Graph Matching: Relax or Not?

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Joint work with Yonathan Aflalo and Ron Kimmel

Minimum-distortion correspondences



Minimum-distortion correspondences



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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 $\mbox{Graph isomorphism:}$ determine whether ${\bf A}$ and ${\bf B}$ are isomorphic

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

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

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

$$\boldsymbol{\Pi}^* = \underset{\boldsymbol{\Pi} \in \mathcal{P}}{\operatorname{argmin}} \| \boldsymbol{A} - \boldsymbol{\Pi}^T \boldsymbol{B} \boldsymbol{\Pi} \|_F^2$$

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Convex Relaxation

$$\begin{split} \mathbf{P}^* &= \underset{\mathbf{P} \in \mathcal{D}}{\operatorname{argmin}} \| \mathbf{P} \mathbf{A} - \mathbf{B} \mathbf{P} \|_{\mathrm{F}}^2 \\ \mathcal{D} &= \{ \mathbf{P} \geq \mathbf{0} : \mathbf{P} \mathbf{1} = \mathbf{P}^{\mathrm{T}} \mathbf{1} = \mathbf{1} \} \text{ space of } \\ n \times n \text{ double-stochastic matrices} \end{split}$$

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Generally, \mathbf{P}^* is not a permutation!

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

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

Solved by Hungarian algorithm

Obviously, Π^{\ast} is a solution of the relaxation

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

Convex Relaxation

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s.t.
$$\mathbf{P}\mathbf{1} = \mathbf{P}^{\mathrm{T}}\mathbf{1} = \mathbf{1}$$

double-stochastic matrices

An even bigger relaxation

$$\begin{aligned} \mathbf{P}^* &= \underset{\mathbf{P}}{\operatorname{argmin}} \| \mathbf{P} \mathbf{A} - \mathbf{B} \mathbf{P} \|_{\mathrm{F}}^2 \\ \text{s.t. } \mathbf{P} \mathbf{1} &= \mathbf{1} \end{aligned}$$

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no inequality constraints

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$\mathbf{P}^* = \underset{\mathbf{P}}{\operatorname{argmin}} \|\mathbf{P}\mathbf{A} - \mathbf{B}\mathbf{P}\|_{\mathrm{F}}^2 \text{ s.t. } \mathbf{P}\mathbf{1} = \mathbf{1}$

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

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

Property: friendly graphs are asymmetric

Property: *friendly graphs are asymmetric* (have trivial automorphism group)

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- **Property:** friendly graphs are asymmetric *Proof:* Let $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{\mathrm{T}}$ be friendly. Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$. $\Rightarrow \forall i : \mathbf{A} \mathbf{\Pi} \mathbf{u}_i = \lambda_i \mathbf{\Pi} \mathbf{u}_i$ $\Rightarrow \Pi \mathbf{u}_i$ is an eigenvector of A corresponding to λ_i . A has simple spectrum $\Rightarrow \Pi \mathbf{u}_i = \pm \mathbf{u}_i$. $\Pi \neq \mathbf{I} \Rightarrow \exists \mathbf{u}_i \text{ for which } \Pi \mathbf{u}_i = -\mathbf{u}_i$ $\Rightarrow \mathbf{1}^{\mathrm{T}} \mathbf{\Pi} \mathbf{u}_{i} = -\mathbf{1}^{\mathrm{T}} \mathbf{u}_{i}.$
- $\begin{aligned} \Pi \text{ is a permutation} &\Rightarrow \mathbf{1}^{\mathrm{T}} \Pi \mathbf{u}_{i} = \mathbf{1}^{\mathrm{T}} \mathbf{u}_{i} \\ &\Rightarrow \mathbf{1}^{\mathrm{T}} \mathbf{u}_{i} = 0 \text{ in contradiction to friendliness} \end{aligned}$

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- *Proof:* Let $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{\mathrm{T}}$ be friendly.
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- Π is a permutation $\Rightarrow \mathbf{1}^{\mathrm{T}} \Pi \mathbf{u}_i = \mathbf{1}^{\mathrm{T}} \mathbf{u}_i$
- $\Rightarrow \mathbf{1}^{\mathrm{T}}\mathbf{u}_{i} = 0$ in contradiction to friendliness

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

Checking isomorphism is hard

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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.

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

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

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

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$$\min_{\mathbf{P}} \|\mathbf{P} \mathbf{\Pi}^{*T} \mathbf{B} \mathbf{\Pi}^{*} - \mathbf{B} \mathbf{P}\|_{\mathrm{F}}^{2} \text{ s.t. } \mathbf{P} \mathbf{1} = \mathbf{1}$$

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$\min_{\mathbf{P}} \|\mathbf{P}\boldsymbol{\Pi}^{*T}\mathbf{B} - \mathbf{B}\mathbf{P}\boldsymbol{\Pi}^{*T}\|_{\mathrm{F}}^2 \ \mathrm{s.t.} \ \mathbf{P}\mathbf{1} = \mathbf{1}$

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

Input: two friendly graphs B and $A = \Pi^{*T}B\Pi^{*}$ Convex quadratic program reparametrized with $Q = P\Pi^{*T}$

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

with global minimizer $\mathbf{Q} = \mathbf{\Pi}^* \mathbf{\Pi}^{*T} = \mathbf{I}$.

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

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

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

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 $0 = \mathbf{Q}\mathbf{U}\mathbf{\Lambda}^{2}\mathbf{U}^{\mathrm{T}} + \mathbf{U}\mathbf{\Lambda}^{2}\mathbf{U}^{\mathrm{T}}\mathbf{Q}$ $-2\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathrm{T}}\mathbf{Q}\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathrm{T}} + \boldsymbol{\alpha}\mathbf{1}^{\mathrm{T}}$

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

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

$$0 = \mathbf{U}^{\mathrm{T}}\mathbf{Q}\mathbf{U}\mathbf{\Lambda}^{2} + \mathbf{\Lambda}^{2}\mathbf{U}^{\mathrm{T}}\mathbf{Q}\mathbf{U}$$
$$-2\mathbf{\Lambda}\mathbf{U}^{\mathrm{T}}\mathbf{Q}\mathbf{U}\mathbf{\Lambda} + \mathbf{U}^{\mathrm{T}}\boldsymbol{\alpha}\mathbf{1}^{\mathrm{T}}\mathbf{U}$$

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

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

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

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

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

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 $1 = \mathbf{Q}\mathbf{1} = \mathbf{U}\mathbf{F}\mathbf{U}^{\mathrm{T}}\mathbf{1}$

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Friendliness:

- ullet A has simple spectrum
- ${\scriptstyle \bullet}$ no eigenvectors of ${\bf A}$ are orthogonal to the constant vector ${\bf 1}$

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

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

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Proof using results from regular perturbation theory of linear equations

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- 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 $\hat{\Pi} = \Pi^*$.

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 $1000 \ {\rm strongly} \ {\rm friendly} \ {\rm graphs}$









Basis vectors of each eigenspace are selected such that either

none of them is orthogonal to ${\bf 1}$; or all are orthogonal to ${\bf 1}$



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Unfriendliness degree: m + k

Matching of unfriendly graphs

First-order optimality condition:

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

$$\sum_{j} F_{ij} v_j = v_i$$

Matching of unfriendly graphs

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$$\left(egin{array}{ccc} (\lambda_i-\lambda_1)^2 & & \ & \ddots & \ & & (\lambda_i-\lambda_n)^2 \end{array}
ight) {f f}_i+\gamma_i {f v}={f 0}$$

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 $n+1 \ {\rm equations}$ and variables each

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

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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!

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Case II: hostile eigenspace

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

First-order optimality condition:

$$\left(egin{array}{ccc} (\lambda_i-\lambda_1)^2 & & \ & \ddots & \ & & (\lambda_i-\lambda_n)^2 \end{array}
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ight)$$

Pseudo-stochasticity constraint:

$$\mathbf{v}^{\mathrm{T}}\mathbf{f}_{i} = 0$$

Rank- $(m_i + 1)$ deficient!

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

is rank-(m+k) deficient!

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Solution space is (m + k)-dimensional.

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Solution space is (m + k)-dimensional.

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

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

is rank-(m+k) deficient!

Convex relaxation + projection can produce wrong solutions!

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

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

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Columns of C and Π^*D are corresponding functions (e.g., indicator of vertices).

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Rows of C and Π^*D are corresponding attributes.

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

Convex Relaxation

$$\min_{\mathbf{P}} \|\mathbf{P}\mathbf{A} - \mathbf{B}\mathbf{P}\|_{\mathrm{F}}^2 \text{ s.t. } \mathbf{P}\mathbf{1} = \mathbf{1}$$
Convex Relaxation of seeded/attributed matching

$\min_{\mathbf{P}} \|\mathbf{P}\mathbf{A} - \mathbf{B}\mathbf{P}\|_{\mathrm{F}}^{2} + \mu \|\mathbf{P}\mathbf{C} - \mathbf{D}\|_{\mathrm{F}}^{2} \text{ s.t. } \mathbf{P}\mathbf{1} = \mathbf{1}$

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penalty on attributes disagreement penalty on seeds correspondence

Main result

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

DD^T**u**_j ≠ 0 ∀j = i,...,i + m_i if eigenspace is hostile; or

•
$$\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_{j} \neq \mathbf{1} \frac{\mathbf{u}_{i}^{\mathrm{T}}\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_{j}}{\mathbf{1}^{\mathrm{T}}\mathbf{u}_{i}} \ \forall j = i+1,\ldots,i+m_{i}$$

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

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

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Convex quadratic program

 $\min_{\mathbf{P}} \|\mathbf{P}\mathbf{A} - \mathbf{B}\mathbf{P}\|_{\mathrm{F}}^{2} + \mu \|\mathbf{P}\mathbf{C} - \mathbf{D}\|_{\mathrm{F}}^{2} \text{ s.t. } \mathbf{P}\mathbf{1} = \mathbf{1}$

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

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

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

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

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Show that the minimizer is unique

First-order optimality condition:

$$\mathbf{Q}\mathbf{B}^{2} + \mathbf{B}^{2}\mathbf{Q} - 2\mathbf{B}\mathbf{Q}\mathbf{B} + \mu\mathbf{Q}\mathbf{D}\mathbf{D}^{\mathrm{T}} - \mu\mathbf{D}\mathbf{D}^{\mathrm{T}} + \alpha\mathbf{1}^{\mathrm{T}} = \mathbf{0}$$

Pseudo-stochasticity constraint: Q1 = 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: $\mathbf{F}\mathbf{v} = \mathbf{v}$

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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

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

• $\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_{j} \neq \mathbf{0} \ \forall j = i, \dots, i + m_{i}$ if eigenspace is hostile; or

•
$$\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_{j} \neq \mathbf{1} \frac{\mathbf{u}_{i}^{\mathrm{T}}\mathbf{D}\mathbf{D}^{\mathrm{T}}\mathbf{u}_{j}}{\mathbf{1}^{\mathrm{T}}\mathbf{u}_{i}} \forall j = i+1, \dots, i+m_{i}$$

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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





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- **Symmetry breaking:** add low-rank noise to unfriendly eigenspaces of **A** to make it friendly. Will the relaxation still work?
- **Finding all isomorphisms** (in particular, all symmetries of a graph).