

Diffusion Maps and Spectral Clustering

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1 Spectral Clustering

1.1 Graph Laplacians

Spectral clustering is a clustering algorithm which is far more expressive than k -means, and is not limited to convex clusters.

Definition 1.1 (Undirected weighted graph). *A weighted graph is an undirected graph $G = (V, E)$ where $V = \{v_1, \dots, v_n\}$ and each two vertices v_i, v_j are connected with an edge with non-negative weight $w_{ij} \geq 0$. We denote the weight matrix as W .*

Remark 1.2. *When data lies in Euclidean space and the weights are not given, it is a common practice to use Gaussian kernel to compute the weights*

$$w_{ij} = \frac{\exp(-\|x_i - x_j\|^2)}{2\sigma^2},$$

for such bandwidth parameter σ .

Remark 1.3. *A common practice is to connect each point only to its k nearest neighbors, which is known as k nn graph. The graph can be easily made symmetric, for example by using $W \leftarrow \frac{1}{2}(W + W^T)$.*

Definition 1.4 (Degree and Degree matrix). *The degree d_i of a vertex v_i and the graph degree matrix D are defined as*

- d_i is the sum of weights on the edges of v_i , i.e., $d_i = \sum_j w_{ij}$.
- D is a diagonal matrix with elements $D_{ii} = d_i$.

Definition 1.5 (Unnormalized graph Laplacian). *The unnormalized graph Laplacian is defined as $L_{un} = D - W$.*

Observe that L_{un} is symmetric.

Proposition 1.6. *For every vector $f \in \mathbb{R}^n$, $f^T L_{un} f = \frac{1}{2} \sum_{i,j} w_{ij} (f_i - f_j)^2$.*

Proof. Exercise. □

It follows that L_{un} is positive semi-definite

Proposition 1.7. *The smallest eigenvalue of L_{un} is 0, and its corresponding eigenvector is the constant vector $\frac{1}{\sqrt{n}}\mathbf{1}$.*

Proof. Let $f = \frac{1}{\sqrt{n}} \mathbf{1}$. Then by proposition 1.6

$$f^T L_{\text{un}} f = 0,$$

hence $f, 0$ are an eigenpair. \square

Proposition 1.8. *The multiplicity of the zero eigenvalue equals the number k of connected components of G , and the corresponding eigenvectors are indicator vectors of the components.*

Proof. We know that 0 is an eigenvalue. Let f be a corresponding eigenvector. Then since $f^T L_{\text{un}} f = 0$, we have that $f_i = f_j$ whenever $w_{ij} > 0$. For $k > 1$ connected components, L_{un} is block diagonal, so its spectrum is the union of the spectra of all blocks. \square

Definition 1.9 (Normalized graph Laplacian). *We define two versions of normalized Laplacians:*

- *The random walk graph Laplacian is $L_{\text{rw}} = D^{-1} L_{\text{un}} = I - D^{-1} W$.*
- *The Symmetric graph Laplacian is $L_{\text{sym}} = D^{-\frac{1}{2}} L_{\text{un}} D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$.*

Remark 1.10. *Observe that L_{rw} and L_{sym} are similar matrices, and hence share the same spectrum. In particular, all eigenvalues of L_{rw} are real.*

Proposition 1.11. *L_{sym} is positive semi-definite (and hence also L_{rw})*

Proof. Exercise. \square

Proposition 1.12. *0 is an eigenvalue of L_{rw} (and hence also of L_{sym}), associated with the constant eigenvector.*

Proof. Exercise. \square

Proposition 1.13. *The multiplicity of the zero eigenvalue in L_{rw} and L_{sym} equals the number k of connected components of G , and the corresponding eigenvectors are indicator vectors of the components.*

Proof. Analogous to the proof of proposition 1.8. \square

1.2 Spectral Clustering

We have seen that eigenvectors corresponding to the zero eigenvalues (to whom we refer from now the first eigenvectors) of the Laplacian indicate the connected components. It therefore makes sense to use these eigenvectors to represent the data and identify the cluster structure.

Spectral clustering works by representing the data using the first k eigenvectors, and running k -means on this representation. Unlike k -means it can handle non-convex data (see Figure 1. Spectral clustering can interestingly be motivated by a graph cut point of view (see section 5 in Von Luxburg's excellent tutorial).

Remark 1.14. *Since the first eigenvector is constant in L_{un} and L_{rw} , it is often omitted.*

Further Reading

A excellent spectral clustering tutorial is <https://link.springer.com/content/pdf/10.1007/s11222-007-9033-z.pdf>.



Figure 1: Spectral clustering (top) versus k -means on non-convex clusters.

2 Diffusion Maps

Diffusion map is a dimensionality reduction technique, that captures geometrical properties of data. In order to do so, it utilizes weighted graphs, which encode local similarity between pairs of points. This local interaction then allows to obtain global representations of the entire data.

Observe that $P := D^{-1}W$ is a Markov matrix, and hence encodes transition probabilities between the vertices. P is a diffusion (averaging) operator, and defines directions of propagation. powers of P corresponds to multi-step walks.

Proposition 2.1. P has stationary distribution π , with $\pi_i = \frac{d_i}{\sum_j d_j}$, i.e., $\pi^T P = \pi^T$.

Proof. Exercise. □

Corollary 2.2. a stationary distribution π is a left eigenvector of P , with eigenvalue 1. Since left and right eigenvalues are the same, P has a 1 eigenvalue.

Corollary 2.3. Let u be an arbitrary vector of length n . Each entry of Pu is a convex combination of the entries of u , and hence cannot be larger than the maximal one. Therefore any eigenvalue of P can be at most 1.

Let $1 = \lambda_0 \geq |\lambda_1| \geq |\lambda_2| \geq \dots$ and ψ_0, ψ_1, \dots be the eigenvalues and eigenvectors of P (exercise: why $\lambda_0 = 1$?)

Definition 2.4 (Diffusion distance). The diffusion distance at time t between vertices v_i and v_j is defined as:

$$D_t(v_i, v_j) = \|P_i^t - P_j^t\|_{\ell^2/d}^2 = \sum_{k=1}^n (P_{ik}^t - P_{jk}^t)^2 / d_k,$$

where P_i^t is the i 'th row of P^t .

Remark 2.5. The notation $\|x\|_{\ell^2/d}^2$ means that the length is $\sqrt{\sum_i x_i^2 / d_i}$.

Intuitively, if v_i and v_j are connected by a large number of paths, their diffusion probabilities will be similar, and hence their diffusion distance will be small.

The following theorem shows that the diffusion distance squared is in fact the Euclidean distance in the eigenspace of P

Theorem 2.6.

$$D_t(v_i, v_j) = \left(\sum_{l=1}^n \lambda_l^{2t} (\psi_{l,i} - \psi_{l,j})^2 \right)^{\frac{1}{2}},$$

where ψ_1, \dots, ψ_n are the eigenvectors of P .

Proposition 2.7. Let $P = D^{-1}W$ and $A = D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$. Let (λ, ϕ) be an eigenpair of A . Then $(\lambda, D^{-\frac{1}{2}}\phi)$ are an eigenpair of P .

Proof. Exercise. □

Proof. Consider $A = D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$. We already know that P has real eigenvalues (since P is similar to A , and A is symmetric). Let $A = \sum \lambda_l \phi_l \phi_l^T$. Then

$$\begin{aligned} P &= D^{-\frac{1}{2}}AD^{\frac{1}{2}} \\ &= \sum_l \lambda_l D^{-\frac{1}{2}}\phi_l \phi_l^T D^{\frac{1}{2}} \end{aligned} \tag{1}$$

The vectors $D^{\frac{1}{2}}\phi_l$, $l = 1, \dots, n$ are orthogonal in $\|\cdot\|_{\ell^2/d}$. This means that we can view the i 'th row of P as an expansion in that basis with coefficients $\lambda_l D^{-\frac{1}{2}}\phi_l := \lambda_l \psi_{li}$. Consequently,

$$\|P_i - P_j\|_{\ell^2/d}^2 = \sum_l \lambda^2 (\psi_{li} - \psi_{lj})^2.$$

Analogously, for P^t we have

$$\|P_i^t - P_j^t\|_{\ell^2/d}^2 = \sum_l \lambda^{2t} (\psi_{li} - \psi_{lj})^2.$$

□

2.1 Representation

The above suggests that we can represent a node v_i using a feature vector

$$\Psi_t(v_i) = (\lambda_1^t \psi_{1,i}^t, \dots, \lambda_L^t \psi_{L,i}^t)^T,$$

for some $L \leq n$.

Recall that by proposition 1.11, L_{sym} is positive semi-definite. The entire spectrum of L_{rw} lies between 0 and 2, and consequently, the spectrum of $P = I - L_{\text{rw}}$ lies between -1 and 1. Since the spectrum decays, for each t only a few eigenvalues λ^t have a significant effect on the diffusion distances, which means that we can use dimensionality L such that λ_L^t is sufficiently small, and achieve dimensionality reduction.