Advanced Graph Algorithms and Optimization	Spring 2020

Introduction to Spectral Graph Theory

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The incidence matrix, the Laplacian matrix, and the adjacency matrix. In Lecture 1, we looked at undirected graphs and we introduce the incidence matrix and the Laplacian of the graph. Let us recall these.

We consider an undirected weighted graph $G = (V, E, \boldsymbol{w})$, with $n = |V|$ vertices and $m = |E|$ edges, where $\boldsymbol{w} \in \mathbb{R}_{+}^{E}$ assigns positive weight for every edge. Let's assume G is connected.

To introduce the *edge-vertex incidence matrix* of the graph, we first have to associate an arbitrary direction to every edge. We then let $\boldsymbol{B} \in \mathbb{R}^{V \times E}$.

$$\boldsymbol{B}(v, e) = \begin{cases} 1 & \text{if } e = (u, v) \\ -1 & \text{if } e = (v, u) \\ 0 & \text{o.w.} \end{cases}$$

The edge directions are only there to help us track the meaning of signs of quantities defined on edges: The math we do should not depend on the choice of sign.

Let $\boldsymbol{W} \in \mathbb{R}^{E \times E}$ be the diagonal matrix given by $\boldsymbol{W} = \operatorname{diag}(\boldsymbol{w})$, i.e $\boldsymbol{W}(e, e) = \boldsymbol{w}(e)$. We define the Laplacian of the graph as $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{W}\boldsymbol{B}^{\top}$. Note that in the first lecture, we define the Laplacian as $\boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^{\top}$, where $\boldsymbol{R}$ is the diagonal matrix with edge resistances on the diagonal. We want to think of high *weight* on an edge as expressing that two vertices are highly connected, whereas we think of high resistance on an edge as expressing that the two vertices are poorly connected, so we let $\boldsymbol{w}(e) = 1/\boldsymbol{R}(e, e)$.

The weighted adjacency matrix $\boldsymbol{A} \in \mathbb{R}^{V \times V}$ of a graph is given by

$$\boldsymbol{A}(u, v) = \begin{cases} \boldsymbol{w}(u, v) & \text{if } \{u, v\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

Note that we treat the edges as undirected here, so $\boldsymbol{A}^{\top} = \boldsymbol{A}$. The weighted degree of a vertex is defined as $\boldsymbol{d}(v) = \sum_{\{u,v\} \in E} w(u, v)$. Again we treat the edges as undirected. Let $\boldsymbol{D} = \operatorname{diag}(\boldsymbol{d})$ be the diagonal matrix in $\mathbb{R}^{V \times V}$ with weighted degrees on the diagonal.

In Problem Set 1, you showed that $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$, and that for $\boldsymbol{x} \in \mathbb{R}^{V}$,

$$\boldsymbol{x}^{\top}\boldsymbol{L}\boldsymbol{x} = \sum_{\{a,b\} \in E} \boldsymbol{w}(a, b)(\boldsymbol{x}(a) - \boldsymbol{x}(b))^2.$$

Now we can express the net flow constraint that $\boldsymbol{f}$ routes $\boldsymbol{d}$ by

$$\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}.$$

This is also called a conservation constraint. In our examples so far, we have $\boldsymbol{d}(s) = -1$, $\boldsymbol{d}(t) = 1$ and $\boldsymbol{d}(u) = 0$ for all $u \in V \setminus \{s, t\}$.

If we let $\boldsymbol{R} = \operatorname{diag}_{e \in E} \boldsymbol{r}(e)$ then Ohm's law tells us that $\boldsymbol{f} = \boldsymbol{R}^{-1}\boldsymbol{B}^{\top}\boldsymbol{x}$.

The Courant-Fisher Theorem. Let us also recall the Courant-Fischer theorem that proved in Lecture 2.

Theorem 0.1 (The Courant-Fischer Theorem)**.** *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n\times n}$, with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. Then*

1.
$$\lambda_i = \min_{\substack{\text{subspace } W\subseteq\mathbb{R}^n \\ \dim(W)=i}} \max_{\boldsymbol{x}\in W, \boldsymbol{x}\neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

2.
$$\lambda_i = \max_{\substack{\text{subspace } W\subseteq\mathbb{R}^n \\ \dim(W)=n+1-i}} \min_{\boldsymbol{x}\in W, \boldsymbol{x}\neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

In fact, from our proof of the Courant-Fischer theorem in Lecture 2, we can also extract a slightly different statement:

Theorem 0.2 (The Courant-Fischer Theorem, eigenbasis version)**.** *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n\times n}$, with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, and corresponding eigenvectors $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ which form an othernormal basis. Then*

1.
$$\lambda_i = \min_{\substack{\boldsymbol{x}\perp\boldsymbol{x}_1,\ldots\boldsymbol{x}_{i-1} \\ \boldsymbol{x}\neq\boldsymbol{0}}} \frac{\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

2.
$$\lambda_i = \max_{\substack{\boldsymbol{x}\perp\boldsymbol{x}_{i+1},\ldots\boldsymbol{x}_{n} \\ \boldsymbol{x}\neq\boldsymbol{0}}} \frac{\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

Of course, we also have $\lambda_i(\boldsymbol{A}) = \frac{\boldsymbol{x}_i^\top \boldsymbol{A}\boldsymbol{x}_i}{\boldsymbol{x}_i^\top \boldsymbol{x}_i}$.

1 Understanding Eigenvalues of the Laplacian

We would like to understand the eigenvalues of the the Laplacian.

Let us start by considering the n vertex complete graph with unit weights, which we denote by K_n. The adjacency matrix of K_n is $\boldsymbol{A} = \boldsymbol{1}\boldsymbol{1}^\top - \boldsymbol{I}$, since it has ones everywhere, except for the diagonal, where entries are zero. The degree matrix $\boldsymbol{D} = (n-1)\boldsymbol{I}$. Thus the Laplacian is $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A} = n\boldsymbol{I} - \boldsymbol{1}\boldsymbol{1}^\top$.

Thus for any $\boldsymbol{y} \perp \boldsymbol{1}$, we have $\boldsymbol{y}^\top \boldsymbol{L}\boldsymbol{y} = n\boldsymbol{y}^\top\boldsymbol{y} - (\boldsymbol{1}^\top\boldsymbol{y})^2 = n\boldsymbol{y}^\top\boldsymbol{y}$.

From this, we can conclude that any $\boldsymbol{y} \perp \boldsymbol{1}$ is an eigenvector of eigenvalue n, and that all $\lambda_2 = \lambda_3 = \ldots = \lambda_n = n$.

Next, let us try to understand λ_2 and λ_n for P_n, the n vertex path graph with unit weight edges. I.e. the graph has edges $E = \{\{i, i+1\} \text{ for } i = 1 \text{ to } (n-1)\}$.

This is in a sense the least well-connected unit weight graph on n vertices, whereas K_n is the most well-connected.

1.1 Test Vector Bounds on λ_2 and λ_n

We can use the eigenbasis version of the Courant-Fisher theorem to observe that the second-smallest eigenvalue of the Laplacian is given by

$$\lambda_2(\boldsymbol{L}) = \min_{\substack{\boldsymbol{x} \neq \boldsymbol{0} \\ \boldsymbol{x}^\top \boldsymbol{1} = 0}} \frac{\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}. \tag{1}$$

We can get a better understand this particular case through a couple of simple observations. Suppose $\boldsymbol{x} = \boldsymbol{y} + \alpha \boldsymbol{1}$, where $\boldsymbol{y} \perp \boldsymbol{1}$. Then $\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x} = \boldsymbol{y}^\top \boldsymbol{L} \boldsymbol{y}$, and $\|\boldsymbol{x}\|_2^2 = \|\boldsymbol{y}\|^2 + \alpha^2 \|\boldsymbol{1}\|^2$. So for any given vector, you can increase the value of $\frac{\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$, by instead replacing $\boldsymbol{x}$ with the component orthogonal to $\boldsymbol{x}$, which we denoted by $\boldsymbol{y}$.

We can conclude from Equation (2) that for *any* vector $\boldsymbol{y} \perp \boldsymbol{1}$,

$$\lambda_2 \leq \frac{\boldsymbol{y}^\top \boldsymbol{L} \boldsymbol{y}}{\boldsymbol{y}^\top \boldsymbol{y}}$$

When we use a vector $\boldsymbol{y}$ in this way to prove a bound on an eigenvalue, we call it a *test vector*.

Now, we'll use a test vector to give an upper bound on $\lambda_2(\boldsymbol{L}_{P_n})$. Let $\boldsymbol{x} \in \mathbb{R}^V$ be given by $\boldsymbol{x}(i) = (n+1) - 2i$, for $i \in [n]$. This vector satisfies $\boldsymbol{x} \perp \boldsymbol{1}$. We picked this because we wanted a sequence of values growing linearly along the path, while also making sure that the vector is orthogonal to $\boldsymbol{1}$. Now

$$\begin{aligned}
\lambda_2(\boldsymbol{L}_{P_n}) &\leq \frac{\sum_{i \in [n-1]} (\boldsymbol{x}(i) - \boldsymbol{x}(i+1))^2}{\sum_{i=1}^n \boldsymbol{x}(i)^2} \\
&= \frac{\sum_{i=1}^{n-1} 2^2}{\sum_{i=1}^n (n+1-2i)^2} \\
&= \frac{4(n-1)}{(n+1)n(n-1)/3} \\
&= \frac{12}{n(n+1)} \leq \frac{12}{n^2}.
\end{aligned}$$

Later, we will prove a lower bound that shows this value is right up to a constant factor. But the test vector approach based on the Courant-Fischer theorem doesn't immediately work when we want to prove lower bounds on $\lambda_2(\boldsymbol{L})$.

We can see from either version of the Courant-Fischer theorem that

$$\lambda_n(\boldsymbol{L}) = \max_{\boldsymbol{v} \neq \boldsymbol{0}} \frac{\boldsymbol{v}^\top \boldsymbol{L} \boldsymbol{v}}{\boldsymbol{v}^\top \boldsymbol{v}}. \tag{2}$$

Thus for *any* vector $\boldsymbol{y} \neq 0$,

$$\lambda_n \geq \frac{\boldsymbol{y}^\top \boldsymbol{L} \boldsymbol{y}}{\boldsymbol{y}^\top \boldsymbol{y}}.$$

This means get a test vector-based lower bound on λ_n. Let us apply this to the Laplacian of P_n. We'll try the vector $\boldsymbol{x} \in \mathbb{R}^V$ be given by $\boldsymbol{x}(1) = -1$, and $\boldsymbol{x}(n) = 1$ and $\boldsymbol{x}(i) = 0$ for $i \neq 0, 1$.

Here we get

$$\lambda_n(\boldsymbol{L}_{P_n}) \geq \frac{\boldsymbol{y}^\top \boldsymbol{L} \boldsymbol{y}}{\boldsymbol{y}^\top \boldsymbol{y}} = \frac{2}{2} = 1.$$

Again, it's not clear how to use the Courant-Fischer theorem to prove an upper bound on $\lambda_n(\boldsymbol{L})$. But, later we'll see how to prove an upper that shows that for P_n, the lower bound we obtained is right up to constant factors.