Laplacians of Graphs, Spectra and Laplacian polynomials

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Laplacian matrix

The Laplacian matrix of a graph and its eigenvalues can be used in several areas of mathematical research and have a physical interpretation in various physical and chemical theories. The related matrix - the adjacency matrix of a graph and its eigenvalues were much more investigated in the past than the Laplacian matrix. In the same time, the Laplacian spectrum is much more natural and more important than the adjacency matrix spectrum because of it numerous application in mathematical physics, chemistry and financial mathematics.

Since the classical paper by Mark Kac "Can one hear the shape of a drum?" (1966), the question of what geometric properties of a manifold are determined by its Laplace operator has inspired many intriguing results. See papers by S. Wolpert (1979), P. Buser (1986), R. Brooks (1987), R. Isangulov (2000) for Riemann surfaces and survey by by E.R.van Dam and W.H.Haemers (2003) for graphs.

Laplacian matrix. Laplacian spectrum

The graphs under consideration are supposed to be unoriented and finite. They may have loops, multiple edges and to be disconnected.
Let a_{uv} be the number of edges between two given vertices u and v of G.
The matrix $A = A(G) = [a_{uv}]_{u,v \in V(G)}$, is called the *adjacency matrix* of the graph G.
Let $d(v)$ denote the degree of $v \in V(G)$, $d(v) = \sum_u a_{uv}$, and let $D = D(G)$ be the diagonal matrix indexed by $V(G)$ and with $d_{vv} = d(v)$.
The matrix $L = L(G) = D(G) - A(G)$ is called the *Laplacian matrix* of G.
It should be noted that loops have no influence on $L(G)$. The matrix $L(G)$ is sometimes called the *Kirchhoff matrix* of G.
It should be mentioned here that the rows and columns of graph matrices are indexed by the vertices of the graph, their order being unimportant.

Let G be a given graph. Orient its edges arbitrarily, i.e. for each $e \in E(G)$ choose one of its ends as the *initial* vertex, and name the other end the *terminal* vertex. The *oriented incidence matrix* of G with respect to the given orientation is the $|V| \times |E|$ matrix $C = \{c_{ve}\}$ with entries

$$c_{ve} = \begin{cases} +1, & \text{if } v \text{ is the terminal vertex of } e, \\ -1, & \text{if } v \text{ is the initial vertex of } e, \\ 0, & \text{if } v \text{ and } e \text{ are not incident.} \end{cases}$$

It is well known that $L(G) = C\,C^t$ independently of the orientation given to the edges of G. Since

$$(L(G)x,\, x) = (C\,C^t x,\, x) = (C^t x,\, C^t x)$$

we have

$$(L(G)x,\, x) = \sum_{v\,u \in E(G)} a_{vu}(x_v - x_u)^2.$$

Laplacian polynomial and Laplacian spectrum

We denote by $\mu(G, x)$ the characteristic polynomial of $L(G)$. We will call it the *Laplacian polynomial.* Its roots will be called the *Laplacian eigenvalues* (or sometimes just eigenvalues) of G. They will be denoted by $\lambda_1(G) \leq \lambda_2(G) \leq \ldots \leq \lambda_n(G)$, $(n = |V(G)|)$, always enumerated in increasing order and repeated according to their multiplicity.

We note that λ_1 is always equal to 0.
Graph G is connected if and only if $\lambda_2 > 0$.

If G consists of k components then

$$\lambda_1(G) = \lambda_2(G) = \ldots = \lambda_k(G) = 0 \text{ and } \lambda_{k+1}(G) > 0.$$

Laplacian for Graphs

We summarise the above results in the following theorem.

Theorem

Let G be a graph. Then:

(a) *$L(G)$ has only real eigenvalues,*

(b) *$L(G)$ is positive semidefinite,*

(c) *its smallest eigenvalue is $\lambda_1 = 0$ and a corresponding eigenvector is $(1, 1, \dots, 1)^t$. The multiplicity of 0 as an eigenvalue of $L(G)$ is equal to the number of components of G.*

Many published works relate the Laplacian eigenvalues of graphs with the eigenvalues of graphs obtained by means of some operations on the graphs we start with. The first result is obvious but very useful.

Theorem

Let G be the disjoint union of graphs $G_1, G_2, \ldots, G_k$. Then

$$\mu(G, x) = \prod_{i=1}^{k} \mu(G_i, x).$$

The *complement* of a graph G is a graph $\overline{G}$ on the same vertices such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G.
The next two results were first observed by A. K. Kelmans.

Theorem (Kelmans, 1966)

If $\overline{G}$ denotes the complement of the graph G then

$$\mu(\overline{G}, x) = (-1)^{n-1}\frac{x}{n-x}\mu(G, n-x)$$

and so the eigenvalues of $\overline{G}$ are $\lambda_1(\overline{G}) = 0$, and

$$\lambda_{i+1}(\overline{G}) = n - \lambda_{n-i+1}(G),\ i = 1, 2, \ldots, n-1.$$

Laplacian for Graphs.

As a corollary from the previous result one can get the following beautiful theorem.

Theorem (Kel'mans, 1965)

Let $X_1 * X_2$ denote the join of X_1 and X_2, i.e. the graph obtained from the disjoint union of X_1 and X_2 by adding all possible edges uv, $u \in V(X_1)$, $v \in V(X_2)$. Then

$$\mu(X_1 * X_2, x) = \frac{x(x - n_1 - n_2)}{(x - n_1)(x - n_2)} \mu(X_1, x - n_2)\mu(X_2, x - n_1).$$

where n_1 and n_2 are orders of X_1 and X_2, respectively and $\mu(X, x)$ is the characteristic polynomial of the Laplacian matrix of X.

Let G be a simple graph (without multiple edges). The *line graph* $L(G)$ of G is the graph whose vertices correspond to the edges of G with two vertices of $L(G)$ being adjacent if and only if the corresponding edges in G have a vertex in common. The *subdivision graph* $S(G)$ of G is obtained from G by inserting, into each edge of G, a new vertex of degree 2. The *total graph* $T(G)$ of G has its vertex set equal to the union of vertices and edges of G, and two of them being adjacent if and only if they are incident or adjacent in G.

Laplacian for Graphs.

Theorem (Kel'mams, 1967)

Let G be a d-regular simple graph with m edges and n vertices. Then

(a) $\mu(L(G), x) = (x - 2d)^{m-n}\mu(G, x)$,

(b) $\mu(S(G), x) = (-1)^m(2 - x)^{m-n}\mu(G, x(d + 2 - x))$,

(c) $\mu(T(G), x) = (-1)^m(d + 1 - x)^n(2d + 2 - x)^{m-n}\mu(G, \frac{x(d+2-x)}{d+1-x})$.

Laplacian for Graphs

The *Cartesian product* $G \times H$ (simetimes $G \Box H$) of graphs G and H is a graph such that the vertex set of $G \times H$ is the Cartesian product $V(G) \times V(H)$; and any two vertices (u, u') and (v, v') are adjacent in $G \times H$ if and only if either $u = v$ and u' is adjacent with v' in H, or $u' = v'$ and u is adjacent with v in G.

Examples :

(a) The Cartesian product of two edges is a cycle on four vertices: $K_2 \times K_2 = C_4$.

(b) The Cartesian product of K_2 and a path graph is a ladder graph.

(c) The Cartesian product of two path graphs is a grid graph.

(d) The Cartesian product of two hypercube graphs is another hypercube: $Q_i \times Q_j = Q_{i+j}$.

(e) The graph of vertices and edges of an n-prism is the Cartesian product graph $K_2 \times C_n$.

Laplacian for Graphs

Theorem (M. Fiedler (1973))

The Laplacian eigenvalues of the Cartesian product $X_1 \times X_2$ of graphs X_1 and X_2 are equal to all the possible sums of eigenvalues of the two factors:

$$\lambda_i(X_1) + \lambda_j(X_2),\ i = 1, \ldots, |V(X_1)|,\ j = 1, \ldots, |V(X_2)|.$$

Using this theorem we can easily determine the spectrum of "lattice" graphs. The $m \times n$ lattice graph is just the Cartesian product of paths, $P_m \times P_n$. Below we will show that the spectrum of path-graph P_k is

$$\ell_i^{(k)} = 4\sin^2\frac{\pi i}{2k},\ i = 0, 1, \ldots, k-1.$$

So $P_m \times P_n$ has eigenvalues

$$\lambda_{i,j} = \ell_i^{(m)} + \ell_j^{(n)} = 4\sin^2\frac{\pi i}{2m} + 4\sin^2\frac{\pi j}{2n},\ i = 0, 1, \ldots, m-1, j = 0, 1, \ldots, n-1.$$

Circulant matrices

Fix a positive integer $n \geq 2$ and let $v = (v_0,\, v_1,\, \ldots,\, v_{n-1})$ be a row vector in $\mathbb{C}^n$. Define the shift operator $T : \mathbb{C}^n \to \mathbb{C}^n$ by

$$T(v_0,\, v_1,\, \ldots,\, v_{n-1}) = (v_{n-1},\, v_0,\, \ldots,\, v_{n-2}).$$

The circulant matrix associated to v is the $n \times n$ matrix whose rows are given by iteration of the shift operator acting on v, that is to say the k-th row is given by $T^{k-1}v,\ k = 1,\, \ldots,\, n$. Such a matrix will be denoted by

$$V = circ\{v\} = circ\{v_0,\, v_1,\, \ldots,\, v_{n-1}\}.$$

The following theorem shows how one can calculate eigenvalues and eigenvectors of V.

Theorem (Eigenvalues of circulant matrix)

Let $v = (v_0, v_1, \ldots, v_{n-1})$ be a row vector in $\mathbb{C}^n$, and $V = circ\{v\}$. If ε is primitive $n-$th root of unity, then

$$\det V = \det \begin{pmatrix} v_0 & v_1 & \ldots & v_{n-2} & v_{n-1} \\ v_{n-1} & v_0 & \ldots & v_{n-3} & v_{n-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ v_2 & v_3 & \ldots & v_0 & v_1 \\ v_1 & v_2 & \ldots & v_{n-1} & v_0 \end{pmatrix} = \prod_{l=0}^{n-1}(\sum_{j=0}^{n-1} \varepsilon^{j\ell} v_j).$$

Corollary

Eigenvalues of circulant matrix V is given by the formulae

$$\lambda_\ell = \sum_{j=0}^{n-1} \varepsilon^{j\ell} v_j,\ \ell = 0, \ldots, n-1.$$

Proof. We view the matrix V as a a self map (linear operator) of $\mathbb{C}^n$. For each integer ℓ, $0 \le \ell \le n-1$, let $x_\ell \in \mathbb{C}^n$ be a transpose of the row vector $(1, \varepsilon^\ell, \varepsilon^{2\ell}, \ldots, \varepsilon^{(n-1)\ell})$ and

$$\lambda_\ell = v_0 + \varepsilon^\ell v_1 + \ldots + \varepsilon^{(n-1)\ell} v_{n-1}.$$

A quite simple calculation shows that

$$\begin{pmatrix} v_0 & v_1 & \ldots & v_{n-2} & v_{n-1} \\ v_{n-1} & v_0 & \ldots & v_{n-3} & v_{n-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ v_2 & v_3 & \ldots & v_0 & v_1 \\ v_1 & v_2 & \ldots & v_{n-1} & v_0 \end{pmatrix} \begin{pmatrix} 1 \\ \varepsilon^\ell \\ \vdots \\ \varepsilon^{(n-2)\ell} \\ \varepsilon^{(n-1)\ell} \end{pmatrix} = \lambda_\ell \begin{pmatrix} 1 \\ \varepsilon^\ell \\ \vdots \\ \varepsilon^{(n-2)\ell} \\ \varepsilon^{(n-1)\ell} \end{pmatrix}.$$

Thus λ_ℓ is an eigenvalue of V with eigenvector x_ℓ. Since $\{x_0, x_1, \ldots, x_{n-1}\}$ is linearly independent set, we conclude that $\det V = \prod_{\ell=0}^{n-1} \lambda_\ell$.

Circulant graphs

Circulant graphs can be described in several equivalent ways:

(a) The graph has an adjacency matrix that is a circulant matrix.

(b) The automorphism group of the graph includes a cyclic subgroup that acts transitively on the graph's vertices.

(c) The n vertices of the graph can be numbered from 0 to $n-1$ in such a way that, if some two vertices numbered x and y are adjacent, then every two vertices numbered z and $(z - x + y) \mod n$ are adjacent.

(d) The graph can be drawn (possibly with crossings) so that its vertices lie on the corners of a regular polygon, and every rotational symmetry of the polygon is also a symmetry of the drawing.

(e) The graph is a Cayley graph of a cyclic group.

Examples

(a) The circulant graph $C_n(s_1, \ldots, s_k)$ with jumps $s_1, \ldots, s_k$ is defined as the graph with n vertices labeled $0, 1, \ldots, n-1$ where each vertex i is adjacent to $2k$ vertices $i \pm s_1, \ldots, i \pm s_k \mod n$.

(b) n-cycle graph $C_n = C_n(1)$.

(c) n-antiprism graph $C_{2n}(1, 2)$.

(d) n-prism graph $Y_n = C_{2n}(2, n)$, n odd.

(e) The Moebius ladder graph $M_n = C_{2n}(1, n)$.

(f) The complete graph $K_n = C_n(1, 2, \cdots, [\frac{n}{2}])$.

(g) The complete bipartite graph $K_{n,n} = C_n(1, 3, \cdots, 2[\frac{n}{2}] + 1)$.

Exercise 1.1.
Find Laplacian spectrum of the complete graph on n vertices K_n.

Solution: We want to show that $\mu(K_n, x) = x(x-n)^{n-1}$. To solve this problem we use induction by number of vertices n. For $n = 1$, K_1 is a singular vertex. Its Laplacian matrix $L(K_n) = \{0\}$. Hence $\mu(K_1, x) = x$. Hence the statement is true for $n = 1$. Suppose that for given n the equality $\mu(K_n, x) = x(x-n)^{n-1}$ is already proved. It is easy to see that K_{n+1} is a join of K_n and K_1. By Kel'mans theorem we get

$$\mu(K_{n+1}, x) = \frac{x(x-n-1)}{(x-1)(x-n)}\mu(K_1, x-n)\mu(K_n, x-1) =$$

$$= \frac{x(x-n-1)}{(x-1)(x-n)}(x-n)(x-1)(x-n-1)^{n-1} = x(x-n-1)^n.$$

Hence, the Laplacian spectrum of K_n is $\{0^1,\ n^{n-1}\}$.

Exercise 1.2.
Find Laplacian spectrum of the complete bipartite graph $K_{n,m}$.

Solution: Let us note that $K_{n,m}$ is a join of X_m and X_n, where X_k is a disjoint union of k vertices. We have
$L(X_k) = D(X_k) - A(X_k) = O_k - O_k = O_k$, where O_k is $k \times k$ zero matrix.
Hence, $\mu(X_k, x) = x^k$. By Kel'mans theorem we obtain

$$\mu(K_{n,m}, x) = \frac{x(x-m-n)}{(x-n)(x-m)}\mu(X_n, x-m)\mu(X_m, x-n) =$$

$$= \frac{x(x-m-n)}{(x-n)(x-m)}(x-m)^n(x-n)^m = x(x-m-n)(x-n)^{m-1}(x-m)^{n-1}.$$

Hence, the Laplacian spectrum of $K_{n,m}$ is $\{0^1,\ n^{m-1},\ m^{n-1}, (m+n)^1\}$.

Exercise 1.3.
Find Laplacian spectrum of the cycle graph C_n.

Solution: The Laplacian matrix $L(C_n)$ is the circulant matrix with entities

$$v_0 = 2,\ v_1 = -1,\ v_2 = \ldots = v_{n-2} = 0,\ v_{n-1} = -1.$$

Then by properties of circulant matrices its eigenvalues are

$$\lambda_k = v_0 + v_1\varepsilon^k + \ldots + v_{n-1}\varepsilon^{(n-1)k},\ k = 0,\ \ldots,\ n-1,$$

where $\varepsilon = e^{\frac{2\pi i}{n}}$ is the n-th primitive root of the unity. Hence,

$$\lambda_k = 2 - \varepsilon^k - \varepsilon^{(n-1)k}.$$

Since

$$e^{\frac{2\pi i}{n}k} + e^{\frac{2\pi i}{n}(n-1)k} = 2\left(\frac{e^{\frac{2\pi i}{n}k} + e^{-\frac{2\pi i}{n}k}}{2}\right) = 2\cos\frac{2\pi k}{n},$$

we have $\lambda_k = 2 - 2\cos\frac{2\pi k}{n},\ k = 0,\ \ldots,\ n-1.$

Exercise 1.4.
Find Laplacian spectrum of the path graph P_n.

Solution: The Laplacian matrix for path graph P_n has the form

$$L_n = L(P_n) = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ 0 & 0 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & \dots & -1 & 1 \end{pmatrix}.$$

Then its characteristic matrix is given by

$$L_n - \lambda I_n = \begin{pmatrix} 1-\lambda & -1 & 0 & \dots & 0 & 0 \\ -1 & 2-\lambda & 1 & \dots & 0 & 0 \\ 0 & -1 & \lambda-2 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2-\lambda & -1 \\ 0 & 0 & 0 & \dots & -1 & 1-\lambda \end{pmatrix}.$$

Let $V_n = \det(L_n - \lambda I_n)$. Then $\det V_n$ is equal

$$\begin{vmatrix} 1-\lambda & -1 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1-\lambda \end{vmatrix} =$$

$$\begin{vmatrix} 2-\lambda & -1 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1-\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1-\lambda \end{vmatrix} =$$

$$\underbrace{\begin{vmatrix} 2-\lambda & -1 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1-\lambda \end{vmatrix}}_{n\times n} - \underbrace{\begin{vmatrix} 2-\lambda & -1 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1-\lambda \end{vmatrix}}_{n-1\times n-1} =$$

$$D_n - D_{n-1}.$$

In a similar way $D_n = U_n - U_{n-1}$, where

$$U_n = \underbrace{\begin{vmatrix} 2-\lambda & -1 & \dots & 0 \\ -1 & 2-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 2-\lambda \end{vmatrix}}_{n\times n} = U_n(\frac{2-\lambda}{2}).$$

Exercises

Here $U_n(x) = \dfrac{\sin(n+1)\arccos x}{\sin\arccos x}$ is a Chebyshev polynomial of the second kind. Since $U_n(x) - 2xU_{n-1}(x) + U_{n-2}(x) = 0$, we obtain

$$V_n = D_n - D_{n-1} = U_n(x) - 2U_{n-1}(x) + U_{n-2}(x)$$

$$= (2x-2)U_{n-1}(x) = -\lambda U_{n-1}(\frac{\lambda-2}{2}),$$

where $x = \frac{\lambda-2}{2}$. The equation

$$\lambda U_{n-1}(\frac{\lambda-2}{2}) = 0$$

has the following solutions $\lambda_k = 2 - 2\cos(\frac{\pi k}{n}),\ k = 0, \ldots, n-1.$

Exercise 1.5.

Show that Laplacian polynomial of the path graph P_n has the following form

$$\mu(P_n, x) = x\, U_{n-1}(\frac{x-2}{2}),$$

where $U_{n-1}(x) = \frac{\sin(n \arccos x)}{\sin(\arccos x)}$ is the Chebyshev polynomial of the second kind.

Solution:

Follows from the previous exercise.

Exercise 1.6.
Find Laplacian spectrum of the wheel graph $W_n = K_1 * C_n$.

Answer: $\{0,\ n+1,\ 3-2\cos\frac{2\pi k}{n},\ k=1,\ \ldots,\ n-1\}$

Exercise 1.7.

Find Laplacian spectrum of the fan graph $F_n = K_1 * P_n$.
Answer: $\{0,\ n+1,\ 3-2\cos\frac{\pi k}{n},\ k=1,\ \ldots,\ n-1\}$

Exercise 1.8.
Show that the Laplacian polynomial of the fan graph $F_n = K_1 * P_n$ is given by the formula

$$\mu(F_n,\, x) = x(x-n-1)U_{n-1}(\frac{x-3}{2})$$

where $U_{n-1}(x)$ is the Chebyshev polynomial of the second kind.

Exercise 1.9.
Find Laplacian spectrum of the cylinder graph $P_m \times C_n$.

Solution:
The spectrum of P_m is $\lambda_j = 4\sin^2(\frac{\pi j}{2m})$, $j = 0, \ldots, m-1$ and the spectrum of C_n is $\mu_k = 4\sin^2(\frac{2\pi k}{2n})$, $k = 0, \ldots, n-1$. As a result we have the following spectrum for $P_m \times C_n$.

$$\ell_{j,k} = 4\sin^2(\frac{\pi j}{2m}) + 4\sin^2(\frac{2\pi k}{2n}),\ j = 0, \ldots, m-1,\ k = 0, \ldots, n-1.$$

Exercise 1.10.
Find Laplacian spectrum of the Moebius ladder graph M_n. Moebius ladder graph is a cycle graph C_{2n} with additional edges, connecting opposite vertices in cycle.

Solution:
We note that the Laplacian matrix for M_n is circulant $circ\{v_0 \ldots, v_{2n-1}\}$, where $v_0 = 3,\ v_1 = -1,\ v_2 = \ldots = v_{n-1} = 0$,
$v_n = -1,\ v_{n+1} = \ldots = v_{2n-2} = 0,\ v_{2n-1} = -1$. Let $\varepsilon = e^{\frac{2\pi i}{2n}}$ be the $2n$-th primitive root of unity.
Then $L(M_n)$ has the following spectrum

$$\lambda_k = \sum_{j=0}^{2n-1} \varepsilon^{kj} v_j = 3 + (-1)^{k+1} - 2\cos\frac{\pi k}{n},\ k = 0, \ldots, 2n-1.$$