Linear Algebra II
Spectral Drawing and Spectral Clustering

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Graphs

Let $X = (V_X, E_X)$ be a finite undirected graph where $V_X = \{v_1, \cdots, v_n\}$ is the set of vertices and $E_X \subset V_X \times V_X$ is the set of directed edges, i.e. whenever $(v_i, v_j) \in E_X$, we also have $(v_j, v_i) \in E_X$.

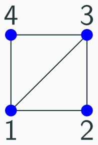
Two vertices v and w are in the same connected component if there exists a sequence of vertices $v_1 = v, v_2, \cdots, v_m = w$ such that $(v_i, v_{i+1}) \in E_X$ for all i.

Adjacency Matrices

Let $A_X = (A_{ij})$ be a matrix of size $n \times n$, such that

$$A_{ij} = \begin{cases} 1 & , \text{ if } (v_i, v_j) \in E_X; \\ 0 & , \text{ if } (v_i, v_j) \notin E_X. \end{cases}$$

The matrix A_X is called the adjacency matrix of X.

$X =$ 

$$A_X = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Since A_X is a real symmetric matrix, it admits a set of real eigenvalues, called the spectrum of the graph.

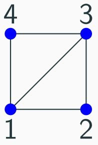
Laplacian Matrices

There is another useful matrix associated to a graph X

$$L_X = D_X - A_X$$

Here D_X is a diagonal matrix which (i,i)-th entry is the number of edges containing the vertex v_i, called the degree of v_i, denoted by $\deg(v_i)$.

The matrix L_X is called the Laplacian matrix of X.

$X =$ 

$$L_X = \begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}$$

We will see later that L is positive semi-definite.

Edge Energy Functions

A graph drawing of X is a map $\rho : V_X \to \mathbb{R}^k$. Especially, we interest in the case $k = 2$ or 3. The spectral drawing is a method of graph drawing which uses the spectrum of the Laplacian.

First, let us consider the regular drawing $\rho : V_X \to \mathbb{R}^n$ such that $\rho(v_i) = \vec{e}_i$, the i-th standard basis of $\mathbb{R}^n$. For a subspace W of $\mathbb{R}^n$, define the edge energy function as

$$\mathcal{E}(W) := \sum_{\substack{(v_i,v_j)\in E_X \\ i<j}} \|\mathrm{proj}_W(\vec{e}_i - \vec{e}_j)\|^2 = \sum_{t=1}^{k} \sum_{\substack{(v_i,v_j)\in E_X \\ i<j}} \|\mathrm{proj}_{\vec{w}_t}(\vec{e}_i - \vec{e}_j)\|^2.$$

Here $\{\vec{w}_1, \cdots, \vec{w}_k\}$ is an orthonormal basis of W. Note that the set $\rho(V_x)$ lies on the hyper plane $x_1 + \cdots + x_n = 1$. Therefore, we shall only consider the case $W \perp (1, \cdots, 1)^t$.

Spectral Drawing

For

$$W \in \operatorname*{arg\,min}_{\substack{W' : \dim W' = k \\ W' \perp (1, \cdots, 1)^t}} \{\mathcal{E}(W')\},$$

the map $(\mathrm{proj}_W \circ \rho) : V_X \mapsto W$ is called the k-dimensional spectral drawing of X.

Suppose $\dim W = 1$, let $\vec{x} = (x_1, \cdots, x_n)^t$ be the unit vector in W. Then

$$\mathrm{proj}_W(\vec{e_i}) = x_i \vec{x}$$

and

$$\mathcal{E}(W) = \sum_{(v_i,v_j)\in E_X, i<j} (x_i - x_j)^2 = \sum_i^n \deg(v_i) x_i^2 - \sum_{(v_i,v_j)\in E_X} x_i x_j = \vec{x}^t L_X \vec{x}.$$

Consider the following quadratic form

$$Q(\vec{x}) = \vec{x}^t L_X \vec{x}.$$

When $\dim W = k$, let $\vec{w}_1, \cdots, \vec{w}_k$ be an orthonormal basis of W, then

$$\mathcal{E}(W) = \sum_{i=1}^k Q(\vec{w}_i).$$

Positive Semi-Definiteness

Since

$$Q(\vec{x}) = \vec{x}^t L_X \vec{x} = \sum_{(v_i, v_j) \in E_X, i<j} (x_i - x_j)^2,$$

We have the following.

- The quadratic form $Q(\vec{x})$ is positive semi-definite.
- Suppose $Q(\vec{x}) = 0$. If v_i and v_j lie in the same connected component of X, then $x_i = x_j$.
- If $x_i = x_j$, whenever v_i and v_j lie in the same connected component of X, then $Q(\vec{x}) = 0$.
- The dimension of the kernel of L_X is equal to the number of connected components of X.

Let $\alpha = \{\vec{v}_1, \cdots, \vec{v}_k\}$ be an orthonormal basis of the zero eigenspace W of L. Write $\vec{v}_i^t = (v_{i1} \cdots v_{in})$. Then

$$\mathrm{proj}_{\vec{v}_i}(\vec{e}_j) = v_{ij} \quad \text{and} \quad \mathrm{Rep}_\alpha(\mathrm{proj}_W(\vec{e}_j))^t = (v_{1j} \cdots v_{kj}).$$

Theorem

Two vertices v_i and v_j are in the same connected component if and only if $\mathrm{proj}_W(\vec{e}_i) = \mathrm{proj}_W(\vec{e}_j)$

In other words, under the projection onto the zero eigenspace, every connected component maps to a single point and distinct connected components map to distinct points.

Similarity Graphs

Clustering is the process of making a group of abstract objects into classes of similar objects. In data analysis, one can regard each data in a data set X as a vertex of the similarity graph. Th graph is characterized by the similarity adjacency matrix $A = (A_{ij})$ such that

- $A_{ij} = K(\vec{v}_i, \vec{v}_j)$ is the similarity between the i-th vertex $\vec{v}_i$ and the j-th vertex $\vec{v}_j$, which is a number between 0 and 1. Here K is the similarity function.
- A_{ij} is closed to one if the i-th vertex and j-th vertex are similar.

Let D be the degree matrix which (i, i)-th entry is equal to $\sum_j A_{ij}$ and $L = D - A$ be the Laplacian of the similarity graph. Using the projection onto the eigenspace of small eigenvalues of the Laplacian to find the clusters is called the method of spectral clustering.

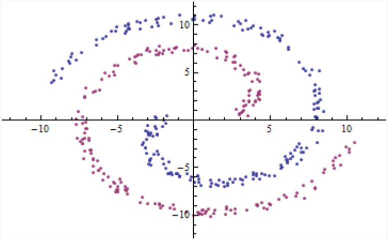
Example of Similarity Functions

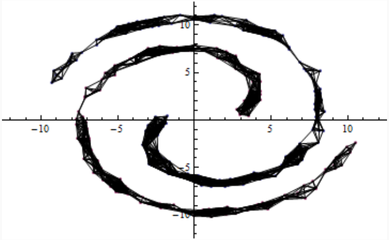
Example

The following are some well-used similarity function.

- Fix a $\sigma > 0$ and set $K(\vec{v}_i, \vec{v}_j) = \exp(-\|v_i - \vec{v}_j\|^2/\sigma^2)$.
- Fix a positive integer k. Let $K(\vec{v}_i, \vec{v}_j) = 1$ if $\vec{v}_i$ and v_j are both one of the k nearest points of each other in X. Let $K(\vec{v}_i, \vec{v}_j) = 0$, otherwise.
- Fix $\epsilon > 0$. Let $K(\vec{v}_i, \vec{v}_j) = 1$ if $\|\vec{v}_i - \vec{v}_j\| < \epsilon$ and $K(\vec{v}_i, \vec{v}_j) = 0$, otherwise.

Example

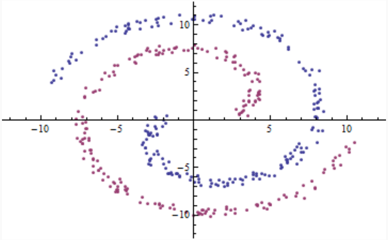


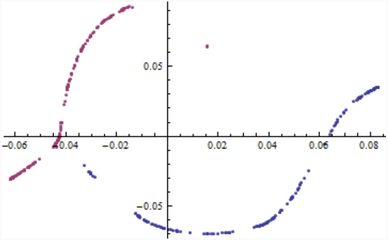


A data set in $\mathbb{R}^2$

Its ϵ-similarity graphs

Example





A data set in $\mathbb{R}^2$

Spectral projection using $K(\vec{v}_i, \vec{v}_j) = \exp(-\| v_i - \vec{v}_j \|^2)$.

Usual Graphs v.s. Similarity Graphs

	Usual Graphs	Similarity Graphs
Matrix	Adjacency Matrix	Similarity Matrix
Eigenvalues for the Proj.	Zero Eigenvalues	Small Eigenvalues
Proj. of a Conn. Comp.	A Point	A Cluster

Suppose X is a connected graph. Then the zero eigenspace of L_X is spanned by $(1, \cdots, 1)^t$. Let $\vec{w}_1, \cdots, \vec{w}_k$ be an orthonormal basis of W, then we have

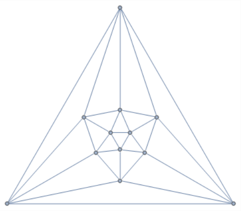
$$E(W) = \sum_{i=1}^{k} Q(\vec{w}_i) = \sum_{i=1}^{k} \vec{w}_i^t L \vec{w}_i.$$

By the previous homework, $E(W)$ is minimal if $\vec{w}_i$ is the eigenvector corresponding to the i-th smallest eigenvalue. Since we also request that $W \perp (1, \cdots, 1)^t$, we conclude that $E(W)$ is minimal if W is $\vec{w}_i$ is the eigenvector corresponding to the i-th smallest nonzero eigenvalue.

Example

Let A be the adjacency matrix of the Icosahedral graph.

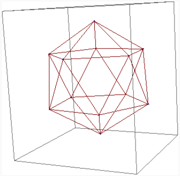
$$A = \begin{pmatrix} 0&0&1&0&1&1&0&0&1&1&0&0 \\ 0&0&0&1&0&0&1&1&0&0&1&1 \\ 1&0&0&0&0&0&1&1&1&1&0&0 \\ 0&1&0&0&1&1&0&0&0&0&1&1 \\ 1&0&0&1&0&1&0&0&1&0&1&0 \\ 1&0&0&1&1&0&0&0&0&1&0&1 \\ 0&1&1&0&0&0&0&1&1&0&1&0 \\ 0&1&1&0&0&0&1&0&0&1&0&1 \\ 1&0&1&0&1&0&1&0&0&0&1&0 \\ 1&0&1&0&0&1&0&1&0&0&0&1 \\ 0&1&0&1&1&0&1&0&1&0&0&0 \\ 0&1&0&1&0&1&0&1&0&1&0&0 \end{pmatrix}$$



The spectrum of its Laplacian is given by

$$0, \color{red}{2.76393}, \color{red}{2.76393}, \color{red}{2.76393}, 6, 6, 6, 6, 6, 7.23607, 7.23607, 7.23607$$

One can get the following spectral drawing on $\mathbb{R}^3$ using the eigenvectors corresponding to the smallest three nonzero eigenvalues of L.

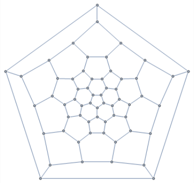


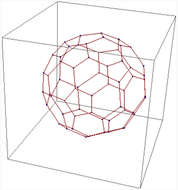
Example

Let X be the graph of truncated Icosahedron. The spectrum of its Laplacian is given by

$$0, 0.243402, 0.243402, 0.243402, 0.697224, 0.697224, \cdots$$

One can get the following spectral drawing on $\mathbb{R}^3$ using the eigenvectors corresponding to the smallest three nonzero eigenvalues of L.





Remark: The adjacency matrix of this graph can compute from the Cayley graph expression. More precisely, the adjacency matrix can be computed only using two permutations (12345) and (12)(34).