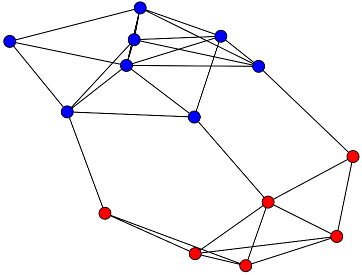
Graph Mining
SD212
7. Graph Embedding

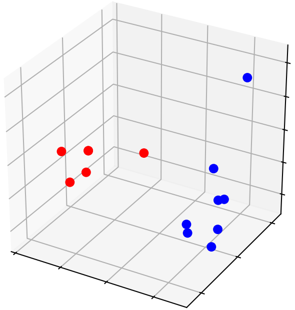
Thomas Bonald

2019 – 2020

Motivation

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

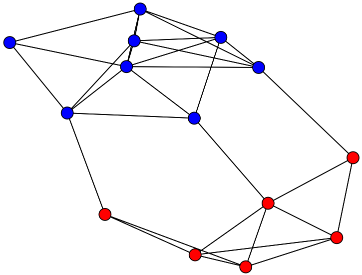
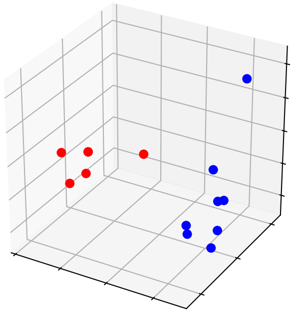




Outline

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

Lemma

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

Spectral decomposition

Proposition

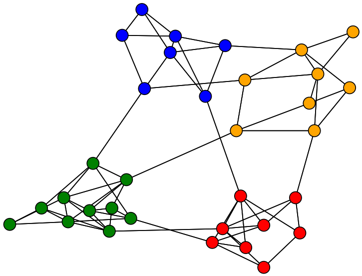
By the spectral theorem,

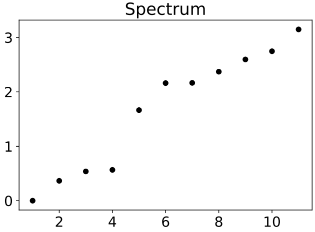
$$LV = V\Lambda$$

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





Spectral embedding

Definition

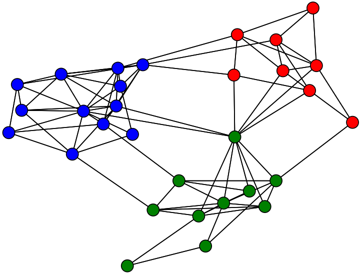
Embedding X given by the first K eigenvectors of the Laplacian (except the first)

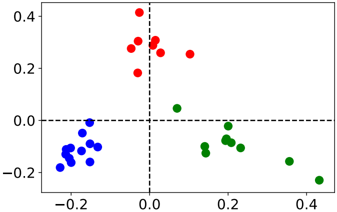
Theorem

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



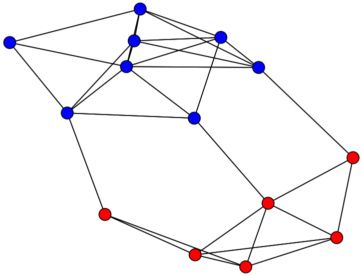


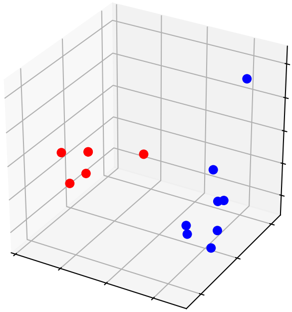
Outline

1. Spectral embedding
2. **Laplacian eigenmaps**
3. Extensions

Back to the optimization problem

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





Generalized eigenvalue problem

Proposition

$$LV = DV\Lambda$$

where

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

Transition matrix

Proposition

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

where

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

Laplacian eigenmap

Definition

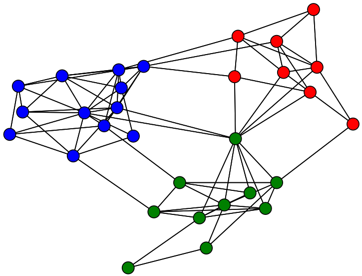
Embedding X given by the K leading eigenvectors of the **transition matrix** (except the first)

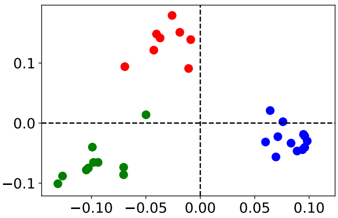
Theorem

The Laplacian eigenmap is optimal:

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

Example

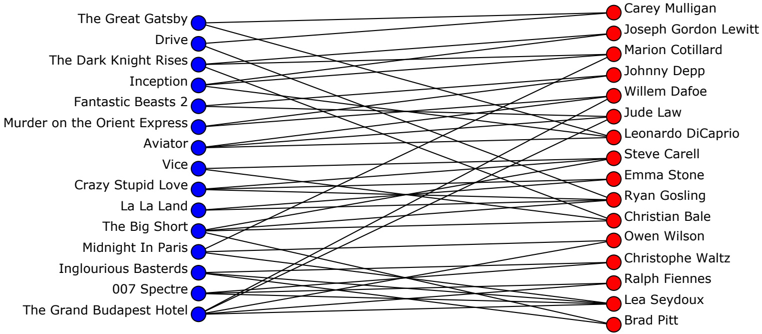




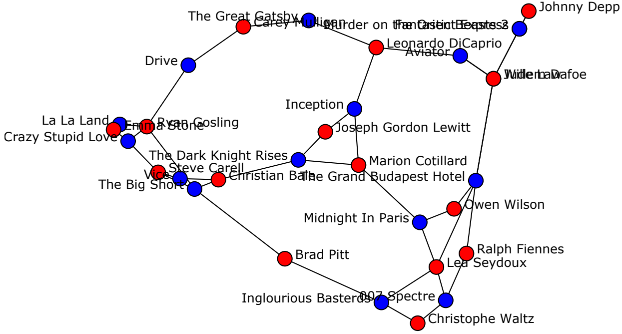
Outline

1. Spectral embedding
2. Laplacian eigenmaps
3. **Extensions**

Bipartite graphs



Co-embedding



Directed graphs as bipartite graphs