The Laplacian and Graph Drawing

We are now going to explore our demonstration of graph drawing a little more deeply.

Suppose we let $\mathbb{R}^V$ - the space of vertex weights - represent positions of the vertices. We'd like to ~~use~~ find a "nice" drawing $\vec{x} \in \mathbb{R}^V$.

Here's a classical approach.

- We want vertices that are nearby on the graph to be nearby in space.

So we choose $\vec{x}$ minimizing

$$Q_{L_G}(\vec{x}) = \sum_{\substack{v_i - v_j \\ \text{an edge of } G}} (\vec{x}(v_i) - \vec{x}(v_j))^2 = \langle \vec{x}, L_G \vec{x} \rangle$$

We know that $Q_{L_G}(\vec{0}) = 0$, so we require the constraint $\langle \vec{x}, \vec{x} \rangle = 1$.

From the Courant-Fischer theorem,

$$\vec{x} = \underset{\langle \vec{x}, \vec{x} \rangle = 1}{\operatorname{argmin}} \langle \vec{x}, \vec{x} \rangle_{L_G}$$

$$= \vec{\psi}_1,$$

the first eigenvector of L_G, with lowest eigenvalue.

However, we saw in homework that

$$\lambda_1 = 0 \quad \text{and} \quad \varphi_1 = (1 \cdots 1)^T = \vec{1}$$

Thus we add the additional constraint that $\langle \vec{x}, \vec{1} \rangle = 0$.

Lemma. If we have vectors $\vec{x}_1, \ldots, \vec{x}_K \in \mathbb{R}^V$ and use them to form a $V \times K$ matrix X, then

1) X determines an embedding of G in $\mathbb{R}^K$ by $X(v_i) =$ ith <u>row</u> of X.

2) $$\sum_{\substack{v_i \leftrightarrow v_j \\ \text{(an edge of } G)}} |X(v_i) - X(v_j)|^2 = \sum_{i=1}^{K} \langle \vec{x}_i, \vec{x}_i \rangle_{L_G}$$

Proof. 1 is basically a definition and does not require proof. In coordinates,

$$\sum_{\substack{v_i \sim v_j \\ \text{(an edge of } G\text{)}}} |X(v_i) - X(v_j)|^2 = \sum_{\substack{v_i \sim v_j \\ \text{(an edge of } G\text{)}}} \sum_{\ell=1}^{K} (X_{i\ell} - X_{j\ell})^2$$

$$= \sum_{\ell=1}^{K} \sum_{v_i \sim v_j} (X_{i\ell} - X_{j\ell})^2$$

theorem in notes

$$= \sum_{\ell=1}^{K} \langle X_{-\ell}, L_G X_{-\ell} \rangle$$

$$= \sum_{\ell=1}^{K} \langle \vec{X}_\ell, \vec{X}_\ell \rangle_{L_G}$$

Note: $X_{-\ell}$ means "the ℓth column of X", or "all entries of X in the form $X_{w\ell}$ for any w".

as required. $\square$

Theorem. Let L be a graph Laplacian and let $\vec{x}_1, \ldots, \vec{x}_k$ be orthonormal vectors in $\mathbb{R}^V$ which are all orthogonal to $\vec{1}$. Then

$$\sum_{i=1}^{k} \langle \vec{x}_i, L\vec{x}_i \rangle \geq \sum_{i=2}^{k+1} \lambda_i$$

(where $\lambda_1 \leq \ldots \leq \lambda_V$ are the eigenvalues of L) with equality only if the $\vec{x}_i$ are all ~~in span~~ $\cancel{(\vec{\phi}_2, \ldots, \vec{\phi}_{k+1})}$ orthogonal to every $\vec{\phi}_j$ with $\lambda_j > \lambda_{k+1}$.

This theorem tells us precisely how to construct the embeddings of G in $\mathbb{R}^k$ which minimize the "spring energy"

$$\sum_{v_i \sim v_j} |X(v_i) - X(v_j)|^2.$$

Proof. We may assume[1] that $\vec{\varphi}_1$ is a constant vector.

Let $\vec{x}_1, \ldots, \vec{x}_K$ be completed to an orthonormal basis $\vec{x}_1, \ldots, \vec{x}_v$ for $\mathbb{R}^v$. Recalling that $\vec{\varphi}_1, \ldots, \vec{\varphi}_v$ are an orthonormal basis for $\mathbb{R}^v$ of eigenvectors of L,

$$\sum_{j=1}^{v} \underbrace{\langle \vec{\varphi}_j, \vec{x}_i \rangle}_{\text{the entries in } \vec{x}_i \text{ if we write it in the } \vec{\varphi}_j \text{ basis}}{}^2 = \|\vec{x}_i\|^2 = 1$$

$$\sum_{j=1}^{v} \underbrace{\langle \vec{x}_j, \vec{\varphi}_i \rangle}_{\text{the entries in } \vec{\varphi}_i \text{ if we write it in the } \vec{x}_j \text{ basis.}}{}^2 = \|\vec{\varphi}_i\|^2 = 1$$

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1. The eigenspace for $\lambda_1 = 0$ could be large if more eigenvalues are 0. But the constant vectors are always in this space.

This means that the matrix

$$\Psi^T X \quad \text{where } (\Psi^T X)_{ij} = \langle \vec{\psi}_j, \vec{x}_i \rangle$$

is said to be "doubly stochastic".

Now $\langle \vec{\psi}_1, \vec{x}_i \rangle = 0$ for all i, so

$$\langle \vec{x}_i, L\vec{x}_i \rangle = \sum_{j=2}^{n} \lambda_j \langle \vec{\psi}_j, \vec{x}_i \rangle^2$$

(This is ~~a~~ ~~[illegible]~~ something we proved in the course of proving Courant-Fischer.)

$$= \lambda_{k+1} + \sum_{j=2}^{n} (\lambda_j - \lambda_{k+1}) \langle \vec{\psi}_j, \vec{x}_i \rangle^2$$

(This is a weird move, but since $\sum_{j=2}^{n} \langle \vec{\psi}_j, \vec{x}_i \rangle^2 = 1$, it's certainly true.)

$$\geq \lambda_{k+1} + \sum_{j=2}^{k+1} (\lambda_j - \lambda_{k+1}) \langle \vec{\psi}_j, \vec{x}_i \rangle^2$$

(for $j > k+1$, $\lambda_j \geq \lambda_{k+1}$, so we only deleted non negative ~~positive~~ terms from the sum)

This is an equality only if

$$\sum_{j=k+2}^{v} (\lambda_j - \lambda_{k+1}) \langle \vec{\varphi}_j, \vec{x}_i \rangle^2 = 0$$

or if $\langle \vec{\varphi}_j, \vec{x}_i \rangle = 0$ when $\lambda_j - \lambda_{k+1} > 0$.

Now we have

$$\sum_{i=1}^{k} \langle \vec{x}_i, L\vec{x}_i \rangle \geq \sum_{i=1}^{k} \left(\lambda_{k+1} + \sum_{j=2}^{k+1} (\lambda_j - \lambda_{k+1}) \langle \vec{\varphi}_j, \vec{x}_i \rangle^2 \right)$$

$$= k\lambda_{k+1} + \sum_{j=2}^{k+1} \underbrace{(\lambda_j - \lambda_{k+1})}_{\text{at least } 0} \underbrace{\sum_{i=1}^{k} \langle \vec{\varphi}_j, \vec{x}_i \rangle^2}_{\text{at most } 1}$$

$$\geq k\lambda_{k+1} + \sum_{j=2}^{k+1} \lambda_j - \lambda_{k+1}$$

$$= \sum_{j=2}^{k+1} \lambda_j$$

If $\lambda_j = \lambda_{k+1}$, the terms we lose in passing to the inequality were 0. If $\lambda_j > \lambda_{k+1}$, we must have $\sum_{i=1}^{K} \langle \vec{\Psi}_j, \vec{X}_i \rangle^2 = 0$, to ~~be~~ have equality, which is exactly the condition in the statement. □

This tells us that the drawings produced by eigenvectors are optimal and also canonical.

Definition. Given two graphs G and G', we say that a map $f: \{v_1, \dots, v_v\} \to \{v'_1, \dots, v'_{v'}\}$ is an <u>isomorphism</u> between graphs if

1) f is a bijection (f is 1-1, onto)
2) The map $v_i - v_j \mapsto f(v_i) - f(v_j)$ is a bijection between the edges of G and the edges of G'.

We will show in homework that

Prop. If G and G' are isomorphic, then they have the same spectrum of eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n = \lambda_1' \leq \cdots \leq \lambda_n'$.

If $\lambda_2 < \lambda_3 \cdots < \lambda_K$, then there are only 2^K optimal drawings of G ~~and G_2~~ one of which must match any optimal drawing of G'.

This means that our drawings can often help us construct isomorphisms (or rule them out!).