

Lecture 15

This is essentially [10, Lecture 2] with small modifications.

8.3.2 Weighted graphs and the graph Laplacian

A weighted graph $G = (V, E, w)$ is a graph $G = (V, E)$ along with a function $w : E \rightarrow \mathbb{R}^+$ (where $\mathbb{R}^+ = (0, \infty)$). The adjacency matrix of a weighted graph, rather than putting ones for the edges, instead puts the weight:

$$(A_G)_{ij} = \begin{cases} w(i, j) & \text{if } (i, j) \in E, \\ 0 & \text{otherwise} \end{cases}$$

The degree matrix is defined the same as before, but $(D_G)_{ii}$ is now the sum of the weights of the weighted edges connected to vertex i :

$$(D_G)_{ii} = \sum_{j=1}^n (A_G)_{ij} = \sum_{j=1}^n w(i, j).$$

Finally, as before, the graph Laplacian is given by:

$$L_G = D_G - A_G. \tag{46}$$

Let us now give a more convenient formulation of the graph Laplacian. Let $G_{1,2}$ be the graph on two vertices $V = \{1, 2\}$ with one edge $(1, 2)$ and $w(1, 2) = 1$ (if in the future we forget to specify the weights, assume they are all one as in an unweighted graph). By definition we have:

$$L_{G_{1,2}} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Note that for a vector $v \in \mathbb{R}^2$,

$$v^T L_{G_{1,2}} v = (v[1] - v[2])^2.$$

Now let $G = (V, E)$ be a graph on n vertices, and suppose $(i, j) \in E$. Define the subgraph $G_{i,j}$ of G as $G_{i,j} = (V, (i, j))$, i.e., it has the same n vertices, but only the edge (i, j) . The graph Laplacian $L_{G_{i,j}}$ is the $n \times n$ matrix whose only non-zero entries are in the intersections of rows and

columns i and j . As an example, consider the graph G on 5 vertices with $(2,5) \in E$. Then:

$$L_{G_{2,5}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix}.$$

Clearly in this example, and generally, the 2×2 matrix at the intersection of rows and columns i and j is

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

For a general weighted graph $G = (V, E, w)$, we now claim that (check this!):

$$L_G = \sum_{(i,j) \in E} w(i,j) L_{G_{i,j}}. \quad (47)$$

Many elementary properties of the graph Laplacian follow from (47). In particular, for $v \in \mathbb{R}^n$, it is immediate that:

$$v^T L_G v = \sum_{(i,j) \in E} w(i,j) (v[i] - v[j])^2.$$

Thus $v^T L_G v \geq 0$ for any $v \in \mathbb{R}^n$, from which it follows that L_G is a positive semidefinite matrix. In particular, all eigenvalues of L_G are nonnegative.

8.3.3 Connectivity

From the definition $L_G = D_G - A_G$, it is immediate that $L_G \mathbf{1} = 0$ and so any constant vector is an eigenvector of L_G with eigenvalue 0.

Proposition 2. *Let $G = (V, E)$ be a graph, and let $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ be the eigenvalues of L_G . Then:*

$$\lambda_2 > 0 \iff G \text{ is connected.}$$

Proof. We first prove that $\lambda_2 > 0 \implies G$ is connected. This statement is equivalent to its contrapositive, which is: G is disconnected $\implies \lambda_2 = 0$. We prove the latter. If G is disconnected, then it can be described as the

union of two graphs G_1 and G_2 . Without loss of generality, we can relabel the vertices such that:

$$L_G = \begin{pmatrix} L_{G_1} & \mathbf{0} \\ \mathbf{0} & L_{G_2} \end{pmatrix}.$$

Thus L_G has two orthogonal eigenvectors both with eigenvalue zero:

$$\varphi_1 = \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \end{pmatrix} \quad \text{and} \quad \varphi_2 = \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix},$$

and so $\lambda_1 = \lambda_2 = 0$.

Now we prove: G is connected $\implies \lambda_2 > 0$. Let φ be an eigenvector of L_G with eigenvalue 0. Since $L_G \varphi = 0$, we have:

$$\varphi^T L_G \varphi = \sum_{(i,j) \in E} (\varphi[i] - \varphi[j])^2 = 0. \quad (48)$$

We prove by induction that $\varphi[i] = \varphi[j]$ for all $i, j \in V$, and hence that φ must be a constant vector (which implies that the dimension of the eigenspace of eigenvalue 0 is one, and so $\lambda_2 > 0$). The inductive argument will be over the length m of the minimum length path connecting i and j . Suppose that $m = 1$. Then $(i, j) \in E$, and by (48) we have $\varphi[i] = \varphi[j]$. Now suppose that $\varphi[k] = \varphi[\ell]$ for all $k, \ell \in V$ that are connected by a path of length $m \leq m_0 - 1$ for $m_0 \leq 2$. Now let $i, j \in V$ be connected by a path of length m_0 , say $i = u_1, u_2, \dots, u_{m_0}, u_{m_0+1} = j$. Then $\varphi(u_1) = \varphi(u_2)$ since $(u_1, u_2) \in E$, and $\varphi(u_2) = \varphi(u_{m_0+1})$ since u_2 and u_{m_0+1} are connected by a path of length $m_0 - 1$. But then $\varphi[i] = \varphi(u_1) = \varphi(u_2) = \varphi(u_{m_0+1}) = \varphi[j]$. \square

Corollary 1. Let $G = (V, E, w)$ be a weighted graph, and let $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ be the eigenvalues of L_G . Then:

$$\lambda_2 > 0 \iff G \text{ is connected.}$$

Corollary 2. Let $G = (V, E, w)$ be a weighted graph, and let $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ be the eigenvalues of L_G . Then:

$$\lambda_1 = \lambda_2 = \dots = \lambda_m = 0 \iff G \text{ has } m \text{ connected components.}$$

References

- [1] Bernhard Schölkopf and Alexander J. Smola. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. Adaptive Computation and Machine Learning. The MIT Press, 2002.
- [2] Afonso S. Bandeira. Ten lectures and forty-two open problems in the mathematics of data science. MIT course *Topics in Mathematics of Data Science*, 2015.
- [3] Jon Shlens. A tutorial on principal component analysis. arXiv:1404.1100, 2014.
- [4] Karl Pearson. On lines and planes of closest fit to systems of points in space. *Philosophical Magazine, Series 6*, 2(11):559–572, 1901.
- [5] V. A. Marchenko and L. A. Pastur. Distribution of eigenvalues in certain sets of random matrices. *Mat. Sb. (N.S.)*, 72(114):507–536, 1967.
- [6] J. Baik, G. Ben-Arous, and S. Péché. Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *The Annals of Probability*, 33(5):1643–1697, 2005.
- [7] Debashis Paul. Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica*, pages 1617–1642, 2007.
- [8] Trevor Hastie, Robert Tibshirani, and Jerome Friedman. *The Elements of Statistical Learning*. Springer-Verlag New York, 2nd edition, 2009.
- [9] Athanasios Tsanas and Angeliki Xifara. Accurate quantitative estimation of energy performance of residential buildings using statistical machine learning tools. *Energy and Buildings*, 49:560–567, 2012.
- [10] Daniel A. Spielman. Spectral graph theory. *Yale Course Notes*, Fall, 2009.