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:

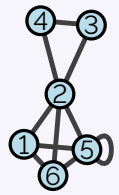
- The adjacency matrix of an undirected simple graph is symmetric, and therefore has a complete set of real eigenvalues and an orthogonal eigenvector basis.
- The set of eigenvalues of a graph is the spectrum of the graph.
- Eigenvalues are denoted as $\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \lambda_n$
- The largest eigenvalue λ_0 lies between the average and maximum degrees
- The number of closed walks of length k in G equals $\sum_i^n = 0\lambda_i^k$
- 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 2nd 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 clsutering*, *graph matching*, *embedding*, etc. Assuming G undirected with eigenvalues $\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \lambda_n$, 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).

[5] Daniel Spielman. "Spectral graph theory". In: *Combinatorial scientific computing*. 18. Citeseer, 2012.