MAT 280: Harmonic Analysis on Graphs & Networks
Lecture 3: Baiscs of Graph Theory: Graph Laplacians

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Outline

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1. Basic Definitions in Graph Theory
2. Matrices Associated with a Graph
3. Why Graph Laplacians?

Basic Definitions

- A *graph* G consists of a set of *vertices* (or nodes) V and a set of *edges* E connecting some pairs of vertices in V. We write $G = (V, E)$.
- An edge connecting a vertex $x \in V$ and itself is called a *loop*.
- For $x, y \in V$, if $\exists$ more than one edge connecting x and y, they are called *multiple edges*.
- A graph having loops or multiple edges is called a *multiple graph* (or *multigraph*); otherwise it is called a *simple* graph.

- In this class, we shall only deal with simple graphs. So, when we say a graph, we mean a simple graph.

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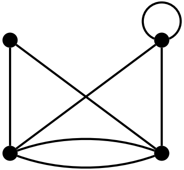
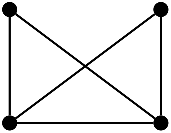


A multiple graph



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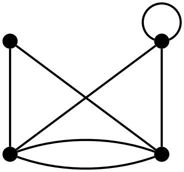

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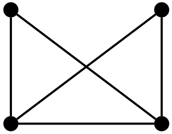

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- If two distinct vertices $x, y \in V$ are connected by an edge e, then x, y are called the *endpoints* (or *ends*) of e, and x, y are said to be *adjacent*, and we write $x \sim y$. We also say an edge e is *incident with* x and y, and e *joins* x and y.
- The number of edges that are incident with x (i.e., have x as their endpoint) = the *degree* (or *valency*) of x and write $d(x)$ or d_x.
- If the number of vertices $|V| < \infty$, then G is called a *finite* graph; otherwise an *infinite* graph.
- If each edge in E has a direction, G is called a *directed graph* or *digraph*, and such E is written as $\boldsymbol{E}$.
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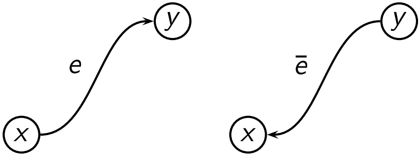

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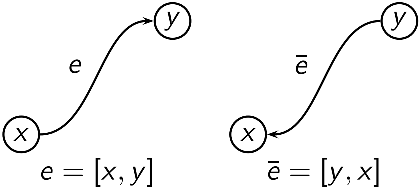

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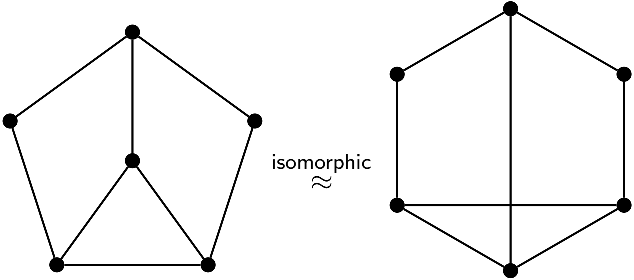
- We say two graphs are *isomorphic* if $\exists$ a one-to-one correspondence between the vertex sets such that if two vertices are joined by an edge in one graph, the corresponding vertices are also joined by an edge in the other graph.



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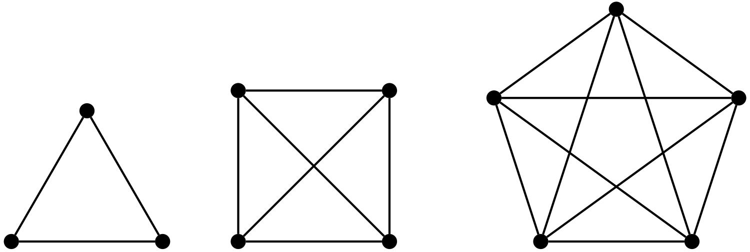
- The *complete graph* K_n on n vertices is a simple graph that has all possible $\binom{n}{2}$ edges.



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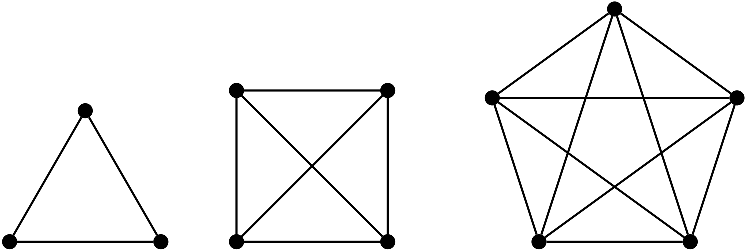

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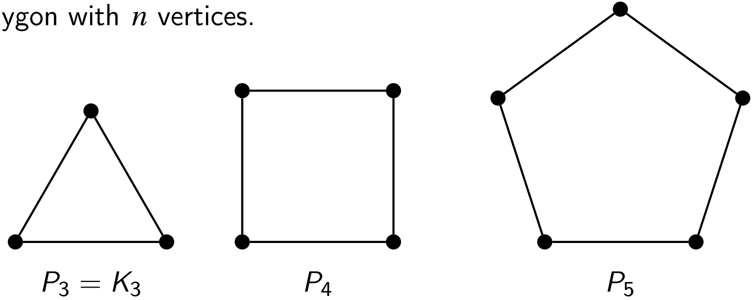
- A *polygon* is a finite connected graph that is regular of degree 2. $P_n =$ a polygon with n vertices.



- The *complete bipartite graph* $K_{n,m}$ has $n+m$ vertices $a_1, \ldots, a_n$, $b_1, \ldots, b_m$, and all nm pairs (a_i, b_j) as edges. An example: $K_{2,3}$:

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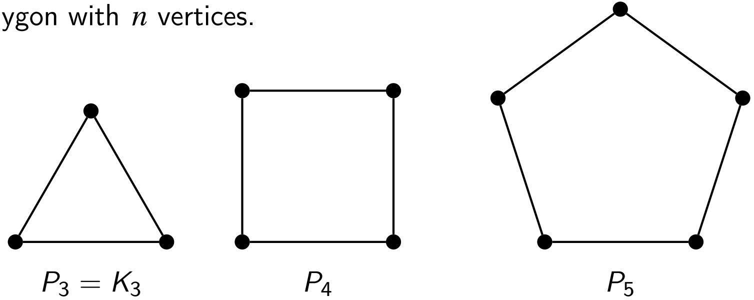

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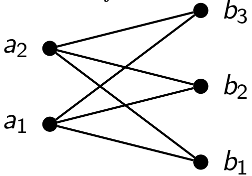

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Matrices Associated with a Graph

- The *adjacency matrix* $A = A(G) = (a_{ij}) \in \mathbb{R}^{n\times n}$, $n = |V|$, for an unweighted graph G consists of the following entries:

$$a_{ij} := \begin{cases} 1 & \text{if } v_i \sim v_j; \\ 0 & \text{otherwise.} \end{cases}$$

- Another typical way to define its entries is based on the *similarity* of information at v_i and v_j:

$$a_{ij} := \exp(-\mathrm{dist}(v_i, v_j)^2/\epsilon^2)$$

where dist is an appropriate distance measure (i.e., metric) defined in V, and $\epsilon > 0$ is an appropriate scale parameter. This leads to a *weighted* graph. We will discuss later more about the weighted graphs, how to determine weights, and how to construct a graph from given datasets in general.

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- The *degree matrix* $D = D(G) = \mathrm{diag}(d_1, \ldots, d_n) \in \mathbb{R}^{n \times n}$ is a diagonal matrix whose entries are:

$$d_i := d(v_i) = d_{v_i} = \sum_{j=1}^{n} a_{ij}.$$

  Note that the above definition works for both unweighted and weighted graphs.

- The *transition matrix* $P = P(G) = (p_{ij}) \in \mathbb{R}^{n \times n}$ consists of the following entries:

$$p_{ij} := a_{ij}/d_i \quad \text{if } d_i \neq 0.$$

- p_{ij} represents the probability of a random walk from v_i to v_j in one step: $\sum_j p_{ij} = 1$, i.e., P is *row stochastic*.
- $A^{\mathsf{T}} = A$, $P^{\mathsf{T}} \neq P$, $P = D^{-1}A$.

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Matrices Associated with a Graph . . .

- Let G be an *undirected* graph. Then, we can define several *Laplacian* matrices of G:

$$L(G) := D - A \qquad \textit{Unnormalized}$$

$$L_{\mathrm{rw}}(G) := I_n - D^{-1}A = I_n - P = D^{-1}L \qquad \textit{Normalized}$$

$$L_{\mathrm{sym}}(G) := I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} \qquad \textit{Symmetrically-Normalized}$$

- The *signless* Laplacian is defined as follows, but we will not deal with this in this course: $Q(G) := D + A$.
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Functions Defined on a Graph

$$
\begin{aligned}
C(V) &:= \{\text{all functions defined on } V\} \\
C_0(V) &:= \{f \in C(V) \,|\, \operatorname{supp} f \text{ is a finite subset of } V\} \\
\operatorname{supp} f &:= \{u \in V \,|\, f(u) \neq 0\} \\
\mathscr{L}^2(V) &:= \{f \in C(V) \,|\, \|f\| := \sqrt{\langle f, f \rangle} < \infty\} \\
\langle f, g \rangle &:= \sum_{u \in V} d(u) f(u) g(u).
\end{aligned}
$$

Lemma

$$\langle Pf, g \rangle = \langle f, Pg \rangle \quad \forall f, g \in \mathscr{L}^2(V);$$

$$\|Pf\| \leq \|f\| \quad \forall f \in \mathscr{L}^2(V).$$

Functions Defined on a Graph . . .

- Let $f \in \mathscr{L}^2(V)$. Then

$$Lf(v_i) = d_i f(v_i) - \sum_{j=1}^{n} a_{ij} f(v_j) = \sum_{j=1}^{n} a_{ij} \left(f(v_i) - f(v_j) \right).$$

  i.e., this is a generalization of the *finite difference approximation* to the Laplace operator.

- On the other hand,

$$L_{\mathrm{rw}} f(v_i) = f(v_i) - \sum_{j=1}^{n} p_{ij} f(v_j) = \frac{1}{d_i} \sum_{j=1}^{n} a_{ij} \left(f(v_i) - f(v_j) \right).$$

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- Note that these definitions of the graph Laplacian corresponds to $-\Delta$ in $\mathbb{R}^d$, i.e., they are *nonnegative operators* (or *positive semi-definite matrices*).

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Functions Defined on a Graph . . .

- A function $f \in C(V)$ is called *harmonic* if

$$Lf = 0, \; L_{\mathrm{rw}} f = 0, \text{ or } \; L_{\mathrm{sym}} f = 0.$$

- A function $f \in C(V)$ is called *superharmonic* at $x \in V$ if

$$Lf(x) \geq 0, \; L_{\mathrm{rw}} f(x) \geq 0, \text{ or } \; L_{\mathrm{sym}} f(x) \geq 0.$$

- These corresponds to:

$$f(v_i) \geq \frac{1}{d_i} \sum_{j=1}^{n} a_{ij} f(v_j), \; f(v_i) \geq \sum_{j=1}^{n} p_{ij} f(v_j), \text{ or } \; f(v_i) \geq \sum_{j=1}^{n} \frac{a_{ij}}{\sqrt{d_i}\sqrt{d_j}} f(v_j).$$

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Derivatives and Green's Identity

Let $C(\boldsymbol{E}) := \{\varphi \text{ defined on } \boldsymbol{E} \,|\, \varphi(\bar{e}) = -\varphi(e), e \in \boldsymbol{E}\}$. For $f \in C(V)$, define the *derivative* $df \in C(\boldsymbol{E})$ of f as

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Theorem (The discrete version of Green's first identity, Dodziuk 1984)

$$\forall f_1, f_2 \in C_0(V),\ \langle df_1, df_2 \rangle = \langle L_{\mathrm{rw}} f_1, f_2 \rangle = \sum_{u \in V} L f_1(u) f_2(u).$$

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Corollary

L, L_{rw}, and L_{sym} are nonnegative operators, e.g.,

$$\langle L_{\mathrm{rw}} f, f \rangle = \sum_{u \in V} Lf(u)\, f(u) = \langle df, df \rangle \geq 0.$$

The Minimum Principle

Theorem (The discrete version of the minimum principle)

Let $f \in C(V)$ be superharmonic at $x \in V$. If $f(x) \le \min_{y \sim x} f(y)$, then $f(z) = f(x)$, $\forall z \sim x$.

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Proof. From the superharmonicity of f at $x \in V$, we have

$$\frac{1}{d_x} \sum_{y\sim x} a_{xy} f(y) \le f(x).$$

On the other hand, from the condition of this theorem, we have

$$\frac{1}{d_x} \sum_{y\sim x} a_{xy} f(y) \ge \frac{1}{d_x} \sum_{y\sim x} a_{xy} f(x) = f(x).$$

Hence, we must have $\frac{1}{d_x} \sum_{y\sim x} a_{xy} f(y) = f(x)$. But this can happen only if $f(z) = f(x)$, $\forall z \sim x$. □

Outline

Why Graph Laplacians?

- After all, *sines* (*cosines*) are the eigenfunctions of the Laplacian on the *rectangular* domain with Dirichlet (Neumann) boundary condition.
- *Spherical harmonics, Bessel functions, and Prolate Spheroidal Wave Functions*, are part of the eigenfunctions of the Laplacian for the *spherical, cylindrical, and spheroidal* domains, respectively.
- Hence, the eigenfunction expansion of data measured at the vertices using the eigenfunctions (in fact, eigenvectors) of a graph Laplacian corresponds to Fourier (or spectral) analysis of the data on that graph.
- They also play a useful role to understand a graph (e.g., the discrete nodal domain theorem useful for grouping vertices; see Bıyıkoğlu, Leydold, & Stadler, LNM, Springer, 2007)

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Why Graph Laplacians? . . .

- Furthermore, the eigenvalues of $L(G)$ reflect various intrinsic geometric and topological information about the graph including
  - connectivity or the number of separated components
  - diameter (the maximum distance over all pairs of vertices)
  - mean distance, . . .
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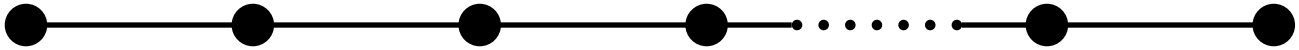
A Simple Yet Important Example: A Path Graph



$$\underbrace{\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}}_{L(G)} = \underbrace{\begin{bmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & \\ & & & & & 1 \end{bmatrix}}_{D(G)} - \underbrace{\begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}}_{A(G)}$$

The eigenvectors of this matrix are exactly the *DCT Type II* basis vectors (used for the JPEG standard) while those of the *symmetrically-normalized Graph Laplacian matrix* $L_{\text{sym}} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$ are the *DCT Type I* basis! (See G. Strang: "The discrete cosine transform," *SIAM Review*, vol. 41, pp. 135–147, 1999).

- $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n),\ k = 0 : n-1.$
- $\boldsymbol{\phi}_k(\ell) = a_{k;n} \cos\left(\pi k \left(\ell + \frac{1}{2}\right)/n\right),\ k, \ell = 0 : n-1;\ a_{k;n}$ is a const. s.t. $\|\boldsymbol{\phi}_k\|_2 = 1.$
- In this simple case, λ (eigenvalue) is a monotonic function w.r.t. the frequency, which is the eigenvalue index k. *For a general graph, however, the notion of frequency is not well defined.*