Machine Learning on Graphs
MDI343
Spectral Embedding

Thomas Bonald

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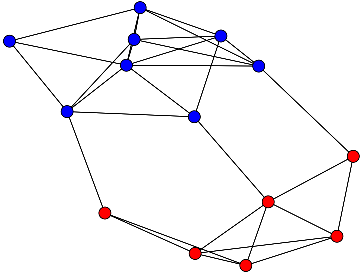
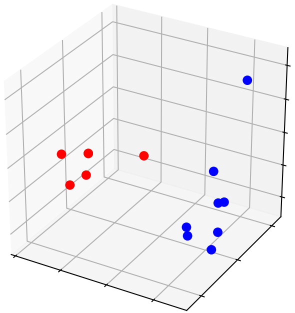
Motivation

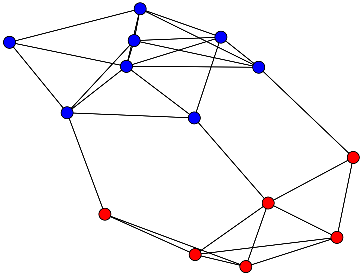
- Representation of a graph in a vector space
- Dimensionality reduction

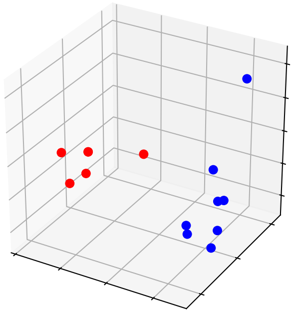




An optimization problem

$$\min_{X : X^T 1 = 0, X^T X = I} \sum_{i,j \in V} A_{ij} ||X_i - X_j||^2$$





Laplacian matrix

Definition

The **Laplacian** matrix is defined by

$$L = D - A$$

A **symmetric**, **positive semi-definite** matrix

Lemma

$$\mathrm{tr}(X^T L X) = \frac{1}{2} \sum_{i,j \in V} A_{ij} ||X_i - X_j||^2$$

Spectral decomposition

Theorem

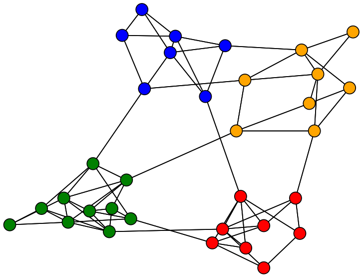
By the spectral theorem,

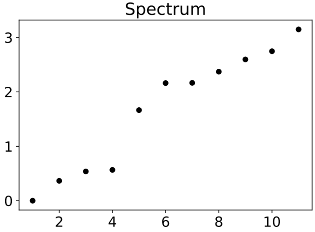
$$LV = V\Lambda$$

where

- $V^T V = I$
- $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 = 0 \leq \lambda_2 \leq \ldots \leq \lambda_n$

Example





First eigenvector

Proposition

$$L1 = 0$$

In particular,

- $V_1 \propto 1$
- $V_2^T 1 = \ldots = V_n^T 1 = 0$

Spectral embedding

Definition

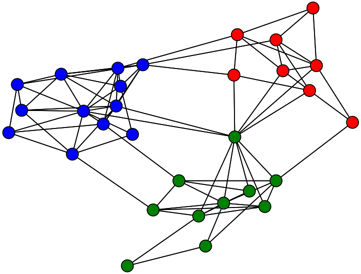
Spectral embedding X in dimension K given by the first K eigenvectors of the Laplacian (except the first)

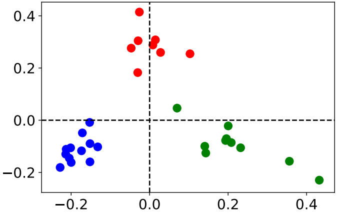
Theorem

The spectral embedding is optimal:

$$X = \arg \min_{X : X^T 1 = 0,\ X^T X = I_K} \mathrm{tr}(X^T L X)$$

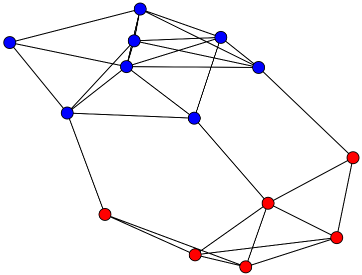
Example

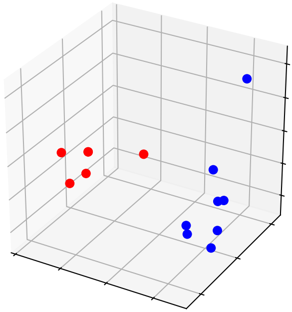




Back to the optimization problem

$$\min_{X : X^T \color{blue}{d} = 0, X^T \color{blue}{D} X = I} \sum_{i,j \in V} A_{ij} ||X_i - X_j||^2$$





Generalized eigenvalue problem

Theorem

We have:

$$LV = DV\Lambda$$

where

- $V^T DV = I$
- $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 = 0 \leq \lambda_2 \leq \ldots \leq \lambda_n$

Random walk

Definition

The **transition matrix** of the random walk is defined by:

$$P = D^{-1}A$$

This is a **stochastic** matrix

Proposition

$$PV = V(I - \Lambda)$$

where

- $V^T DV = I$
- $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 = 0 \le \lambda_2 \le \ldots \le \lambda_n$

Spectral embedding (random walk)

Definition

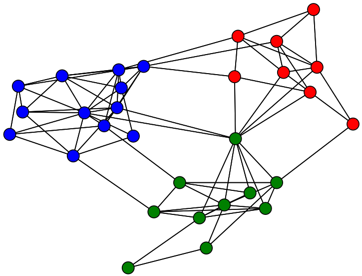
Spectral embedding X in dimension K given by the K leading eigenvectors of the **transition matrix** (except the first)

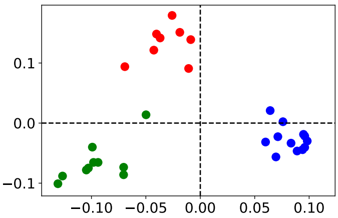
Theorem

The spectral embedding is optimal:

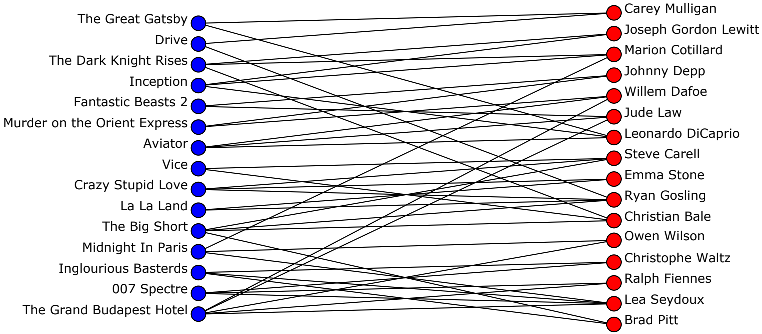
$$X = \arg \min_{X : X^T d = 0, X^T D X = I_K} \mathrm{tr}(X^T L X)$$

Example

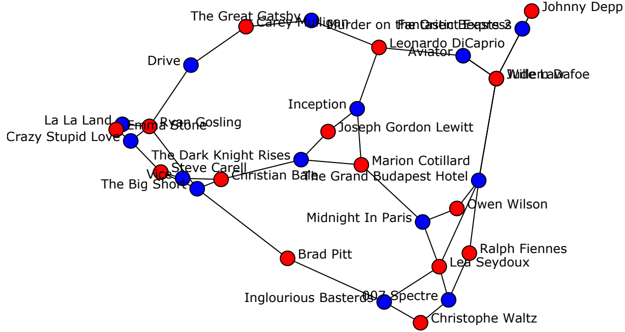




Extension to bipartite graphs



Co-embedding



Directed graphs as bipartite graphs