Joint Optimization of Fidelity And Commensurability for Manifold Alignment

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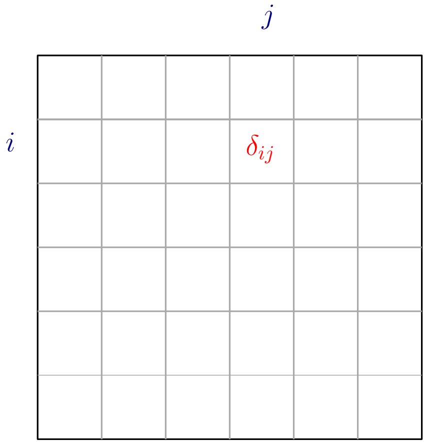
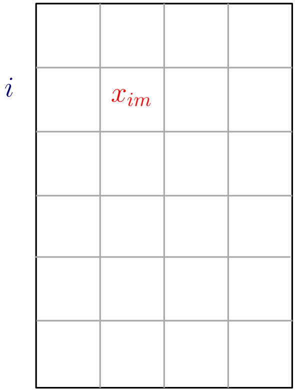
July 8, 2012

Dissimilarity Representation vs Feature Representation





$$\Delta = [\delta_{ij}]$$

$$x_i \in \mathbf{R}^d$$

$$\delta_{ij} >= 0 \;,\; \delta_{ii} = 0 \;,\; \delta_{ij} = \delta_{ji}$$
$$i = \{1, \ldots, n\} \quad j = \{1, \ldots, n\}$$

How do we embed dissimilarities in Euclidean space?

Multidimensional Scaling [BorgGroenen1997]

Given $n \times n$ dissimilarity matrix
$\Delta = [\delta_{st}]; s = 1, \ldots, n;\ t = 1, \ldots, n,$

- Finds an embedding of the dissimilarities in the Euclidean space (with a chosen dimension d) such that the distances between the embeddings are as close as possible (in various senses) to the original dissimilarities in Δ.
- One function to measure closeness is the weighted raw-stress:

$$\sigma_W(X) = \sum_{1 \le s \le n; 1 \le t \le n} w_{st}(d_{st}(X) - \delta_{st})^2$$

where $d_{st}(X)$ is the Euclidean distance between s^{th} and t^{th} embedded points, and
weight matrix $W = [w_{st}]; s = 1, \ldots, n;\ t = 1, \ldots, n.$

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Problem Formulation for Dissimilarity Representation

Given K $n \times n$ dissimilarity matrices

$$\boldsymbol{\Delta}^{(k)} = [\delta_{ij}]^{(k)}; 1 \leq i < j \leq n; k = 1, \cdots, K;$$

- Dissimilarities between n objects are each measured under K different conditions.
- The set of dissimilarities under different conditions for the same object are "matched".

Also given

$\mathbf{D}^{(k)} = \{\delta_i; i = 1, \ldots, n\} \qquad k = 1, \ldots, K$: dissimilarities between K new measurements and previous n objects under the same K conditions.

Question we can answer

Do dissimilarities $\mathbf{D}^{(k)}$ come from K new measurements that represent a single object?

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Meaning of "conditions" and "matched"

	Condition 1	Condition 2
A linked collection of wikipedia articles	Textual content of an article	Hyperlink graph of articles
A linked collection of English and French wikipedia articles	The articles in English	The articles in French
Photos of same objects taken under different condition	Indoor photos	Outdoor photos

Hypotheses

For K=2,

$$H_0 : \mathbf{D}^{(1)} \sim \mathbf{D}^{(2)} \text{ (Matched)}$$

versus

$$H_A : \mathbf{D}^{(1)} \nsim \mathbf{D}^{(2)} \text{ (Not matched)}$$

(Hypothesis testing with α=constraint on the probability of missing a true match)

Omnibus Embedding Approach

$$\overset{2n\times 2n}{M} = \begin{bmatrix} \overset{n\times n}{\Delta_1} & \overset{n\times n}{L} \\ L^{T} & \overset{n\times n}{\Delta_2} \end{bmatrix}$$

- Impute L (dissimilarities between different conditions) to obtain an *omnibus dissimilarity matrix* M
- Embed the omnibus matrix M as $2n$ points (one point for each condition of each object) in commensurate space ($\mathbb{R}^d$)

Out-of-sample Embedding

$$\Delta \longrightarrow X$$

$$[D^{(k)}; k = 1, \ldots, K] \xrightarrow[X]{\text{OOS-embed}} \qquad Y$$

Omnibus Embedding Approach (OOS-embedding)

$$\overset{2n\times 2n}{M} = \begin{bmatrix} \overset{n\times n}{\Delta_1} & \overset{n\times n}{L} \\ L^{T} & \overset{n\times n}{\Delta_2} \end{bmatrix} \begin{matrix} \overset{n\times 1}{D^{(1)}} & \overset{n\times 1}{\vdots} \\ \overset{n\times 1}{\vdots} & \overset{n\times 1}{D^{(2)}} \end{matrix}$$

$$\begin{matrix} y_1 & {D^{(1)}}^{T} & \\ y_2 & & {D^{(2)}}^{T} \end{matrix}$$

General Approach

1. Map/Embed via MDS in-sample ($\mathbf{\Delta}_k; k = 1, \ldots, K$) dissimilarities into commensurate space.
2. Map/Embed (Out-of-sample) test dissimilarities ($\mathbf{D}^{(k)}; k = 1, \ldots, K$) into commensurate space.
3. Compute test statistic τ (the distance between embeddings of test dissimilarities).
4. Reject null hypothesis if τ is large.

Fidelity and Commensurability Criteria

Fidelity is how well the mapping to commensurate space preserves original dissimilarities. Within-condition *fidelity error* is given by

$$\epsilon_{f_k} = \frac{1}{\binom{n}{2}} \sum_{1 \le i < j \le n} (d(\widetilde{\boldsymbol{x}}_{ik}, \widetilde{\boldsymbol{x}}_{jk}) - [\delta_{ij}]^{(k)})^2,$$

where $\widetilde{\boldsymbol{x}}_{ik}$ is the embedded configuration of ith object for kth condition.

Fidelity and Commensurability Criteria

Commensurability is how well the mapping to commensurate space preserves matchedness. Between-condition *commensurability error* is given by

$$\epsilon_{c_{k_1 k_2}} = \frac{1}{n} \sum_{1 \le i \le n} \left(d(\widetilde{\boldsymbol{x}}_{ik_1}, \widetilde{\boldsymbol{x}}_{ik_2}) - [\delta_{ii}]^{(k_1,k_2)} \right)^2$$

for different conditions k_1 and k_2.

Although $[\delta_{ii}]^{(k_1,k_2)}$ is not available (the between-condition dissimilarities), it is not unreasonable in this setting to set $[\delta_{ii}]^{(k_1,k_2)} = 0$ for all i, k_1, k_2. (We want embedded points of the same object to be close.)

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Commensurability and Fidelity Terms in Raw Stress

The weighted raw stress criterion for MDS with different conditions is

$$\sigma_W(X) = \sum_{i \le j, k_1 \le k_2} w_{ijk_1k_2}(d_{ijk_1k_2}(X) - [\delta_{ij}]^{(k1,k2)})^2$$

(i and j are the indices for the object, k_1 and k_2 are condition indices).

Ignoring some error terms (We can set $w_{ijk_1k_2} = 0$ for $i \neq j$ and $k_1 \neq k_2$)

$$\sigma_W(X) = \underbrace{\sum_{i=j, k_1 < k_2} w_{ijk_1k_2}(d_{ijk_1k_2}(X) - [\delta_{ij}]^{(k1,k2)})^2}_{Commensurability} + \underbrace{\sum_{i<j, k_1 = k_2} w_{ijk_1k_2}(d_{ijk_1k_2}(X) - [\delta_{ij}]^{(k1,k2)})^2}_{Fidelity}$$

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Which one is critical for hypothesis testing performance: Fidelity or Commensurability?

Setting $w_{ijk_1k_2}$ to $(1-w)$ for Fidelity terms, and to w for Commensurability terms,

$$\sigma_w(X) = \underbrace{\sum_{i=j,k_1<k_2} w(d_{ijk_1k_2}(X) - [\delta_{ij}]^{(k1,k2)})^2}_{Commensurability} + \underbrace{\sum_{i<j,k_1=k_2} (1-w)(d_{ijk_1k_2}(X) - [\delta_{ij}]^{(k1,k2)})^2}_{Fidelity} .$$

w controls the tradeoff between Fidelity and Commensurability.
Define w^* to be the value of w which maximizes power.

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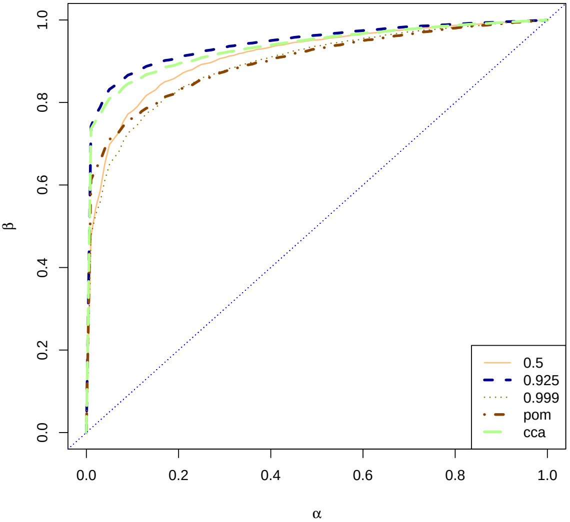
Simulation Results

ROC curves: Power(β) against allowable Type I error(α)



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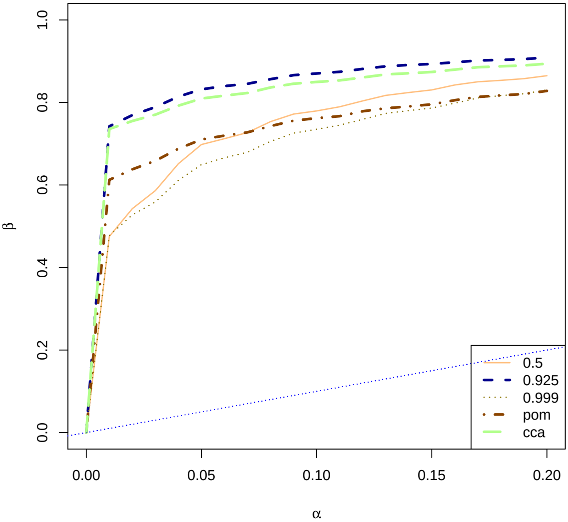

Matching Dissimilarities

If multiple dissimilarities are available $\mathbf{D}_i^{(k)}, i = 1, \ldots, n$ from two different conditions, what is the best matching of dissimilarities from two different conditions?

- Embed the dissimilarities
- Interpret the distances between embeddings as costs in an assignment problem
- Solve the linear assignment problem by the Hungarian algorithm:
  Find the best assignment $f : \{1, \ldots, s\} \to \{1, \ldots, s\}$ that minimizes the cost
  $$\sum_{i=1}^{n} C(i, f(i))$$
  where the cost $C(\cdot, \cdot)$ is the distance between the embeddings of each dissimilarity from the different conditions.

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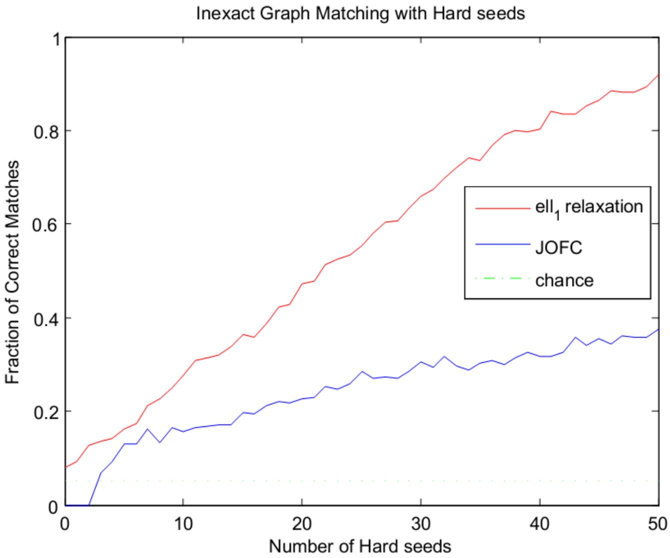
Vertex Correspondence: Graph matching with seeds

To solve the inexact graph matching problem with hard seeds where the objects we want to match are graph vertices,

- Compute dissimilarities between vertices
- Embed the hard seeds which are known to be matched with JOFC.
- OOS-embed the vertices to be matched.
- Compute dissimilarities between embeddings of vertices between different graphs
- Solve the linear assignment problem with dissimilarities as costs.

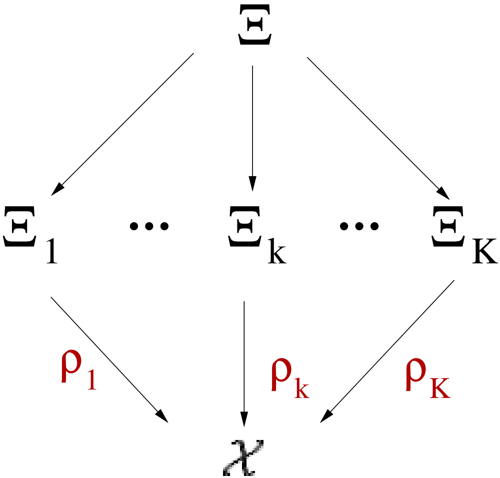
Simulation Results: Graph Matching
Fraction of Correct Matches vs Number of Hard Seeds



Conclusions

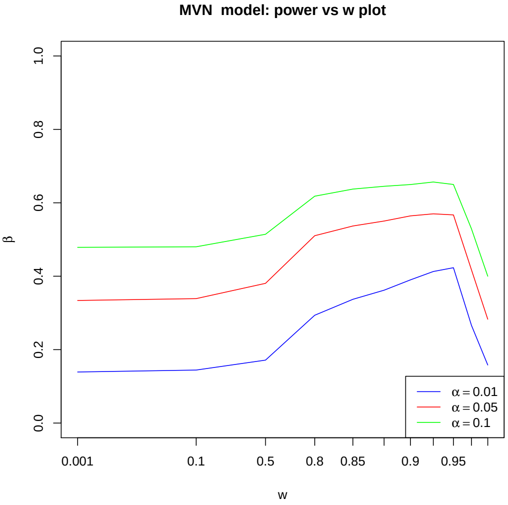
- Our JOFC approach is a general tool that can solve many kinds of related problems.
- The tradeoff between fidelity and commensurability , controlled by the parameter w has a big effect on the performance for the inference task.
- A particular type of graph matching problem can be solved using JOFC followed by the Hungarian algorithm.

Measurement Spaces and Commensurate Space



Simulation Results

Power(β) curves: Power(β) against w at fixed α



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Carey E. Priebe, David J. Marchette, Zhiliang Ma, Sancar Adali
Manifold Matching: Joint Optimization of Fidelity and Commensurability
Brazilian Journal of Probability and Statistics, accepted for publication
February, 2012.