(Robust) Seeded graph matching

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- Given two graphs, the Graph matching problem (GMP) seeks to find an alignment of the vertex sets of the two graphs that best preserves the connectivity structure of the graphs

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THIRTY YEARS OF GRAPH MATCHING IN PATTERN RECOGNITION

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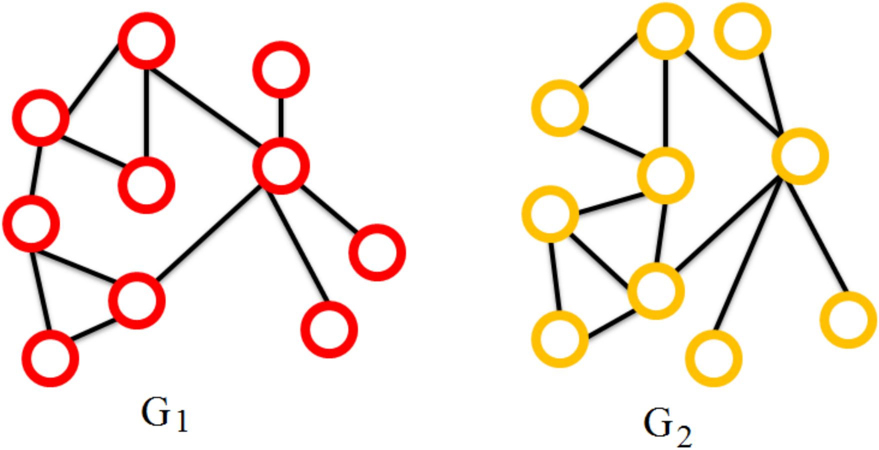
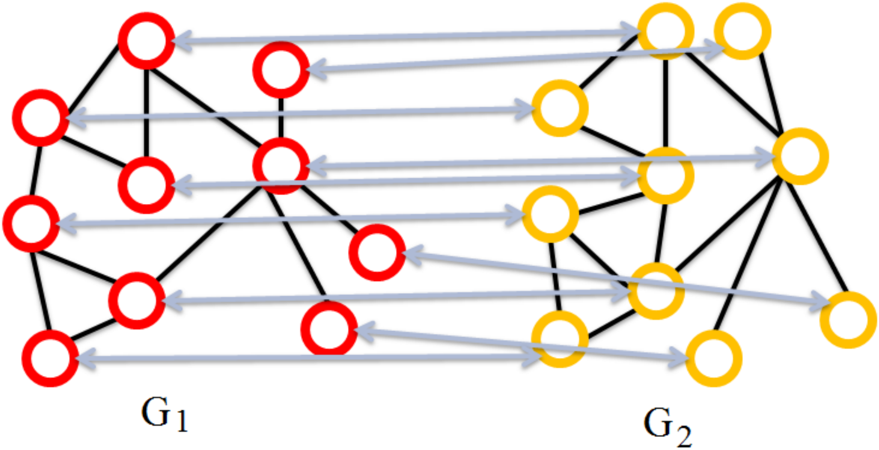

G_1
G_2


G_1
G_2

- Given two graphs, the Graph matching problem (GMP) seeks to find an alignment of the vertex sets of the two graphs that best preserves the connectivity structure of the graphs
- In the seeded graph matching problem, we are further provided subsets of the vertices (Seeds)

  $$S_1 \subset V_1, \ S_2 \subset V_2$$

  and a seeding function

  $$\phi \subset S_1 \times S_2, \quad \text{i.e. } (u, v) \in \phi \Rightarrow \text{ u and v are "matched"}$$

  Goal: Leverage ϕ to match the remaining vertices

- Our proceudre: The Joint Optimization of Fidelity and Commensurabilty (JOFC) graph matching algorithm of Lyzinski et al. (2014)
- Adapted from the manifold matching methodologies of Priebe et al. (2013)
- Is **robust**
- Briefly, the JOFC algorithm proceeds as follows:
  1. Jointly embed the seeded vertices into a common Euclidean space
  2. Separately out-of-sample embed the nonseeded vertices
  3. Match the embedded nonseeded vertices—this is equivalent to solving the generalized assignment problem

- We begin with Δ_1 and Δ_2, dissimilarity representations of the graphs G_1 and G_2 resp.
- Let

$$X_1^{(1)}, X_2^{(1)}, \ldots, X_{s_1}^{(1)} \text{ be the embedded seeded vertices of } G_1,$$

and

$$X_1^{(2)}, X_2^{(2)}, \ldots, X_{s_2}^{(2)} \text{ the embedded seeded vertices of } G_2$$

- We want the embedding to simultaneously preserve:
  1. The within graph dissimilarities amongst the seeded vertices (fidelity)

  1b. The across graph relationship provided by the seeding between non-matched seeded vertices (separability)

  2. The across graph relationship given by the seeding (commensurability)

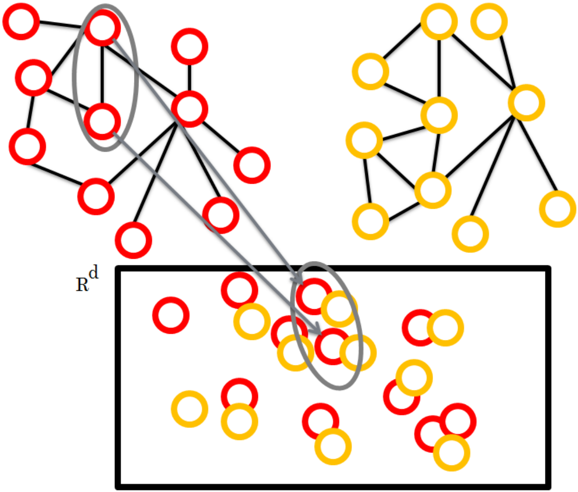
- We want the embedding to simultaneously preserve:
  1. The within graph dissimilarities amongst the seeded vertices i.e. we wish to minimize the within graph squared fidelity error of the embedding given by

$$\varepsilon^2_{F_1} := \sum_{i,j} \left(d(X_i^{(1)}, X_j^{(1)}) - \Delta_1(i,j) \right)^2$$

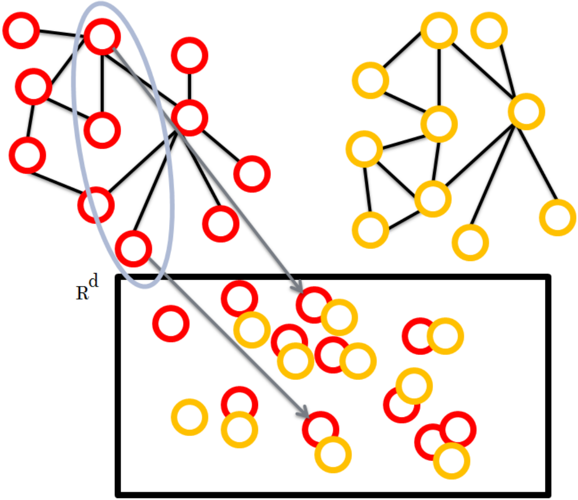
and

$$\varepsilon^2_{F_2} := \sum_{i,j} \left(d(X_i^{(2)}, X_j^{(2)}) - \Delta_2(i,j) \right)^2$$

Minimize the squared fidelity error of the embedding



Minimize the squared fidelity error of the embedding



- We want the embedding to simultaneously preserve:
  1b. The dissimilarities amongst the non-matched seeded vertices across graphs
  i.e. we wish to minimize the across graph squared separability error of the embedding given by

$$\varepsilon_S^2 := \sum_{\substack{\text{i,j s.t. i and j are non-matched} \\ \text{seeded vertices}}} \left(d(X_i^{(1)}, X_j^{(2)}) - \delta(i,j) \right)^2$$

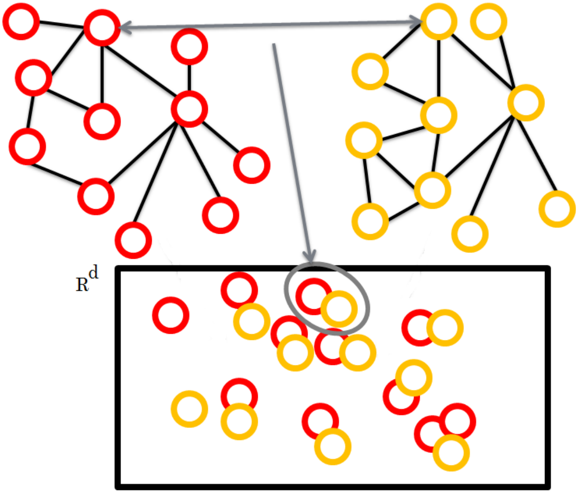
  δ here is an unknown across graph dissimilarity, and must be imputed or treated as missing data

- We want the embedding to simultaneously preserve:
  2. The across graph relationship given by the seeding i.e. we wish to minimize the within graph squared commensurability error of the embedding given by

$$\varepsilon_C^2 := \sum_{\substack{\text{i,j s.t. i and j are matched} \\ \text{by the seeding}}} \left(d(X_i^{(1)}, X_j^{(2)}) - \delta(i,j) \right)^2$$

     Again δ here is an unknown across graph dissimilarity, though if i and j are matched by the seeding, it is reasonable to impute $\delta(i,j) = 0$

2. Minimize the squared commensurability error of the embedding



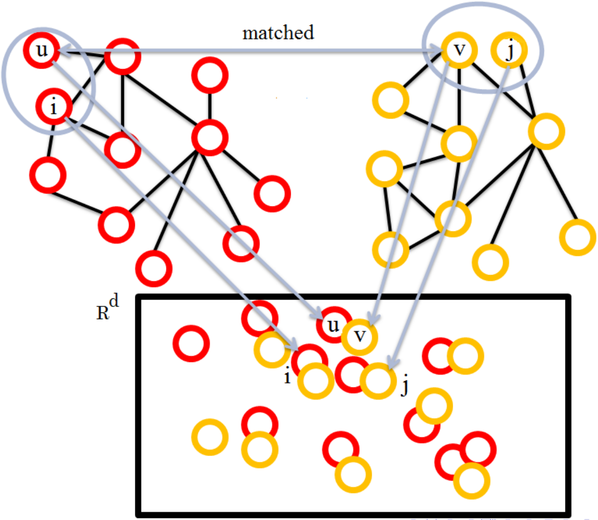
- We embed the seeded vertices using the SMACOF algorithm of de Leeuw (1977)—a version of weighted MDS
- With a judicious choice of weightings here, SMACOF seeks to minimize
$$w(\epsilon_{F_1}^2 + \epsilon_{F_2}^2 + \epsilon_S^2) + (1-w)\epsilon_{C^2}$$
- In our applications, we found best performance with $w = 0.8$; see Adali et al. (2013) for motivation

- We next out-of-sample embed the unseeded vertices of G_1 ($\{Y_i^{(1)}\}$) and of G_2 ($\{Y_i^{(2)}\}$) using the weighted MDS procedure of Tang et al. (2013)
- Through a judicious choice of weightings, we seek to minimize the stress function

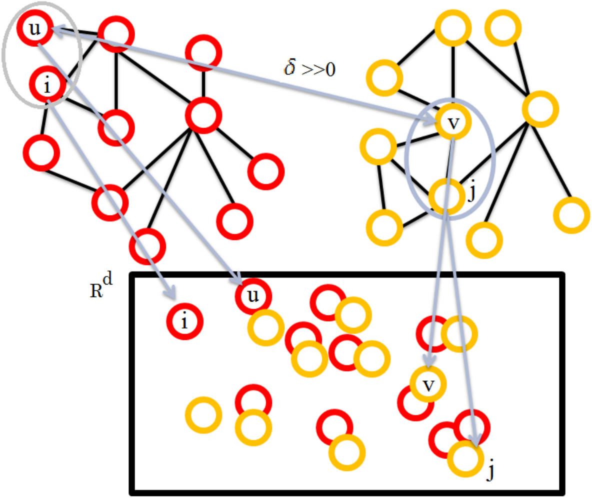
$$\sigma(\mathbf{Y}) = \sum_i \sum_j \left(d(X_i^{(1)}, Y_j^{(1)}) - \Delta^{(1)}(i,j) \right)^2 + \sum_i \sum_j \left(d(X_i^{(2)}, Y_j^{(2)}) - \Delta^{(2)}(i,j) \right)^2$$

  i.e. we wish to preserve the within graph dissimilarities between the seeded and unseeded vertices
- Then match embedded vertices based on Euclidean distance: closer together=more likely to be matched

- Suppose $i \in V(G_1)$ and $j \in V(G_2)$ are unseeded vertices that should be matched to each other



- Suppose $i \in V(G_1)$ and $j \in V(G_2)$ are unseeded vertices that should NOT be matched to each other



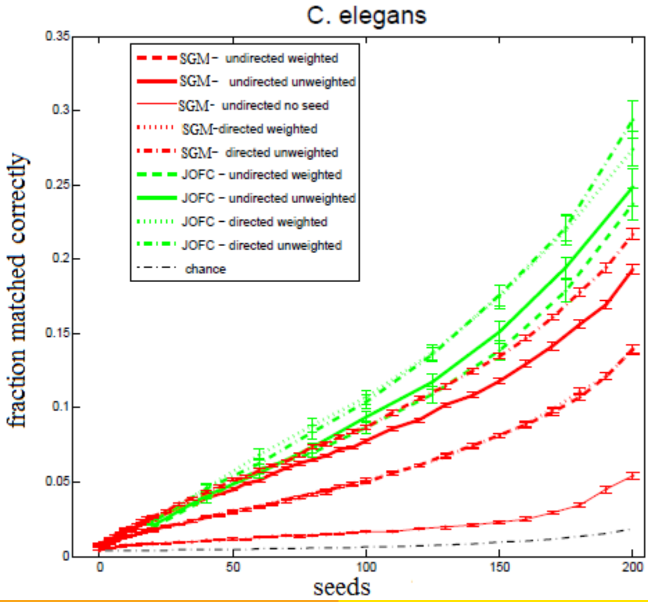
- We then match the unseeded embedded vertices by minimizing

$$\sum_{\substack{i,j \text{ unseeded vertices} \\ \text{matched by M}}} d(Y_i^{(1)}, Y_j^{(2)}).$$

  over all matchings $M \subset V(G_1) \times V(G_2)$ of the unseeded vertices
- This is equivalent to a generalized assignment problem—NP-hard in general, but are good approximation algorithms

Ex Matching C. elegans connectomes

- The C. elegans nervous system is believed to be composed of 302 labelled vertices (279 with synapses to other neurons)
- There are two types of connections between neurons: electrical and chemical
- We match the chemical connectome to the electrical connectome to understand the extent to which connectivity structure alone is enough to identify neurons across the connectomes


C. elegans
SGM- undirected weighted
SGM- undirected unweighted
SGM- undirected no seed
SGM-directed weighted
SGM- directed unweighted
JOFC – undirected weighted
JOFC – undirected unweighted
JOFC – directed weighted
JOFC – directed unweighted
chance
fraction matched correctly
seeds
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0
50
100
150
200

- This procedure is flexible enough to handle:
  1. $|V(G_1)| \neq |V(G_2)|$—allow for many–to–many, many–to–one or many–to–none matchings in the embedded graphs
  2. Weighted directed graphs—use a dissimilarity that allows for weightedness and directedness in the graphs for the embedding
  3. The case of "soft" seeds—suitably weight the MDS embeddings
- Is easily modified for vertex classification
- Working on scaling the SMACOF subroutine—would lead to our algorithm scaling

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