Data Analysis and Manifold Learning
Lecture 10: Spectral Matching

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Outline of Lecture 10

- Graph isomorphism problems
- Solving graph isomorphism with spectral matching
- Problems with standard algorithms
- The ”signature” of an eigenvector
- Graph matching based on point registration
Material for this lecture

The Graph Isomorphism Problem

- Let two graphs $G_A$ and $G_B$ have the same number of nodes, and let $\pi : \mathcal{V}_A \longrightarrow \mathcal{V}_B$ be a bijection;
- $\pi$ is an isomorphism if and only if:

$$u \sim v \iff \pi(u) \sim \pi(v)$$

- The notion of graph isomorphism allows to study the structure of graphs.
- The graph isomorphism problem: an algorithm that determines whether two graphs are isomorphic.
- It is one of only two, out of 12 total, problems listed in Garey & Johnson (1979) whose complexity remains unresolved: It has not been proven to be included in, nor excluded from, P (polynomial) or NP-complete.
The Subgraph Isomorphism Problem

- Let two graphs $G_A$ with $n_A$ nodes and $G_B$ with $n_B$ nodes such that $n_A > n_B$.
- One must determine whether $G_A$ contains a subgraph that is isomorphic to $G_B$.
- The number of possible solutions is: $\binom{n_B}{n_A} n_B!$
- The problem is NP-complete (Nondeterministic polynomial).
The Maximum Subgraph Matching Problem

- Let two graphs $G_A$ with $n_A$ nodes and $G_B$ with $n_B$ nodes such that $n_A > n_B$.
- Determine the largest pair of subgraphs $(G'_A, G'_B)$, with $G'_A \subset G_A$ and $G'_B \subset G_B$, such that $G'_A$ and $G'_B$ are isomorphic.
- The number of possible solutions is:
  \[
  \sum_{i=1}^{n_B} \binom{i}{n_A} \binom{i}{n_B} i!
  \]
- The problem is NP-complete
How to Solve Graph Isomorphism Problems

Let’s consider, as above two undirected graphs (weights are all equal to 1) with the same number of nodes.

Let’s define a metric between the two graphs as:

$$\arg \max_{\pi} \sum_{i=1}^{n} \sum_{j=1}^{n} (e_{ij} - e_{\pi(i)\pi(j)})^2$$
Using Graph matrices

- Let \( W_A \) and \( W_B \) be the adjacency matrices of two graphs with the same number of nodes \( n \).
- Let \( P \in \mathcal{P}_n \) be a permutation matrix: exactly one entry in each row and column is equal to 1, and all the other entries are 0.
- Left multiplication of \( W \) with \( P \) permutes the rows of \( W \) and
- Right multiplication of \( W \) with \( P \) permutes the columns of \( W \).
- What does \( PWP^\top \) stand for?
- \( W = U\Lambda U^\top \)
- \( PWP^\top = (PU) \Lambda (PU)^\top \)
- Think of the rows of \( U \) as the coordinates of the graph’s vertices in spectral space ... the nodes are renamed.
A Simple Example

\[ W_A = \begin{bmatrix}
0 & 1 & 1 & 0 \\
1 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 
\end{bmatrix} \]

\[ P = \begin{bmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 
\end{bmatrix} \]

\[ W_B = PW_A P^\top = \begin{bmatrix}
0 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 
\end{bmatrix} \]

Which corresponds to:

\[ v_1 \leftrightarrow u_2, \ v_2 \leftrightarrow u_1, \ v_3 \leftrightarrow u_4, \ v_3 \leftrightarrow u_4 \]
The Graph Isomorphism Problem with Matrices

- The metric between two graphs becomes:

\[ P^* = \arg \min_P \| W_A - P W_B P^\top \|_2^2 \]

- where the Frobenius norm is being used:

\[ \| A \|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j}^2 = \text{tr}(A^\top A). \]
An Exact Solution

When the metric is equal to zero:

\[ W_A = PW_B P^\top \]

- Two isomorphic graphs have the same eigenvalues;
- The reverse is not always true.
Finding an Exact Solution in the Spectral Domain

- Let’s write an equality:

\[ W_A = P^* W_B P^{*\top} \]

- Consider the spectral decompositions:

\[ W_A = U_A \Lambda_A U_A^\top \quad \text{and} \quad W_B = \tilde{U}_B \Lambda_B \tilde{U}_B^\top \]

- with the notation:

\[ \tilde{U}_B = U_B \mathcal{S} \quad \text{and} \quad \mathcal{S} = \text{Diag}[s_i], \ s_i = \pm 1 \]

- By substitution in the first equation, we obtain:

\[ P^* = U_B \mathcal{S} U_A^\top \]
Short Discussion

- There are as many solutions as the number of possible $S$-matrices, i.e., $2^n$.
- Not all of these solutions correspond to a valid permutation matrix.
- There exist some $S^*$ that exactly make $P^*$ a permutation: these are valid solutions to the graph isomorphism problem.
- Eigenspace alignment:

$$U_A = P^* U_B S^*$$

The rows of $U_A$ can be interpreted as the coordinates of the graph’s vertices in the eigenspace of $W_A$. The above equation can be interpreted as a registration between the embedding of the two graphs. Hence:

- The graph isomorphism problem can be viewed as a rigid registration problem in embedded space.
The Hoffman-Wienlandt Theorem

\[ \sum_{i=1}^{n} (\alpha_i - \beta_i)^2 \leq \|W_A - W_B\|^2 \]

This theorem is the fundamental building block of spectral graph matching.
Corollary

The inequality (1) becomes an equality when the eigenvectors of $W_A$ are aligned with the eigenvectors of $W_B$ up to a sign ambiguity:

$$U_B = U_A S.$$  \hspace{1cm} (2)

Corollary

If $Q$ is an orthogonal matrix, then

$$\sum_{i=1}^{n} (\alpha_i - \beta_i)^2 \leq \|W_A - Q W_B Q^\top\|^2.$$  \hspace{1cm} (3)

Indeed, matrix $Q W_B Q^\top$ has the same eigenvalues as matrix $W_B$. 
Umeyama’s Theorem

**Theorem**

*(Umeyama’1988)* If \( W_A \) and \( W_B \) are real-symmetric matrices with \( n \) distinct eigenvalues (that can be ordered), \( \alpha_1 < \ldots < \alpha_i < \ldots < \alpha_n \) and \( \beta_1 < \ldots < \beta_i < \ldots < \beta_n \), the minimum of:

\[
J(Q) = \| W_A - QW_B Q^\top \|_2^2
\]

is achieved for:

\[
Q^* = U_A S U_B^\top
\]  \hspace{1cm} (4)

and hence (3) becomes an equality:

\[
\sum_{i=1}^{n} (\alpha_i - \beta_i)^2 = \| W_A - Q^* W_B Q^*^\top \|_2^2.
\]
Method Proposed by Umeyama in 1988

- Notice that (4) can be written as:

\[ U_A = Q^* U_B S \]

which is a relaxed version of the permutation matrix in the exact isomorphism case (permutation is replaced by an orthogonal matrix).

- For each sign matrix $S$ (remember that there are $2^n$ such matrices) there is an orthogonal matrix that satisfies Umeyama’s theorem, but not all these matrices can be easily relaxed to a permutation, and not all these permutations correspond to an isomorphism.
Umeyama’s Heuristic

- Take the absolute values of the eigenvector’s components:
  \[ \overline{U}_A(i, j) = |u_{ij}| \]

- It can be shown that the problem can be written as the following maximization problem:
  \[ \max_{Q} \text{tr}(\overline{U}_A \overline{U}_B^\top Q^\top) \]

This is not, however, such an easy problem to solve (See Umeyama’1988 for more details).

- It can be looked at as an assignment problem, namely extracting a permutation matrix \( P \) from the nonnegative matrix \( \overline{Q} = \overline{U}_A \overline{U}_B^\top \).
The method just described has serious limitations:

- It applies to graphs with the same number of nodes;
- It assumes that there are no eigenvalue multiplicities and that the eigenvalues can be reliably ordered;
- The heuristic proposed is weak and it does not necessarily lead to a simple algorithm;
- Other heuristics were proposed.
The Laplacian eigenvector associated with the smallest non-null eigenvalue is the direction of maximum variance of a graph (principal component).

The histogram of this eigenvector’s entries is invariant to vertex ordering.
Characterization of These Histograms

- If $\mathbf{L} \mathbf{u} = \lambda \mathbf{u}$ then: $\mathbf{P} \mathbf{L} \mathbf{P}^\top \mathbf{P} \mathbf{u} = \lambda \mathbf{P} \mathbf{u}$
- The vectors $\mathbf{u}$ and $\mathbf{P} \mathbf{u}$ have the same histograms;
- Remind that for each eigenvector $\mathbf{u}_i$ of $\mathbf{L}$ we have $-1 < u_{ik} < +1$, $\bar{u}_k = 0$, and $\sigma_k = 1/n$.
- The number of bins and the bin-width are invariant:
  
  $w_k = \frac{3.5\sigma_k}{n^{1/3}} = \frac{3.5}{n^{4/3}}$
  
  $b_k = \frac{\sup_i u_{ik} - \inf_i u_{ik}}{w_k} \approx \frac{n^{4/3}}{2}$

- The histogram is not invariant to the sign change, i.e., $H\{\mathbf{u}\} \neq H\{-\mathbf{u}\}$. 

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Shape Matching (1)

\[ t = 200, \quad t' = 201.5 \]

\[ t = 90, \quad t' = 1005 \]
Shape Matching (2)
Shape Matching (3)
Sparse Shape Matching

- Shape/graph matching is equivalent to matching the embedded representations [Mateus et al. 2008]
- Here we use the projection of the embeddings on a unit hyper-sphere of dimension $K$ and we apply rigid matching.
- How to select $t$ and $t'$, i.e., the scales associated with the two shapes to be matched?
- How to implement a robust matching method?
Let $C_X$ and $C_{X'}$ be the covariance matrices of two different embeddings $X$ and $X'$ with respectively $n$ and $n'$ points:

$$\det(C_X) = \det(C_{X'})$$

$det(C_X)$ measures the volume in which the embedding $X$ lies. Hence, we impose that the two embeddings are contained in the same volume.

From this constraint we derive:

$$t' \ tr(L') = t \ tr(L) + K \log n/n'$$
Robust Matching

- Build an association graph.
- Search for the largest set of mutually compatible nodes (maximal clique finding).
- See [Sharma and Horaud 2010] (Nordia workshop) for more details.