Network Science Cheatsheet

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Networks as Matrices

Matrices in short

Matrices are mathematical objects that can be thought as *tables* of numbers. The size of a matrix is expressed as $m \times n$, for a matrix with m rows and n columns. **The order (row/column) is important**.
M_{ij} is a notation representing the element on **row** i and **column** j.

A - Adjacency matrix

The most natural way to represent a graph as a matrix is called the Adjacency matrix A. It is defined as a square matrix, such as the number of rows (and the number of columns) is equal to the number of nodes N in the graph. Nodes of the graph are numbered from 1 to N, and there is an edge between nodes i and j if the corresponding position of the matrix A_{ij} is not 0.

- A value on the diagonal means that the corresponding node has a **self-loop**
- the graph is **undirected**, the matrix is **symmetric**: $A_{ij} = A_{ji}$ for any i, j.
- In an **unweighted** network, and edge is represented by the value 1.
- In a **weighted** network, the value A_{ij} represents the **weight** of the edge (i, j)

Typical operations on A

Some operations on Adjacency matrices have straightforward interpretations and are frequently used, such as **Multiplying** A by **itself** and **Multiplying** A by a **column vector**

Multiplying A by itself

Multiplying A by **itself** allows to know the number of walks of a given length that exist between any pair of nodes: A^2_{ij} corresponds to the number of walks of length 2 from node i to node j, A^3_{ij} to the number of walks of length 3, etc.

Multiplying A by a column vector

Multiplying A by a **column vector** W of length $1 \times N$ can be thought as setting the i th value of the vector to the ith node, and each node *sending* its value to its neighbors (for undirected graphs). The result is a column vector with N elements, the ith element corresponding to the sum of the values of its neighbors in W. This is convenient when working with **random walks** or **diffusion** phenomenon.

Spectral properties of A

Spectral Graph Theory is a whole field in itself, and beyond the scope of this class. A few elements for those with a *linear algebra* background:

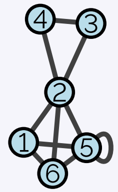
- The adjacency matrix of an undirected simple graph is symmetric, and therefore has a complete set of real eigenvalues and an orthogonal eigenvector basis.
- The set of eigenvalues of a graph is the spectrum of the graph.
- The n eigenvalues are denoted as $\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \lambda_{\max}$
- The largest eigenvalue $\lambda_{\max}$ lies between the average and maximum degrees.
- In a large, sparse random graph, $\lambda_{\max} \approx \langle k \rangle$
- The number of closed walks of length k in G equals $\sum_{i=0}^{n} \lambda_i^k$
- A graph is bipartite if and only if its spectrum is symmetric (i.e., if λ is an eigenvalue, then so is $-\lambda$
- If G is connected, then the diameter of G is strictly less than its number of distinct eigenvalues

Graph Laplacian

The **Graph Laplacian**, or **Laplacian Matrix** of a graph is a variant of the Adjacency matrix, often used in *Spectral Graph Theory*.
It is defined as $D - A$, with D the *Degree matrix* of the graph, defined as a $N \times N$ matrix with $D_{ii} = k_i$ and zeros everywhere else.

Matrix notation - Example

Graph



A - Adjacency Mat.

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

D - Degree Matrix

$$\begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

L - Laplacian

$$\begin{pmatrix} 3 & -1 & 0 & 0 & -1 & -1 \\ -1 & 5 & -1 & -1 & -1 & -1 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 2 & 0 & 0 \\ -1 & -1 & 0 & 0 & 4 & -1 \\ -1 & -1 & 0 & 0 & -1 & 3 \end{pmatrix}$$

A^2

$$\begin{pmatrix} 3 & 2 & 1 & 1 & 3 & 2 \\ 2 & 5 & 1 & 1 & 3 & 2 \\ 1 & 1 & 2 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 1 & 1 \\ 3 & 3 & 1 & 1 & 4 & 3 \\ 2 & 2 & 1 & 1 & 3 & 3 \end{pmatrix}$$

Random W. mat.

$$\begin{pmatrix} 0 & \frac{1}{5} & 0 & 0 & \frac{1}{4} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} & \frac{1}{3} \\ 0 & \frac{1}{5} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{5} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{5} & 0 & 0 & \frac{1}{4} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{5} & 0 & 0 & \frac{1}{4} & 0 \end{pmatrix}$$

Laplace Operator

Intuitively, the Laplace operator is a generalization of the second derivative, and is defined in discrete situations, for each value, as the sum of differences between the value and its "neighbors". e.g., in time, the 2^{nd} derivative *acceleration* is the difference between current speed and previous speed. In a B&W picture, it's the difference between the greylevel on current pixel and the greylevel of 4 or 8 closest pixels, and perform *edge detection*. On a graph, with W a column vector representing values on nodes, LW computes for each node the difference to neighbors.

Spectral properties of L

Eigenvalues of the Laplacian have many applications, such as *spectral clustering*, *graph matching*, *embedding*, etc. Assuming G undirected with eigenvalues $\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots \lambda_n$, here are some interesting properties:

- The smallest eigenvalue λ_i equals 0
- The number of 0 eigenvalues gives the number of connected components

Random Walk matrix

Another useful matrix of a graph is the **Random Walk Transition Matrix** R. It is the column normalized version of the adjacency matrix. R_{ij} can be understood as the probability for a random walker located on node i to move to j.

Going Further

- Introduction to spectral graph theory (Nica 2016)
- Survey on Graph Spectral Theory (Spielman 2012)
- Book on Graph Spectral Theory (Chung and Graham 1997)
- Spectral graph Clustering (Nascimento and De Carvalho 2011)
- Wavelets on graph (Hammond, Vandergheynst, and Gribonval 2011)

References

[1] Fan RK Chung and Fan Chung Graham. *Spectral graph theory*. 92. American Mathematical Soc., 1997.

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[3] Maria CV Nascimento and Andre CPLF De Carvalho. "Spectral methods for graph clustering–a survey". In: *European Journal of Operational Research* 211.2 (2011), pp. 221–231.

[4] Bogdan Nica. "A brief introduction to spectral graph theory". In: *arXiv preprint arXiv:1609.08072* (2016).

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