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, an 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: \(A_{ij}^2\) corresponds to the number of walks of length 2 from node \(i\) to node \(j\), \(A_{ij}^3\) 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 \(i\)th node, and each node sending its value to its neighbors (for undirected graphs). The result is a column vector with \(N\) elements, the \(i\)th 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 \(\lambda_n\) lies between the average and maximum degrees.
- The number of closed walks of length \(k\) in \(G\) equals \(\sum i = \omega \lambda_i^k\).
- A graph is bipartite if and only if its spectrum is symmetric (i.e., if \(A\) is an eigenvalue, then so is \(-A\)).
- 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 \(D_{ii} = d_i\) and zeros everywhere else.
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 greylvel 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 \( \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \lambda_n \), here are some interesting properties:

- The smallest eigenvalue \( \lambda_1 \) 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