elements.
 Given d, d' ∈ MET_n and λ ≥ 0, we have λ(d + d') ∈ MET_n, so

 MET_n is a convex cone.

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- CUT_n in DL97: For $S \subseteq N$ define the cut-semimetric

$$d_{\mathcal{S}}(i,j) = \begin{cases} 1 & \text{for } ij \in \delta(\mathcal{S}) := \{ij : |\mathcal{S} \cap \{i,j\}| = 1\}, \\ 0 & \text{otherwise}, \end{cases}$$

then $\sum_{S \subseteq N} \lambda_S d_S$ with $\lambda_S \ge 0$ is again a semimetric. \rightarrow the cut cone $\text{CUT}_n := \{\sum_{S \subseteq N} \lambda_S d_S : \lambda_S \ge 0 \ \forall S \subseteq N\}$

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For a normed space (E, || · ||), d_{||·||}(x, y) = ||x - y|| is the associated norm metric. In particular, we use d_{Ip} = ||x - y||_p

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Embeddings and Distortion

Given two distance spaces (N, d), (N', d') a mapping $\phi : N \to N'$ is called a Lipschitz embedding of (N, d) into (N', d') with distortion $c \ge 1$ if

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An embedding with distortion c = 1 is an isometric embedding.

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A distance space is l_p embeddable if there is an isometric embedding into (\mathbb{R}^m, d_{l_p}) for some $m \ge 1$.

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[Bourgain1985]: Any *n*-point metric space (N, d) can be embedded in $O(\log n)$ -dimensional Euclidean space with distortion $O(\log n)$.

• *d*-cube: $n = 2^d$ vertices, distortion $\sqrt{d} \in O(\log n)$ for l_2 .

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[JohnsonLindenstrauss1984]: Any *n* points in an Euclidean space can be mapped to \mathbb{R}^t with $t = O(\frac{\log n}{\varepsilon^2})$ and distortion $\leq 1 + \varepsilon$.

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Example: Isometric I_{∞} embedding

d is a semimetric on $N = \{1, ..., n\} \Leftrightarrow (N, d)$ is I_{∞} embeddable [$\Leftrightarrow d \in \mathsf{MET}_n$]

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<u>"</u> \Rightarrow ": setting $v_i = (d(1, i), \dots, d(n-1, i)) \in \mathbb{R}^{n-1}$ for $i \in N$ defines an isometry:

$$\|v_i - v_j\|_{\infty} = \max\{\underbrace{|d(k,i) - d(k,j)|}_{\triangle \text{-ineq } \leq d(i,j)} : k \in \{1,\ldots,n-1\}\} \stackrel{k \in \{i,j\}}{=} d(i,j)$$

Example: I_1 Embeddability and the Cut Cone

A cut semimetric d_S , $S \subseteq N$ is l_1 embeddable: $\phi(i) = 1$ for $i \in S$, $\phi(i) = 0$ for $i \in N \setminus S$.



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Checking I_1 embeddability is *NP*-complete!

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Minimum Distortion Euclidean Embeddings [LLR1995]

Semidefinite programming allows to find a minimum distortion Euclidean embedding in \mathbb{R}^n :

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- Put $v_i = \rho(i)$, $V = [v_1, \dots, v_n]$ and consider the
 - Gram matrix $X = V^T V \succeq 0$ $(x_{ij} = v_i^T v_j)$ $E_{ij} = \begin{vmatrix} 1 & -1 & i \\ -1 & 1 & j \end{vmatrix}$

Note: $||v_i||^2 = x_{ii}$ and $||v_i - v_j||^2 = x_{ii} - 2x_{ij} + x_{jj} = \langle E_{ij}, X \rangle$

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Use $[JL84] \rightarrow$ embedding in $\mathbb{R}^{O(\log n)}$ with distortion $O(D_{opt})$

 [Vallentin2007] optimal distortion embeddings for classes of distance regular graphs (Hamming/Johnson=Graphs/悪.) = → = → へ ペ

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Minimum Distortion Embeddings of Finite Metric Spaces

Further Embedding Problems

Generalized Laplacians and Nodal Domains

Low Rank Approaches

Sensor Network Localization Euclidean Distance Matrix Completion

 Given a graph G = (N, E), a few node positions v_i ∈ ℝ^d, i ∈ N' ⊂ N and (approximate) edge lengths,

is there a distance preserving embedding of all nodes in \mathbb{R}^d ?

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• various relaxation variants exist [SoYe2004,DKQW2006], e.g.,

$$\begin{array}{ll} \min & \frac{1}{2} \sum_{ij \in E} \left(\langle E_{ij}, X \rangle - d(i,j)^2 \right)^2 \\ \text{s.t.} & x_{ij} = v_i^{\mathsf{T}} v_j \qquad \forall 1 \leq i \leq j \leq k \\ & X \succeq 0 \end{array}$$

• almost identical to the Euclidean Distance Matrix Completion Problem [DingKrislockQianWolkowicz2006]

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 [DingKrislockQianWolkowicz2006]
- Questions of uniqueness lead to rigidity/tensegrity theory. [SoYe2005]
- main difficulty: $\mathbb{R}^d \Leftrightarrow \operatorname{rank}(X^*) \leq d$ (nonconvex!)
- ightarrow general interest in "existence of low rank optimal solutions"

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Graph Realizations

[BelkConnelly07]

• A graph G = (N, E) with given distances d_{ij} , $ij \in E$ is realizable in \mathbb{R}^d if there exist $v_1, \ldots, v_n \in \mathbb{R}^d$ with $||v_i - v_j|| = d_{ij} \forall ij \in E$

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 1-realizable: no K₃ minor (forests)
 - \circ 2-realizable: no K_4 minor (series parallel)
 - \circ 3-realizable: no K_5 and $K_{2,2,2}$ minor

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- [SoYe06] give a polynomial algorithm for constructing an (approx.) realization for 3-realizable graphs
Tensegrities [Connelly1998]

• A tensegrity consists of bars, cables, and struts that link vertices that are *pinned* or *not pinned* \rightarrow graph with edges of fixed/max/min length





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 \rightarrow stress matrix Ω , $\Omega_{ij} = -w_{ij}$ for $ij \in E$, $\Omega_{ii} = \sum_{ii \in F} w_{ij}$ and = 0 otherwise.



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• The tensegrity is super stable if $w_{ii} > 0$ (< 0) for all cables (struts), $\Omega \succeq 0$ has max. rank n-d-1 and there are no (infinitesimal) affine flexes

Maximum Variance Unfolding [WeinbergerSaul2004]

- visualization-technique for graphs G = (N, E) in data mining
- \bullet Spread out a graph as much as possible, edges = cables of length 1

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 $\rightarrow\,$ "rotate" the graph around its barycenter

[GHW05]

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- Also equivalent to redistributing edge weights so as to

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• Corresponds to finding a fastest mixing (symmetric) Markov chain on *G*

[SBXD04]

[GHW05] [GHW05]

Low Rank Approaches

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Laplace matrix of a graph

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



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May be viewed as a discrete version of the Laplace operator $\Delta u = u_{xx} + u_{yy}$:

For the wave equation
$$\Delta u = u_{tt}$$
 solve $\Delta u + \lambda u = 0 \leftrightarrow u_{xx}(x, y) \approx \frac{u(x-h,y)-2u(x,y)+u(x+h,y)}{h^2}$,
 $u_{yy}(x, y) \approx \frac{u(x-h,y)-2u(x,y)+u(x+h,y)}{h^2}$,
 $u_{yy}(x, y) \approx \frac{u(x,y-h)-2u(x,y)+u(x,y+h)}{h^2}$,
 $4u(x,y)-u(x-h,y)-u(x+h,y)-u(x,y-h)-u(x,y+h) \approx h^2\lambda u(x,y)$

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

• Properties: $L_w \succeq 0$ (sym., pos. semidef.), $\lambda_1(L_w) = 0$ with EV 1.

Nodal Domains

In the wave equation of a string or drum, eigenfunctions represent modes of vibration.

For each eigenfunction, the zeros represent nodes/nodal lines, along which the string/drum does not move. The moving regions in between are the nodal domains, all points in a nodal domain have the same sign.

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For an eigenvector v of $L_w(G)$ of a connected graph G = (N, E) there are

- strong nodal domains: each connected component of the subgraph induced by all *i* ∈ *N* with *v_i* > 0 (and likewise by *v_i* < 0)
- weak nodal domains: each connected component of the subgraph induced by all $i \in N$ with $v_i \ge 0$ (and likewise by $v_i \le 0$)



For the depicted values of the eigenvector

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For the depicted values of the eigenvector there are 4 strong nodal domains

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For the depicted values of the eigenvector there are 4 strong nodal domains and 2 weak nodal domains.

Nodal Domains of Generalized Laplacians [BLS2000]

A symmetric matrix M is called a generalized Laplacian or discrete Schrödinger operator of a graph G = (N, E), if

$$M_{ij} \text{ is } \begin{cases} < 0 & \text{ for } ij \in E, \\ = 0 & \text{ for } ij \notin E, i \neq j, \\ \in \mathbb{R} & \text{ for } i = j. \end{cases}$$

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Theorem. Let *M* be a generalized Laplacian of a connected graph and let λ_k be an eigenvalue of *M* of multiplicity *r*, i. e., $\lambda_1 \leq \cdots \leq \lambda_{k-1} < \lambda_k = \cdots = \lambda_{k+r-1} < \lambda_{k+r} \leq \cdots$.

Any eigenvector to λ_k induces at most k weak nodal domains and at most k + r - 1 strong nodal domains.

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Fiedler1974 proved that for any eigenvector v of $\lambda_2(G)$ and $\alpha \leq 0$, the node set $N_{\alpha} := \{i \in N : v_i \geq \alpha\}$ induces a connected subgraph. He showed tight relations between $\lambda_2(G)$ and the connectivity of the graph. \rightarrow Fiedler-vector in spectral graph partitioning heuristics.

Rough sketch for strong nodal domains: idea goes back to Courant. Let v^k to λ_k induce strong domains D_1, \ldots, D_m . Define *m* new vectors g^j via $g_i^j := \begin{cases} v_i^k & \text{for } i \in D_j, \\ 0 & \text{otherwise,} \end{cases} j = 1, \ldots, m.$ They are linearly independent, because their support is distinct.

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Let w^1, \ldots, w^{m-1} be eigenvectors to $\lambda_1, \ldots, \lambda_{m-1}$, span dim. m-1 $\Rightarrow \exists \alpha_j \in \mathbb{R}$ so that $g = \sum_{j=1}^m \alpha_j g^j \neq 0$ and $g^T w^h = 0$, $h = 1, \ldots, m-1$. w.l.o.g., $\|g\| = 1 \Rightarrow g^T Mg \geq \lambda_m$ (orthog. to the first $m-1 w^h$)

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Exploit
$$g = a \circ v$$
 with $a_i = \begin{cases} \alpha_j & \text{if } i \in D_j, \\ 0 & \text{otherwise,} \end{cases}$
in order to show $g^T Mg \leq \lambda_k$
(e.g., for $ij \in E$ with $v_i v_j > 0 \Rightarrow \alpha_i - \alpha_j = 0$).

Rough sketch for strong nodal domains: idea goes back to Courant. Let v^k to λ_k induce strong domains D_1, \ldots, D_m . Define *m* new vectors g^j via $g_i^j := \begin{cases} v_i^k & \text{for } i \in D_j, \\ 0 & \text{otherwise,} \end{cases} j = 1, \ldots, m.$ They are linearly independent, because their support is distinct.

Let w^1, \ldots, w^{m-1} be eigenvectors to $\lambda_1, \ldots, \lambda_{m-1}$, span dim. m-1 $\Rightarrow \exists \alpha_j \in \mathbb{R}$ so that $g = \sum_{j=1}^m \alpha_j g^j \neq 0$ and $g^T w^h = 0$, $h = 1, \ldots, m-1$. w.l.o.g., $\|g\| = 1 \Rightarrow g^T Mg \geq \lambda_m$ (orthog. to the first $m-1 w^h$)

Exploit
$$g = a \circ v$$
 with $a_i = \begin{cases} \alpha_j & \text{if } i \in D_j, \\ 0 & \text{otherwise,} \end{cases}$
in order to show $g^T Mg \leq \lambda_k$
(e.g., for $ij \in E$ with $v_i v_j > 0 \Rightarrow \alpha_i - \alpha_j = 0$).
Now $\lambda_m \leq g^T Mg \leq \lambda_k < \lambda_{k+r}$ implies $m < k + r$.

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Given a graph G = (N, E) the parameter $\mu(G)$ is the largest corank of any matrix M satisfying

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 $\mu(G)$ is bounded above by the tree width +1 and it is minor monotone!

- $\mu(G) \leq 1 \Leftrightarrow G$ is a disjoint union of paths
- $\mu(G) \leq 2 \Leftrightarrow G$ is outerplanar
- $\mu(G) \leq 3 \Leftrightarrow G$ is planar
- $\mu(G) \leq 4 \Leftrightarrow G$ is linklessly embeddable

Low Rank Approaches

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Minimum Distortion Embeddings of Finite Metric Spaces

Further Embedding Problems

Generalized Laplacians and Nodal Domains

Low Rank Approaches

SDP Rank Reduction [SoYeZhang2006]

• Given distance constraints $\langle E_{ij}, X \rangle = d_{ij}$, how much do we have to violate them to find low-rank solutions?



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Theorem. Given $A_1, \ldots, A_m \in S^n_+$, $b_1, \ldots, b_m \in \mathbb{R}_+$, suppose there is an $X \succeq 0$ with

$$\langle A_i, X \rangle = b_i, \qquad i = 1, \ldots, m.$$

For $r = \min\{\sqrt{2m}, n\}$ and any $d \ge 1$ there is an $X_0 \succeq 0$, $\operatorname{rank}(X_0) \le d$ so that

$$\beta(m,n,d) \cdot b_i \leq \langle A_i, X_0 \rangle \leq \alpha(m,n,d) \cdot b_i \qquad i = 1, \dots, m$$

with $\alpha(m,n,d) = \begin{cases} 1 + \frac{12 \ln(4mr)}{d} & \text{for } 1 \leq d \leq 12 \ln(4mr) \\ 1 + \sqrt{\frac{12 \ln(4mr)}{d}} & \text{for } d > 12 \ln(4mr) \end{cases}$
and $\beta(m,n,d) = \begin{cases} \frac{1}{(2m)^{2/d}e} & \text{for } 1 \leq d \leq 4 \ln(2m) \\ \max\left\{\frac{1}{(2m)^{2/d}e}, 1 - \sqrt{\frac{4 \ln(2m)}{d}}\right\} & \text{for } d > 4 \ln(2m). \end{cases}$

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• [Barvinok2002]: $(1 - \varepsilon)b_i \le \langle A_i, X_0 \rangle \le (1 + \varepsilon)b_i$ for $d = 8\varepsilon^{-2}\ln(4m)$

• includes [JohnsonLindenstrauss1984]

Finding Low-Rank Solutions by Norm Minimization [RechtFazelParrilo2007]

• rank version of sparsest vector/compressed sensing is

min rank(Y) s.t. $\mathcal{A}Y = b, Y \in \mathbb{R}^{m \times n}$



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• e.g. for finding low-rank Euclidean distance matrices, solve

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How to represent $X \succeq 0$?

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How to represent $X \succeq 0$?

$$\operatorname{rank}\left(Y = \left[\begin{array}{cc}I_d & V\\V^{\mathsf{T}} & X\end{array}\right]\right) = d \qquad \Leftrightarrow \qquad X = V^{\mathsf{T}}V \succeq 0$$

 \Rightarrow EDM-Completion in \mathbb{R}^d may be cast as the problem

min rank(Y) s.t. AY = b
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Nuclear Norm Minimization [RechtFazelParrilo2007]

- Solve relaxation of min rank(Y) s.t. $AY = b, Y \in \mathbb{R}^{m \times n}$
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• They also show that this holds for a certain random family of matrices.

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SDPLR by [BurerMonteiro2003/5]