Graph Matching: Relax or Not?

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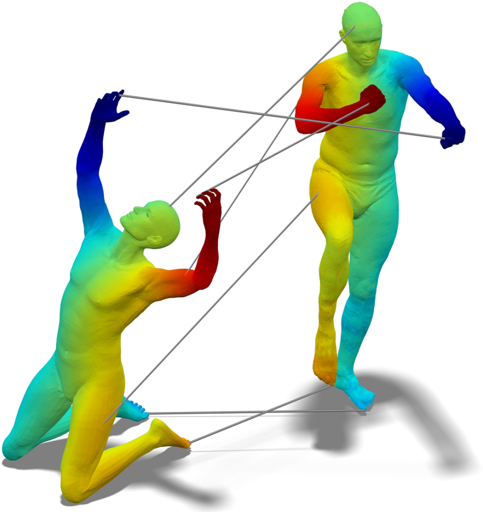
Joint work with Yonathan Aflalo and Ron Kimmel

Minimum-distortion correspondences



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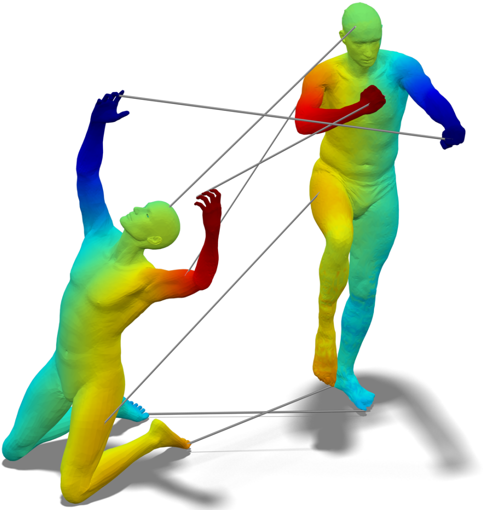
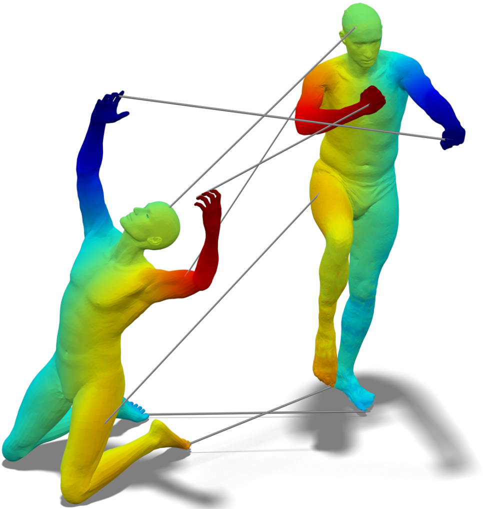


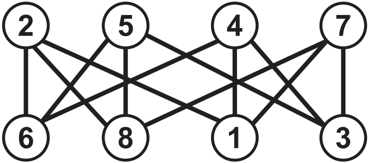
Find the best structure-preserving correspondence

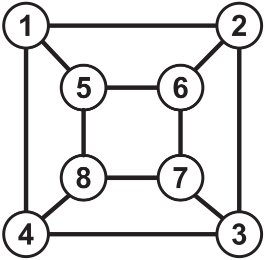
Minimum-distortion correspondences



Find $\varphi : (X, d_X) \mapsto (Y, d_Y)$ **minimizing** $\|d_X - d_Y \circ (\varphi \times \varphi)\|$

'Graph matching' problems





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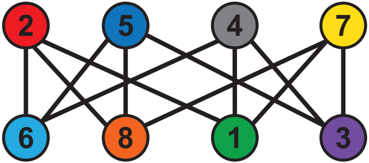

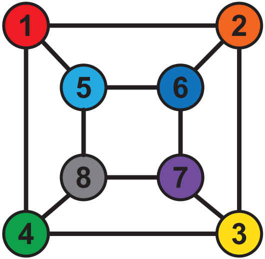

'Graph matching' problems

Given two undirected weighted graphs represented by adjacency matrices $\mathbf{A}$ and $\mathbf{B}$

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Exact graph 'matching': find isomorphism relating $\mathbf{A}$ and $\mathbf{B}$

Inexact graph 'matching': find best approximate isomorphism relating $\mathbf{A}$ and $\mathbf{B}$

Graph Matching (NP)

$$\mathbf{\Pi}^* = \underset{\mathbf{\Pi} \in \mathcal{P}}{\operatorname{argmin}} \|\mathbf{A} - \mathbf{\Pi}^{\mathrm{T}} \mathbf{B} \mathbf{\Pi}\|$$

$\mathcal{P}$ = space of $n \times n$ permutation matrices

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Convex Relaxation

$$\mathbf{P}^* = \underset{\mathbf{P} \in \mathcal{D}}{\operatorname{argmin}} \|\mathbf{PA} - \mathbf{BP}\|_{\mathrm{F}}^2$$

$\mathcal{D} = \{\mathbf{P} \geq \mathbf{0} : \mathbf{P1} = \mathbf{P}^{\mathrm{T}}\mathbf{1} = \mathbf{1}\}$ space of $n \times n$ double-stochastic matrices

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2. **Projection onto $\mathcal{P}$ (LAP)**

$$\hat{\mathbf{\Pi}} = \operatorname*{argmax}_{\mathbf{\Pi}\in\mathcal{P}} \operatorname{tr}(\mathbf{\Pi}^{\mathrm{T}}\mathbf{P}^*)$$

Solved by Hungarian algorithm

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Surprisingly, not so much is known about the relation between $\mathbf{\Pi}^*$ and $\hat{\mathbf{\Pi}}$!

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double-stochastic matrices

An even bigger relaxation

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no inequality constraints

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Friendly graphs: an undirected weighted graph $\mathbf{A}$ is friendly if

- $\mathbf{A}$ has simple spectrum
- no eigenvectors of $\mathbf{A}$ are orthogonal to the constant vector $\mathbf{1}$

Friendly graphs

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(have trivial automorphism group)

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Converse is not true (think of a regular asymmetric graph), but such graphs should be rare

Main result

Theorem: *Let* A *and* B *be friendly isomorphic graphs. Then* $\mathbf{P}^* = \mathbf{\Pi}^*$.

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Checking isomorphism is hard

Checking friendliness is easy

Solve the relaxation: if $\mathbf{P}^*\mathbf{A} = \mathbf{B}\mathbf{P}^*$ then the unique isomorphism is $\mathbf{\Pi}^* = \mathbf{P}^*$. Otherwise, no isomorphism exists.

Sketch of the proof

Input: two friendly graphs $\mathbf{B}$ and $\mathbf{A} = \mathbf{\Pi}^{*\mathrm{T}}\mathbf{B}\mathbf{\Pi}^{*}$

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Convex quadratic program

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Show that the minimizer is unique

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Convex quadratic program reparametrized with $\mathbf{Q} = \mathbf{P}\mathbf{\Pi}^{*\mathrm{T}}$

$$\min_{\mathbf{Q}} \|\mathbf{QB} - \mathbf{BQ}\|_{\mathrm{F}}^2 \ \text{ s.t. } \ \mathbf{Q1} = \mathbf{1}$$

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First-order optimality condition: There exit n Lagrange multipliers $\boldsymbol{\alpha}$ such that

$$\mathbf{0} = \nabla_{\mathbf{Q}} \mathcal{L} = \mathbf{QB}^2 + \mathbf{B}^2\mathbf{Q} - 2\mathbf{BQB} + \boldsymbol{\alpha}\mathbf{1}^{\mathrm{T}}$$

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First-order optimality condition: using spectral representation $\mathbf{B} = \mathbf{U\Lambda U}^{\mathrm{T}}$

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$$\mathbf{0} \;=\; \mathbf{F}\boldsymbol{\Lambda}^2 + \boldsymbol{\Lambda}^2\mathbf{F} - 2\boldsymbol{\Lambda}\mathbf{F}\boldsymbol{\Lambda} + \boldsymbol{\gamma}\mathbf{v}^{\mathrm{T}}$$

where $\mathbf{F} = \mathbf{U}^{\mathrm{T}}\mathbf{Q}\mathbf{U}$, $\boldsymbol{\gamma} = \mathbf{U}^{\mathrm{T}}\boldsymbol{\alpha}$, $\mathbf{v} = \mathbf{U}^{\mathrm{T}}\mathbf{1}$

Sketch of the proof

First-order optimality condition:

$$\mathbf{F}\boldsymbol{\Lambda}^2 + \boldsymbol{\Lambda}^2\mathbf{F} - 2\boldsymbol{\Lambda}\mathbf{F}\boldsymbol{\Lambda} + \boldsymbol{\gamma}\mathbf{v}^{\mathrm{T}} = \mathbf{0}$$

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$$F_{ij}(\lambda_i - \lambda_j)^2 + v_j\gamma_i = 0$$

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Due to friendliness $v_i = \mathbf{u}_i^{\mathrm{T}}\mathbf{1} \neq 0$

First-order optimality condition:

$$F_{ij}(\lambda_i - \lambda_j)^2 + v_j \gamma_i = 0$$

In particular, for $i = j$: $v_i \gamma_i = 0$

Due to friendliness $v_i = \mathbf{u}_i^{\mathrm{T}} \mathbf{1} \neq 0 \Rightarrow \boldsymbol{\gamma} = \mathbf{0}$

First-order optimality condition:

$$F_{ij}(\lambda_i - \lambda_j)^2 = 0 \quad \text{for } i \neq j$$

Sketch of the proof

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$\mathbf{1} = \mathbf{Q}\mathbf{1}$

Sketch of the proof

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$\Rightarrow \mathbf{v} = \mathbf{F}\mathbf{v}$ with $v_i \neq 0$

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$\Rightarrow \mathbf{v} = \mathbf{F}\mathbf{v}$ with $v_i \neq 0 \Rightarrow \mathbf{F} = \mathbf{I}$
$\Rightarrow \mathbf{Q} = \mathbf{U}\mathbf{F}\mathbf{U}^{\mathrm{T}} = \mathbf{I}$

Friendliness:

- $\mathbf{A}$ has simple spectrum
- no eigenvectors of $\mathbf{A}$ are orthogonal to the constant vector $\mathbf{1}$

Theorem: *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be friendly isomorphic graphs. Then* $\hat{\mathbf{\Pi}} = \mathbf{P}^* = \mathbf{\Pi}^*$.

Strong friendliness:

- $\mathbf{A}$ has δ-separated spectrum
- every eigenvector $\mathbf{u}_i$ of $\mathbf{A}$ satisfied $|\mathbf{u}_i^{\mathrm{T}}\mathbf{1}| > \epsilon$

Theorem: *Let* A *and* B *be strongly friendly* ρ*-isomorphic graphs with* $\rho = \rho(\epsilon, \delta)$*. Then* $\|\mathbf{P}^* - \mathbf{\Pi}^*\|_\infty < \frac{1}{2}$.

ρ-isomorphic $\Leftrightarrow \exists \mathbf{\Pi}^* : \|\mathbf{\Pi}^*\mathbf{A} - \mathbf{B}\mathbf{\Pi}^*\|_{\mathrm{F}}^2 \leq \rho$

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Proof using results from regular perturbation theory of linear equations

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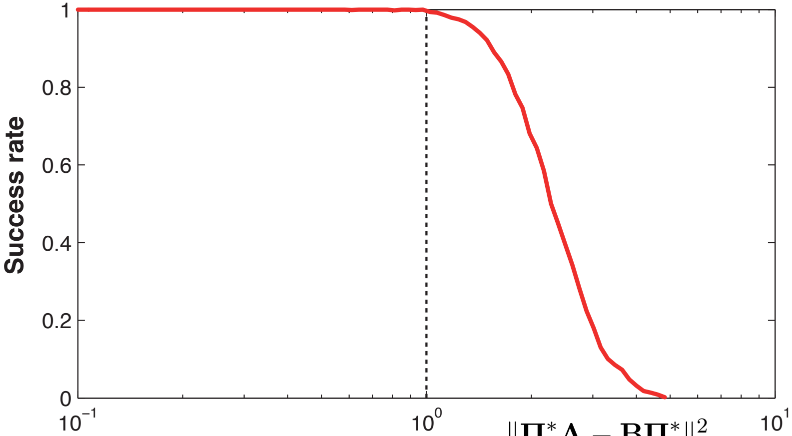
If $\|\mathbf{P}^*\mathbf{A} - \mathbf{B}\mathbf{P}^*\|_{\mathrm{F}}^2 < \rho(\epsilon, \delta)$ then $\hat{\mathbf{\Pi}}$ is the globally optimal approximate isomorphism. Otherwise, no ρ-isomorphism exists.

Experimental validation on 1000 strongly friendly graphs



$$\textbf{Noise} = \frac{\|\mathbf{\Pi}^*\mathbf{A} - \mathbf{B}\mathbf{\Pi}^*\|_{\mathrm{F}}^2}{\rho(\epsilon, \delta)}$$

Adjacency matrix has d non-simple eigenspaces

$$\underbrace{\lambda_1 = \lambda_2 = \cdots = \lambda_{i_1}}_{\text{multiplicity } m_1 + 1} < \underbrace{\lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2}}_{\text{multiplicity } m_2 + 1} < \cdots$$

Unfriendly graphs

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$$m = m_1 + m_2 + \cdots + m_d$$

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Basis vectors of each eigenspace are selected such that either

none of them is orthogonal to $\mathbf{1}$; or

all are orthogonal to $\mathbf{1}$

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Basis vectors of each eigenspace are selected such that either

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Unfriendliness degree: $m + k$

First-order optimality condition:

$$F_{ij}(\lambda_i - \lambda_j)^2 + v_j \gamma_i = 0 \qquad v_i = \mathbf{u}_i^{\mathrm{T}} \mathbf{1}$$

Pseudo-stochasticity constraint:

$$\sum_j F_{ij} v_j = v_i$$

First-order optimality condition:

$$\begin{pmatrix} (\lambda_i - \lambda_1)^2 & & \\ & \ddots & \\ & & (\lambda_i - \lambda_n)^2 \end{pmatrix} \mathbf{f}_i + \gamma_i \mathbf{v} = \mathbf{0}$$

Pseudo-stochasticity constraint:

$$\mathbf{v}^{\mathrm{T}} \mathbf{f}_i = v_i$$

for each i-th row $\mathbf{f}_i = (F_{i1}, \ldots, F_{in})^{\mathrm{T}}$

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n systems with $n + 1$ equations and variables each

$\mathbf{u}_i$ belongs to a non-hostile eigenspace

First-order optimality condition:

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Case I: non-hostile eigenspace

$\mathbf{u}_i$ belongs to a non-hostile eigenspace $\Rightarrow v_i \neq 0$
$\Rightarrow \gamma_i = 0$

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Rank-m_i deficient!

Case II: hostile eigenspace

$\mathbf{u}_i$ belongs to a hostile eigenspace

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Pseudo-stochasticity constraint:

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Case II: hostile eigenspace

$\mathbf{u}_i$ belongs to a hostile eigenspace $\Rightarrow v_i = 0$

First-order optimality condition:

$$\begin{pmatrix} (\lambda_i - \lambda_1)^2 & & \\ & \ddots & \\ & & (\lambda_i - \lambda_n)^2 \end{pmatrix} \mathbf{f}_i + \gamma_i \mathbf{v} = \mathbf{0}$$

Pseudo-stochasticity constraint:

$$\mathbf{v}^{\mathrm{T}} \mathbf{f}_i = v_i$$

$\mathbf{u}_i$ belongs to a hostile eigenspace $\Rightarrow v_i = 0$
$\Rightarrow \gamma_i$ undetermined

First-order optimality condition:

$$\begin{pmatrix} (\lambda_i - \lambda_1)^2 & & \\ & \ddots & \\ & & (\lambda_i - \lambda_n)^2 \end{pmatrix} \mathbf{f}_i = -\gamma_i \begin{pmatrix} \vdots \\ \mathbf{0} \\ \vdots \end{pmatrix}$$

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Rank-$(m_i + 1)$ deficient!

For an $(m+k)$-unfriendly graph, the system

$$F_{ij}(\lambda_i - \lambda_j)^2 + v_j\gamma_i = 0$$
$$\sum_j F_{ij}v_j = v_i$$

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Some solutions may belong to Voronoi cells of permutations that are not isomorphisms!

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is rank-$(m+k)$ deficient!

Convex relaxation + projection can produce wrong solutions!

Seeds (known correspondences): collection of q real functions $\mathbf{C} = (\mathbf{c}_1, \ldots, \mathbf{c}_q)$ on the vertex set of $\mathbf{A}$ with corresponding functions $\mathbf{D} = (\mathbf{d}_1, \ldots, \mathbf{d}_q)$ on $\mathbf{B}$.

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Attributes: q-dimensional vector-valued vertex attributes $\mathbf{C} = (\mathbf{c}_1^{\mathrm{T}}, \ldots, \mathbf{c}_n^{\mathrm{T}})^{\mathrm{T}}$.

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Seeds and attributes

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Columns of $\mathbf{C}$ and $\mathbf{\Pi}^*\mathbf{D}$ are corresponding functions (e.g., indicator of vertices).

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Rows of $\mathbf{C}$ and $\mathbf{\Pi}^*\mathbf{D}$ are corresponding attributes.

Covariant with a preferred isomorphism: $\mathbf{\Pi}^*\mathbf{C} = \mathbf{D}$.

Convex Relaxation

$$\min_{\mathbf{P}} \|\mathbf{PA} - \mathbf{BP}\|_{\mathrm{F}}^2 \ \text{ s.t. } \ \mathbf{P1} = \mathbf{1}$$

Convex Relaxation of seeded/attributed matching

$$\min_{\mathbf{P}} \|\mathbf{PA} - \mathbf{BP}\|_{\mathrm{F}}^2 + \mu \|\mathbf{PC} - \mathbf{D}\|_{\mathrm{F}}^2 \;\; \text{s.t.} \;\; \mathbf{P1} = \mathbf{1}$$

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penalty on attributes disagreement

penalty on seeds correspondence

Main result

Theorem: *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be isomorphic graphs related by* $\mathbf{\Pi}^*$*. Let* $\mathbf{C}$ *and* $\mathbf{D} = \mathbf{\Pi}^*\mathbf{C}$ *be corresponding seeds/attributes, with* $\mathbf{D}$ *further satisfying for every non-simple eigenspace of* $\mathbf{B}$ *spanned by* $\mathbf{u}_i, \ldots, \mathbf{u}_{i+m_i}$

- $\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_j \neq \mathbf{0}\ \forall j = i, \ldots, i + m_i$ *if eigenspace is hostile; or*
- $\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_j \neq \mathbf{1}\dfrac{\mathbf{u}_i^{\mathrm{T}}\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_j}{\mathbf{1}^{\mathrm{T}}\mathbf{u}_i}\ \forall j = i+1, \ldots, i + m_i$ *otherwise.*

Then, $\mathbf{P}^* = \mathbf{\Pi}^*$ is the unique solutuon of the relaxation for every $\mu > 0$.

Sketch of the proof

Input: two graphs $\mathbf{B}$ and $\mathbf{A} = \mathbf{\Pi}^{*\mathrm{T}}\mathbf{B}\mathbf{\Pi}^{*}$ with seeds/attributes $\mathbf{C}$ and $\mathbf{D} = \mathbf{\Pi}^{*}\mathbf{C}$

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Convex quadratic program

$$\min_{\mathbf{P}} \|\mathbf{PA} - \mathbf{BP}\|_{\mathrm{F}}^2 + \mu\|\mathbf{PC} - \mathbf{D}\|_{\mathrm{F}}^2 \text{ s.t. } \mathbf{P1} = \mathbf{1}$$

with global minimizer $\mathbf{P} = \mathbf{\Pi}^*$.

Sketch of the proof

Input: two graphs $\mathbf{B}$ and $\mathbf{A} = \mathbf{\Pi}^{*\mathrm{T}}\mathbf{B}\mathbf{\Pi}^{*}$ with seeds/attributes $\mathbf{C}$ and $\mathbf{D} = \mathbf{\Pi}^{*}\mathbf{C}$

Convex quadratic program reparametrized with $\mathbf{Q} = \mathbf{P}\mathbf{\Pi}^{*\mathrm{T}}$

$$\min_{\mathbf{Q}} \|\mathbf{QB} - \mathbf{BQ}\|_{\mathrm{F}}^2 + \mu\|\mathbf{QD} - \mathbf{D}\|_{\mathrm{F}}^2 \ \text{ s.t. } \ \mathbf{Q1} = \mathbf{1}$$

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with global minimizer $\mathbf{Q} = \mathbf{I}$.

Show that the minimizer is unique

Sketch of the proof

First-order optimality condition:

$$\mathrm{QB}^2 + \mathrm{B}^2\mathrm{Q} - 2\mathrm{BQB} + \mu\mathbf{QDD}^{\mathrm{T}} - \mu\mathbf{DD}^{\mathrm{T}} + \boldsymbol{\alpha}\mathbf{1}^{\mathrm{T}} = \mathbf{0}$$

Pseudo-stochasticity constraint: $\mathrm{Q}\mathbf{1} = \mathbf{1}$

First-order optimality condition:

$$\mathbf{F}\mathbf{\Lambda}^2 + \mathbf{\Lambda}^2\mathbf{F} - 2\mathbf{\Lambda}\mathbf{F}\mathbf{\Lambda} + \mu\mathbf{F}\mathbf{G} - \mu\mathbf{G} + \boldsymbol{\gamma}\mathbf{v}^{\mathrm{T}} = \mathbf{0}$$

with $\mathbf{G} = \mathbf{U}^{\mathrm{T}}\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{U}$

Pseudo-stochasticity constraint: $\mathbf{F}\mathbf{v} = \mathbf{v}$

Sketch of the proof

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with $\mathbf{G} = \mathbf{U}^{\mathrm{T}}\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{U} \succeq 0$

Pseudo-stochasticity constraint: $\mathbf{F}\mathbf{v} = \mathbf{v}$

Adding attributes/seeds increases rank

Main result

Theorem: *Let* $\mathrm{D} = \mathbf{\Pi}^* \mathrm{C}$ *satisfying for every non-simple eigenspace* $\mathrm{sp}\{\mathbf{u}_i, \ldots, \mathbf{u}_{i+m_i}\}$

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Main result

Theorem: *Let* $\mathrm{D} = \Pi^*\mathrm{C}$ *satisfying for every non-simple eigenspace* $\mathrm{sp}\{\mathbf{u}_i, \ldots, \mathbf{u}_{i+m_i}\}$

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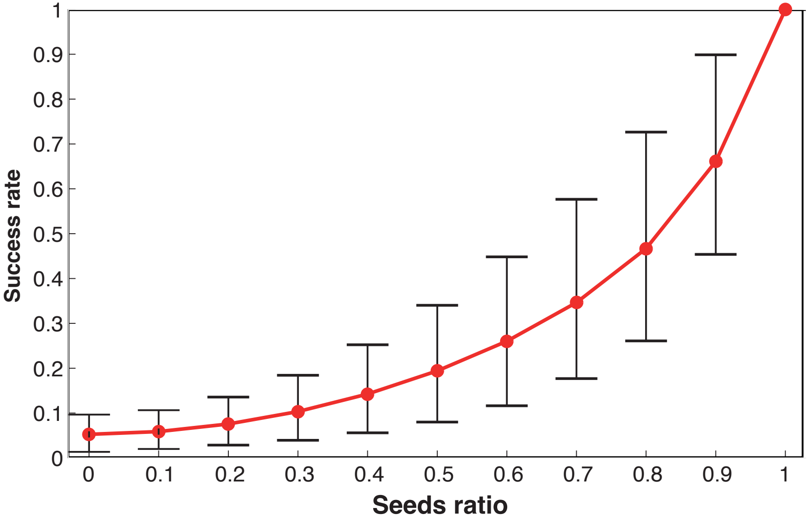
Then, $\mathbf{P}^* = \mathbf{\Pi}^*$ is the unique solutuon of relaxation.

$m + k$ **linearly independent seeds are required.**

Experimental validation on 1000 symmetric graphs



$$= \frac{\#\text{seeds}}{\#\text{symmetries}}$$

Questions

- **Relaxation space:** We used $\mathbf{P1} = \mathbf{1}$. Do we need $\mathbf{P} \geq 0$? do we need $\mathbf{P}^{\mathrm{T}}\mathbf{1} = \mathbf{1}$? Practical consequences?

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- **Better use of geometry:** adjacency matrices are, e.g., metric? low dimensional? smooth? bounded curvature?
- **Symmetry breaking:** add low-rank noise to unfriendly eigenspaces of $\mathbf{A}$ to make it friendly. Will the relaxation still work?
- **Finding all isomorphisms** (in particular, all symmetries of a graph).