Spectral Graph Theory and Algorithms, Summer 2017	19 June 2017

Lecture 1

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1 Eigenvectors, Eigenvalues, and Graph Theory

Consider $A \in \mathbf{R}^{n\times x}$, $A = A^T$ (symmetric). If $Ax = \lambda x$, then for $x \in \mathbf{R}^n$, $\lambda \in \mathbf{R}$,

- x is an *eigenvector*;
- λ is the corresponding *eigenvalue*.

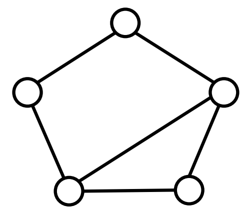
Eigenvectors and eigenvalues have applications in differential equations, mechanics, harmonic analysis, and many others.

An undirected graph G is represented as a tuple (V, E) consisting of a set of vertices V and a set of edges E. We are interested in paths, flows, cuts, colorings, cliques, spanning trees, etc. of the graph G.

This semester we will ask what graphs and eigenvalues have to do with each other.

2 An Introductory Example

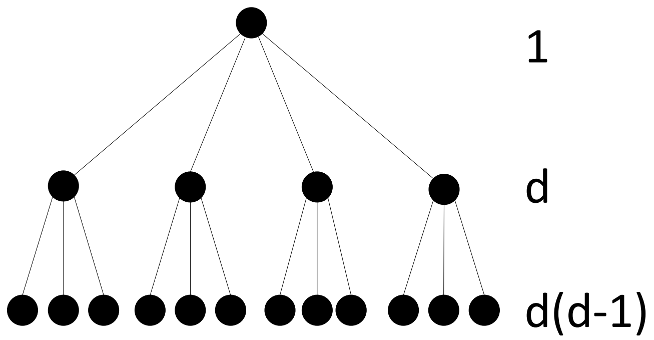
The diameter D of a graph is minimum length you would have to be able to travel to guarantee that you could go from any node in the graph to any other node. Formally, $D = \max_{i,j\in V}$[length of shortest i-j path]. A graph is said to be d-regular if all nodes are of degree d, where degree is defined as the number of edges incident on each vertex. The below graph has diameter 2 but is not d-regular since some nodes are of degree 2 and some are of degree 3.



For our introductory example[1], we will consider d-regular graphs of diameter 2 with as many nodes as possible. By starting at any node i, the graph could look like

[0]This lecture was drawn from Hoffman and Singleton, "Moore Graphs with Diameter 2 and 3", *IBM Journal of Research and Development* 5, 497–504, 1960; Trevisan, *Lecture Notes on Expansion, Sparsest Cut, and Spectral Graph Theory*, Chapter 1, and Lau's 2015 lecture notes, Lecture 1:`https://cs.uwaterloo.ca/~lapchi/cs798/notes/L01.pdf`. These notes are from scribe notes written by Matthew Zalesak and Qinru Shi.

[1]This material is taken from the article A.J. Hoffman, R.R. Singleton, "On Moore Graphs with Diameters 2 and 3," *IBM Journal*, pp. 497–504, November 1960.



In this graph, note that there are no connections between adjacent nodes in the first layer since we want to maximize the number of nodes in the graph. Also, the connections between the leaf nodes are omitted from the diagram. Based on the diagram, such a graph would have $n = 1 + d + d(d-1) = d^2 + 1$ nodes.

Let $A = (a_{ij})$ be the adjacency matrix of G, defined as

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

If $B = A^2$, then

$$b_{ij} = \sum_k a_{ik} a_{kj} = \text{ number of walks of 2 steps in graph } G \text{ from } i \text{ to } j.$$

Since this is a d-regular graph, we have that $b_{ii} = d$ since starting at i we can reach d vertices in one step and then immediately return.

Starting at i we reach every other vertex in G in exactly 0 steps, exactly 1 step, or exactly 2 steps (exclusive or). Thus,

$$I + A + A^2 - dI = J,$$

where I is the identity matrix and J is the matrix of all ones.

We'll need the following facts from linear algebra.

Fact 1 *For $A \in \mathbf{R}^{n\times n}$ symmetric, the following are true:*

- *All of the eigenvalues of A are real.*
- *There exist eigenvalues $\lambda_1, \ldots, \lambda_n$ (called the spectrum) and eigenvectors $x_1, \ldots, x_n$ such that $\langle x_i, x_j \rangle = x_i^T x_j = 0$ for $i \neq j$.*
- *The trace* $\operatorname{tr}(A) = \sum_{i=1}^n a_{ii} = \sum_{i=1}^n \lambda_i$.

We've discussed the notion of a d-regular graph with diameter two, but does such a graph exist? To answer this problem we can use linear algebra to tell us what such a graph would might look like.

First notice that $Ae = de$, where $e = (1, \ldots, 1)^T$ is the vector of all ones. This is true since A is d-regular. Thus, e is an eigenvector of A and d is the eigenvalue. Also notice that

$$A^2 e = A(Ae) = A(de) = d(Ae) = d^2 e.$$

Thus,

$$\begin{aligned}(I + A + A^2 - dI)e &= Je \\ e + de + d^2e - de &= ne\end{aligned}$$

So $n = d^2 + 1$, though we already knew that.

Now let v be any other eigenvector of A orthogonal to e. Then $v^T e = 0$, and thus $Jv = 0$. We have that $Av = \lambda v$ for some eigenvalue λ. Also, $A^2 v = A(Av) = A(\lambda v) = \lambda^2 v$. Thus

$$\begin{aligned}(I + A + A^2 - dI)v &= Jv \\ v + \lambda v + \lambda^2 v - \lambda v &= 0 \\ \implies 1 + \lambda + \lambda^2 - d &= 0\end{aligned}$$

So for all eigenvalues not corresponding to e, we have $\lambda = \frac{-1 \pm \sqrt{4d-3}}{2}$.

Given what we now know about the eigenvalues, what can we tell? We can invoke the trace! Notice that $tr(A) = 0$: $a_{ii} = 0$ for all i since there are no self-loops in the graph. Now we consider two possible cases.

1. If $\sqrt{4d-3}$ is irrational,

   then in order for the trace to sum to zero, the eigenvalues $\frac{-1+\sqrt{4d-3}}{2}$ and $\frac{-1-\sqrt{4d-3}}{2}$ must each have multiplicity $\frac{n-1}{2}$. Plugging this in gives

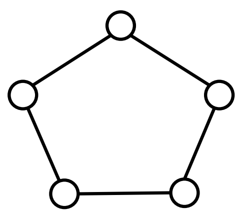
   $$\begin{aligned}tr(A) = 0 &= d + \frac{n-1}{d}\left(\frac{-1+\sqrt{4d-3}}{2} + \frac{-1-\sqrt{4d-3}}{2}\right) \\ &= d - \frac{n-1}{2} \\ &= d - \frac{d^2}{2} \\ \implies & d = 0 \text{ or } d = 2.\end{aligned}$$

   So the only possible graphs would be:

   (a) $d = 0$ A single node, which does not have diameter two.

   (b) $d = 2$ In this case $n = 5$, which gives the 5 cycle; the 5-cycle is a 2-regular graph of diameter 2.

2. If $\sqrt{4d-3}$ *is* rational,

then let $s^2 = 4d-3$. Let m be the multiplicity of the eigenvalue $\frac{-1+s}{2}$. Then

$$\begin{aligned} tr(A) &= d + m\left(\frac{-1+s}{2}\right) + (n-1-m)\left(\frac{-1-s}{2}\right) \\ &= 0 \end{aligned}$$

Using the fact that $d = \frac{1}{4}(s^2+3)$, we get $n-1 = d^2 = \frac{1}{16}(s^4+6s^2+9)$. So continuing

$$= \frac{1}{4}(s^2+3) + m\left(\frac{-1+s}{2}\right) + \left(\frac{1}{16}(s^4+6s^2+9) - m\right)\left(\frac{-1-s}{2}\right)$$

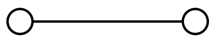
After simplifying the algebra, we find that

$$-s^5 - s^4 - 6s^3 + 2s^2 + (32m-9)s + 15 = 0.$$

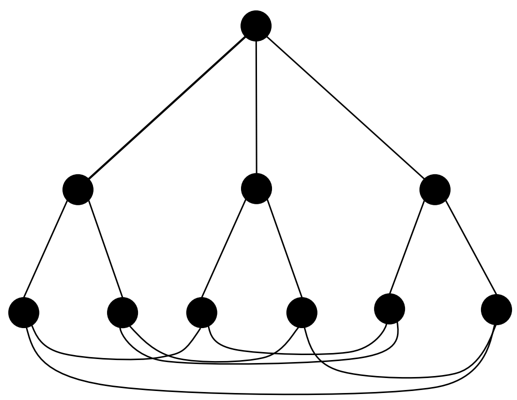
By the rational root theorem, we know that any solution to this polynomial must be a factor of 15. Thus, we can enumerate all possible roots.

Possibilities

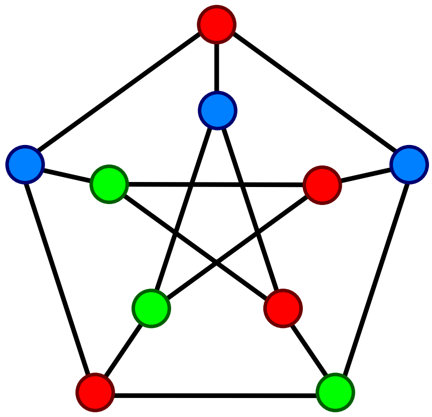
(a) $s = 1, d = 1, n = 2$
A 1-regular graph on 2 nodes is a single edge, but its diameter is not 2.



(b) $s = 3, d = 3, n = 10$
We can represent this graph in two ways:



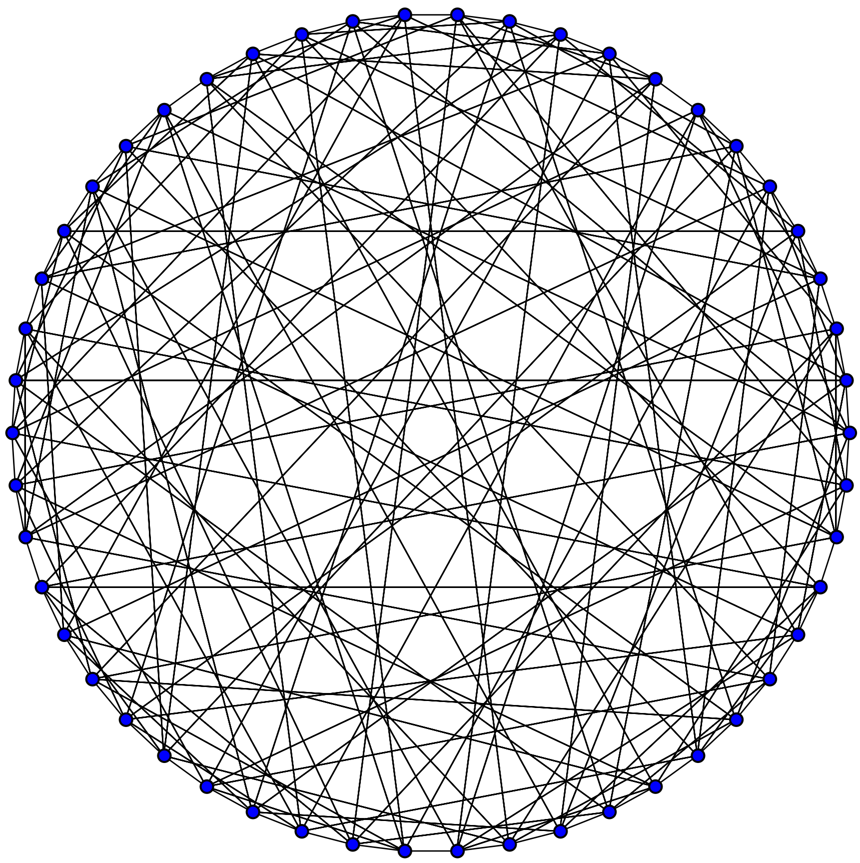
This first representation shows what the graph would look like using the same type of diagram we used earlier.



This second representation is often called the Petersen representation (*Image source: Wikipedia*), and the graph is called the *Petersen graph.* Petersen found it in the course of trying to find the smallest cubic (that is, 3-regular) bridgeless graph that could not be 3-edge-colored. A bridgeless graph is one such that the graph is still connected after removing any edge. A 3-edge-colorable graph is one in which we can color every edge with one of three colors such that at each vertex, all incident edges have different colors. The Petersen graph is also the smallest cubic bridgeless graph that does not have a Hamiltonian cycle. Knuth has called the Petersen graph "a remarkable configuration that serves as a counterexample to many optimistic predictions about what might be true for graphs in general."

(c) $s = 5, d = 7, n = 50$

This graph is known to exist and is called the Hoffman-Singleton graph (Hoffman, Singleton 1960).



(Image source: Wikipedia)

(d) $s = 15, d = 57, n = 3250$.

Does this graph exist? We don't know. This is a good research question!

This example is to give you a small taste of how eigenvectors can be useful in graph theory. By looking at the spectrum of d-regular graphs of diameter 2 with as many nodes as possible, we were able to come up with very strong restrictions on the possible values of d.

3 Definitions and Eigenvalue Basics

Let $x = a + ib \in \mathbb{C}$ be a complex number, then we define $\overline{x} = a - ib$ to be its *conjugate*. For a matrix of complex numbers $A = (x_{ij}) \in \mathbb{C}^{m\times n}$, we define $A^* = (z_{ij}) \in \mathbb{C}^{n\times m}$ where $z_{ij} = \overline{x}_{ji}$ for all $i \leq n$ and $j \leq m$. A^* is then called the *conjugate transpose* of A.

For $x, y \in \mathbb{C}^n$, their inner product is defined as

$$\langle x, y\rangle \equiv x^* y = \sum_{i=1}^{n} \overline{x}_i y_i$$

For $A \in \mathbb{C}^{n\times n}$, $\lambda \in \mathbb{C}$ and $x \neq 0 \in \mathbb{C}^n$, if $Ax = \lambda x$, then x is an *eigenvector* of A and λ is the associated *eigenvalue.*

Note that $Ax = \lambda x$ if and only if $Ax - \lambda I x = 0$, which is equivalent to $(\lambda I - A)x = 0$. For $x \neq 0$, we have

$$\det(\lambda I - A) = 0.$$

$\det(\lambda I - A)$ for fixed A is a polynomial of degree n in λ. We call it the *characteristic polynomial* of A. There are exactly n solutions to $\det(\lambda I - A) = 0$ (with multiplicity). Each solution is an eigenvalue.

A matrix A is *Hermitian* if $A = A^*$. If $A \in \mathbf{R}^{n\times n}$, then A is symmetric. ($A = A^T$)

Hermitian matrices have the following two nice properties.

Lemma 1 *If A is Hermitian, then all its eigenvalues are real.*

Proof: Suppose λ and $x \neq 0$ satisfy $Ax = \lambda x$. Then,

$$\begin{aligned}\langle Ax, x\rangle = (Ax)^* x = x^* A^* x \\ = x^* A x \\ = \langle x, Ax\rangle.\end{aligned}$$

Also, we have

$$\langle Ax, x\rangle = \langle \lambda x, x\rangle = \overline{\lambda}\langle x, x\rangle = \overline{\lambda}\|x\|^2$$

and

$$\langle x, Ax\rangle = \langle x, \lambda x\rangle = \lambda\langle x, x\rangle = \lambda\|x\|^2.$$

Since $x \neq 0$, $\lambda = \overline{\lambda}$, which means that λ is real. □

Lemma 2 *Let A be a Hermitian matrix. Suppose x and y are eigenvectors of A with different eigenvalues λ and λ' ($\lambda \neq \lambda'$). Then, x and y are orthogonal.*

Proof: Since A is Hermitian, we have

$$\langle Ax, y\rangle = (Ax)^* y = x^* A^* y = x^* A y = \langle x, Ay\rangle$$

By Lemma 1, λ and λ' are real, so

$$\langle Ax, y\rangle = \langle \lambda x, y\rangle = \lambda\langle x, y\rangle$$

and

$$\langle x, Ay\rangle = \langle x, \lambda' y\rangle = \lambda'\langle x, y\rangle.$$

Then,

$$(\lambda - \lambda')\langle x, y\rangle = 0.$$

Because $\lambda \neq \lambda'$, x and y must be orthogonal. □

4 Rayleigh Quotients and the Spectral Theorem

For the rest of the class, we are going to focus on real symmetric matrices. We assume that all matrices A that appear in this section are symmetric and $n \times n$. Our goal is to prove the following theorem, which will be extremely useful for the rest of the semester.

Theorem 3 *Let $A \in \mathbf{R}^{n\times n}$ be a symmetric matrix. Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be its eigenvalues (all real by Lemma 1) and $x_1, x_2, \cdots, x_n$ be orthonormal vectors (e.g. $\|x_i\|^2 = 1,\ \langle x_i, x_j\rangle = 0\ \ \forall i \neq j$) such that $Ax_i = \lambda_i x_i$ for $i = 1, 2, \cdots, n$. Then, for all $0 \leq k \leq n-1$,*

$$\lambda_{k+1} = \min_{x\in \mathrm{R}^n : x \perp span(x_1,\cdots,x_k)} \frac{x^T Ax}{x^T x}$$

and any minimizer is the associated eigenvector.

The expression $\frac{x^T Ax}{x^T x}$ is called the *Rayleigh quotient*. One reason this theorem is very useful is that it allows us to get an upper bound on λ_{k+1}: the Rayleigh quotient of x for any $x \perp \mathrm{span}(x_1, \cdots, x_k)$ yields an upper bound. We will be using this technique for bounding eigenvalues *ad nauseum.*

In order to prove the theorem, we first prove the following lemma.

Lemma 4 *Let $A \in \mathbf{R}^{n\times n}$ be symmetric and $k \leq n-1$. Let $x_1, \cdots, x_k$ be orthogonal eigenvectors of A. Then there exists an eigenvector x_{k+1} orthogonal to $x_1, \cdots, x_k$.*

Proof: Let V be a $(n-k)$-dimensional subspace of $\mathbf{R}^n$ that contains all $x \in \mathbf{R}^n$ such that $x \perp \mathrm{span}(x_1, \cdots, x_k)$. For any $x \in V$, $Ax \in V$ since for all $i = 1, \cdots, k$,

$$\langle x_i, Ax\rangle = x_i^T Ax = (A^T x_i)^T x = (Ax_i)^T x = (\lambda x_i)^T x = \lambda\langle x_i, x\rangle = 0.$$

Let $b_1, \cdots, b_{n-k}$ be an orthonormal basis of V. Define

$$B = \begin{bmatrix} | & | & & | \\ b_1 & b_2 & \cdots & b_{n-k} \\ | & | & & | \end{bmatrix} \in \mathbf{R}^{n\times(n-k)}.$$

For any $z \in \mathbf{R}^{n-k}$, $Bz \in V$ since Bz is a linear combination of vectors in V.

Also, for all $z \in V$,

$$BB^T z = B \begin{bmatrix} b_1^T z \\ b_2^T z \\ \vdots \\ b_{n-k}^T z \end{bmatrix} = \langle b_1, z\rangle b_1 + \cdots + \langle b_{n-k}, z\rangle b_{n-k} = z \tag{1}$$

since B is a orthonormal basis of V.

Let λ be an eigenvalue of $A' = B^T AB \in \mathbf{R}^{(n-k)\times(n-k)}$ with associated eigenvector y. Then,

$$B^T ABy = \lambda y.$$

We know $By \in V$, so $A(By) \in V$. By (1),

$$BB^T(ABy) = ABy.$$

On the other hand,

$$BB^T ABy = B(B^T ABy) = \lambda By,$$

so

$$ABy = \lambda By.$$

Since B is non-singular and $y \neq 0$, $By \neq 0$, so By is an eigenvector of A. Note that By is orthogonal to $x_1, \cdots, x_k$ because $By \in V$. $\square$

An easy corollary of Lemma 4 is the Spectral Theorem.

Corollary 5 *(Spectral Theorem) For a symmetric matrix $A \in \mathbf{R}^{n\times n}$ with (real) eigenvalues $\lambda_1, \cdots, \lambda_n$, there exist orthonormal vectors $x_1, \cdots, x_n$ such that x_i is the eigenvector associated with λ_i.*