MAT 280: Laplacian Eigenfunctions: Theory, Applications, and Computations
Lecture 18: Introduction to Spectral Graph Theory – I. Basics of Graph Theory

Lecturer: Naoki Saito
Scribe: Adam Dobrin/Allen Xue

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We introduce the graph theory for multiple reasons. First, graphs are very general. They can be adapted to deal with numerous general situations and can represent very complicated objects (e.g., high-dimensional dataset $\{\boldsymbol{x}_k\}_{k=1}^N \subset \mathbb{R}^d$). Graph theory has been used in many different fields, such as clustering (and image segmentation), classification, data mining, search engines, and statistical learning theory.

The following section is based on [1, Chap. 1] and [2].

1 Basics of the graph theory

1.1 A Series of Definitions and Notations

- A **graph** G consists of a set of **vertices** V and a set of **edges** E connecting some pairs of vertices in V. We write $G = (V, E)$.
- An edge connecting a vertex (or node) $x \in V$ to itself is called a **loop**.
- For $x, y \in V$, if there exist more than one edges connecting x and y, then they are called **multiple edges**.

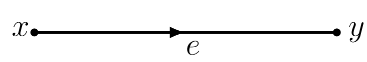

Figure 1: Directed Edge

- A graph containing loops or multiple edges is called a **multiple graph**, or a **multigraph**. Otherwise, it is called a **simple graph**.

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

- If two distinct vertices $x, y \in V$ are connected by an edge $e \in E$, then x and y are called the **endpoints** (or ends) of e, and x and y are said to be **adjacent**, written as $x \sim y$. In this situation, we also say that e is **incident** with x and y and that e **joins** x and y.

- The **degree**, or **valency**, of a vertex x is the number of edges incident with x, denoted as deg(x) or $m(x)$.

- For each $x \in V$, if $m(x)$ is finite, then the graph G is called a **locally finite graph**. However, $m_\infty(G) \triangleq \sup_{x \in V} m(x)$ could be infinite. A **finite graph** G is one in which $\#(V) = |V| < \infty$. An **infinite graph** is one in which $|V| = \infty$.

- If each edge in E has a direction associated with it, then we call the graph G a **directed graph**, or **digraph**. As in Figure 1, e is called **directed edge**, x is called the **tail** of e and the destination of e, y, is called the **head** of e. We write $e = [x, y]$, and $\overline{e} = [y, x]$ for reverse direction. If there is no direction associated with an edge e joining x, y, then we write $e = (x, y) = (y, x)$. Also we define $\mathbb{E} \triangleq \{$a set of all directed edges$\}$.

- For a given $x, y \in V$, a sequence $c = \{v_1, v_2, \ldots, v_{n+1}\}$ of vertices in V is called a **path** connecting x and y if $v_1 = x$, $v_{n+1} = y$, and $v_1 \sim v_2 \sim \ldots \sim v_n \sim v_{n+1}$. We define the **length** of a **path** c is n in this case and write $\ell(c) = n$.

- For any two vertices in V, if there exists a path connecting them, such a graph G is called a **connected graph**.

- The **graph distance** between x and y is given by

$$d(x,y) \triangleq \inf\{\ell(c) \,|\, c \text{ is a path connecting } x \text{ and } y\}.$$

- The **diameter** of a graph G is given by

$$\text{diam}(G) \triangleq \sup\{d(x,y) \,|\, x, y \in V\}.$$

- G is **finite** $\iff$ $\text{diam}(G) < \infty$.

- We say two graphs are **isomorphic** if there 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 joined by an edge in the other graph. In Figure 2, G_1, G_2 are isomorphic.

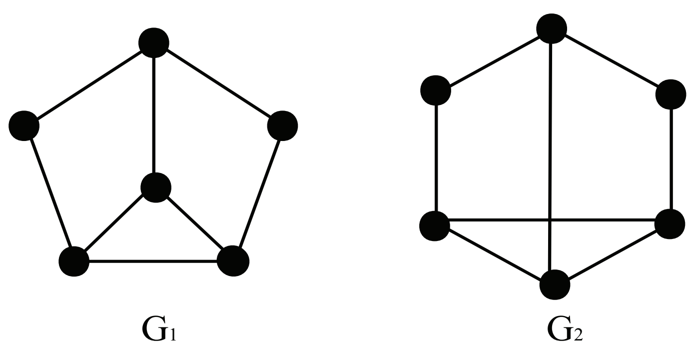

Figure 2: Two graphs are *isomorphic*.

- A **complete graph** on n vertices, K_n, is a simple graph that has all possible $\binom{n}{2}$ edges (i.e., every vertex is connected to every other vertex). See Figure 3 for some examples.

- If all of the vertices of a graph G have the same degree, then G is called a **regular graph**. Note that K_n is regular for all $n = 2, 3, \ldots$.

- A **polygon** on n vertices, P_n, is a finite connected graph that is regular of degree 2. See Figure 4 for some simple examples.

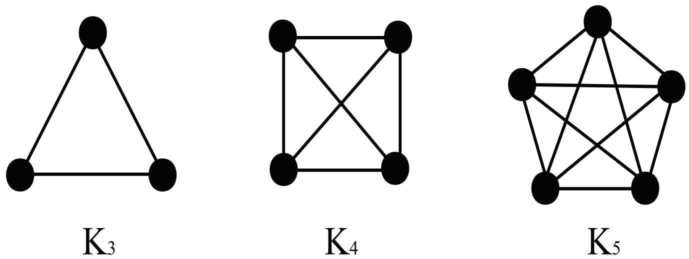

Figure 3: Some examples of *complete graph*.

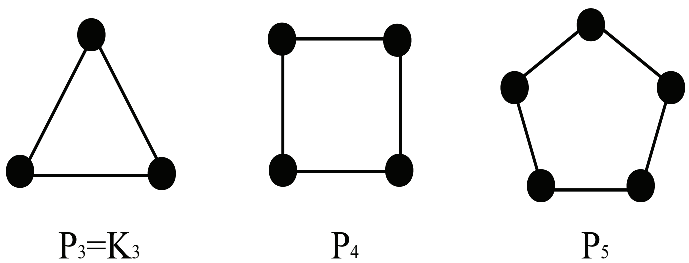

Figure 4: Some examples of *polygon*.

- A **complete bipartite graph**, $K_{n,m}$, is a simple graph on $n + m$ vertices $\{a_1, \ldots, a_n, b_1, \ldots, b_m\}$ such that $a_i \sim b_j$ for all $1 \leq i \leq n$, $1 \leq j \leq m$. Note that a complete bipartite graph is regular if and only if $n = m$. A simple example is shown in Figure 5.

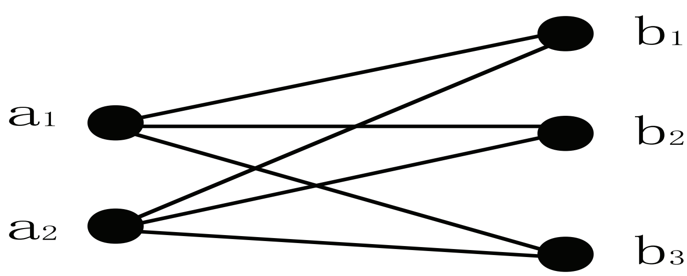

Figure 5: A *complete bipartite graph* with vertices a_1, a_2, b_1, b_2, b_3.

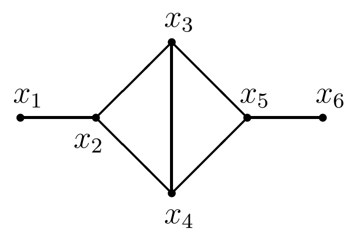

Figure 6: An example graph with 6 vertices

1.2 Matrices Associated with a Graph $G = (V, E)$

Definition 1.1. The **adjacency matrix** A of G consists of the following entries:

$$a_{uv} \triangleq \begin{cases} 1 & \text{if } u \sim v \\ 0 & \text{otherwise.} \end{cases}$$

So $A = (a_{uv}) \in \mathbb{R}^{N \times N}$, where $N = |V|$. Notice that for a multiple graph, we set $a_{uv} = \#(u, v)$ if $u \sim v$.

Definition 1.2. The **transition matrix** P of G consists of the following entries:

$$p_{uv} \triangleq \begin{cases} \frac{1}{m(u)} & \text{if } u \sim v \\ 0 & \text{otherwise.} \end{cases}$$

Then $P = (p_{uv}) \in \mathbb{R}^{N \times N}$, where $N = |V|$. Notice that for a multiple graph, $p_{uv} = \frac{a_{uv}}{m(u)}$ if $u \sim v$. It is not difficult to observe that p_{uv} represents the probability of a random walk from u to v in on step if we view the random walk to take each edge of a vertex with equal probability. And we have $\sum_{v \in V}^{N} p_{uv} = 1$ for all $u \in V$. We call such a matrix P a **stochastic matrix**.

Example 1.3. Given a graph G as shown in Figure 6. We can construct both the adjacency matrix A and the transition matrix P as:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \qquad P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Note that while $A^T = A$, $P^T \neq P$. The graph G is completely determined by A.

Now consider a function f on V, i.e., $f : V \to \mathbb{R}$. Let $B = A$ or P, then

$$Bf(u) = \sum_{v \in V} b_{uv} f(v), \quad u \in V.$$

Let

$$C(V) \triangleq \{\text{all functions defined on } V\}$$

and

$$C_0(V) \triangleq \{f \in C(V) \mid \operatorname{supp} f \text{ is a finite subset of } V\},$$

where $\operatorname{supp} f \triangleq \{u \in V \mid f(u) \neq 0\}$. Also define

$$L^2(V) \triangleq \{f \in C(V) \mid \|f\| = \sqrt{\langle f, f \rangle} < \infty\},$$

where $\langle f, g \rangle \triangleq \sum_{u \in V} m(u) f(u) g(u)$.

Lemma 1.4. *For all* $f, g \in L^2(V)$, $\langle Pf, g \rangle = \langle f, Pg \rangle$ *and* $\|Pf\| \leq \|f\|$.

Proof.

$$\begin{aligned} \langle Pf, g \rangle &= \sum_{u \in V} m(u) Pf(u) g(u) \\ &= \sum_{u \in V} (Af(u)) g(u) \\ &= \sum_{u \in V} f(u)(Ag(u)) \\ &= \sum_{u \in V} m(u) f(u) Pg(u) \\ &= \langle f, Pg \rangle . \end{aligned}$$

The proof that $\|Pf\| \leq \|f\|$ will be left as an exercise. (Hint: use the fact that P is a stochastic matrix, where $\sum_j p_{ij} = 1$ and $p_{ij} \geq 0$.)

$\square$

References

[1] J. H. VAN LINT AND R. M. WILSON, *A Course in Combinatorics*, 2nd Ed., Cambridge Univ. Press, 2001.

[2] H. URAKAWA, "Spectral geometry and graph theory," *Ouyou Suuri (Bulletin of the Japan Society of Industrial and Applied Mathematics)*, vol. 12, no. 1, pp. 29-45, 2002. In Japanese.