Graph matrices and eigenvalues

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1 Some linear algebra concepts

Recall that the *eigenvalues* of a real matrix M are the values $\lambda \in \mathbb{C}$ such that $Mx = \lambda x$ for some nonzero vector $x \in \mathbb{C}^n$. Such a vector x is called an *eigenvector* associated to λ, and (λ, x) is called an *eigenpair* of M. Recall that:

1. An $n \times n$ matrix M has exactly n eigenvalues (counted with their multiplicity).
2. The eigenvalues of M are the roots of the *characteristic polynomial* of M, that is, the polynomial $\det(M - zI)$ of degree n, in the variable z.
3. A real matrix can have *complex* eigenvalues; for example the matrix $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ has eigenvalues $+\boldsymbol{i}$, and $-\boldsymbol{i}$ where $\boldsymbol{i}$ is the imaginary root of -1.
4. Complex eigenvalues appear in *conjugate pairs*: if $a + b\boldsymbol{i}$ is an eigenvalue of M (with $a, b \in \mathbb{R}$), then $a - b\boldsymbol{i}$ is an eigenvalue of M.
5. A real *symmetric* matrix has n *real* eigenvalues.

A *diagonal* matrix is a square matrix D such that $i \neq j$ implies $D_{ij} = 0$. An *upper triangular* matrix is a square matrix T such that $i > j$ implies $T_{ij} = 0$.

An *orthogonal* matrix Q is a square matrix such that the products $QQ^\top$ and $Q^\top Q$ are both equal to the identity matrix I. (With $Q^\top$ we denote the transpose of Q if Q is a real matrix; if it is complex, we mean the *conjugate* transpose, that is, the transpose of a matrix in which each element $a + b\boldsymbol{i}$ is replaced by $a - b\boldsymbol{i}$).

A *permutation* matrix A has entries $A_{ij} = 1$ iff $j = \pi(i)$ and 0 otherwise, for some bijective function $\pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$. Every permutation matrix is orthogonal.

Theorem 1.1 (Diagonal form). *If $A \in \mathbb{R}^{n \times n}$ is a real and symmetric matrix, then there exist a real orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ and a real diagonal matrix $D \in \mathbb{R}^{n \times n}$ such that $A = QDQ^\top$. The elements on the diagonal of D correspond to the eigenvalues of A.*

Theorem 1.2 (Schur form). *If $A \in \mathbb{R}^{n\times n}$ is a real matrix, then there exist a complex orthogonal matrix $Q \in \mathbb{C}^{n\times n}$ and a complex upper triangular matrix $T \in \mathbb{C}^{n\times n}$ such that $A = QTQ^\top$. The elements on the diagonal of T correspond to the eigenvalues of A.*

Theorem 1.3 (Gershgorin's Circle Theorem). *Let $A \in \mathbb{C}^{n\times n}$, and let R_i be the sum of the moduli of the off-diagonal elements in the ith row of A: $R_i = \sum_{j\neq i} |A_{ij}|$. Then each eigenvalue of A lies in the union of the circles*

$$\lambda \in \mathbb{C} \,:\, |\lambda - A_{ii}| \leq R_i, \qquad i = 1, 2, \ldots, n.$$

Additionally, if the ith disk is disjoint from the others, then it contains precisely one of A's eigenvalues.

Proof. For the first part, is enough to show that for any eigenvalue λ of A, there exists some $i = 1, 2, \ldots, n$ such that $|\lambda - A_{ii}| \leq R_i$. Consider an eigenpair (λ, x) of A and let i be an index such that $|x_i|$ is maximum. Note that $|x_i| > 0$ since $x \neq 0$. Also, $\sum_{j=1}^{n} A_{ij}x_j = \lambda x_i$, or equivalently,

$$\sum_{j\neq i} A_{ij}x_j = (\lambda - A_{ii})x_i.$$

If we take absolute values of both sides, and use the triangular inequality $|a + b| \leq |a| + |b|$,

$$|\lambda - A_{ii}|\,|x_i| = \left|\sum_{j\neq i} A_{ij}x_j\right| \leq \sum_{j\neq i} |A_{ij}|\,|x_j| \leq |x_i| \sum_{j\neq i} |A_{ij}| = |x_i|\,R_i.$$

Dividing by $|x_i|$ gives the first claim. We will not prove the second claim. □

2 The adjacency matrix and the incidence matrix

The *adjacency matrix* of a digraph $G(V, E)$ is a matrix $A \in \mathbb{R}^{n\times n}$ $(n = |V|)$ defined by

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

The same definition is used for (undirected) graphs; in that case, A is symmetric and has an all-zero diagonal. If the edges have weights w_{ij}, it is natural to define A_{ij} to be the weight of edge (i, j) if an edge (i, j) exists, and 0 if there is no edge (i, j):

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

The *incidence matrix of a digraph* $G(V, E)$ is a matrix $B \in \mathbb{R}^{n\times m}$ $(n = |V|,\ m = |E|)$ defined by

$$B_{ve} = \begin{cases} +1 & \text{if } v \text{ is the tail of } e \\ -1 & \text{if } v \text{ is the head of } e \\ 0 & \text{if otherwise.} \end{cases}$$

In the case of an undirected graph, we can orient its edges arbitrarily, and use the incidence matrix of the resulting digraph. For some purposes, the choice of orientation will not matter.

2.1 A taste of spectral graph theory: an example

We will show that the adjacency matrix A of a directed graph has the following property: the eigenvalues of A are all 0 if and only if A represents an acyclic digraph.

Exercise 2.1. Prove the easy direction: if A is the adjacency matrix of a directed acyclic graph, then all eigenvalues of A are 0. Hint: find a suitable Schur decomposition $A = QTQ^\top$, with $Q^\top = Q^{-1}$, and use the fact that if $A = QTQ^{-1}$, the matrices A and T have the same eigenvalues.

What is the number $N_{ij}^{(r)}$ of walks of given length r between two nodes i and j in a given graph or directed graph? If $r = 1$, the answer is simply A_{ij}. If $r = 2$, the answer is

$$N_{ij}^{(2)} = \sum_{k=1}^{n} A_{ik}A_{kj} = [A^2]_{ij}$$

where $[A^2]_{ij}$ denotes the ijth element of the matrix A^2. Similarly, $N_{ij}^{(3)} = [A^3]_{ij}$, and one can show by induction that

$$N_{ij}^{(r)} = [A^r]_{ij}.$$

A special case is when $i = j$, so we are counting the number of closed walks of length r that start and end in i. The total number L_r of closed walks of length r in the network is the sum of this quantity over all possible starting points i:

$$L_r = \sum_{i=1}^{n}[A^r]_{ii} = \operatorname{tr} A^r,$$

where $\operatorname{tr} M$ is the *trace* of M (the sum of the elements on M's main diagonal).

Exercise 2.2. (Circularity of the trace operator.) Prove that $\operatorname{tr}(XY) = \operatorname{tr}(YX)$ for any pair of matrices $X \in \mathbb{R}^{a\times b}$, $Y \in \mathbb{R}^{b\times a}$.

By using the Schur decomposition of A, we can show that $L_r = \sum_{i=1}^{n} \kappa_i^r$, where $\kappa_1, \ldots, \kappa_n$ are the eigenvalues of A. Indeed, notice that if x is an eigenvector of A with eigenvalue κ, then $QTQ^\top x = Ax = \kappa x$, and multiplying by $Q^\top$ both sides we get $(Q^\top Q)TQ^\top x = \kappa Q^\top x$, that is, $TQ^\top x = \kappa Q^\top x$, so $Q^\top x$ is an eigenvector of T with the same eigenvalue κ. So (using $\operatorname{tr}(XY) = \operatorname{tr}(YX)$ for square matrices X,Y),

$$L_r = \operatorname{tr} A^r = \operatorname{tr}(QT^rQ^\top) = \operatorname{tr}(Q^\top QT^r) = \operatorname{tr} T^r = \sum_i \kappa_i^r.$$

This fact can be used to complete the proof, as the following exercise asks.

Exercise 2.3. Using the above formula for L_r, show that if A is the adjacency matrix of a directed graph and all of the eigenvalues of A are 0, then the digraph is acyclic.

Exercise 2.4. A matrix A is *nilpotent* if there is some integer $k > 0$ such that A^k is an all-zero matrix. Prove that a nonnegative matrix A is nilpotent if and only if the support digraph of A is acyclic.

3 The graph Laplacian

3.1 Undirected, unweighted graphs

Given an undirected graph $G(V, E)$, let $\deg(i)$ be the number of edges incident to node $i \in V$ (the *degree* of v). We define the *degree matrix* of G as follows:

$$D = \begin{pmatrix} \deg(1) & 0 & 0 & \cdots \\ 0 & \deg(2) & 0 & \cdots \\ 0 & 0 & \deg(3) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Then if A is the adjacency matrix of G, the matrix $L \stackrel{\text{def}}{=} D - A$ is called the *Laplacian* of G. Note that we have

$$L_{ij} = \begin{cases} \deg(i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } \{i, j\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

If we orient arbitrarily the edges of G, obtaining a digraph $\overrightarrow{G}$, and let B be the signed incidence matrix of $\overrightarrow{G}$, we have

$$L(G) = B(\overrightarrow{G})B(\overrightarrow{G})^\top.$$

Exercise 3.1. Check that, for an unweighted graph G, $BB^\top = D - A = L$, independently of the orientation of the edges of $\overrightarrow{G}$.

A graph can be built by combining edges together; the Laplacian can be built by adding simple matrices together, one for each edge. Namely, for any (oriented) edge $e \in E$, consider its incidence vector χ_e defined by $\chi_e(i) = +1$ if i is the tail of e, $\chi_e(i) = -1$ if i is the head of i, and $\chi_e(i) = 0$ otherwise (note that χ_e is a column of the B matrix).

If $e = (i, j)$, the rank-1 matrix $\chi_e \chi_e^\top$ is given by:

$$\chi_e \chi_e^\top = \begin{array}{c} \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{pmatrix} \dots & \vdots & \dots & \vdots & \dots \\ \dots & 1 & \dots & -1 & \dots \\ \dots & \vdots & \dots & \vdots & \dots \\ \dots & -1 & \dots & 1 & \dots \\ \dots & \vdots & \dots & \vdots & \dots \end{pmatrix} \end{array}$$

Note that the orientation of e is relevant for the signs in χ_e, but is irrelevant for the signs in $\chi_e \chi_e^\top$.

Now, the Laplacian can be alternatively expressed as the combination of the rank-1 matrix elements $\chi_e \chi_e^\top$:

$$L = \sum_{e \in E} \chi_e \chi_e^\top.$$

The graph Laplacian, being a real and symmetric matrix, has n real eigenvalues. The decomposition $L = BB^\top$ implies that L can only have non-negative eigenvalues: if v is any eigenvector of L, say with eigenvalue λ, then

$$\lambda v^\top v = v^\top L v = (v^\top B)(B^\top v) = (B^\top v)^\top (B^\top v) \geq 0$$

and dividing both sides by $v^\top v > 0$ shows that λ is nonnegative. (In other words, L is a positive semidefinite matrix. This can also be seen by Gershgorin's circle theorem.)

The *Laplacian potential* associated with a graph is the positive semidefinite quadratic form

$$\Phi(x) = x^\top L x = \frac{1}{2} \sum_{i,j=1}^{n} A_{ij}(x_i - x_j)^2 = \sum_{\{i,j\} \in E} (x_i - x_j)^2.$$

The eigenvalues of the Laplacian of a graph are conventionally indexed from the smallest to the largest: $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. The eigenvalues of $L(G)$ contain useful information about the graph G. For example, if a graph has exactly c connected components, then $\lambda_1 = \lambda_2 = \ldots = \lambda_c = 0$, while $\lambda_{c+1} > 0$. In other words, the number of connected components equals the dimension of the null space of L: $c = \dim \ker(L) = n - \operatorname{rank}(L)$.

Note that since a graph has always at least one connected component, λ_1 is always 0. In fact, the vector $\mathbf{1} = (1, 1, \ldots, 1)$ is always an eigenvector of L, with eigenvalue 0 (exercise: verify this).

As a special case, $\lambda_2 > 0$ if and only if the graph is connected. The second eigenvalue is also known as the *algebraic connectivity* of the graph.

3.2 Weighted graphs

The Laplacian can be extended to weighted graphs in a straightforward way. Instead of letting A be the adjacency matrix, we define A to be a weighted adjacency matrix, with $A_{ij} = w_{ij}$ if $\{i, j\}$ is an edge with weight w_{ij}, and $A_{ij} = 0$ if $\{i, j\}$ is not an edge. Similarly, instead of letting D be the diagonal degree matrix, we let D be the diagonal matrix of node *volumes*,

$$D = \begin{pmatrix} \mathrm{vol}(1) & 0 & 0 & \cdots \\ 0 & \mathrm{vol}(2) & 0 & \cdots \\ 0 & 0 & \mathrm{vol}(3) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where $\mathrm{vol}(i)$ is the total weight of the edges incident to node i. Then we define $L \stackrel{\text{def}}{=} D - A$, as before, so that

$$L_{ij} = \begin{cases} \mathrm{vol}(i) & \text{if } i = j \\ -w_{ij} & \text{if } i \neq j \text{ and } \{i, j\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

In this case, $L = BCB^\top$, where C is an $m \times m$ diagonal matrix with diagonal entries $(w_e)_{e \in E}$, where w_e is the weight associated to edge e. If $w_e \geq 0$ for all edges $e \in E$, we can show that all eigenvalues of L are nonnegative, exactly like in the unweighted case.

We also have $L = \sum_{e \in E} w_e \chi_e \chi_e^\top$. Finally, the Laplacian potential becomes $\sum_{\{i,j\} \in E} w_{ij}(x_i - x_j)^2$.

3.3 Digraphs

Can we extend the Laplacian matrix to directed graphs? The most natural way to do so is to define

$$L_{ij} = \begin{cases} \deg^+(i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } (i,j) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Here $\deg^+(i)$ is the number of arcs leaving node i (the *out-degree* of i). Thus $L = D_+ - A$, where D_+ is the diagonal matrix with the out-degrees of the nodes on the diagonal. Note that, when the digraph is symmetric ($(i,j) \in E$ iff $(j,i) \in E$), then this coincides with the Laplacian of the corresponding undirected graph.

Unfortunately, many convenient properties of the graph Laplacian do not hold for the digraph Laplacian: for example, in general L is not symmetric and its eigenvalues may be complex numbers. However, they have a nonnegative real part.

Let $\Delta^+ = \max_i \deg^+(i)$. Then, by Gershgorin's circle theorem, all eigenvalues of L are located in the disk of radius Δ^+ centered at $(\Delta^+, 0)$ in the complex plane. In particular, they have nonnegative real part.

In general, it is still true that $\text{rank}(L) = n - c$, where c is the number of strongly connected components of the digraph. If the digraph is strongly connected, then $\text{rank}(L) = n - 1$. It is also the case that 0 is always an eigenvalue of L, since $L \cdot \mathbf{1} = \mathbf{0}$. However, $\mathbf{1}^\top L$ does not necessarily equal $\mathbf{0}^\top$.