1 Symmetric matrices and adjacency of a graph

In this section, we shall introduce the basic theory of symmetric matrices, including a result generally overlooked in a first or second linear algebra course. We shall define the adjacency matrix of a graph, and then make connections between the algebraic properties of this matrix and the combinatorial properties of the graph.

1.1 Symmetric matrices

We shall work over the vector space $\mathbb{R}^n$. If $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, then $\langle \mathbf{v}, \mathbf{u} \rangle = \mathbf{v}^T\mathbf{u}$ is an inner product (meaning, it is a positive-definite commutative bilinear form). A linear operator $\mathbf{M} : \mathbb{R}^n \to \mathbb{R}^n$ is self-adjoint if $\langle \mathbf{Mv}, \mathbf{u} \rangle = \langle \mathbf{v}, \mathbf{Mu} \rangle$ for all $\mathbf{u}$ and $\mathbf{v}$, and, because $\mathbf{M}$ can (and will) be seen as a square matrix, it follows that $\mathbf{M}$ is a self-adjoint operator if and only if $\mathbf{M} = \mathbf{M}^T$, that is, $\mathbf{M}$ is a symmetric matrix. Symmetric matrices enjoy two key important properties: they are diagonalizable by orthogonal eigenvectors, and all of their eigenvalues are real. We start proving both properties.

Lemma 1.1. *The eigenvalues of a real symmetric matrix are real numbers.*

Proof. Let $\mathbf{Mu} = \lambda\mathbf{u}$, with $\mathbf{u} \neq \mathbf{0}$. Some of these things could be complex numbers, so we can take the conjugate on both sides, recovering

$$\mathbf{M}\overline{\mathbf{u}} = \overline{\lambda}\overline{\mathbf{u}}.$$

Thus $\overline{\mathbf{u}}$ is an eigenvector with eigenvalue $\overline{\lambda}$. Thus

$$\lambda\mathbf{u}^T\overline{\mathbf{u}} = (\mathbf{Mu})^T\overline{\mathbf{u}} = \mathbf{u}^T(\mathbf{M}\overline{\mathbf{u}}) = \overline{\lambda}\mathbf{u}^T\overline{\mathbf{u}}.$$

Because $\mathbf{u}^T\overline{\mathbf{u}} \neq 0$ if $\mathbf{u} \neq 0$, then $\lambda = \overline{\lambda}$. □

Now simply assume whenever we are dealing with a symmetric matrix, its eigenvalues are real, and any eigenvector can be assumed to be real.

Lemma 1.2. *Let $\mathbf{M}$ be a real symmetric matrix, and assume $\mathbf{u}$ and $\mathbf{v}$ are eigenvectors associated to different eigenvalues. Then $\mathbf{v}^T\mathbf{u} = 0$, that is, they are orthogonal.*

Proof. Say $\mathbf{Mu} = \lambda\mathbf{u}$ and $\mathbf{Mv} = \mu\mathbf{v}$, with $\lambda \neq \mu$. It follows that

$$\lambda(\mathbf{v}^T\mathbf{u}) = \mathbf{v}^T\mathbf{Mu} = (\mathbf{v}^T\mathbf{Mu})^T = \mathbf{u}^T\mathbf{M}^T\mathbf{v} = \mathbf{u}^T\mathbf{Mv} = \mu(\mathbf{u}^T\mathbf{v}) = \mu(\mathbf{v}^T\mathbf{u}).$$

As $\lambda \neq \mu$, it must be that $\mathbf{v}^T\mathbf{u} = 0$. □

The lemma above already implies that if $\mathbf{M}$ is diagonalizable, then it is diagonalizable with orthogonal eigenvectors — as, in fact, we eigenvectors corresponding to distinct eigenvalues are orthogonal, and inside each eigenspace we can always find an orthogonal basis. We move forward.

A subspace U of $\mathbb{R}^n$ is said to be $\mathbf{M}$-invariant if, for all $\mathbf{u} \in U$, $\mathbf{Mu} \in U$. This is a key fundamental concept in linear algebra, and several results are proven by noting that certain subspaces are invariant for certain operator.

Lemma 1.3. *Let $\mathbf{M}$ be a real symmetric matrix. If U is $\mathbf{M}$-invariant, then $U^\perp$ is also $\mathbf{M}$-invariant.*

Proof. Note that $\mathbf{v} \in U^\perp$, by definition, if $\mathbf{v}^T\mathbf{u} = 0$ for all $\mathbf{u} \in U$. For all $\mathbf{u} \in U$ and $\mathbf{v} \in U^\perp$, note that

$$(\mathbf{Mv})^T\mathbf{u} = \mathbf{v}^T\mathbf{Mu} = \mathbf{v}^T(\mathbf{Mu}) = 0,$$

because $\mathbf{u} \in U$, U is $\mathbf{M}$-invariant, and so $\mathbf{Mu} \in U$, and $\mathbf{v} \in U^\perp$. Thus $\mathbf{Mv} \in U^\perp$, as we wanted. □

Let λ be such that $\det(\lambda\mathbf{I} - \mathbf{M}) = 0$. Then $\lambda\mathbf{I} - \mathbf{M}$ is singular, and therefore it contains at least one non-zero vector in its kernel. This is saying that all square matrices $\mathbf{M}$ contain at least one eigenvector for each root of $\phi_{\mathbf{M}}(x) = \det(x\mathbf{I} - \mathbf{M})$. As $\mathbf{M}$ is symmetric, we now know that all possible roots of $\phi_{\mathbf{M}}$ are real.

Lemma 1.4. *Let U be an $\mathbf{M}$-invariant subspace with dimension ≥ 1. Then there is one eigenvector of $\mathbf{M}$ in U.*

Proof. Let $\mathbf{P}$ be a matrix whose columns form an orthonormal basis for U. As U is $\mathbf{M}$-invariant, it follows that there is a matrix $\mathbf{N}$ so that

$$\mathbf{MP} = \mathbf{PN}.$$

(Stop now and think carefully why this equality is true.) In particular, $\mathbf{N} = \mathbf{P}^T\mathbf{MP}$, so $\mathbf{N}$ is symmetric. Let $\mathbf{u}$ be one eigenvector of $\mathbf{N}$ with eigenvalue λ. Then

$$\mathbf{MPu} = \mathbf{PNu} = \lambda\mathbf{Pu},$$

and, moreover $\mathbf{Pu} \neq \mathbf{0}$, as the columns of $\mathbf{P}$ are linearly independent. Thus $\mathbf{Pu}$ is an eigenvector for $\mathbf{M}$ in U. □

These four lemmas above are all you need to prove the following result by induction as an exercise.

Theorem 1.5. *Let $\mathbf{M}$ be a real symmetric matrix. Then $\mathbf{M}$ is diagonalizable by set of orthogonal eigenvectors, all of them corresponding to real eigenvalues.*

Exercise 1.6. Write the proof of this theorem as an exercise.

Corollary 1.7. *Let $\mathbf{v}_1, ..., \mathbf{v}_n$ be an orthonormal basis of eigenvectors for $\mathbf{M}$, each corresponding to an eigenvalue $\lambda_1, ..., \lambda_n$ (these are not necessarily distinct). Let $\mathbf{P}$ be the matrix whose ith column is $\mathbf{v}_i$, and Λ the diagonal matrix whose ith diagonal element is λ_i. Then*

$$\mathbf{P}^T\mathbf{MP} = \mathbf{\Lambda},$$

and

$$\mathbf{M} = \lambda_1(\mathbf{v}_1\mathbf{v}_1^T) + ... + \lambda_n(\mathbf{v}_n\mathbf{v}_n^T).$$

Proof. A linear operator is defined and determined by its action on a basis. The first equality follows from the fact that both sides act equally on the canonical basis of $\mathbb{R}^n$. The second follows from

$$\mathbf{M} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^T,$$

and, by definition of matrix product, $\mathbf{M} = \mathbf{v}_1(\lambda_1\mathbf{v}_1^T) + ... + \mathbf{v}_n(\lambda_n\mathbf{v}_n^T)$. □

You should recall right now that, because $\mathbf{v}_i$ is normalized, then $\mathbf{P}_i = \mathbf{v}_i\mathbf{v}_i^T$ is the matrix that represents the orthogonal projection onto the line spanned by $\mathbf{v}_i$, that is, $\mathbf{P}_i$ is a projection as $\mathbf{P}_i^2 = \mathbf{P}_i$, and it is an orthogonal projection as $\mathbf{P}_i$ is symmetric. Note that $\mathbf{P}_i\mathbf{P}_j = \mathbf{0}$ whenever $i \neq j$, and so any sum of the $\mathbf{P}_i$s for distinct indices will correspond to the orthogonal projection onto the space spanned by the $\mathbf{v}_i$s of the same indices. In particular $\sum_{i=1}^n \mathbf{P}_i = \mathbf{I}$.

Exercise 1.8. Assume $\mathbf{P}_i$s are orthogonal projections. Show that $\mathbf{P}_1 + \mathbf{P}_2$ is an orthogonal projection if and only if $\mathbf{P}_1\mathbf{P}_2 = \mathbf{0}$.

Show now that $\mathbf{P}_1 + ... + \mathbf{P}_k$ is an orthogonal projection if and only if $\mathbf{P}_i\mathbf{P}_j = \mathbf{0}$ for $i \neq j$.

Say $\mathbf{M}$ is an $n \times n$ symmetric matrix with distinct eigenvalues $\theta_0, ..., \theta_d$. When we write the second equation from the statement of Corollary 1.7, we can collect the terms corresponding to equal eigenvalues, and have

$$\mathbf{M} = \sum_{r=0}^{d} \theta_r \mathbf{E}_r, \tag{1}$$

where, according to the discussion above, each $\mathbf{E}_r$ corresponds to the orthogonal projection onto the θ_r eigenspace. Equation (1) is usually referred to the as the *spectral decomposition* of the matrix $\mathbf{M}$.

Exercise 1.9. Find the spectral decomposition of

$$\mathbf{M} = \begin{pmatrix} 1+\sqrt{2} & 0 & 1-\sqrt{2} & 0 \\ 0 & 1+\sqrt{2} & 0 & 1-\sqrt{2} \\ 1-\sqrt{2} & 0 & 1+\sqrt{2} & 0 \\ 0 & 1-\sqrt{2} & 0 & 1+\sqrt{2} \end{pmatrix}$$

Hint: do not try to compute the characteristic polynomial. It is easier to simply try to look and guess which are the eigenvectors and eigenvalues.

Note that the $\mathbf{E}_r$ are symmetric matrices satisfying $\mathbf{E}_r\mathbf{E}_s = \delta_{rs}\mathbf{E}_r$, and $\sum_{r=0}^d \mathbf{E}_r = \mathbf{I}$.

Exercise 1.10. Prove (or at least convince yourself) that for any polynomial $p(x)$, it follows that

$$p(\mathbf{M}) = \sum_{r=0}^{d} p(\theta_r)\mathbf{E}_r.$$

Exercise 1.11. Let $\mathbf{M}$ be a symmetric matrix, with spectral decomposition as in (1).
(A) What is the minimal polynomial of $\mathbf{M}$? (B) Prove that for each $\mathbf{E}_r$, there is a polynomial p_r of degree d so that $p_r(\mathbf{M}) = \mathbf{E}_r$. Describe this polynomial as explicitly as you can.

Exercise 1.12. Prove that two symmetric matrices $\mathbf{M}$ and $\mathbf{N}$ commute if and only if they can be simultaneously diagonalized by the same set of orthonormal eigenvectors. Is it true that if $\mathbf{M}$ and $\mathbf{N}$ commute, then there is always a polynomial p so that $p(\mathbf{M}) = \mathbf{N}$? Characterize what else you need to observe to guarantee that such polynomial exists.

Exercise 1.13. Let $\mathbf{A}$ and $\mathbf{B}$ be matrices (not necessarily squared shaped), so that both products $\mathbf{AB}$ and $\mathbf{BA}$ are defined. Prove that

$$\operatorname{tr} \mathbf{AB} = \operatorname{tr} \mathbf{BA},$$

and conclude that if $\mathbf{M}$ is a symmetric matrix with eigenvalues $\lambda_1, ..., \lambda_n$, then $\operatorname{tr} \mathbf{M}$ is equal to $\lambda_1 + ... + \lambda_n$. How about $\operatorname{tr} \mathbf{M}^2$?

1.2 The adjacency matrix of a graph

Given a graph G on a vertex set V, one can always define an arbitrary ordering to the vertices, that is, let $V = \{a_1, ..., a_n\}$, and encode the graph as a symmetric 01-matrix as follows. *The adjacency matrix* $\mathbf{A}$ of G is defined as $\mathbf{A}_{ij} = 1$ of $a_i \sim a_j$, and $\mathbf{A}_{ij} = 0$ otherwise (including the diagonal elements).

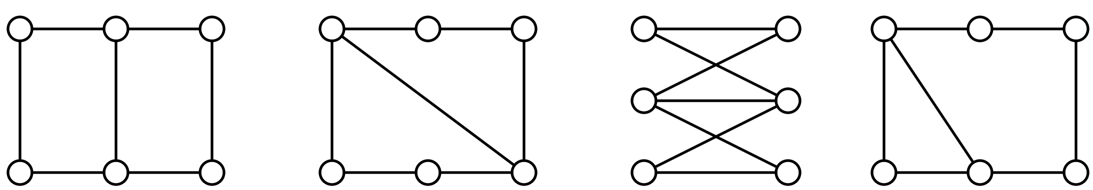
The field of spectral graph theory concerns itself with the main problem of relating spectral properties of matrices that encode adjacency in a graph (such as $\mathbf{A}$) with the combinatorial properties of the graph. We shall see several examples of such relations.

Exercise 1.14. Let G be a graph, suppose the vertices V are ordered, and let $\mathbf{A}$ be the corresponding adjacency matrix of G. Suppose you reorder the vertices by means of a permutation. Let $\mathbf{P}$ be the 01 matrix representing this permutation. Show that the new adjacency matrix obtained from this re-ordering is $\mathbf{PAP}^T$. Conclude that the eigenvalues are the same, and the only change in the eigenvectors is a permutation of its entries.

Because of this exercise, we shall simply ignore the underlying ordering, and speak of "the" adjacency matrix of G.

Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ on the same number of vertices, a very natural question is whether or not they encode the same combinatorial structure, which can be translated as: is there a function $f : V_1 \to V_2$ that maps edges to edges and non-edges to non-edges? Such a function, if it exists, is called a *graph isomorphism*. You can think of an isomorphism like this: draw both graphs in the plane, and try to move the vertices of one of them (without creating or destroying edges) so that the two drawings look exactly the same.

Example 1.15. Graphs G_1, G_2 and G_3 are all isomorphic, but G_4 is "different".



G_1 G_2 G_3 G_4

Two isomorphic graphs can always be seen as graphs on the same vertex set, and the isomorphism is a re-ordering that preserves adjacency and non-adjacency. Thus:

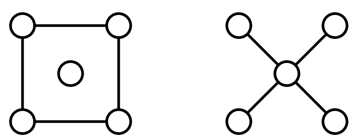
Theorem 1.16. *Let G and H be isomorphic graphs. Order their vertex sets from 1 to n, and let $\mathbf{P}$ be the permutation matrix that corresponds to the isomorphism from G to H. Then*

$$\mathbf{P}\mathbf{A}(G)\mathbf{P}^T = \mathbf{A}(H).$$

As a consequence, $\mathbf{A}(G)$ and $\mathbf{A}(H)$ have the same eigenvalues. □

Exercise 1.17. Order the vertices of G_1 and G_2 equally in terms of their geometric position. Then find the matrix $\mathbf{P}$ so that $\mathbf{P}\mathbf{A}(G_1)\mathbf{P} = \mathbf{A}(G_2)$. Compute the eigenvalues of G_1 and G_4 (using a software?) and conclude that they cannot be isomorphic.

One of the motivations of the development of spectral graph theory was the hope that two graphs would be isomorphic if and only if they had the same eigenvalues. Such a claim would immediately provide an efficient polynomial time algorithm to decide whether two graphs are isomorphic (and yet no such algorithm is known to this day). Two graphs with the same eigenvalues are called *cospectral graphs*. The following pair of graphs are the smallest known cases of cospectral but (clearly) non-isomorphic graphs. They have spectrum $2, 0^{(3)}, -2$.



G_1 G_2

This example also shows that the spectrum of a graph does not determine whether the graph is connected or not. This immediately raises the general question: what graph properties can be determined from the spectrum?

A *walk* of length r in a graph G is a sequence of $r+1$ (possibly repeated) vertices $a_0, ..., a_r$ with the property that $a_i \sim a_j$. A walk is *closed* if $a_0 = a_r$.

Lemma 1.18. *The number of distinct walks of length r from a to b in G is precisely equal to $(\mathbf{A}^r)_{ab}$.*

Exercise 1.19. Verify this result on at least 3 different graphs checking powers $r = 1, 2, 3$ for each. Then, sketch a proof by induction of this result.

Corollary 1.20. *If G has diameter D, then it must have at least $D+1$ distinct eigenvalues.*

Proof. Let

$$\mathbf{A}(G) = \sum_{r=0}^{d} \theta_r \mathbf{E}_r$$

be the spectral decomposition of $\mathbf{A}(G)$. Let W be the subspace of $\mathrm{Sym}_n(\mathbb{R})$ generated by $\{\mathbf{A}^0, \mathbf{A}, \mathbf{A}^2, ...\}$. As we saw in the past section, all powers of $\mathbf{A}$ are a linear combinations of the $\mathbf{E}_r$s, and each $\mathbf{E}_r$ is a polynomial in $\mathbf{A}$. Moreover, the matrices $\mathbf{E}_r$ are pairwise orthogonal, thus they are all linearly independent. As a consequence, $\dim W = d + 1$, and $\{\mathbf{E}_0, ..., \mathbf{E}_d\}$ form a basis for W. Now observe that if $r \leq D$, then at least one entry of $\mathbf{A}^r$ is non-zero "for the first time", meaning that it was equal to 0 for all smaller powers of $\mathbf{A}$. Thus $\{\mathbf{A}^0, \mathbf{A}, \mathbf{A}^2, ..., \mathbf{A}^D\}$ form a linearly independent set in W, and $D \leq d$. □

Let us now return to the problem of deciding what can be determined by the spectrum of a graph alone. Clearly the number of vertices in a graph is determined by the spectrum. An immediate consequence of the Lemma 1.18 is that the number of edges is also determined by the spectrum.

Corollary 1.21. *Let G be a graph on n vertices, with m edges, and let $\lambda_1, ..., \lambda_n$ the eigenvalues of $\mathbf{A}(G)$. Then*

$$\lambda_1^2 + ... + \lambda_n^2 = 2m.$$

Proof. Both sides are equal to $\operatorname{tr} \mathbf{A}^2$. □

Exercise 1.22. Find a formula for the number of triangles (cycles of length 3) found as subgraphs of G that depends only on the eigenvalues of G. Explain why the number of cycles of length 4 is not determined by the spectrum alone (as you witnessed in the example above).

Exercise 1.23. Does the spectrum alone determines the length of the shortest odd cycle of a graph? Explain.

Exercise 1.24. If G has n vertices, prove that all eigenvalues lie in the interval $(-n, n)$.

Exercise 1.25. Let G be a k-regular graph (that is, all vertices have k neighbours). Prove that k is an eigenvalue for G by describing a corresponding eigenvector.

Let $\mathbf{J}$ stand for the matrix whose all entries are equal to 1. If G is a graph, let $\overline{G}$ stand for the complement graph of G, that is, the graph whose edges are precisely the non-edges of G. Then, clearly,

$$\mathbf{A}(\overline{G}) = \mathbf{J} - \mathbf{A}(G) - \mathbf{I}.$$

As immediate consequence of the past exercise, we have:

Lemma 1.26. *Let G be a k-regular graph, with eigenvalues $k = \lambda_1, ..., \lambda_n$. Then the eigenvalues of $\overline{G}$ are*

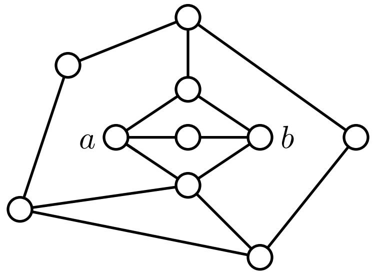
$$n - k - 1,\ -\lambda_2 - 1,\ ...,\ -\lambda_n - 1.$$

Proof. The all 1s vector $\mathbf{1}$ is an eigenvector of G. Let $\mathbf{v}_2, ..., \mathbf{v}_n$ complete a basis of orthogonal eigenvectors. Then

$$(\mathbf{J} - \mathbf{A}(G) - \mathbf{I})\mathbf{1} = (n - k - 1)\mathbf{1} \quad \text{and} \quad (\mathbf{J} - \mathbf{A}(G) - \mathbf{I})\mathbf{v}_i = -\lambda_i - 1,$$

as $\mathbf{J}\mathbf{v}_i = \mathbf{0}$ because $\mathbf{1}$ and $\mathbf{v}_i$ are orthogonal. □

Exercise 1.27. Assume G contains a pair of vertices a and b so that the neighbourhood of a is equal to neighbourhood of b (the rest of the graph can be anything). For example:



(a) Prove that 0 is an eigenvalue of this graph (Hint: look at a and b and try to produce one eigenvector for 0). If the example looks too complicate, forget about the 5-cycle and focus only on a, b and their neighbours.

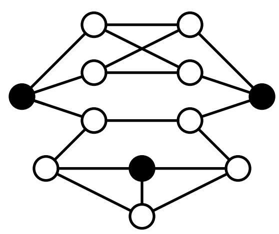
(b) What could you say if a and b shared the same neighbourhood, but were also neighbours themselves?

Exercise 1.28. Assume $G = (V, E)$ is a k-regular graph which contains a subset of vertices $U \subseteq V$ satisfying the following properties:

(a) No two vertices in U are neighbours.

(b) Any vertex in $V \backslash U$ contains exactly one neighbour in U.

Prove that if such U exists, then -1 is an eigenvalue of the graph. (Hint: recall G is assumed to be k-regular, and, again, try to produce one eigenvector. Try first in the example below, where the dark vertices are the vertices in U.)



In this next section, we shall see that two important properties about a graph can be determined from its spectrum alone: whether the graph is regular, and whether the graph is bipartite.

1.3 Perron-Frobenius (a special case)

Let $\mathbf{M}$ be a real $n \times n$ matrix with nonnegative entries. For example, the adjacency matrix of a graph. This matrix is called primitive if, for some integer k, $\mathbf{M}^k > 0$, and it is called irreducible if for all indices i and j, there is an integer k so that $(\mathbf{M}^k)_{ij} > 0$. All primitive matrices are irreducible, but the converse is not necessarily true.

Example 1.29. Consider

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad , \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Verify that the first is primitive, the second and third are both irreducible, but not primitive, and the fourth is neither.

Exercise 1.30. Prove that if $\mathbf{M}$ is irreducible, then $\mathbf{I} + \mathbf{M}$ is primitive.

Exercise 1.31. Let G be a graph. Show that

(a) $\mathbf{A}(G)$ is irreducible if and only if G is connected.

(b) $\mathbf{A}(G)$ is not primitive if G is bipartite.

Over the next few results, we shall actually see, amongst other things, that $\mathbf{A}(G)$ is irreducible but not primitive if and only if G is connected and bipartite. Results below are known as the Perron-Frobenius theory. This theory applies generally to matrices which are assumed to be irreducible and nothing else. We shall however add the hypothesis that the matrices are also symmetric, for the proofs become simpler and more meaningful, and our matrices will almost always be symmetric anyway.

Our first observation.

Lemma 1.32. *Let $\mathbf{M}$ be a nonnegative symmetric matrix, $\mathbf{M} \neq \mathbf{0}$. If λ is the largest eigenvalue of $\mathbf{M}$, then $\lambda > 0$.*

Proof. Follows immediately from $\operatorname{tr} \mathbf{M} \geq 0$. □

For any nonzero vector $\mathbf{u} \in \mathbb{R}^n$, and symmetric matrix $\mathbf{M}$, define

$$R_{\mathbf{M}}(\mathbf{u}) = \frac{\mathbf{u}^T \mathbf{M} \mathbf{u}}{\mathbf{u}^T \mathbf{u}}.$$

This is known as the Rayleigh quotient of $\mathbf{u}$ with respect to $\mathbf{M}$. Note that $R_{\mathbf{M}}(\alpha \mathbf{u}) = R_{\mathbf{M}}(\mathbf{u})$ for all $\alpha \neq 0$, so we shall typically assume $\mathbf{u}$ has been normalized. In a sense, this is a measurement of how much $\mathbf{M}$ displaces $\mathbf{u}$, also proportional to how much $\mathbf{M}$ stretches or shrinks $\mathbf{u}$. Therefore one should expect that this is maximum when $\mathbf{u}$ is an eigenvector of $\mathbf{M}$, corresponding to a large eigenvalue.

Lemma 1.33. *If $\mathbf{u}$ is eigenvector of $\mathbf{M}$ with eigenvalue θ, then $R_{\mathbf{M}}(\mathbf{u}) = \theta$. If λ is the largest eigenvalue of $\mathbf{M}$, then, for all $\mathbf{v} \in \mathbb{R}^n$, $R_{\mathbf{M}}(\mathbf{v}) \leq \lambda$. Equality holds for some $\mathbf{v}$ only if $\mathbf{v}$ is eigenvector for λ.*

Proof. Only the second and third assertions deserve a proof. Let $\mathbf{M} = \sum_{r=0}^{d} \theta_r \mathbf{E}_r$ be the spectral decomposition of $\mathbf{M}$. Assume θ_0 is the largest eigenvalue, and that $\mathbf{v}$ is a normalized vector. Then

$$\begin{aligned} R_{\mathbf{M}}(\mathbf{v}) = \mathbf{v}^T \mathbf{M} \mathbf{v} &= \theta_0(\mathbf{v}^T E_0 \mathbf{v}) + \theta_1(\mathbf{v}^T E_1 \mathbf{v}) + ... + \theta_d(\mathbf{v}^T E_d \mathbf{v}) \\ &\leq \theta_0((\mathbf{v}^T E_0 \mathbf{v}) + (\mathbf{v}^T E_1 \mathbf{v}) + ... + (\mathbf{v}^T E_d \mathbf{v}) = \theta_0. \end{aligned}$$

Equality holds if and only if $(\mathbf{v}^T E_r \mathbf{v}) = 0$ for all $r > 0$, which is the same as saying that $\mathbf{v}$ belongs to the θ_0 eigenspace. □

Lemma 1.34. *Let* $\mathbf{M}$ *be symmetric, non-negative and irreducible, with largest eigenvalue* λ*. There is a corresponding eigenvector* $\mathbf{u}$ *to* λ *so that* $\mathbf{u} > \mathbf{0}$*.*

Proof. Let $\mathbf{v}$ be a normal eigenvector for λ, and define $\mathbf{u}$ to be made from $\mathbf{v}$ by taking the absolute value at each entry (also denoted by $\mathbf{u} = |\mathbf{v}|$). Note that $\mathbf{u}$ is still normal, and, moreover

$$\lambda = R_{\mathbf{M}}(\mathbf{v}) = |R_{\mathbf{M}}(\mathbf{v})| \leq R_{\mathbf{M}}(\mathbf{u}) \leq \lambda.$$

(Second equality follows from $\lambda > 0$. First inequality from is simply the triangle inequality. Second follows from Lemma 1.33.)

Hence $R_{\mathbf{M}}(\mathbf{u}) = \lambda$, and $\mathbf{u}$ is an eigenvector for λ, with $\mathbf{u} \geq \mathbf{0}$. To see that $\mathbf{u} > \mathbf{0}$, note that as $\mathbf{M}$ is irreducible, it follows from Exercise 1.30 that $\mathbf{I} + \mathbf{M}$ is primitive, and so there is a k so that $(\mathbf{I}+\mathbf{M})^k > \mathbf{0}$. The vector $\mathbf{u}$ is also eigenvector for this matrix (with eigenvalue $(1+\lambda)^k$, but

$$\mathbf{0} < (\mathbf{I}+\mathbf{M})^k\mathbf{u} = (1+\lambda)^k\mathbf{u},$$

implying $\mathbf{u} > \mathbf{0}$. □

Lemma 1.35. *The largest eigenvalue* λ *of a symmetric, non-negative and irreducible matrix is simple (meaning, its eigenspace has dimension 1).*

Proof. From the proof of the past lemma, we know that no eigenvector for λ contains an entry equal to 0. No subspace of dimension larger than 1 can be such that all of its non-zero vectors have no non-zero entries. □

And finally:

Lemma 1.36. *Let* $\mathbf{M}$ *be symmetric, non-negative and irreducible. Let* λ *be its largest eigenvalue. Let* μ *be any other eigenvalue. Then* $\lambda \geq |\mu|$*, and, moreover, if* $-\lambda$ *is an eigenvalue, then* $\mathbf{M}^2$ *is not irreducible.*

Proof. Let $\mathbf{v}$ be an eigenvector for μ. As $\mathbf{v}$ is orthogonal to the positive eigenvector corresponding to λ, at least one entry of $\mathbf{v}$ is negative. Thus

$$|\mu| = |R_{\mathbf{M}}(\mathbf{v})| < R_{\mathbf{M}}(|\mathbf{v}|) \leq \lambda.$$

Now note that λ^2 is the largest eigenvalue of $\mathbf{M}^2$ (which is, still, symmetric and non-negative). If $-\lambda$ is eigenvalue of $\mathbf{M}$, then the eigenspace of λ^2 in $\mathbf{M}^2$ is at least 2-dimensional, thus $\mathbf{M}^2$ cannot be irreducible. □

It is quite surprising at first sight that the hypothesis on $\mathbf{M}$ being symmetric can be dropped entirely from the results above. The geometric intuition remains the same: a nonnegative irreducible matrix acts in the nonnegative orthant and there it encounters a unique direction which is an eigenvector. The proofs of these results are not hard per se, but I didn't feel they would add much to this notes. You are however invited to check any reference on spectral graph theory or non-negative matrix theory to find your favourite version of these results.

Now, to the applications.

Theorem 1.37. *Let $\mathbf{A}$ be the adjacency matrix of a connected graph G, and $\lambda_1 \geq ... \geq \lambda_n$ its spectrum.*

(a) G is k-regular if and only if $(1/n)(\lambda_1^2 + ... + \lambda_n^2) = \lambda_1$, and, in this case, $k = \lambda_1$.

(b) G is bipartite if and only if $\lambda_1 = -\lambda_n$. If this is the case, then for all λ_i, $-\lambda_i$ is also an eigenvalue.

Proof.

(a) Let $\mathbf{1}$ be the all 1s vector. The equality is equivalent to

$$R_{\mathbf{A}}(\mathbf{1}) = \lambda_1,$$

which, as we saw, is equivalent to $\mathbf{1}$ being an eigenvector of λ_1. This vector is eigenvector if and only if all row sums of $\mathbf{A}$ are equal, or, equivalently, all vertices have the same degree, which is going to be precisely equal to the eigenvalue λ_1.

(b) If G is bipartite, its adjacency matrix can always be written as

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{0} \end{pmatrix}.$$

If $\begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{pmatrix}$ is eigenvector for λ_i, then it is easy to see that $\begin{pmatrix} \mathbf{v}_1 \\ -\mathbf{v}_2 \end{pmatrix}$ is eigenvector for $-\lambda_i$. On the other hand, if $-\lambda_1$ is eigenvalue, then, from Lemma 1.36, it follows that $\mathbf{A}^2$ is not irreducible. Thus there are at least two vertices you can never walk from one to another with an even number of steps. Therefore there can be no odd cycles in this graph.

□

Corollary 1.38. *Let λ be the largest eigenvalue of $\mathbf{A}(G)$. Let Δ be the largest degree of G, and let ∂ be its average degree. Then*

$$\partial \leq \lambda \leq \Delta.$$

Proof. The first inequality follows from the fact that

$$\partial = R_{\mathbf{A}}(\mathbf{1}) \leq \lambda.$$

(Note in particular that this implies $\lambda \geq \delta$, where δ is the smallest degree of G). For the second, we have $\mathbf{A1} \leq \Delta\mathbf{1}$, and with $\mathbf{v}$ eigenvector for λ, we can multiply by $\mathbf{v}^T$ on the left. As $\mathbf{v} > \mathbf{0}$, the sign is preserved, and

$$\lambda \mathbf{v}^T \mathbf{1} = \mathbf{v}^T \mathbf{A} \mathbf{1} \leq \Delta \mathbf{v}^T \mathbf{1},$$

so $\theta \leq \Delta$. □

Exercise 1.39. Prove that $\lambda \geq \sqrt{\Delta}$. (Hint: look at $\mathbf{A}^2$ and the proof above).

1.4 Eigenvalues of some classes of graphs

Consider the following classes of graphs:

(a) K_n - complete graphs on n vertices.

(b) $K_{a,b}$ - complete bipartite graphs with a vertices on one side, and b vertices on the other (in particular if $a = 1$, these are the stars).

(c) C_n - cycle graphs on n vertices.

(d) P_n - path graphs on n vertices.

Our goal here is to determine the eigenvalues (and eigenvectors) of these classes.

(a) This is easy. $\mathbf{A}(K_n) = \mathbf{J} - \mathbf{I}$. The eigenvalues of $\mathbf{J}$ are n (simple, with eigenvector $\mathbf{1}$) and 0 (all others). Thus the spectrum of K_n is $n-1$ and -1.

(b) Write

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{J}_{a,b} \\ \mathbf{J}_{b,a} & \mathbf{0} \end{pmatrix}.$$

There are $b-1$ vectors in the kernel of $\mathbf{J}_{a,b}$ and $a-1$ vectors in the kernel of $\mathbf{J}_{b,a}$. Each corresponding to an eigenvector for the eigenvalue 0 of $\mathbf{A}$. The two eigenvectors remaining are

$$\begin{pmatrix} \sqrt{b}\mathbf{1} \\ \sqrt{a}\mathbf{1} \end{pmatrix} \text{ and } \begin{pmatrix} \sqrt{b}\mathbf{1} \\ -\sqrt{a}\mathbf{1} \end{pmatrix},$$

corresponding to the eigenvalues $\sqrt{ab}$ and $-\sqrt{ab}$ respectively.

(c) This one is trickier. $\mathbf{A}(C_n)$ is the sum of two permutation matrices corresponding to the cycle $(123...n)$ and its inverse, say $\mathbf{P}$ and $\mathbf{P}^{-1}$. An eigenvector for a cyclic matrix can be easily built from an n-root of unity ω:

$$\mathbf{P}\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix} = \begin{pmatrix} \omega^{n-1} \\ 1 \\ \vdots \\ \omega^{n-2} \end{pmatrix} = \omega^{n-1}\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix} \text{ and}$$

$$\mathbf{P}^{-1}\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix} = \begin{pmatrix} \omega \\ \omega^2 \\ \vdots \\ 1 \end{pmatrix} = \omega\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{n-1} \end{pmatrix},$$

thus the eigenvalues are $\omega^{n-1} = \omega^{-1}$ and ω, hence the eigenvalues of $\mathbf{A}(C_n) = \mathbf{P} + \mathbf{P}^{-1}$ are $\omega^{-1} + \omega$ for all nth roots of unity, that is, $\omega = \mathrm{e}^{2\pi\mathrm{i}(k/n)}$, $k = 0, ..., n-1$. Thus the eigenvalues of C_n are

$$2\cos\left(2\pi\frac{k}{n}\right) \quad \text{for } k = 0, ..., n-1.$$

Note that 2 is always the largest (and simple) eigenvalue, and that -2 is an eigenvalue if and only if n is even. All other eigenvalues have multiplicity 2.

(d) We provide one way of finding this now. The other will come later as an exercise. Look at the cycle C_{2n+2}. Let ω be a $(2n+2)$th root of unity. Then

$$\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{2n+1} \end{pmatrix} \text{ and } \begin{pmatrix} 1 \\ \omega^{-1} \\ \vdots \\ \omega^{-(2n+1)} \end{pmatrix}$$

are both eigenvalues of $\mathbf{A}(C_{2n+2})$ for $\omega+\omega^{-1}$, and so is any linear combination of them. In particular

$$\begin{pmatrix} 1 \\ \omega \\ \vdots \\ \omega^{2n+1} \end{pmatrix} - \begin{pmatrix} 1 \\ \omega^{-1} \\ \vdots \\ \omega^{-(2n+1)} \end{pmatrix} = \begin{pmatrix} 0 \\ \omega-\omega^{-1} \\ \vdots \\ \omega^{2n+1}+\omega^{-2n-1} \end{pmatrix}.$$

Note that there will be another 0 at position $n+2$, corresponding to $\omega^{n+1}-\omega^{-n-1} = -1-(-1) = 0$. The n non-zero entries (only when $\omega \neq 1$) from positions 2 to $n+1$ are part of an eigenvector of C_{2n+2} which do not get interfered by the rest of the graph (those 0s at positions 1 and $n+2$ "disconnect" the eigenvector). Hence this part of the eigenvector is also an eigenvector for P_n (subgraph of C_{2n+2} from positions 2 to $n+1$). Therefore the spectrum of $\mathbf{A}(P_n)$ is

$$\omega+\omega^{-1} = 2\cos\left(\pi\frac{k}{n+1}\right) \quad \text{for } k=1,...,n.$$

1.5 Bounds to the largest and smallest eigenvalues

Later in this course we will study a powerful technique called interlacing, which allows for several interesting results relating eigenvalues and combinatorics. For now, however, we will see some examples of results one could obtain by means of ad-hoc ideas, applied to the largest and smallest eigenvalues.

Exercise 1.40. Let G be a graph with m edges, and let $\theta_1,...,\theta_n$ be the eigenvalues of $\mathbf{A}$. Assume that they are numbered so that $\theta_i^2 \geq \theta_{i+1}^2$. Show that

$$\theta_i \leq \sqrt{\frac{2m}{i}}.$$

Recall now our usual notation for the eigenvalues of $\mathbf{A}$ with $\lambda_1 \geq ... \geq \lambda_n$. A consequence of the exercise above is that $\lambda_1 \leq \sqrt{2m}$. We can do better.

Theorem 1.41 (Hong)**.** *For a graph with n vertices and m edges,*

$$\lambda_1 \leq \sqrt{2m-(n-1)}.$$

Proof. Let $\mathbf{x}$ be an unit length eigenvector corresponding to λ_1, and let $\mathbf{x}(i)$ be the vector obtained from $\mathbf{x}$ by erasing all entries which do not correspond to neighbours of i. In particular, the ith entry of $\mathbf{x}(i)$ is also zeroed.

Note though that we still have

$$\mathbf{e}_i^\mathsf{T} \mathbf{A} \mathbf{x}(i) = \lambda_1 \mathbf{x}_i.$$

By Cauchy-Schwarz,

$$\lambda_1^2 \mathbf{x}_i^2 = |\mathbf{e}_i^\mathsf{T} \mathbf{A} \mathbf{x}(i)|^2 \leq |\mathbf{e}_i^\mathsf{T} \mathbf{A}|^2 |\mathbf{x}(i)|^2 = d_i \left(1 - \sum_{j \not\sim i} {\mathbf{x}_j}^2 \right)$$

and summing over all i, we get

$${\lambda_1}^2 \leq 2m - \sum_{i=1}^{n} d_i \left(\sum_{j \not\sim i} {\mathbf{x}_j}^2 \right).$$

It is not difficult to show that the subtracted term upper bounds $n-1$, with equality if and only if $d_i = 1$ or $d_i = n-1$ for all i. It follows that

$${\lambda_1}^2 \leq \sqrt{2m - (n-1)}.$$

Equality holds if and only if $X = K_n$ or $X = K_{1,n-1}$. $\square$

We can also provide an interesting lower bound to λ_n.

Theorem 1.42 (Constantine, Hong, Powers)**.** *For a given graph with smallest eigenvalue λ_n,*

$$\lambda_n \geq -n/2.$$

Proof. Let $\mathbf{x}$ be a unit length eigenvector for λ_n, and suppose there are precisely a vertices whose coordinate is positive and b with negative. Then

$$\begin{aligned}
\lambda_n = \mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x} &\geq \sum_{\mathbf{x}_i \mathbf{x}_j < 0} \mathbf{A}_{ij} \mathbf{x}_i \mathbf{x}_j \\
&\geq \sum_{\mathbf{x}_i \mathbf{x}_j < 0} \mathbf{x}_i \mathbf{x}_j \\
&\geq \lambda_n(K_{a,b}) \\
&= -\sqrt{ab} \\
&\geq -n/2.
\end{aligned}$$

$\square$

1.6 A result for regular graphs

The theorem in this subsection will reappear when we talk about interlacing. But it contains the nice, elementary proof below.

If the graph is regular, the size of the largest coclique can be associated with the smallest eigenvalue.

Theorem 1.43 (Delsarte)**.** *Let G be a k-regular graph, eigenvalues $k = \lambda_1 \geq .... \geq \lambda_n$. Say the size of the largest coclique of G is α. Then*

$$\alpha \leq \frac{n(-\lambda_n)}{k - \lambda_n}.$$

Proof. Let $\mathbf{x}$ be the characteristic vector of a largest coclique, meaning, $\mathbf{x}_i = 1$ if and only if i belongs to the coclique, and 0 otherwise. Note that

$$\mathbf{x}^\mathsf{T}\mathbf{A}\mathbf{x} = 0, \text{ thus } \mathbf{x}^\mathsf{T}(\mathbf{A} - \lambda_n\mathbf{I})\mathbf{x} = -\lambda_n \cdot \alpha.$$

On the other hand,

$$\mathbf{x}^\mathsf{T}(\mathbf{A} - \lambda_n\mathbf{I})\mathbf{x} = \sum_{i=1}^{n}(\lambda_i - \lambda_n)\mathbf{x}^\mathsf{T}\mathbf{E}_i\mathbf{x}.$$

All terms in the sum are non-negative, as $(\lambda_i - \lambda_n) \geq 0$ and $\mathbf{x}^\mathsf{T}\mathbf{E}_i\mathbf{x} \geq 0$. We can discard all of them but the first, and recalling that $\mathbf{1}$ is the eigenvector for λ_1, we have that $\mathbf{E}_1 = (1/n)\mathbf{J}$. Thus

$$-\lambda_n \cdot \alpha \geq \frac{\lambda_1 - \lambda_n}{n}\alpha^2,$$

and the result follows. □

1.7 Graphs with largest eigenvalue at most 2

It is still a common topic of research in spectral graph theory to classify all graphs whose spectrum lie within a constant given interval. One of the earliest and simplest results classifies all graphs whose largest eigenvalue does not surpass 2.

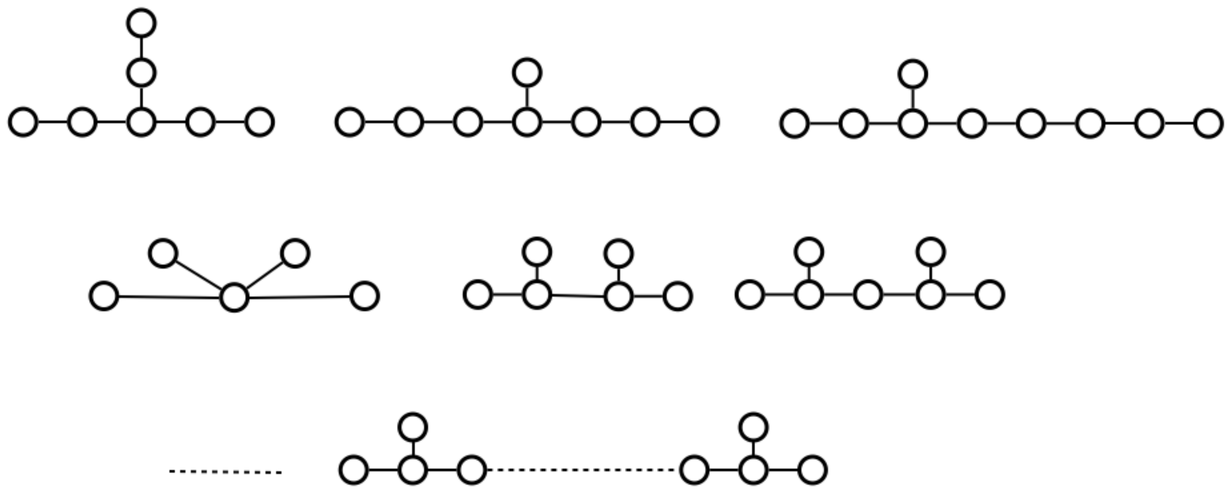
Lemma 1.44. *Let G be a connected graph, and assume H is a proper subgraph of G. Let $\lambda(G)$ be the largest eigenvalue of G, and $\lambda(H)$ the largest eigenvalue of H. Then*

$$\lambda(H) < \lambda(G).$$

Proof. Exercise! □

Exercise 1.45. Argue why any graph with largest eigenvalue at most 2 is either a tree or a cycle.

Exercise 1.46. Show that the following graphs all have largest eigenvalue equal to 2, by exhibiting a suitable eigenvector.



From the previous exercises, it follows that any graph with largest eigenvalue at most two is either a cycle, one of the trees above, or possibly a tree that contains none of the above as a subgraph. It is not difficult to see that any such tree must be a proper subgraph of the ones above.

1.8 References

Here is the set of references used to write the past few pages.

I used Chapter 8 of Godsil and Royle to write about the spectral decomposition of a symmetric matrix. This was also my reference for the basics and some exercises on the adjacency matrix.

(a) Chris Godsil and Gordon Royle. *Algebraic Graph Theory.* Springer-Verlag, New York, 2001.

Exercise 1.28 comes from Chan and Godsil "Symmetry and Eigenvectors".

I looked extensively for a nice intuitive proof of Perron-Frobenius in its full form, but the best I could do relied on using fixed point theorems. I then came up with the simplified version assuming matrices in question are symmetric. A good reference is Brouwer and Haemers, Chapter 2.

(b) Andries E Brouwer and Willem H Haemers. *Spectra of Graphs.* Universitext. Springer, New York, 2012

I also used the reference above for the spectrum of paths and cycles.