11 Laplacians and graph drawings

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Def 18.17: Given a weighted graph $G=(V,W)$, with $V=\{v_1,\dots,v_m\}$, if $\{e_1,\dots,e_n\}$ are the edges, for any orientation σ of underlying graph G, the incidence matrix B^σ is the $m\times n$ matrix

$$b_{ij} = \begin{cases} \sqrt{w_{ij}} & \text{if } s(e_j)=v_i \\ -\sqrt{w_{ij}} & \text{if } t(e_j)=v_i \\ 0 & \text{otherwise.} \end{cases}$$

Prop. 18.3 $\underset{\text{diagonal degree matrix}}{B^\sigma(B^\sigma)^T = D} - W = \underset{\text{Laplacian}}{L}$ for any orientation σ of a weighted graph $G=(V,W)$.

We can also directly prove that L is positive semidefinite by evaluating the quadratic form.

Prop 18.4 For any $m\times m$ symmetric matrix $W=(w_{ij})$, if $L=D-W$, where $D=\mathrm{diag}(L\vec{1})$, then

$$x^T L x = \frac{1}{2}\sum_{i,j=1}^{m} w_{ij}(x_i-x_j)^2 \quad \forall x\in\mathbb{R}^m.$$

Thus, $x^T L x$ does not depend on the diagonal entries w_{ii}, and if $w_{ij}\geq 0$ $\forall i,j$, then L is positive semidefinite.

proof.

$$\begin{aligned} x^T L x &= x^T D x - x^T W x \\ &= \sum_{i=1}^{m} d_i x_i^2 - \sum_{i,j} w_{ij} x_i x_j \\ &= \frac{1}{2}\left(\sum_{i=1}^{m} d_i x_i^2 - 2\sum_{i,j} w_{ij} x_i x_j + \sum_{j=1}^{m} d_j x_j^2\right) \\ &= \frac{1}{2}\left(\sum_{i=1}^{m}\sum_{j=1}^{m} w_{ij}x_i^2 - 2w_{ij}x_i x_j + w_{ij}x_j^2\right) \\ &= \frac{1}{2}\sum_{i,j} w_{ij}(x_i-x_j)^2. \end{aligned}$$

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Corollaries: For any weighted symmetric graph $G=(V,W)$,

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(1) The eigenvalues $0=\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_m$ of L are real and nonnegative, and there is an orthonormal basis of eigenvectors.

(2) The smallest eigenvalue $\lambda_1 = 0$ and $\vec{1}$ is a corresponding eigenvector.

Prop 18.5 Let $G=(V,W)$, $L=D-W$. Then $\dim(\operatorname{Ker} L) = \#$ connected components of G. Furthermore, $\operatorname{Ker} L$ has a basis consisting of indicator vectors of the connected components of G.

proof sketch: $L = BB^{T}$, so L and B^{T} have the same nullspace.

Corollary: If G is connected, then $\lambda_2 > 0$.

λ_2 is known as the Fiedler number of the graph, and is super important in spectral graph theory.

(one application is to graph partitioning)

Def. 18.19 Let $G=(V,W)$ with no isolated vertex (ie. no vertex without edges to some other vertex). Then the normalized graph Laplacians

$$L_{sym} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} W D^{-\frac{1}{2}} \qquad \text{(symmetric)}$$

$$L_{rw} = D^{-1} L = I - D^{-1} W. \qquad \text{(random walk)}$$

Prop. 18.6 Let $G=(V,W)$ with no isolated vertices. The graph Laplacians L, L_{sym}, L_{rw} have the following properties.

(1) L_{sym} is symmetric and positive semidefinite, and

$$x^{T} L_{sym} x = \frac{1}{2} \sum_{i,j} w_{ij} \left(\frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}} \right)^2 \qquad \forall x \in \mathbb{R}^m$$

$$x^{T} L_{sym} x = x^{T} D^{-\frac{1}{2}} L D^{-\frac{1}{2}} x$$

$x^T L_{sym} x = x^T D^{-\frac{1}{2}} L D^{-\frac{1}{2}} x$

(2) L_{sym} and L_{rw} have the same spectrum $(0 = \nu_1 \leq \cdots \leq \nu_m)$, and (u, λ) is an eigenpair of L_{rw} iff $(D^{\frac{1}{2}} u, \lambda)$ is an eigenpair of L_{sym}.

$L_{rw} = D^{-\frac{1}{2}} L_{sym} D^{\frac{1}{2}}$, so similar matrices

$$L_{rw} u = \lambda u \Rightarrow D^{-\frac{1}{2}} L_{sym} D^{\frac{1}{2}} u = \lambda u$$
$$\Rightarrow L_{sym} D^{\frac{1}{2}} u = \lambda D^{\frac{1}{2}} u .$$

(3) L and L_{sym} are symmetric and positive semidefinite. (already shown)

(4) A vector $u \neq 0$ is a solution to the generalized eigenvector problem $Lu = \lambda D u$ iff $D^{\frac{1}{2}} u$ is an eigenvector of L_{sym} for eigenvalue λ iff u is an eigenvector of L_{rw} for eigenvalue λ.

$$Lu = \lambda D u \Rightarrow L_{rw} u = D^{-1} L u = \lambda u .$$

(5) L and L_{rw} have the same nullspace.

$$L_{rw} = D^{-1} L .$$

(6) $L_{rw} \vec{1} = 0$ and $L_{sym} (D^{\frac{1}{2}} \vec{1}) = 0$.

*(7) For every eigenvalue ν_i of L_{sym}, $0 \leq \nu_i \leq 2$.
Furthermore $\nu_m = 2$ iff G has a nontrivial connected bipartite component.

*(8) If $m \geq 2$ and G is not a complete graph, then $\nu_2 \leq 1$.
G is complete iff $\nu_2 = \frac{m}{m-1}$.

*(9) If $m \geq 2$, and G is connected, then $\nu_2 > 0$.

*(10) If $m \geq 2$, and if G has no isolated vertices, then $\nu_m \geq \frac{m}{m-1}$.

* Fun properties we do not prove here, but are basic theorems in algebraic graph theory.

Graph clustering using normalized cuts (brief overview)

Def. 18.20 Given any subset of nodes $A \subseteq V$, the volume $vol(A)$ is the sum of the weights of all edges adjacent to nodes in A

$$vol(A) = \sum_{v_i \in A} \sum_{j=1}^{m} w_{ij}$$

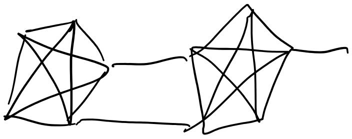
Given any two subsets $A, B \subseteq V$, we define

$$links(A, B) = \sum_{\substack{v_i \in A \\ v_j \in B}} w_{ij}.$$

And let $cut(A) = links(A, \bar{A})$, $(\bar{A} = V - A)$

(measuring links escaping A)

When we are partitioning a graph, the initial intuition is to minimize the cut. (classical min-cut for two clusters)



Problem arises because often we get very unbalanced cuts.

Several ways to balance cut size, but here we focus on the idea of normalized cuts [Shi, Malik, 2000]

$$Ncut(A_1, \dots, A_k) = \sum_{i=1}^{k} \frac{cut(A_i)}{vol(A_i)}$$

The case of $k=2$ is easier. Let's encode a bipartition A, B in a vector $\vec{x}$ s.t. $x_i = 1$ if $i \in A$ and $x_i = -1$ if $i \in B$.

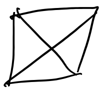
Then

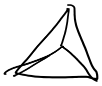
$$Ncut(A, B) = \frac{cut(A)}{vol(A)} + \frac{cut(B)}{vol(B)}$$

$$= \frac{\sum_{x_i>0,\ x_j<0} -w_{ij}x_ix_j}{\sum_{x_i>0} d_i} + \frac{\sum_{x_i<0,\ x_j>0} -w_{ij}x_ix_j}{\sum_{x_i<0} d_i}$$

[Shi, Malik, 2000] We can relax the problem to min $Ncut(\vec{x})$, to get real valued solutions. The solution to that real-valued system is precisely the eigenvector associated with the 2nd smallest eigenvalue. (proof makes extensive use of Rayleigh ratios)

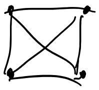
Spectral graph drawing

 or  are the same graph.

or 

How do we compute a "good" drawing?

Def 19.1 Let $G=(V,E)$ be an undirected graph with $|V|=m$. A graph drawing is a function $\rho: V \to \mathbb{R}^n$. The matrix of a graph drawing ρ is a $m \times n$ matrix R whose ith row $\rho(v_i)$ corresponds to the point representing v_i in $\mathbb{R}^n$.

Ex $R = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$ 

We let $\rho(v_i) = e_iR$, where $e_i = (0 \cdots \underset{\text{pos. } i}{1} \cdots 0)$

Def. 19.2 A graph drawing is balanced iff the sum of the entries of

Def. 19.2 A graph drawing is balanced iff the sum of the entries of every column of the matrix of the graph drawing is 0.

i.e. $\vec{1}^T R = 0$

(i.e. if the drawing is centred at the origin.)

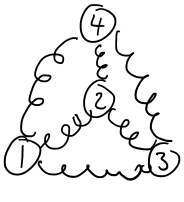
Aside: We may assume that that the cols of R are lin ind., because if not, we can choose a different smaller col basis and have the drawing be to that smaller space.

Aside: Sometimes also called graph embeddings (watch out for injectivity) or graph immersion.

Define: The energy of a drawing R be

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} \|\rho(v_i) - \rho(v_j)\|^2 .$$

Analogy:



Connect nodes by springs and then minimize the potential energy of the system.

"Good" drawings are ones that minimize energy (but are not trivial)

Define: The energy of a drawing R of a weighted graph $G=(V,W)$ is

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} w_{ij} \|\rho(v_i) - \rho(v_j)\|^2 .$$

(think of w_{ij} as spring stiffness)

Prop. 19.1 Let $G=(V,W)$ be a weighted graph, with $|V| = m$ and $W \in \mathbb{R}^{m \times m}$ symmetric, and let R be the matrix of a graph drawing ρ of G in $\mathbb{R}^n$ (an $m \times n$ matrix). If $L = D - W$ is the unnormalized Laplacian matrix, then

$$\mathcal{E}(R) = \mathrm{tr}(R^T L R).$$

Proof. $\mathcal{E}(R) = \sum \; w_{ij} \|\rho(v_i) - \rho(v_j)\|^2$

proof.

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} w_{ij} \| e(v_i) - e(v_j) \|^2$$

$$= \sum_{k=1}^{n} \sum_{\{v_i, v_j\} \in E} w_{ij} (R_{ik} - R_{jk})^2$$

$$= \sum_{k=1}^{n} \cdot \frac{1}{2} \sum_{i,j=1}^{m} w_{ij} (R_{ik} - R_{jk})^2$$

$$= \sum_{k=1}^{n} (R^k)^T L R^k$$

(where R^k is the kth col of R)
(by Prop. 18.4)

$$= tr(R^T L R). \qquad \square$$

So the energy $\mathcal{E}(R)$ is the sum of the (nonnegative) eigenvalues of $R^T L R$.

Note that for any invertible matrix M, $e(v_i)M$ is another graph drawing that conveys the same amount of information. So we may as well choose R + have pairwise orthogonal unit length cols, $R^T R = I$.

Def. 19.3 If a matrix R of a graph drawing satisfies $R^T R = I$, then the corresponding drawing is an orthogonal graph drawing

(this rules out trivial drawings)

Thm 19.1/19.2 Let $G = (V, W)$ be a weighted graph connected graph with $|V| = m$. If the eigenvalues of $L = D - W$ are $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_m$, then the minimal energy of any balanced orthogonal graph drawing of G in $\mathbb{R}^n$ is $\lambda_2 + \cdots + \lambda_{n+1}$. The $m \times n$ matrix R consisting of any unit eigenvectors $u_2, \ldots, u_{n+1}$ associated with $\lambda_2, \ldots, \lambda_{n+1}$ yields a balanced orthogonal graph drawing of minimal energy.

proof. By the Poincare separation theorem/eigenvalue interlacing,

$$\lambda_k = \lambda_k(L) \leq \lambda_k(R^T L R)$$

$$\Rightarrow \sum_{k=1}^{n} \lambda_k \leq Tr(R^T L R).$$

$\sum_{k=1} \lambda_k = \text{Tr}(R^T L R)$.

And if $R = [u_1 \cdots u_n]$, then $R^T L R = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$, so $\text{Tr}(R^T L R) = \sum_{k=1}^{n} \lambda_k$.

But $\lambda_1 = 0$ and $\lambda_2 > 0$, so $u_1 = \frac{\vec{1}}{\sqrt{m}}$.

Because $\langle u_i, u_1 \rangle = 0 \ \forall i \neq 1$, $u_i^T \vec{1} = 0$.

Thus, we can get a balanced orthogonal drawing in $\mathbb{R}^{n-1}$ by removing u_1 and just using $R = [u_2 \cdots u_n]$, which has the same energy

i.e. Balanced orthogonal drawing in $\mathbb{R}^n$ $\Longleftrightarrow$ orthogonal drawing in $\mathbb{R}^{n+1}$,

with energy $\lambda_2 + \cdots + \lambda_{n+1}$.

▨

Aside, using the first eigenvector $u_1 = \frac{\vec{1}}{\sqrt{m}}$ is undesirable because it means all pts have the same first coordinate, another reason to remove it.