Graph Matching: Relax or Not?

Alex Bronstein
School of Electrical Engineering
Tel Aviv University
College of Electrical and Computer Engineering
Duke University

Simons Institute, Berkeley, 2014

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
'Graph matching' problems
'Graph matching' problems

Given two undirected weighted graphs represented by adjacency matrices $A$ and $B$
Graph matching problems

Given two undirected weighted graphs represented by adjacency matrices $A$ and $B$

**Graph isomorphism:** determine whether $A$ and $B$ are isomorphic
Given two undirected weighted graphs represented by adjacency matrices $A$ and $B$

**Graph isomorphism:** determine whether $A$ and $B$ are isomorphic

**Exact graph ’matching’:** find isomorphism relating $A$ and $B$
Given two undirected weighted graphs represented by adjacency matrices \( A \) and \( B \)

**Graph isomorphism:** determine whether \( A \) and \( B \) are isomorphic

**Exact graph ’matching’:** find isomorphism relating \( A \) and \( B \)

**Inexact graph ’matching’:** find best approximate isomorphism relating \( A \) and \( B \)
Graph Matching (NP)

$$\Pi^* = \arg\min_{\Pi \in \mathcal{P}} \| A - \Pi^T B \Pi \|$$

$$\mathcal{P} = \text{space of } n \times n \text{ permutation matrices}$$
Graph Matching (NP)

\[ \Pi^* = \arg\min_{\Pi \in \mathcal{P}} \| A - \Pi^T B \Pi \|_F^2 \]

\[ \mathcal{P} = \text{space of } n \times n \text{ permutation matrices} \]
Graph Matching (NP)

$$\Pi^* = \underset{\Pi \in \mathcal{P}}{\arg \min} \| \Pi A - B \Pi \|_F^2$$

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

Graph Matching (NP)

$$\Pi^* = \arg\min_{\Pi \in \mathcal{P}} \| \Pi A - B \Pi \|_F^2$$

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

Convex Relaxation

$$P^* = \arg\min_{P \in \mathcal{D}} \| PA - BP \|_F^2$$

$$\mathcal{D} = \{ P \geq 0 : P1 = P^T1 = 1 \} \text{ space of } n \times n \text{ double-stochastic matrices}$$
Convex relaxation

Graph Matching (NP)

\[ \Pi^* = \arg\min_{\Pi \in \mathcal{P}} \| \Pi A - BP \|_F^2 \]

\[ \mathcal{P} = \text{space of } n \times n \text{ permutation matrices} \]

Convex Relaxation (QP)

\[ P^* = \arg\min_{P \in \mathcal{D}} \| PA - BP \|_F^2 \]

\[ \mathcal{D} = \{ P \geq 0 : P1 = P^T1 = 1 \} \text{ space of } n \times n \text{ double-stochastic matrices} \]
Convex Relaxation (QP)

\[ \mathbf{P}^* = \arg \min_{\mathbf{P} \in \mathcal{D}} \| \mathbf{P} \mathbf{A} - \mathbf{B} \mathbf{P} \|_F^2 \]

Generally, \( \mathbf{P}^* \) is not a permutation!
1. Convex Relaxation (QP)

\[ P^* = \arg\min_{P \in \mathcal{D}} \| PA - BP \|^2_F \]

Generally, \( P^* \) is not a permutation!

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

\[ \hat{\Pi} = \arg\max_{\Pi \in \mathcal{P}} \langle \Pi, P^* \rangle \]
1. Convex Relaxation (QP)

\[ P^* = \arg\min_{P \in \mathcal{D}} \| PA - BP \|_F^2 \]

Generally, \( P^* \) is not a permutation!

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

\[ \hat{\Pi} = \arg\max_{\Pi \in \mathcal{P}} \text{tr}(\Pi^T P^*) \]
1. Convex Relaxation (QP)

\[ P^* = \arg\min_{P \in \mathcal{D}} \| PA - BP \|_F^2 \]

Generally, \( P^* \) is not a permutation!

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

\[ \hat{\Pi} = \arg\max_{\Pi \in \mathcal{P}} \text{tr}(\Pi^T P^*) \]

Solved by Hungarian algorithm
What is the relation between $\Pi^*$ and $\hat{\Pi}$?
Relax or not?

What is the relation between $\Pi^*$ and $\hat{\Pi}$?

Obviously, $\Pi^*$ is a solution of the relaxation.
What is the relation between $\Pi^*$ and $\hat{\Pi}$?

Obviously, $\Pi^*$ is a solution of the relaxation

However, the relaxation might produce some $P^*$ which is not a permutation and its projection $\hat{\Pi}$ can have $\|\hat{\Pi}A - B\hat{\Pi}\| > 0$
What is the relation between $\Pi^*$ and $\hat{\Pi}$?

Obviously, $\Pi^*$ is a solution of the relaxation.

However, the relaxation might produce some $\mathbf{P}^*$ which is not a permutation and its projection $\hat{\Pi}$ can have $\|\hat{\Pi}\mathbf{A} - \mathbf{B}\hat{\Pi}\| > 0$

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

\[ P^* = \arg\min_{P \geq 0} \| PA - BP \|_F^2 \]

s.t. \( P1 = P^T1 = 1 \)

double-stochastic matrices
An even bigger relaxation

\[ P^* = \arg\min_P \|PA - BP\|_F^2 \]

s.t. \( P1 = 1 \)

pseudo-stochastic matrices
Convex relaxation

An even bigger relaxation

\[ P^* = \arg\min_P \|PA - BP\|_F^2 \]
\[ \text{s.t. } P1 = 1 \]

pseudo-stochastic matrices

\( n \) non-overlapping equality constraints instead of \( 2n \) overlapping constraints
An even bigger relaxation

\[ P^* = \arg \min_P \|PA - BP\|_F^2 \]

s.t. \( P1 = 1 \)

pseudo-stochastic matrices

\( n \) non-overlapping equality constraints instead of \( 2n \) overlapping constraints

no inequality constraints
Convex Relaxation

\[ P^* = \arg\min_P \| PA - BP \|_F^2 \quad \text{s.t.} \quad P1 = 1 \]
Friendly graphs

Convex Relaxation

\[ P^* = \argmin_{P} \|P A - B P\|_F^2 \quad \text{s.t.} \quad P 1 = 1 \]

**Friendly graphs:** an undirected weighted graph \( A \) is friendly if

- \( A \) has simple spectrum
- no eigenvectors of \( A \) are orthogonal to the constant vector \( 1 \)
Property: friendly graphs are asymmetric
Property: *friendly graphs are asymmetric*
(have trivial automorphism group)
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly. Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$. 
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly.
Assume $\Pi \neq I$ permutation such that $\Pi A = A\Pi$.
$\Rightarrow \forall i : Au_i = \lambda_i u_i$
**Property:** friendly graphs are **asymmetric**

**Proof:** Let \( A = U \Lambda U^T \) be friendly. Assume \( \Pi \neq I \) permutation such that \( \Pi A = A \Pi \). 
\[ \Rightarrow \forall i : \Pi A u_i = \lambda_i \Pi u_i \]
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly. Assume $\Pi \neq I$ permutation such that $\Pi A = A\Pi$. Then:

$$\Rightarrow \forall i : \ A\Pi u_i = \lambda_i \Pi u_i$$
Property: friendly graphs are asymmetric

Proof: Let \( A = U\Lambda U^T \) be friendly.
Assume \( \Pi \neq I \) permutation such that \( \Pi A = A\Pi \).
\[ \Rightarrow \forall i : \ A\Pi u_i = \lambda_i \Pi u_i \]
\[ \Rightarrow \Pi u_i \text{ is an eigenvector of } A \text{ corresponding to } \lambda_i. \]
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly.
Assume $\Pi \neq I$ permutation such that $\Pi A = A\Pi$.
$\Rightarrow \forall i : A\Pi u_i = \lambda_i \Pi u_i$
$\Rightarrow \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$.
$A$ has simple spectrum $\Rightarrow \Pi u_i = \pm u_i$. 
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly.
Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$.
$\Rightarrow \forall i : A\Pi u_i = \lambda_i \Pi u_i$
$\Rightarrow \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$.
$A$ has simple spectrum $\Rightarrow \Pi u_i = \pm u_i$.
$\Pi \neq I \Rightarrow \exists u_i$ for which $\Pi u_i = -u_i$
Property: **friendly graphs are asymmetric**

Proof: Let $A = U\Lambda U^T$ be friendly.

Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$.

$\implies \forall i: A\Pi u_i = \lambda_i \Pi u_i$

$\implies \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$.

$A$ has simple spectrum $\implies \Pi u_i = \pm u_i$.

$\Pi \neq I \implies \exists u_i$ for which $\Pi u_i = -u_i$

$\implies 1^T \Pi u_i = -1^T u_i$. 
**Property:** friendly graphs are asymmetric

**Proof:** Let \( A = U \Lambda U^T \) be friendly.
Assume \( \Pi \neq I \) permutation such that \( \Pi A = A \Pi \).
\[ \Rightarrow \forall i : \ A\Pi u_i = \lambda_i \Pi u_i \]
\[ \Rightarrow \Pi u_i \text{ is an eigenvector of } A \text{ corresponding to } \lambda_i. \]
\( A \) has simple spectrum \( \Rightarrow \Pi u_i = \pm u_i. \)
\( \Pi \neq I \Rightarrow \exists u_i \text{ for which } \Pi u_i = -u_i \)
\[ \Rightarrow 1^T \Pi u_i = -1^T u_i. \]
\( \Pi \) is a permutation \( \Rightarrow 1^T \Pi = 1^T \)
**Property:** friendly graphs are asymmetric

**Proof:** Let $A = U\Lambda U^T$ be friendly. Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$.

$\Rightarrow \forall i : A\Pi u_i = \lambda_i \Pi u_i$

$\Rightarrow \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$.

$A$ has simple spectrum $\Rightarrow \Pi u_i = \pm u_i$.

$\Pi \neq I \Rightarrow \exists u_i$ for which $\Pi u_i = -u_i$

$\Rightarrow 1^T \Pi u_i = -1^T u_i$

$\Pi$ is a permutation $\Rightarrow 1^T \Pi u_i = 1^T u_i$
Property: friendly graphs are asymmetric

Proof: Let $A = U\Lambda U^T$ be friendly. Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$. 
$\Rightarrow \forall i : A\Pi u_i = \lambda_i \Pi u_i$ 
$\Rightarrow \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$. 
$A$ has simple spectrum $\Rightarrow \Pi u_i = \pm u_i$. 
$\Pi \neq I \Rightarrow \exists u_i$ for which $\Pi u_i = -u_i$ 
$\Rightarrow 1^T \Pi u_i = -1^T u_i$. 
$\Pi$ is a permutation $\Rightarrow 1^T \Pi u_i = 1^T u_i$ 
$\Rightarrow 1^T u_i = 0$ in contradiction to friendliness
**Property:** friendly graphs are **asymmetric**

**Proof:** Let $A = U \Lambda U^T$ be friendly.

Assume $\Pi \neq I$ permutation such that $\Pi A = A \Pi$.

$\Rightarrow \forall i : A \Pi u_i = \lambda_i \Pi u_i$

$\Rightarrow \Pi u_i$ is an eigenvector of $A$ corresponding to $\lambda_i$.

$A$ has simple spectrum $\Rightarrow \Pi u_i = \pm u_i$.

$\Pi \neq I \Rightarrow \exists u_i$ for which $\Pi u_i = -u_i$

$\Rightarrow 1^T \Pi u_i = -1^T u_i$.

$\Pi$ is a permutation $\Rightarrow 1^T \Pi u_i = 1^T u_i$

$\Rightarrow 1^T u_i = 0$ in contradiction to friendliness

Converse is not true (think of a regular asymmetric graph), but such graphs should be rare.
Theorem: Let $A$ and $B$ be friendly isomorphic graphs. Then $P^* = \Pi^*$. 
Theorem: Let $A$ and $B$ be friendly isomorphic graphs. Then $\hat{\Pi} = P^* = \Pi^*$. 
Theorem: Let $A$ and $B$ be friendly isomorphic graphs. Then $\hat{\Pi} = P^* = \Pi^*$.

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

Checking isomorphism is hard

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

Checking **isomorphism** is hard

Checking **friendliness** is easy

Solve the relaxation: if $P^*A = BP^*$ then the unique isomorphism is $\Pi^* = P^*$. Otherwise, no isomorphism exists.
Sketch of the proof

**Input:** two friendly graphs \( B \) and \( A = \Pi^T B \Pi^* \)
Input: two friendly graphs $B$ and $A = \Pi^*^T B \Pi^*$

Convex quadratic program

$$\min_P \|PA - BP\|_F^2 \quad \text{s.t.} \quad P1 = 1$$

with global minimizer $P = \Pi^*$. 
Sketch of the proof

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

Convex quadratic program

$$\min_{P} \left\| P A - B P \right\|_F^2 \quad \text{s.t.} \quad P 1 = 1$$

with global minimizer $P = \Pi^*$.

Show that the minimizer is unique
Sketch of the proof

**Input:** two friendly graphs $B$ and $A = \Pi^* B \Pi^*$

Convex quadratic program

$$\min_{P} \| P \Pi^* T B \Pi^* - B P \|_F^2 \quad \text{s.t.} \quad P 1 = 1$$

with global minimizer $P = \Pi^*$.

Show that the minimizer is unique
Sketch of the proof

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

Convex quadratic program

$$\min_P \|P \Pi^T B - B P \Pi^T \|_F^2 \quad \text{s.t.} \quad P1 = 1$$

with global minimizer $P = \Pi^*$.

**Show that the minimizer is unique**
**Input:** two friendly graphs $B$ and $A = \Pi^T B \Pi^*$

Convex quadratic program

\[
\min_{P} \| P \Pi^T B - B P \Pi^T \|_F^2 \quad \text{s.t.} \quad P \Pi^T 1 = 1
\]

with global minimizer $P = \Pi^*$.

**Show that the minimizer is unique**
Sketch of the proof

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

Convex quadratic program reparametrized with $Q = P \Pi^T$

$$\min_Q \|QB - BQ\|_F^2 \quad \text{s.t.} \quad Q1 = 1$$

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

Show that the minimizer is unique
Sketch of the proof

\[
\min_Q \|QB - BQ\|_F^2 \quad \text{s.t.} \quad Q1 = 1
\]
Sketch of the proof

\[
\min_Q \|QB - BQ\|_F^2 \quad \text{s.t.} \quad Q1 = 1
\]

First-order optimality condition: There exist \( n \) Lagrange multipliers \( \alpha \) such that

\[
0 = \nabla_Q \mathcal{L} = QB^2 + B^2Q - 2BQB + \alpha 1^T
\]
Sketch of the proof

\[
\min_Q \|QB - BQ\|^2_F \quad \text{s.t.} \quad Q1 = 1
\]

**First-order optimality condition:** using spectral representation \( B = U\Lambda U^T \)

\[
0 = \nabla_Q \mathcal{L} = QB^2 + B^2Q - 2BQB + \alpha 1^T
\]
Sketch of the proof

\[
\min_{Q} \|QB - BQ\|_F^2 \quad \text{s.t.} \quad Q1 = 1
\]

**First-order optimality condition:** using spectral representation \(B = U\Lambda U^T\)

\[
0 = QU\Lambda^2 U^T + U\Lambda^2 U^T Q - 2U\Lambda U^T QU\Lambda U^T + \alpha 1^T
\]
Sketch of the proof

\[
\min_Q \|QB - BQ\|_F^2 \quad \text{s.t.} \quad Q1 = 1
\]

**First-order optimality condition:** Using spectral representation \( B = U\Lambda U^T \)

\[
0 = U^TQU\Lambda^2 + \Lambda^2 U^TQU - 2\Lambda U^TQU\Lambda + U^T\alpha 1^T U
\]
Sketch of the proof

\[ \min_Q \| QB - BQ \|_F^2 \quad \text{s.t.} \quad Q1 = 1 \]

First-order optimality condition: using spectral representation \( B = U\Lambda U^T \)

\[ 0 = F\Lambda^2 + \Lambda^2 F - 2\Lambda F\Lambda + \gamma v^T \]

where \( F = U^T Q U, \gamma = U^T \alpha, v = U^T 1 \)
First-order optimality condition:

\[ F\Lambda^2 + \Lambda^2 F - 2\Lambda F\Lambda + \gamma v^T = 0 \]
First-order optimality condition:

\[ F_{ij} (\lambda_i - \lambda_j)^2 + v_j \gamma_i = 0 \]
First-order optimality condition:

\[ F_{ij} (\lambda_i - \lambda_j)^2 + \nu_j \gamma_i = 0 \]

In particular, for \( i = j \): \( \nu_i \gamma_i = 0 \)
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 \( v_i = u_i^T 1 \neq 0 \)
Sketch of the proof

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 $v_i = u_i^T 1 \neq 0 \Rightarrow \gamma = 0$
First-order optimality condition:

\[ F_{ij}(\lambda_i - \lambda_j)^2 = 0 \quad \text{for } i \neq j \]
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \)
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow F \) is diagonal
First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow F \) is diagonal

\[ 1 = Q_1 \]
First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow \) \( F \) is diagonal

\[ 1 = Q1 = UFU^T1 \]
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow \textbf{F} \) is diagonal

\[ 1 = \textbf{Q}1 = \textbf{U} \textbf{F} \textbf{U}^T 1 \Rightarrow \textbf{U}^T 1 = \textbf{F} \textbf{U}^T 1 \]
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow F \) is diagonal

\[ 1 = Q1 = UFU^T 1 \Rightarrow U^T 1 = FU^T 1 \]
\[ \Rightarrow v = Fv \text{ with } v_i \neq 0 \]
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow F \) is diagonal

\[ 1 = Q1 = UFU^T 1 \Rightarrow U^T 1 = FU^T 1 \]
\[ \Rightarrow v = Fv \quad \text{with} \quad v_i \neq 0 \Rightarrow F = I \]
Sketch of the proof

First-order optimality condition:

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

Due to friendliness \( \lambda_i \neq \lambda_j \Rightarrow F \) is diagonal

\[ 1 = Q1 = UFU^T 1 \Rightarrow U^T 1 = FU^T 1 \]
\[ \Rightarrow v = Fv \text{ with } v_i \neq 0 \Rightarrow F = I \]
\[ \Rightarrow Q = UFU^T = I \]
Friendliness:

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

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

**Strong friendliness:**

- $A$ has $\delta$-separated spectrum
- every eigenvector $u_i$ of $A$ satisfied $|u_i^T 1| > \epsilon$

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

$\rho$-isomorphic $\iff \exists \Pi^* : \| \Pi^* A - B \Pi^* \|_F^2 \leq \rho$
**Strong friendliness:**

- $A$ has $\delta$-separated spectrum
- every eigenvector $u_i$ of $A$ satisfied $|u_i^T 1| > \epsilon$

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

Proof using results from regular perturbation theory of linear equations
**Strong friendliness:**

- $A$ has $\delta$-separated spectrum
- every eigenvector $u_i$ of $A$ satisfied $|u_i^T 1| > \epsilon$

**Theorem:** Let $A$ and $B$ be strongly friendly $\rho$-isomorphic graphs with $\rho = \rho(\epsilon, \delta)$. Then $\hat{\Pi} = \Pi^*$.

Proof using results from regular perturbation theory of linear equations
Inexact graph matching

**Strong friendliness:**

- $A$ has $\delta$-separated spectrum
- every eigenvector $u_i$ of $A$ satisfied $|u_i^T1| > \epsilon$

**Theorem:** Let $A$ and $B$ be strongly friendly $\rho$-isomorphic graphs with $\rho = \rho(\epsilon, \delta)$. Then $\hat{\Pi} = \Pi^*$. If $\|P^*A - BP^*\|_F^2 < \rho(\epsilon, \delta)$ then $\hat{\Pi}$ is the globally optimal approximate isomorphism. Otherwise, no $\rho$-isomorphism exists.
Experimental validation on 1000 strongly friendly graphs

Noisy Success rate

\[ \text{Noise} = \frac{\| \Pi^* A - B\Pi^* \|_F^2}{\rho(\epsilon, \delta)} \]
Unfriendly graphs

Adjacency matrix has \( d \) non-simple eigenspaces

\[
\lambda_1 = \lambda_2 = \cdots = \lambda_{i_1} < \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots
\]

\( \lambda_1, \lambda_2, \cdots \) are eigenvalues with multiplicities \( m_1 + 1 \) and \( m_2 + 1 \) respectively.
Unfriendly graphs

Adjacency matrix has $d$ non-simple eigenspaces

\[ \lambda_1 = \lambda_2 = \cdots = \lambda_{i_1} < \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots \]

\[
\begin{align*}
\text{multiplicity } m_1 + 1 & \\
m & = m_1 + m_2 + \cdots + m_d
\end{align*}
\]
Unfriendly graphs

Adjacency matrix has \( d \) non-simple eigenspaces

\[
\lambda_1 = \lambda_2 = \cdots = \lambda_{i_1} < \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots
\]

\[\text{multiplicity } m_1 + 1 \quad \text{multiplicity } m_2 + 1\]

\( m = m_1 + m_2 + \cdots + m_d \)

Basis vectors of each eigenspace are selected such that either

- none of them is orthogonal to \( 1 \); or
- all are orthogonal to \( 1 \)
Unfriendly graphs

Adjacency matrix has $d$ non-simple eigenspaces

\[
\begin{align*}
\lambda_1 &= \lambda_2 = \cdots = \lambda_{i_1} < \\
&\quad< \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots
\end{align*}
\]

multiplicity $m_1 + 1$

multiplicity $m_2 + 1$

\[
m = m_1 + m_2 + \cdots + m_d
\]

Basis vectors of each eigenspace are selected such that either

- none of them is orthogonal to $1$ (non-hostile); or
- all are orthogonal to $1$ (hostile)
Unfriendly graphs

Adjacency matrix has $d$ non-simple eigenspaces

$$\lambda_1 = \lambda_2 = \cdots = \lambda_{i_1} < \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots$$

multiplicity $m_1 + 1$ multiplicity $m_2 + 1$

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

Basis vectors of each eigenspace are selected such that either

- none of them is orthogonal to $1$ (non-hostile); or
- all are orthogonal to $1$ (hostile)

$k = \# \text{ of hostile eigenspaces}$
Unfriendly graphs

Adjacency matrix has $d$ non-simple eigenspaces

\[
\lambda_1 = \lambda_2 = \cdots = \lambda_{i_1} < \lambda_{i_1+1} = \cdots = \lambda_{i_1+i_2} < \cdots
\]

multiplicity $m_1 + 1$

multiplicity $m_2 + 1$

\[
m = m_1 + m_2 + \cdots + m_d
\]

Basis vectors of each eigenspace are selected such that either

- none of them is orthogonal to 1 (non-hostile); or
- all are orthogonal to 1 (hostile)

$k = \# \text{ of hostile eigenspaces}$

Unfriendliness degree: $m + k$
Matching of unfriendly graphs

**First-order optimality condition:**

$$F_{ij}(\lambda_i - \lambda_j)^2 + v_j \gamma_i = 0 \quad v_i = u_i^T 1$$

**Pseudo-stochasticity constraint:**

$$\sum_j F_{ij} v_j = v_i$$
Matching of unfriendly graphs

First-order optimality condition:

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2 
\end{pmatrix}
\mathbf{f}_i + \gamma_i \mathbf{v} = 0
\]

Pseudo-stochasticity constraint:

\[
\mathbf{v}^T \mathbf{f}_i = \nu_i
\]

for each \(i\)-th row \(\mathbf{f}_i = (F_{i1}, \ldots, F_{in})^T\)
Matching of unfriendly graphs

First-order optimality condition:

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\mathbf{f}_i + \gamma_i \mathbf{v} = 0
\]

Pseudo-stochasticity constraint:

\[\mathbf{v}^T \mathbf{f}_i = \nu_i\]

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

\(n\) systems with \(n + 1\) equations and variables each
Case I: non-hostile eigenspace

\( u_i \) belongs to a non-hostile eigenspace

**First-order optimality condition:**

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix} f_i + \gamma_i v = 0
\]

**Pseudo-stochasticity constraint:**

\[ v^T f_i = \nu_i \]
Case I: non-hostile eigenspace

\[ u_i \text{ belongs to a non-hostile eigenspace } \Rightarrow v_i \neq 0 \]

First-order optimality condition:

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\] \[ f_i + \gamma_i v = 0 \]

Pseudo-stochasticity constraint:

\[ v^T f_i = v_i \]
Case I: non-hostile eigenspace

\( u_i \) belongs to a non-hostile eigenspace \( \Rightarrow v_i \neq 0 \)
\( \Rightarrow \gamma_i = 0 \)

First-order optimality condition:

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix} f_i = 0
\]

Pseudo-stochasticity constraint:

\( v^T f_i = v_i \)
Case I: non-hostile eigenspace

\( u_i \) belongs to a non-hostile eigenspace \( \Rightarrow v_i \neq 0 \)

\( \Rightarrow \gamma_i = 0 \)

First-order optimality condition:

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\begin{pmatrix}
f_i 
\end{pmatrix} = 0
\]

Pseudo-stochasticity constraint:

\( v^T f_i = v_i \)

Rank-\( m_i \) deficient!
Case II: hostile eigenspace

\( u_i \) belongs to a hostile eigenspace

**First-order optimality condition:**

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\begin{pmatrix}
f_i \\
\gamma_i\mathbf{v}
\end{pmatrix} = 0
\]

**Pseudo-stochasticity constraint:**

\[ \mathbf{v}^T f_i = v_i \]
Case II: hostile eigenspace

\( u_i \) belongs to a hostile eigenspace \( \Rightarrow v_i = 0 \)

**First-order optimality condition:**

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix} f_i + \gamma_i v = 0
\]

**Pseudo-stochasticity constraint:**

\[ v^T f_i = v_i \]
**Case II: hostile eigenspace**

\( \mathbf{u}_i \) belongs to a hostile eigenspace \( \implies \nu_i = 0 \)

\( \implies \gamma_i \) undetermined

**First-order optimality condition:**

\[
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\begin{pmatrix}
f_i \\
0
\end{pmatrix} = -\gamma_i
\begin{pmatrix}
\vdots \\
0
\end{pmatrix}
\]

**Pseudo-stochasticity constraint:**

\( \mathbf{v}^T \mathbf{f}_i = 0 \)
Case II: hostile eigenspace

$u_i$ belongs to a hostile eigenspace $\Rightarrow v_i = 0$
$\Rightarrow \gamma_i$ undetermined

**First-order optimality condition:**

$$
\begin{pmatrix}
(\lambda_i - \lambda_1)^2 \\
\vdots \\
(\lambda_i - \lambda_n)^2
\end{pmatrix}
\begin{pmatrix}
f_i \\
\vdots
\end{pmatrix}
= -\gamma_i
\begin{pmatrix}
0 \\
\vdots
\end{pmatrix}
$$

**Pseudo-stochasticity constraint:**

$$v^T f_i = 0$$

**Rank-$(m_i + 1)$ deficient!**
For an \((m + k)\)-unfriendly graph, the system

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

\[
\sum_j F_{ij}v_j = v_i
\]

is rank-\((m + k)\) deficient!
For an \((m + k)\)-unfriendly graph, the system

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

\[
\sum_j F_{ij}v_j = v_i
\]

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

Solution space is \((m + k)\)-dimensional.
Matching of unfriendly graphs

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

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

\[
\sum_j F_{ij} v_j = v_i
\]

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

Solution space is \((m + k)\)-dimensional.

Some solutions may belong to Voronoi cells of permutations that are not isomorphisms!
For an \((m + k)\)-unfriendly graph, the system

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

\[ \sum_j F_{ij} v_j = v_i \]

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

Convex relaxation \pm projection can produce wrong solutions!
Seeds and attributes

**Seeds (known correspondences):** collection of $q$ real functions $C = (c_1, \ldots, c_q)$ on the vertex set of $A$ with corresponding functions $D = (d_1, \ldots, d_q)$ on $B$. 
Seeds (known correspondences): collection of $q$ real functions $C = (c_1, \ldots, c_q)$ on the vertex set of $A$ with corresponding functions $D = (d_1, \ldots, d_q)$ on $B$.

Attributes: $q$-dimensional vector-valued vertex attributes $C = (c_1^T, \ldots, c_n^T)^T$. 
Seeds (known correspondences): collection of $q$ real functions $\mathbf{C} = (c_1, \ldots, c_q)$ on the vertex set of $\mathbf{A}$ with corresponding functions $\mathbf{D} = (d_1, \ldots, d_q)$ on $\mathbf{B}$.

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

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

**Seeds** *(known correspondences):* collection of $q$ real functions $C = (c_1, \ldots, c_q)$ on the vertex set of $A$ with corresponding functions $D = (d_1, \ldots, d_q)$ on $B$.

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

**Attributes:** $q$-dimensional vector-valued vertex attributes $C = (c_1^T, \ldots, c_n^T)^T$.

Covariant with a preferred isomorphism: $\Pi^*C = D$. 
Seeds (known correspondences): collection of \( q \) real functions \( C = (c_1, \ldots, c_q) \) on the vertex set of \( A \) with corresponding functions \( D = (d_1, \ldots, d_q) \) on \( B \).

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

Attributes: \( q \)-dimensional vector-valued vertex attributes \( C = (c_1^T, \ldots, c_n^T)^T \).

Rows of \( C \) and \( \Pi^*D \) are corresponding attributes.

Covariant with a preferred isomorphism: \( \Pi^*C = D \).
Convex Relaxation

$$\min_P \|PA - BP\|_F^2 \quad \text{s.t.} \quad P1 = 1$$
Convex Relaxation of seeded/attributed matching

\[
\min_{P} \| PA - BP \|^2_F + \mu \| PC - D \|^2_F \quad \text{s.t.} \quad P1 = 1
\]
Seeded/attributed graph matching

**Convex Relaxation** of seeded/attributed matching

\[
\min_P \| PA - BP \|^2_F + \mu \| PC - D \|^2_F \quad \text{s.t.} \quad P1 = 1
\]

penalty on attributes disagreement

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

- $\mathbf{D} \mathbf{D}^T \mathbf{u}_j \neq 0 \quad \forall j = i, \ldots, i + m_i$ if eigenspace is hostile; or

- $\mathbf{D} \mathbf{D}^T \mathbf{u}_j \neq 1 \frac{\mathbf{u}_i^T \mathbf{D} \mathbf{D}^T \mathbf{u}_j}{1^T \mathbf{u}_i} \quad \forall j = i + 1, \ldots, i + m_i$ otherwise.

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

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

Convex quadratic program

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

with global minimizer $\mathbf{P} = \Pi^*$. 
Sketch of the proof

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

Convex quadratic program reparametrized with $Q = PP^T$

$$\min_Q \|QB - BQ\|^2_F + \mu \|QD - D\|^2_F \quad \text{s.t.} \quad Q1 = 1$$

with global minimizer $Q = I$. 
**Input:** two graphs $B$ and $A = \Pi^* B \Pi^*$ with seeds/attributes $C$ and $D = \Pi^* C$

Convex quadratic program reparametrized with $Q = R \Pi^* T$

$$\min_Q \|QB - BQ\|^2_F + \mu \|QD - D\|^2_F \quad \text{s.t.} \quad Q1 = 1$$

with global minimizer $Q = I$.

**Show that the minimizer is unique**
First-order optimality condition:

\[ QB^2 + B^2Q - 2BQB + \mu QDD^T - \mu DD^T + \alpha 1^T = 0 \]

Pseudo-stochasticity constraint: \( Q1 = 1 \)
First-order optimality condition:

\[ F \Lambda^2 + \Lambda^2 F - 2 \Lambda F \Lambda + \mu F G - \mu G + \gamma v^T = 0 \]

with \( G = U^T D D^T U \)

Pseudo-stochasticity constraint: \( F v = v \)
First-order optimality condition:

\[ F \Lambda^2 + \Lambda^2 F - 2 \Lambda F \Lambda + \mu FG - \mu G + \gamma v^T = 0 \]

with \( G = U^T DD^T U \succeq 0 \)

Pseudo-stochasticity constraint: \( Fv = v \)

Adding attributes/seeds increases rank
Theorem: Let $D = \Pi^* C$ satisfying for every non-simple eigenspace $\text{sp}\{u_i, \ldots, u_{i+m_i}\}$

- $DD^T u_j \neq 0 \quad \forall j = i, \ldots, i + m_i$ if eigenspace is hostile; or

- $DD^T u_j \neq 1 \frac{u_i^T DD^T u_j}{1^T u_i} \quad \forall j = i + 1, \ldots, i + m_i$ otherwise.

Then, $P^* = \Pi^*$ is the unique solution of relaxation.
Theorem: Let $D = \Pi^* C$ satisfying for every non-simple eigenspace $\text{sp}\{u_i, \ldots, u_{i+m_i}\}$

- $DD^T u_j \neq 0 \quad \forall j = i, \ldots, i + m_i$ if eigenspace is hostile; or

- $DD^T u_j \neq 1 \frac{u_i^T DD^T u_j}{1^T u_i} \quad \forall j = i + 1, \ldots, i + m_i$ otherwise.

Then, $P^* = \Pi^*$ is the unique solution of relaxation.

$m + k$ linearly independent seeds are required.
Experimental validation on 1000 symmetric graphs

Success rate = \#seeds / \#symmetries
**Relaxation space:** We used $P1 = 1$. Do we need $P \geq 0$? do we need $P^T 1 = 1$? Practical consequences?
Questions

- **Relaxation space:** We used $P1 = 1$. Do we need $P \geq 0$? do we need $P^T1 = 1$? Practical consequences?

- **Better use of geometry:** adjacency matrices are, e.g., metric? low dimensional? smooth? bounded curvature?
Questions

- **Relaxation space:** We used $P1 = 1$. Do we need $P \geq 0$? do we need $P^T1 = 1$? Practical consequences?

- **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 $A$ to make it friendly. Will the relaxation still work?
Questions

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

- **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 $A$ to make it friendly. Will the relaxation still work?

- **Finding all isomorphisms** (in particular, all symmetries of a graph).