An introduction to graph spectra and applications

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Social network

Photo credit: Analytics Vidhya

Plans of the lecture

1. Backgrounds on graph theory.
2. Graph spectra.
3. Graph spectra and the Kuramoto model.
4. Circulant graphs.
5. The Circulant Diagonalization Theorem.

What is a a graph?

A (undirected) graph is an ordered pair $G = (V, E)$ where

- V is a finite set whose elements are called vertices.
- E is a set of is a set of paired vertices.

Suppose the vertex set of G is $\{v_1, v_2, \ldots, v_n\}$. A convenient way to represent G is to use its adjacency matrix $A = (A_{ij})$ where

$$A_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{else.} \end{cases}$$

With this presentation, we can then use tools from linear algebra, representation theory, and number theory to study the structure of G.

Counting walks on G

A walk of length k in a graph is a sequence of (not neccesarily distinct) vertices $v_0, v_1, \ldots, v_k$ such that $(v_i, v_{i+1}) \in E$. A walk is closed if $v_0 = v_k$.

Proposition

The number of walks of length k that start at vertex i and end at vertex j is equal to $(A^k)_{ij}$ where A is the adjacency matrix of G.

Corollary

The number of closed walks of length k on G is equal to the trace $Tr(A^k)$ of the matrix A^k.

Example 1: Complete graph

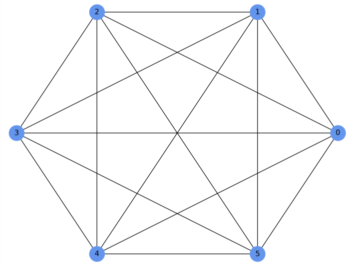

Figure 1: The complete graph K_6 on $N = 6$ nodes

$$\begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

The adjacency matrix of K_6

Example 2: Cycle graph

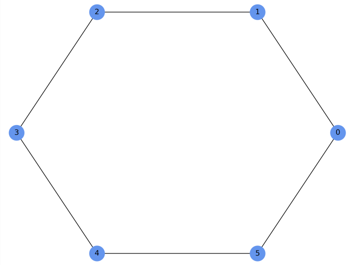

Figure 2: The cycle graph C_6 on $N = 6$ nodes

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

The adjacency matrix of C_6

Example 3: An Erdős–Rényi random graph

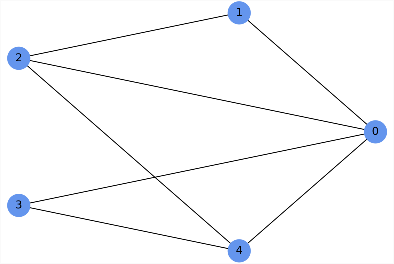

Figure 3: A random graph on $N = 5$ nodes

$$\begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

The adjacency matrix of this graph.

Graph spectra

The spectrum of G, denoted by $\mathrm{Spec}(G)$, is the set of all eigenvalues of its adjacency matrix A. Equivalently, it is the set of all roots of the characteristic polynomial $p_A(t)$ of A where

$$p_A(t) = \det(tI_n - A).$$

A concrete example

Let us consider the spectrum of the complete graph K_3 on three nodes. Its adjacency matrix is given by

$$A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

The characteristics polynomial of A is given by

$$p_A(t) = \det(tI_3 - A) = \begin{vmatrix} t & -1 & -1 \\ -1 & t & -1 \\ -1 & -1 & t \end{vmatrix} = t^3 - 3t - 2 = (t-2)(t+1)^2.$$

Therefore, the spectrum of K_3 is $\{[2]_1, [-1]_2\}$.

What are the spectrum of graphs good for?

Graph spectra plays a fundamental roles in many real-life applications. Some of them are

- Spectral graph theory is important for many search algorithms such as the Google's famous PageRank algorithm.
- Spectral graph theory has been widely used to analyze diverse data sets in the fields of computational chemistry and bioinformatics.
- Many spectral clustering techniques use the spectrum to perform dimensionality reduction on big data sets.
- As we will soon see, the spectra of a network directly influences its (non-linear) dynamics.
- And much more!

The Kuramoto model

Let G be a graph/network with adjacency matrix $A = (a_{ij})$. The Kuramoto model on G is described by the following differential equations

$$\dot{\theta}_i = \omega + \epsilon \sum_{j=1}^{N} a_{ij} \sin(\theta_j - \theta_i) \,, \tag{0.1}$$

where $\theta_i(t) \in [-\pi, \pi]$ is the state of oscillator $i \in [1, N]$ at time t, ω is the angular frequency, ϵ is the coupling strength. By considering a rotating frame, we can often assume that $\omega = 0$.

The complex-valued Kuramoto model

We recently introduced the following complex-valued Kuramoto model

$$\dot{\psi}_i = \epsilon \sum_{j=1}^{N} a_{ij} \big[\sin(\psi_j - \psi_i) - \mathrm{i} \cos(\psi_j - \psi_i) \big], \tag{0.2}$$

Letting $x_i = e^{\mathrm{i}\psi_i}$ and using Euler formula, this equation becomes

$$\dot{x}_i = \epsilon \sum_{j=1}^{N} a_{ij} x_j, \tag{0.3}$$

The general solution of this equation is

$$\vec{x}(t) = e^{Kt} \vec{x}(0), \tag{0.4}$$

where $\vec{x}(t) = (x_1(t), x_2(t), \ldots, x_N(t))$ and $K = \epsilon A$.

The complex-valued Kuramoto model

In a recent work, we showed that there is a strong correspondence

$$\arg(x_i(t)) \longleftrightarrow \theta_i.$$

Specifically, we showed that

- The trajectories of the two systems (the original, nonlinear Kuramoto model and the complex-valued system) can match precisely for long times and
- This approach can thus provide a unified, geometrical insight into the transient behavior of the networks.

The complex-valued Kuramoto model

To evaluate e^{Kt} efficiently, we use its spectrum. More precisely, we can write

$$K = VDV^{-1},$$

where V is the matrix obtained from a choosen eigenbasis of for K and D is the diagonal matrix whose entries are eigenvalues of K. We then have

$$\vec{x}(t) = e^{Kt}\vec{x}(0) = Ve^{Dt}V^{-1}\vec{x}(0).$$

We see from this formula that the spectrum of A is strongly connected with the dynamics of the Kuramoto model on A.

A special type of network that appears often in the literature is the ring graph.

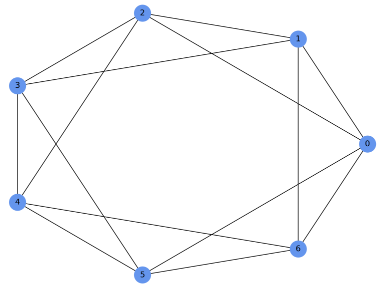

Figure 4: The ring graph with $N = 7$ and $k = 2$.

The adjacency matrix of this graph is given by

$$\begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

We see that all row vectors are composed of the same elements and each row vector is rotated one element to the right relative to the preceding row vector. This is an example of a circulant matrix.

More generally, a circulant matrix is a matrix of the form

$$C = \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-2} & c_{n-1} \\ c_{n-1} & c_0 & c_1 & & c_{n-2} \\ \vdots & c_{n-1} & c_0 & \ddots & \vdots \\ c_2 & & \ddots & \ddots & c_1 \\ c_1 & c_2 & \cdots & c_{n-1} & c_0 \end{bmatrix}.$$

In particular, a circulant matrix is completely determined by the first row vector $\vec{c} = (c_0, c_1, \ldots, c_{n-1})$.

The Circulant Diagonalization Theorem

Let us take a concrete example of a circulant matrix of size 3×3.

$$C = \begin{pmatrix} c_0 & c_1 & c_2 \\ c_2 & c_0 & c_1 \\ c_1 & c_2 & c_0 \end{pmatrix}.$$

Let ω_3 be 3-root of unity. Then we have

$$C \begin{pmatrix} 1 \\ \omega_3 \\ \omega_3^2 \end{pmatrix} = \begin{pmatrix} c_0 + c_1\omega_3 + c_2\omega_3^2 \\ c_2 + c_0\omega_3 + c_1\omega_3^2 \\ c_1 + c_2\omega_3 + c_0\omega_3^2 \end{pmatrix} = \begin{pmatrix} (c_0 + c_1\omega_3 + c_2\omega_3^2)1 \\ (c_0 + c_1\omega_3 + c_2\omega_3^2)\omega_3 \\ (c_0 + c_1\omega_3 + c_2\omega_3^2)\omega_3^2 \end{pmatrix}.$$

We see that $(1, \omega_3, \omega_3^2)^t$ is an eigenvector of C associated with the eigenvalue $c_0 + c_1\omega_3 + c_2\omega_3^2$.

Theorem (The Circulant Diagonalization Theorem)

Let

$$C = \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-2} & c_{n-1} \\ c_{n-1} & c_0 & c_1 & & c_{n-2} \\ \vdots & c_{n-1} & c_0 & \ddots & \vdots \\ c_2 & & \ddots & \ddots & c_1 \\ c_1 & c_2 & \cdots & c_{n-1} & c_0 \end{bmatrix}.$$

be the circulant matrix formed by the vector $(c_0, c_1, \ldots, c_{n-1})$*.*
Let $\omega_n = e^{\frac{2\pi i}{n}}$ *and*

$$v_{n,j} = \left(1, \omega_n^j, \omega_n^{2j}, \ldots, \omega_n^{(n-1)j}\right)^T, \quad j = 0, 1, \ldots, n-1.$$

Then $v_{n,j}$ *is an eigenvector of* C *associated with the eigenvalue*

$$\lambda_j^C = c_0 + c_1\omega_n^j + c_2\omega_n^{2j} + \cdots + c_{n-1}\omega_n^{(n-1)j}$$

An example: Paley graph

Let q be a prime number such that $q \equiv 1 \pmod 4$. The Paley graph G_q associated with q is constructed as follow.

- The vertices of G_q is the set $\mathbb{F}_q$.
- Two vertices u, v are connected by an edge iff

$$(u - v) \in (\mathbb{F}_q^\times)^2.$$

Note that $(\mathbb{F}_q^\times)^2$ is the set of all quadratic residue in $\mathbb{F}_q$.

Paley graph for $q = 13$

Let us consider $q = 13$. We have

$$(\mathbb{F}_{13}^{\times})^2 = \{1^2, 2^2, 3^2, 4^2, \ldots, 12^2\} = \{1, 3, 4, 9, 10, 12\}.$$

The vertices of P_{13} are $V(P_{13}) = \{0, 1, 2, \ldots, 12\}$. We observe that

- $(0, 1) \in E(P_{13})$ because

$$1 - 0 = 1^2 \in (\mathbb{F}_{13})^{\times},$$

  and

$$0 - 1 = 8^2 \in (\mathbb{F}_{13})^{\times}.$$

- $(0, 2) \notin E(P_5)$ because $2 - 0 = 2 \notin (\mathbb{F}_{13}^{\times})^2$.

Paley graph for $q = 13$

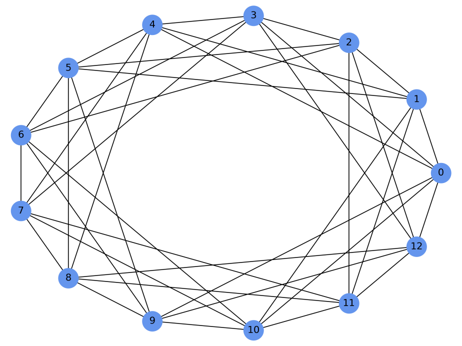

Figure 5: The Paley graph P_{13}

Spectra of P_q

Using the Circulant Diagonalization Theorem and the theory of Gauss sums, we can show the following.

Theorem

The eigenvalues of Paley graphs P_q are $\frac{1}{2}(q-1)$ (with multiplicity 1) and $\frac{1}{2}(-1 \pm \sqrt{q})$ (both with multiplicity $\frac{q-1}{2}$).

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Thank you