Graph Theory I MA1S1

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December 2, 2014

Anton & Rorres: Ch 10.6

Application of matrices to graphs

Graph theory is a subject that is somehow abstract, but at the same time rather close to applications.

Fairly simple minded examples would be an intercity rail network (nodes would be stations and the edges would correspond to the existence of a direct line from one station to another), or an airline route network, or an ancestral tree graph, or a telecommunications network.

Mathematically a graph is something that has vertices (also known as nodes) and edges (also called paths) joining some of the nodes to some others.

For our situation, we consider something more like an airline network (joining different airports by direct flights), but we will take account of the fact that some airports might not be connected by flights that go direct in both directions. Here is a route network for a start-up airline that has two routes it flies. One goes Dublin \rightarrow London and London \rightarrow Dublin, while another route makes a round trip Dublin \rightarrow Galway \rightarrow Shannon \rightarrow Dublin.



The arrows on the edges mean that this is an example of a *directed graph*. Here we allow one-way edges and bi-drectional edges between nodes (or vertices) of the graph, which we draw by indicating arrows. To get the *vertex matrix* for a graph like this, we first number or order the vertices, for instance

Dublin	1
London	2
Galway	3
Shannon	4

and then we make a matrix, a 4×4 matrix in this case since there are 4 vertices, according to the following rules. The entries of the matrix are either 0 or 1. All diagonal entries are 0. The (i, j) entry is 1 if there is a direct edge from vertex i to vertex j (in that direction).

That is we form the matrix M with entries:

$$m_{ij} = \begin{cases} 1, & P_i \to P_j \\ 0, & \text{otherwise} \end{cases}$$
(1)

So in our example graph, the vertex matrix is

$$M = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

For instance the first row in 0110 because there is a direct link $1 \rightarrow 2$ and $1 \rightarrow 3$, but no direct link $1 \rightarrow 4$ (Dublin to Galway is not directly linked).

In more precise terms: A directed graph is a finite set of elements, $\{P_1, P_2, \ldots, P_n\}$ together with a collection of ordered pairs (P_i, P_j) of distinct elements of this set with no ordered pair being repeated.

The elements of this set are called vertices, and the ordered pairs are called directed edges. We also use the notation $P_i \rightarrow P_j$ to indicate a directed edge in a graph.

In general a graph can have separate components.



In science very complicated graphs and networks commonly appear: e.g. metabolic pathways



Image from http://www2.ufp.pt/~pedros/bq/integration.htm

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Image from http://potatometabolicpathways.webs.com

Having a matrix description of graphs is often very useful. Here is one result that makes a connection to matrix multiplication.

Theorem

If M is the vertex matrix of a directed graph, then the entries of M^2 give the numbers of 2-step (or 2-hop) connections.

More precisely, the (i, j) entry of M^2 gives the number of ways to go from vertex *i* to vertex *j* with exactly 2 steps (or exactly one intermediate vertex). Similarly M^3 gives the number of 3-step connections, and so on for higher powers of M.

Consider again the graph:



with the vertex matrix

$$M = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

In our example

$$M^{2} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

The diagonal 1's in the matrix correspond to the fact that there is a round trip Dublin \rightarrow London \rightarrow Dublin (or $1 \rightarrow 2 \rightarrow 1$) and also London \rightarrow Dublin \rightarrow London. The 1 in the top right corresponds to the connection Dublin \rightarrow Galway \rightarrow Shannon.

If we add $M+M^2$ we get nonzero entries in every place where there is a connection in 1 or 2 steps

$$M + M^2 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

and the zeros off the diagonal there correspond to the connections that can't be made in either a direct connection of a 2-hop connection (which is Gaway \rightarrow London and London \rightarrow Shannon in our example). Although we don't see it here the numbers in the matrix M^2 can be bigger than 1 if there are two routes available using 2-hops.

Clique

Definition A subset of a directed graph is called a clique if it satisfies the following three conditions:

- 1 The subset contains at least three vertices.
- **2** For each pair of vertices P_i and P_j in the subset, both $P_i \to P_j$ and $P_j \to P_i$ are true.
- The subset is as large as possible; that is, it is not possible to add another vertex to the subset and still satisfy condition (ii).

A clique is in some sense the largest possible subgroup of vertices that are maximally connected to each other.

For simple graphs we can find cliques by inspection but for more complicated diagrams it is useful to have a tool. For a graph we can form the matrix S with the entries:

$$s_{ij} = \begin{cases} 1, & P_i \leftrightarrow P_j \\ 0, & \text{otherwise} \end{cases}$$
(2)

This is similar to the vertex matrix but only has non-zero entries where both vertices are connected. That is $s_{ij} = 1$ if $m_{ij} = m_{ji} = 1$ but $s_{ij} = 0$ if $m_{ij} = 0$ and/or $m_{ji} = 0$.

We note that this matrix is automatically symmetric as

$$S = S^t$$

We can then identify cliques by using the fact that if $s_{ij}^{(3)}$ are the entries of the matrix S^3 , then a vertex P_i belongs to some clique if and only if $s_{ii}^{(3)} \neq 0$.

Consider the vertex matrix

$$M = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$
(3)

we can find the graph corresponding to the with a bit of work or by using sage \ldots

Graphs and Matrices

<pre>M = Matrix([[0,</pre>	1, 1,	1, 0],[1,	0,	0, 1,	0],[0,	1,	Ο,	1,	1],[0,	1,
1, 0, 0],[0, 1,	1, 1,	0]]); M								
[0 1 1 1 0]										
[1 0 0 1 0]										
[0 1 0 1 1]										
[0 1 1 0 0]										
[0 1 1 1 0]										
G=DiGraph(M)										
P = G.plot()										
P.show(figsize=5)										



Does this matrix have any cliques? The S matrix is

$$S = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$
(4)

and so (can calculate using for example SAGE)

$$S^{3} = \begin{pmatrix} 0 & 2 & 1 & 0 & 0 \\ 2 & 0 & 0 & 3 & 1 \\ 1 & 0 & 0 & 3 & 2 \\ 0 & 3 & 3 & 0 & 0 \\ 0 & 1 & 2 & 0 & 0 \end{pmatrix}$$
(5)

and as there are no non-zero diagonal elements there are no cliques.