Lecture 11: Spectral graph theory.

Previously:

- PCA
- SVD
- tensor decomposition

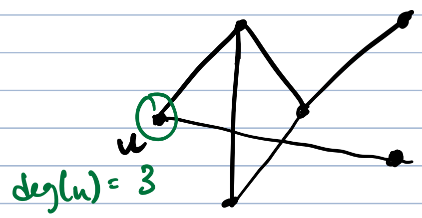
very "analytic" "continuous"

This lecture:

Combinatorial properties of graphs $\Longleftrightarrow$ Linear algebraic properties of matrices

Recall: (undirected) graph $G = (V, E)$

vertices — edges, which are pairs of vertices



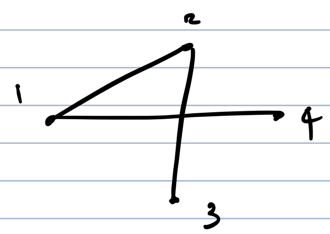
$n = |V|$, $m = |E|$

$V \Leftrightarrow \{1, \dots, n\}$

For any node u, $\deg(u) = \#$ neighbors of u

Def: For any graph G, we can associate to it an $n \times n$ matrix A called the adjacency matrix.

For all $u, v \in V$, $A_{uv} = \begin{cases} 1 & \text{if } (u,v) \in E \\ 0 & \text{o.w.} \end{cases}$



$$A = \begin{array}{c c} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \qquad D = \begin{bmatrix} 2 & & & \\ & 2 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

We can also define degree matrix D, D is diagonal

$$D_{uu} = \deg(u)$$

Def: For any graph G, its Laplacian is defined to be

$$L_G = D - A.$$

$$(L_G)_{u,v} = \begin{cases} \deg(u) & \text{if } u = v \\ -1 & \text{if } (u,v) \in E \\ 0 & \text{o.w.} \end{cases}$$

e.g. for above

$$L_G = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Another useful, related notion: normalized Laplacian.

normalize each row/column so that diagonal entries are 1.

If $\deg(u) = d$ for all $u \in V$ ("d-regular" graph)

$$\mathcal{L}_G := \frac{1}{d} L_G = \frac{1}{d}(D - A)$$

$= d \cdot I$

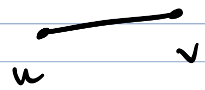
$$= I - \frac{1}{d} A.$$

More generally, is slightly more annoying. to maintain symmetry, the "right" way to normalize is

$$\mathcal{L}_G := D^{-1/2} L_G D^{-1/2}$$
$$= I - D^{-1/2} A D^{-1/2}.$$

Properties of Laplacian:

- If G has a single edge (u,v), then



$$L_G = \begin{array}{c} \\ u \\ \\ v \\ \end{array} \begin{array}{c} \begin{array}{cccc} & u & & v \end{array} \\ \begin{pmatrix} & & & \\ & 1 & & -1 \\ & & & \\ & -1 & & 1 \end{pmatrix} \end{array} \qquad \begin{array}{c|cc} & u & v \\ \hline u & 1 & -1 \\ v & -1 & 1 \end{array}$$

Consequently, for any graph G,

$$L_G = \sum_{(u,v)\in E} L_{\{u,v\}}.$$

- For any vector $x \in \mathbb{R}^n$, and any $w \in V$,

$$(L_G x)_w = \sum_{(u,v)\in E} (L_{\{u,v\}} x)_w$$

$$L_{\{u,v\}}\, x = \begin{array}{c} u \\ \\ v \end{array} \begin{pmatrix} 1 & -1 \\ & \\ -1 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 \\ \vdots \\ 0 \\ x_u - x_v \\ 0 \\ \vdots \\ 0 \\ x_v - x_u \\ 0 \\ \vdots \end{pmatrix} \begin{array}{c} \\ \\ \\ u \\ \\ \\ \\ v \\ \\ \\ \end{array}$$

so $$(L_G(x))_w = \sum_{(w,v)\in E} (L_{\{w,v\}} x)_w = \sum_{v:(w,v)\in E} (x_w - x_v)$$

$$= \deg(w)\cdot x_w - \sum_{v:(w,v)\in E} x_v$$

Also, $$x^T L_G x = \langle x, L_G x \rangle$$

$$= \sum_{(u,v)\in E} \langle x, L_{\{u,v\}} x \rangle$$

$$= \sum_{(u,v)\in E} \underbrace{x_u(x_u - x_v) + x_v(x_v - x_u)}_{\substack{= x_u^2 - 2x_u x_v + x_v^2 \\ = (x_u - x_v)^2}}$$

$$= \sum_{(u,v)\in E} (x_u - x_v)^2$$

Aside: why is this called a "Laplacian"?

In calc or physics, there's a Laplace operator

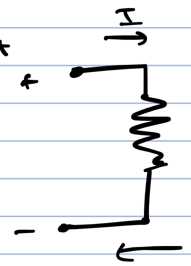
$$\Delta f = \sum \frac{\partial^2 f}{\partial x_i^2}$$ ← measures deviation of temperature at a point x.

this is really a continuous limit of graph Laplacians.

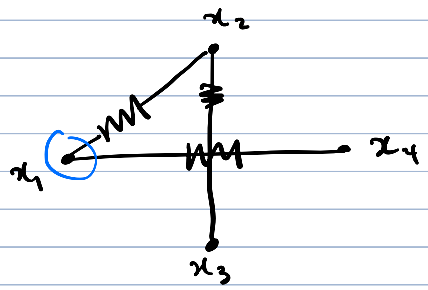
Another interpretation: as an electrical circuit.

Recall Ohm's law:

$$\underbrace{\Delta V}_{\text{change in voltage}} = \overbrace{I}^{\text{current}} R$$



put unit resistors on edge of network



Induced current at x_1

$= x_2 - x_1 + x_4 - x_1$

$= (-L_G x)_1$.

so Laplacian is map from voltage → current.

Power dissipation of a resistor $= I^2 R = (\Delta V)^2$

So total power dissipation of network is

$$\sum_{(u,v)} (x_u - x_v)^2 = x^T L_G x.$$

(end of aside).

Lemma: For any graph G, L_G is positive semi-definite ← all of its eigenvalues are ≥ 0.

pf. Suppose $x \in \mathbb{R}^n$ is an eigenvector w/ eigenvalue λ.

$$x^T L_G x = \sum_{(u,v) \in E} (x_u - x_v)^2 \geq 0.$$

but

$$x^T L_G x = \langle x, L_G x \rangle = \langle x, \lambda x \rangle = \lambda \underbrace{\|x\|_2^2}_{\geq 0}.$$

so $\lambda \geq 0$.

Lemma: For any graph G, if $\vec{1}$ is the all-ones vector,

$$L_G \vec{1} = 0.$$

pf:
$$L_G \vec{1} = \sum_{(u,v)\in E} (\vec{1}_u - \vec{1}_v) = 0.$$

Cor: 0 is an eigenvalue of L_G.

We can arrange the eigenvalues in ascending order
$$0 = \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n.$$

Key idea of spectral graph theory:

Analytic properties of $\lambda_1, \cdots, \lambda_n$ $\Longleftrightarrow$ Discrete/Combinatorial properties of G.

For instance:

Theorem: The multiplicity of the eigenvalue 0 is the # of connected components of G.

pf: We will need the variational/minimax characterization of eigenvalues.

$$\lambda_1 = \min_{\|x\|_2 = 1} x^T L_G x. \qquad v_1 = \text{argmin}.$$

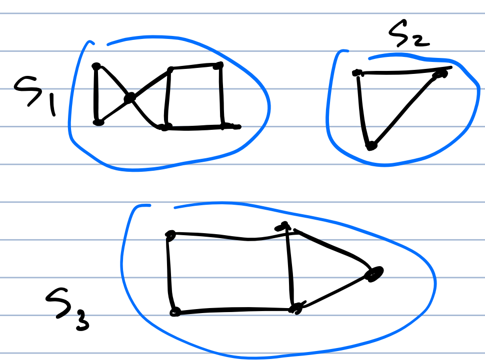
$$\lambda_2 = \min_{\substack{\|x\|_2 = 1 \\ x \perp v_1}} x^T L_G x \qquad v_2 = \text{argmin}$$

$$\vdots$$

$$\lambda_k = \min_{\substack{\|x\|_2 = 1 \\ x \perp v_1, \cdots, v_{k-1}}} x^T L_G x, \qquad v_k = \text{argmin}.$$

1). multiplicity $\ge$ # connected components.

just need to demonstrate k orthogonal vectors $x_1, \cdots, x_k$ s.t. $x_i^T L_G x_i = 0$ $\forall i$



$$(x_1)_u = \begin{cases} 1, & u \in S_1 \\ 0 & \text{o.w.} \end{cases}$$

$$(x_2)_u = \begin{cases} 1, & u \in S_2 \\ 0, & \text{o.w.} \end{cases}$$

$$\vdots$$

$$(x_k)_u = \begin{cases} 1, & u \in S_k \\ 0, & \text{o.w.} \end{cases}$$

$\langle x_i, x_j \rangle = 0$ $\forall i \ne j$ since they have disjoint support

Then, for all i,

$$x_i^T L_G x_i = \sum_{(u,v)\in E} ((x_i)_u - (x_i)_v)^2 = 0$$

2). # connected components $\geq$ multiplicity of 0.

Suppose L_G had $k+1$ 0 eigenvalues. We know that $x_1, \ldots, x_k$ are eigenvectors, so variational characterization says there is x_{k+1} which is orthogonal to all $x_1, \ldots, x_k$ s.t. $x_{k+1} \neq 0$, and $x_{k+1} L_G x_{k+1} = 0$.

$$= \sum_{(u,v)\in E} ((x_{k+1})_u - (x_{k+1})_v)^2$$

$$= \sum_{i=1}^{k} \sum_{(u,v)\in S_i} ((x_{k+1})_u - (x_{k+1})_v)^2 = 0.$$

x_{k+1} must be constant on every connected component.

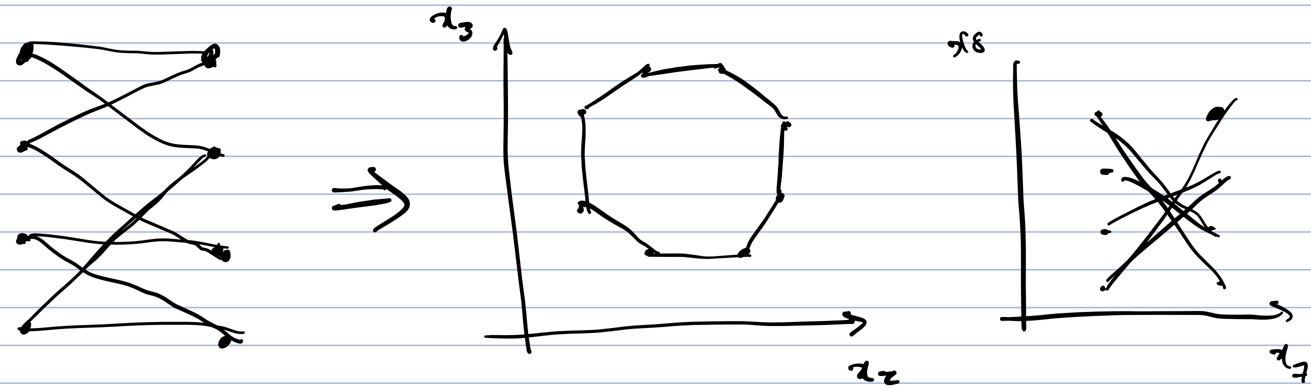
but $x_{k+1} \neq 0 \Rightarrow (x_{k+1})_u = c \neq 0$ for some u.

Say $u \in S_i$. Then $(x_{k+1})_v = c \ \forall\, v \in S_i$. But then $\langle x_{k+1}, x_i \rangle \neq 0$, which is a contradiction!

Spectral embeddings.

An eigenvector x assigns real numbers to vertices. We can take pairs of eigenvectors and plot where the points lie.

e.g.



Why? Recall again, for any eigenvector x_i w/ $\|x_i\|_2 = 1$,

$$x_i^T L_G x_i = \lambda_i.$$

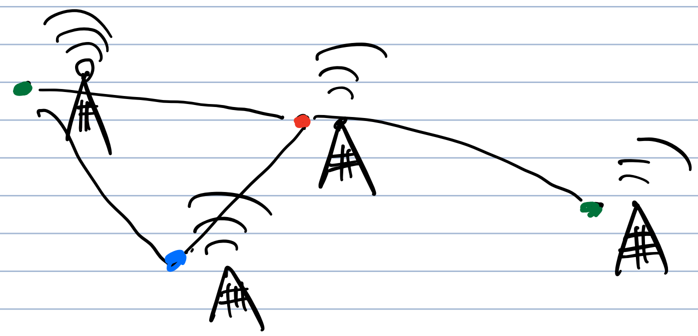
$$\sum_{(u,v)\in E} ((x_i)_u - (x_i)_v)^2$$

small eigenvectors want to make edges short

large eigenvectors want edges long

Application: graph coloring.

Def: A k-coloring of a graph $G = (V, E)$ is a map $f: V \to \{1, \dots, k\}$ s.t. $f(u) \neq f(v)$ $\forall (u,v) \in E$.



nearby radio towers should use different frequencies.

color of node = frequency. want adjacent nodes to have different colors.

In general, determining if G has a k-coloring is NP-hard.

heuristic based on spectral

If you take embedding w/ large eigenvalues

nearby in embedding $\approx$ "far" in graph.

Idea:

1. plot embedding onto large eigenvalues
2. partition space into k regions
3. Assign each region a different color.

Can then locally fix coloring afterwards.