Spectral Graph Theory

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March 4, 2019

1 Introduction

1.1 Adjacency Matrix Representation of A Graph

We represent a Graph G with a square adjacency matrix A, where entry

$$a_{ij} = \begin{cases} 1 & \text{if (i, j) is an edge in } G \\ 0 & \text{otherwise} \end{cases}$$

Evidently, the matrix is symmetric, or $a_{ij} = a_{ji}$. Therefore by spectral theorem, we have a orthonormal basis of eigenvectors, with real eigenvalues associated.

2 Counting Paths with Adjacency Matrix

Theorem L. et G be a graph on labeled vertices, let A be its adjacency matrix, and let k be a positive integer. Then $A_{i,j}^k$ is equal to the number of walks from i to j that are of length k .

Proof. The proof is fairly simple, and we will do it by induction.

When $k = 1$, we look at the original adjacency matrix, and $A_{i,j}$ indicates whether there's an edge between i, j, which is a path of length 1.

Now assume that the statement is true for k, and prove it for $k + 1$.

Let's first think about it intuitively, A^k gives the number of paths walks from i to all other points. If one such point is v, then we just need to determine if there's and edge from v to j, if so then we just add the number of walks from i to k.

Let z be any vertex of G. If there are $b_{i,z}$ walks of length k from i to z, and there are $a_{z,j}$ walks of length one (in other words, edges) from z to j, then there are $b_{i,z}a_{z,j}$ walks of

length $k + 1$ from i to j whose next-to-last vertex is z. Therefore, the number of all walks of length $k + 1$ from i to j is:

$$c(i, j) = \sum_{z \in G} b_{i,z} a_{z,j}$$

Since $b_{i,z}$ correspond to an entry in A^k, the formula above is basically a matrix multiplication.

$\square$

At this point, it's a good habit to check our proof again. Ask ourselves this question:

We know $A_{i,j}^k$ represents some number of walks from i to j, but does it count all of them?

We'll leave it as a quick thought exercise.

2.1 Connectivity

Theorem L. et G be a simple graph on n vertices, and let A be the adjacency matrix of G. Then G is connected iff $(I + A)^{n-1}$ consists of strictly positive entries.

Proof. We will only give the central idea of the proof here

A path from one point to another consists at most n vertices, or $n - 1$ edges. Therefore, if we cannot find a path between two points within $n - 1$ edges, the graph is not connected

Using the previous theorem, we know that A_{n-1} gives the number of paths if length $n - 1$ between any two points, however, this is **not enough**.

Notice that the theorem indicates it's $(I + A)^{n-1}$ instead of A^{n-1}. So what does the I do?

Graphically, it means that we assume any vertex is connected to itself. What is $(I + A)^{n-1}$ then?

For simplicity, call $(I + A) = A'$. With $A'_{i,i} = 1$, A'^k no longer counts the number of paths of length **strictly** k, but the number of paths of length $\leq k$. This is because we don't have to move to another point every time we multiply A', we can choose to stay at the same point since $A'_{i,i} = 1$.

Therefore $(I + A)^{n-1}$ counts the number of paths of length $\leq n - 1$, and if there still exist an 0 entry $A'^{n-1}_{i,j}$, then it means if we cannot find a path between two points within $n - 1$ edges, the graph is not connected. $\square$

Some Remarks: Bellman-Ford algorithm also uses the property that a path between two vertices in a connected graph has edge count at most $n - 1$ to check for negative cycles.

3 Matrix Tree Theorem (Many Versions)

It turns out that we can use matrix to count the number of spanning trees with matrices. There are many matrix tree theorems, and we here will just talk about a few of them.

3.1 Incidence Matrix

We first define the incidence matrix A for a graph G

The incidence matrix of $G(V, E)$ is a $n \times m$ matrix, where $n = |V|, m = |E|$. We label the edges $e_1, \cdots, e_m$ and vertices $v_1, \cdots, v_n$. Then

$$A_{i,k} = \begin{cases} 1 \text{ if } i \text{ is the head of the edge of } e_k \\ -1 \text{ if } i \text{ is the tail of the edge of } e_k \\ 0 \text{ otherwise} \end{cases}$$

Theorem L. et G be a directed graph without loops, and let A be the incidence matrix of G. Remove any row from A, and let A_0 be the remaining matrix. Then the number of spanning trees of G is det $A_0 A_0^T$

Proof. Let us assume, without loss of generality, that the last row of A was omitted. Let B be an $(n-1) \times (n-1)$ submatrix of A_0. (If $m < n - 1$), then G cannot be connected, and it has no spanning trees.) We claim that $|\det B| = 1$ if and only if the subgraph G' corresponding to the columns of B is a spanning tree (including the last row), and det $B = 0$ otherwise.

First we need to notice that G' is basically a subgraph with all the vertices but only $n - 1$ edges.

We induct on n. First, let us assume that there is a vertex $v_i (i \neq n)$ of degree one in G'. (The degree of a vertex in an undirected graph is the number of all edges adjacent to that vertex.) Then the i th row of B contains exactly one nonzero element, and that element is 1 or -1. Expanding det B by this row, and using the induction hypothesis, the claim follows. Indeed, G' is a spanning tree of G if and only if $G' - v_i$ is a spanning tree of $G - v_i$.

If G' has no vertices of degree one (except possibly v_n, the vertex associated to the deleted last row). Then G' is not a spanning tree (cus no leaf).

Since G' has $n - 1$ edges, and is not a spanning tree, there must be a vertex in G' that has degree zero. If this vertex is not v_n, then B has a zero row, and det $B = 0$. If this vertex is v_n, then each column of B contains one 1, and one -1 as each edge has a head and a tail. Therefore, the sum of all rows of B is 0, so the rows of B are linearly dependent, and det $B = 0$

The Binet-Cauchy formula, that can be found in most Linear Algebra textbooks, says that

$$\det A_0 A_0^T = \sum (\det B)^2$$

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where the sum ranges over all $(n-1) \times (n-1)$ submatrices B of A_0. However, we have just seen that $(\det B)^2 = 1$ if and only if B corresponds to a spanning tree of A, and $(\det B)^2 = 0$ otherwise. Therefore, the proof follows. $\qquad \square$

Theorem L. et U be a simple undirected graph. Let $\{v_1, v_2, \cdots, v_n\}$ denote the vertices of U. Define the $(n-1) \times (n-1)$ matrix L_0 by

$$l_{i,j} = \begin{cases} \text{degree of } v_i & i = j \\ l_{i,j} = -1 & i \neq j \text{ and } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

Then the theorem states $\det L_0$ counts the number of spanning trees in U

Proof. We turn U into a directed graph with each edge replaced with a **pair** or directed opposited edges.

Let A_0 be the incidency matrix of $G - v_n$. We claim that $A_0 A_0^T = 2L_0$. The entry of $A_0 A_0^T$ in position (i, j) is the scalar product of the ith and j th row of A_0. If $i = j$, then every edge that starts or ends at v_i contributes 1 to this inner product. Therefore, the entry of $A_0 A_0^T$ in position (i, i) is the degree of v_i in G, or, in other words, twice the degree of v_i in U

If $i = j$, then we see that every edge between i and j in U will contribute -2 to $A_0 A_0^T$, but the corresponding entry in L_0 is -1. Therefore all entries in L_0 is half of $A_0 A_0^T$.

Therefore $2^{n-1} \det L_0 = \det \left(A_0 A_0^T \right)$. However, for each spanning tree in G, each of its edge can choose 2 directions in U, so it corresponds to 2^{n-1} spanning trees in U. And also since $A_0 A_0^T$ counts the number of spanning trees in U, we then have $\det L_0$ counts the number of spanning trees in G. $\qquad \square$