A simple nullspace version of the matrix tree theorem

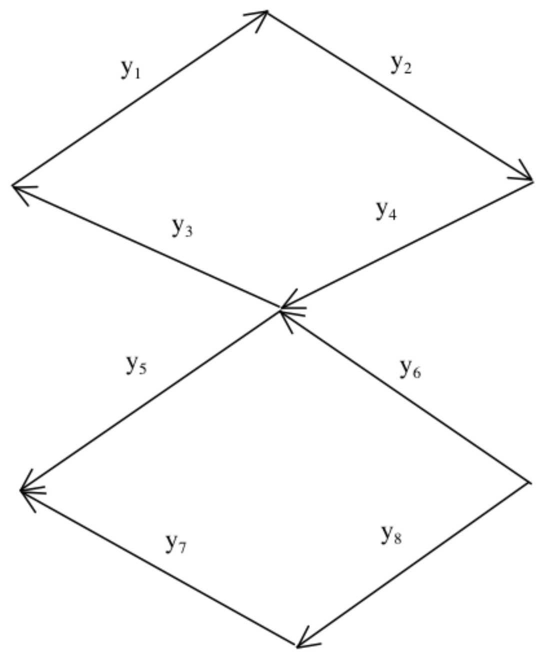
1 Overview

The matrix tree theorem states that the number of spanning trees in an m nodes, n arcs graph of an incidence matrix, A, equals the determinant of $A_0 A_0^T$ where A_0 is the $(m-1) \times n$ matrix formed by dropping any row from A. An incidence matrix is a matrix in which the elements are zeros except each column has one 1 and one -1. A proof follows from the Binet-Cauchy theorem (stated below) and unimodularity of submatrices of A_0 (defined below).

The simple nullspace version of the matrix tree theorem says the number of spanning trees equals $\left|NN^T\right|$ where N is the $r \times n$ simple nullspace of A, simple refers to composing the nullspace entirely of 0's and ± 1, $r = n - m + 1 \geq 1$ is the dimension of the nullspace, and $|\cdot|$ is the determinant of the matrix. Our proof follows the reasoning outlined above for the standard version of the matrix tree theorem. That is, we utilize the Binet-Cauchy theorem and unimodularity of submatrices of N. Since spanning trees are formed by eliminating loops in the graph it's natural to focus on the nullspace (the nullspace is the loops in the graph).

1.1 Non-overlapping arcs

If there are no arcs in multiple loops (no overlaps), then the nullspace version is immediately demonstrated. That is, the number of spanning trees is the product of the number of arcs in each (linearly independent) loop; this is precisely what $\left|NN^T\right|$ gives. Hence, the challenge involves addressing overlapping arcs (arcs in multiple loops). A simple non-overlapping graph is depicted below.



Non-overlapping arcs graph

A simple nullspace for the above graph is $N = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \end{bmatrix}$ and $|NN^T| = \begin{vmatrix} 4 & 0 \\ 0 & 4 \end{vmatrix} = 4^2 = 16$. Also,

$$A = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

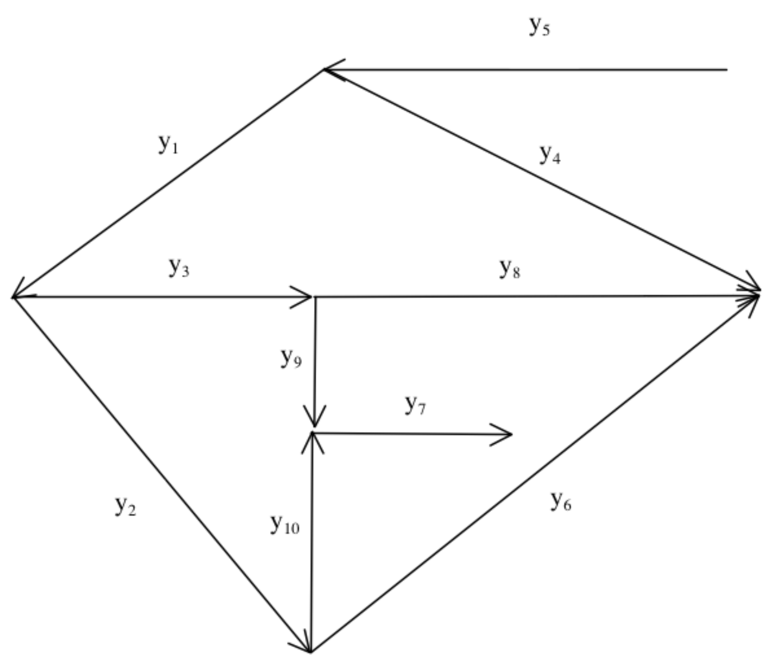
such that $AN^T = 0$. Drop any row (say, the last row) and we have

$$|A_0 A_0^T| = \begin{vmatrix} 2 & -1 & 0 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ -1 & 0 & -1 & 4 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & -1 & 0 & 2 \end{vmatrix} = 16$$

This not only illustrates the equivalence between the standard and nullspace versions of the theorem but also the relative computational simplicity of the nullspace version.

1.2 Overlapping arcs

A simple illustration of three loops with overlapping arcs is instructive.



Overlapping arcs graph

The incidence matrix associated with this graph is 8×10 and the nullspace is 3×10 such that $AN^T = 0$. Arcs 5 and 7 are not in loops and a simple basis for the nullspace is

$$N = \begin{bmatrix} 1 & 0 & 1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 1 & -1 \end{bmatrix}$$

where $\left|A_0 A_0^T\right| = \left|NN^T\right| = 36$. Notice, if each of the three loop involving four arcs did not involve any overlapping arcs there would be $4^3 = 64$ spanning trees. Therefore, the key is to count the reduction in spanning trees due to overlaps (in this example, the reduction is $64 - 36 = 28$).

1.3 Unimodularity and the Binet-Cauchy theorem

To address overlaps, we next define unimodularity and state the Binet-Cauchy theorem.

Definition 1 *Total unimodularity (TU): An $r \times s$ matrix M is totally unimodular if the determinant of every $k \times k$ submatrix S is 0 or ± 1 ($1 \le k \le \min\{r, s\}$).*

Theorem 1 *Binet-Cauchy theorem: Let R be a $p \times q$ matrix and S be a $q \times p$ matrix where $p \le q$. Also, let R_k denote the kth column of R and S_k denote the kth column of S. Then,*

$$|RS| = \sum_{1 \le k_1 < k_2 < \cdots k_p \le q} \left|\left[R_{k_1}, R_{k_2}, \ldots, R_{k_p}\right]\right| \left|\left[S_{k_1}^T, S_{k_2}^T, \ldots, S_{k_p}^T\right]\right|$$

Proof. The row i, column j element of RS is $\sum_{k=1}^{q} r_{ik} s_{kj}$ and the jth column is $(RS)_j = \sum_{k=1}^{q} R_k s_{kj}$.

$$\begin{aligned} |RS| &= |[RS_1, RS_2, \ldots, RS_p]| \\ &= \left|\left[\sum_{k_1=1}^{q} R_{k_1} s_{k_1 1}, \sum_{k_2=1}^{q} R_{k_2} s_{k_2 2}, \ldots, \sum_{k_p=1}^{q} R_{k_p} s_{k_p p}\right]\right| \\ &= \sum_{k_1=1}^{q} s_{k_1 1} \left|\left[R_{k_1}, \sum_{k_2=1}^{q} R_{k_2} s_{k_2 2}, \ldots, \sum_{k_p=1}^{q} R_{k_p} s_{k_p p}\right]\right| \\ &= \sum_{k_1=1}^{q} s_{k_1 1} \sum_{k_2=1}^{q} s_{k_2 2} \cdots \sum_{k_p=1}^{q} s_{k_p p} \left|\left[R_{k_1}, R_{k_2}, \ldots, R_{k_p}\right]\right| \end{aligned}$$

Since $\left|\left[R_{k_1}, R_{k_2}, \ldots, R_{k_p}\right]\right| = 0$ for $k_i = k_j$ when $i \ne j$ (linearly dependent rows), we only sum over the cases in which $k_i \ne k_j$ for $i \ne j$. Hence,

$$|RS| = \sum_{1 \le k_1 < k_2 < \cdots k_p \le q} \left|\left[R_{k_1}, R_{k_2}, \ldots, R_{k_p}\right]\right| \left|\left[S_{k_1}^T, S_{k_2}^T, \ldots, S_{k_p}^T\right]\right|$$

This completes the proof. ■

2 A simple nullspace version of the matrix tree theorem

Unimodularity and the Binet-Cauchy theorem set the main stage for the simple nullspace version of the matrix tree theorem but first we define a simple basis for the nullspace of an incidence matrix then state and prove unimodularity for the simple nullspace.

Definition 2 *Simple basis for the nullspace of an incidence matrix: A simple basis for the nullspace of an incidence matrix is one in which each loop is represented by* ± 1 *associated with the arcs contained in the loop and zeros for arcs not in the loop.*

Since an incidence matrix contains only 0 and ± 1 this is always possible and the sign only provides relative direction. For instance, in the 8×10 graph with overlapping arcs, arc 4 is in the opposite direction to the other arcs (arcs 1, 3, and 8) in the first loop identified. It is a matter of indifference whether we define this loop as

$$\begin{bmatrix} 1 & 0 & 1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

or

$$\begin{bmatrix} -1 & 0 & -1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \end{bmatrix}$$

Lemma 1 *Unimodularity of the simple nullspace: A simple basis for the nullspace of an incidence matrix is totally unimodular.*

Proof. The statement is trivially true for single element submatrices. All 2×2 submatrices, S, are either singular or $|S| = |L|\,|U| = 1\,(\pm 1) = \pm 1$ where $S = LU$ by lower, upper factorization (utilizing the facts that the determinant of a triangular matrix is the product of the diagonals and the determinant of the product of square matrices equals the product of the determinants). This follows as relative direction of the arcs must be maintained for each loop with overlapping arcs. By the same reasoning, all larger submatrices with multiple overlapping arcs in the same two loops are singular and submatrices without multiple overlapping arcs in the same two loops are either singular or have determinant equal to ± 1 since their elements are all 0 or ± 1. ■

The intuition for this is no submatrix from any basis for the nullspace includes overlapping arcs in the same two loops in which relative direction is not preserved such as in $\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ (which has determinant equal to 2), rather we could observe multiple overlapping arcs such as $\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$, $\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, or $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ (all of which are singular). For submatrices without multiple overlapping arcs in the same two loops we could have a singular submatrix such as $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, or nonsingular submatrices such as $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$ or $\begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$. But multiple overlapping arcs such as $\begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & -1 \end{bmatrix}$ is not a submatrix from a basis for the nullspace (loops 1 and 3 are consistent but loops 1 and 2 are not part of any basis for the nullspace of an incidence matrix as relative direction of the first and second arcs, columns, is not maintained).

For the 7×8, 2 loops incidence matrix with non-overlapping arcs identified earlier, there are $\begin{pmatrix} 8 \\ 2 \end{pmatrix} = 28$ — 2×2 submatrices, of which 12 are singular. While for the 8×10, 3 loops incidence matrix with multiple overlapping arcs identified earlier, there are $\begin{pmatrix} 10 \\ 3 \end{pmatrix} = 120$ — 3×3 submatrices, of which 84 are singular. The counting of these singular submatrices is the key for connecting $\left|NN^T\right|$ to the number of spanning trees so long as the nullspace is not empty (in the case of a zero dimension nullspace, there is only one spanning tree).

Lemma 2 *The number of $r \times r$ nonsingular submatrices of N equals the number of spanning trees in the graph based on incidence matrix A.*

Proof. Submatrices involving no pairs of loops with overlapping arcs are either singular (and either disconnect the graph or leave loops in the graph) or are nonsingular and identify spanning trees. Hence, once again the challenge resides with loops involving overlapping arcs. Submatrices involving pairs of loops with multiple overlapping arcs are singular by preservation of relative direction (lemma 1) and fail to identify spanning trees. Submatrices involving pairs of loops with one overlapping arc are either singular (identify disconnected graphs or leave loops in the graph) or nonsingular (identify a spanning tree). ■

We now have the pieces in place and the proof of the simple nullspace version of the matrix tree theorem is almost immediate.

Theorem 2 *Simple nullspace version of the matrix tree theorem: For an $m \times n$ ($m \leq n$ implies $r \geq 1$) incidence matrix, A, with simple (nonempty) nullspace basis $r \times n$, N, the number of spanning trees equals $\left|NN^T\right|$.*

Proof. Let S_k be an $r \times r$ submatrix of N for $k = 1, \ldots, n_r$ where $n_r = \left(\begin{array}{c} n \\ r \end{array} \right)$.

$$\begin{aligned}
\left|NN^T\right| &= \sum_{k=1}^{n_r} |S_k| \left|S_k^T\right| && \text{(Binet-Cauchy)} \\
&= \sum_{k=1}^{n_r} |S_k|^2 \\
&= \sum_{S_k \in \text{singular}} |S_k|^2 + \sum_{S_k \in \text{nonsingular}} |S_k|^2 \\
&= \sum_{S_k \in \text{nonsingular}} |S_k|^2 \\
&= \text{number of } r \times r \text{ nonsingular} && \text{(lemma 1)} \\
&\quad\ \text{submatrices of } N \\
&= \text{number of spanning trees of } A && \text{(lemma 2)}
\end{aligned}$$

This completes the proof. ■

3 Discussion

A proof of the standard version of the matrix tree theorem says that submatrices of A_0 are unimodular and only the nonsingular submatrices are included in the count of spanning trees. In other words, the $(m-1) \times (m-1)$ nonsingular submatrices identify the arcs of spanning trees. The simple nullspace version of the matrix tree theorem says look to the complement of the above strategy. Instead of identifying arcs in the spanning tree, identify arcs to remove from the graph to form spanning trees. Since they are complementary actions they must produce the same results. Further, if $m - 1 > r$ (as is often the case), looking to the nullspace or loops in the graph is computationally simpler.

One final point. If we augment A_0 with N to form an $n \times n$ matrix, its determinant equals the number of spanning trees.

$$\left| \begin{bmatrix} A_0 \\ N \end{bmatrix} \right| = \#\text{ spanning trees}$$

Given this result and the standard version of the matrix tree theorem, it's straightforward to connect with the simple nullspace version.

$$\begin{aligned}
\left| \begin{bmatrix} A_0 \\ N \end{bmatrix} \right|^2 &= (\#\text{ spanning trees})^2 \\
&= \left| \begin{bmatrix} A_0 \\ N \end{bmatrix} \begin{bmatrix} A_0 \\ N \end{bmatrix}^T \right| \\
&= \left| \begin{bmatrix} A_0 A_0^T & 0 \\ 0 & NN^T \end{bmatrix} \right| \\
&= \left|A_0 A_0^T\right| \cdot \left|NN^T\right|
\end{aligned}$$

which implies

$$\begin{aligned} \left|NN^T\right| &= \frac{(\#\text{ spanning trees})^2}{(\#\text{ spanning trees})} \\ &= (\#\text{ spanning trees}) \end{aligned}$$

Of course, this can be reversed so that the results for the simple nullspace version of the matrix tree theorem in combination with the standard version of the matrix tree theory imply $\left|\begin{bmatrix} A_0 \\ N \end{bmatrix}\right| = \#$ spanning trees.