Determinants of Distance Matrices of Trees

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ABSTRACT. A formula for the determinant of the distance matrix for a tree as a function of the number of its vertices, independent of the structure of the tree, has been proven by several mathematicians. We explore the details of the proof by Weigen Yan and Yeong-NanYeh, look at the history of the topic, and see the theorem in action by way of examples.

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1. ACKNOWLEDGMENTS

This paper is in partial fulfillment of the requirements for a Masters of Science degree in Mathematics from Portland State University. This "Mathematics in Literature Problem" is based on the article "A simple Proof of Graham and Pollak's Theorem" by Weigen Yan and Yeong-Nan Yeh [6]. Special thanks to my adviser John Caughman, and my reader Joyce O'Halloran.

2. INTRODUCTION

Graph theory is the mathematical study of networks. These networks are represented by nodes (vertices) and connections (edges). This study has many applications, and it branches to many other disciplines of mathematics, resulting in mathematicians from many different mathematical backgrounds having published results in the topic.

In the 1970's, Ronald L. Graham, the man responsible for Graham's Number, published several results in graph theory. Beyond his work in graph theory, Graham actually began some new areas of study such as worst-case analysis in scheduling theory, and the Grahams Scan in computational geometry. On top of his extensive work in applied mathematics, Graham was at one point the president of the International Jugglers Association, a circus performer, and Chief Scientist at California Institute for Telecommunication and Information Technology, and worked at Bell System Tech Labs [8]. Also working at Bell was Dr. H.O. Pollak, with whom Graham worked with on several graph theory results. In their paper titled On the Addressing Problem for Loop Switching [4], graph theory is used in the study of transmitting messages and calls efficiently at Bell System Tech. It is in this application that the need for the determinant of a distance matrix of a tree is discovered, and proven using rather complicated linear algebra.

In 2005, Weigen Yan and Yeong-Nan Yeh published A simple Proof of Graham and Pollak's Theorem [6]. The theorem they are referring to is the formula for the determinant of a distance matrix for a tree, and their proof is the basis for the work done in this paper.

In Yan and Yeh's proof of the formula, an interesting connection is made to Charles Dodgson (27 January 1832 – 14 January 1898). More commonly known by his pen name Lewis Carroll, author of the beloved classic Alice in Wonderland, Dodgson was a recreational mathematician. Among other things, he developed a new way of evaluating determinants of matrices called Condensation, and his method was based on a theorem that is known as the Desnanot-Jacobi Identity [4]. Consequently, this identity is sometimes referred to as Dodgson's determinant evaluation rule, as was done by Yan and Yeh. This plays a large role in the proof of the main theorem of this paper.

We will begin with a review of graph theory and the linear algebra that applies to the focus of this topic. We shall then explore the proof of the main theorem and see some examples of the theorem in action. The proof of the theorem depends on Dodgson's determinant evaluation rule, so we will take a break from the proof of the main theorem to see the proof of this identity, therein completing the proof of the result.

3. TREES AND DETERMINANTS

Graph theory is the study of networks consisting of vertices and edges. A graph is a collection of vertices, edges, and the connections between them. A graph can be *connected*, or *disconnected* (see Figure 1).

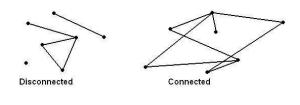
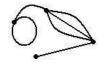


Figure 1

Some graphs can have *loops* or *multi-edges*, (see Figure 2) but a *simple* graph is restricted to exclude these types of edges.



Loops and Multi-edges

Figure 2

Two vertices in a graph are said to be *adjacent* if they are connected by a at least one edge. A *path* is a series of connections in a graph beginning with a vertex and ending with another vertex, with no repeated edges or vertices in the sequence. A *cycle* is a path that ends with the same vertex it began with.

A *tree* is a connected graph with no cycles. (See Figure 3) The vertices at the ends of the tree's branches are called *leaves*. The leaves are circled in Figure 3. A tree of n vertices has n-1 edges [6].

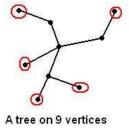


Figure 3

Trees are useful in graph theory since any connected graph has an embedded tree called the *spanning tree*, which uses all the vertices of the graph. There are a lot of nice results

about trees, which can make the work easier if one can restrict attention to the spanning tree of the graph.

The *distance* from one vertex to another in a graph is the length of the shortest path. The way we think about length of a path is the number of "steps" between each vertex. It is the same to count the number of edges between the vertices in such a shortest path. The *distance matrix* of a graph on *n* vertices is an $n \times n$ matrix whose i, jth entry is the distance between the ith and jth vertices [6]. Such a matrix is by definition symmetric with whole number entries. For example, the distance matrix of the tree in figure 3 would be made by naming the vertices v_1, \ldots, v_9 and forming the matrix. Depending on how the tree is labeled, the matrix will look different, but will have the same determinant. The entries will all be the same but will be permuted throughout the matrix by a series of row and column switches. For example, if row 2 and 3 are swapped, then we must also swap column 2 and 3. Each swap results in negation of the determinant, but since all our swaps come in pairs, our determinant will remain unchanged. In Figure 4, a labeling is assigned and the resulting distance matrix is given.

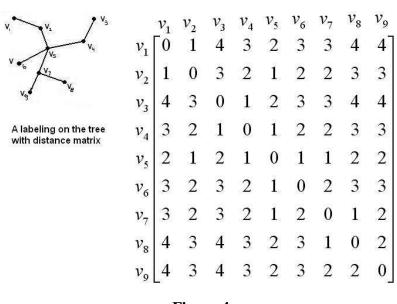


Figure 4

In linear algebra, determinants of square matrices can be found by a method called co-factor expansion. This method utilizes a notion called the minor of an element. The minor of an element a_{ij} is defined as the sub-matrix left after the ith row and jth column are deleted (crossed out). This is denoted as M_{ij} . The cofactor element of a_{ij} is denoted by C_{ij} and is equal to $(-1)^{i+j} |M_{ij}|$.

In cofactor expansion, you may pick any row or column you like to expand along. It is beneficial and eases computation time to pick a row or column rich with zeros. The determinant of the matrix is then equal to the sum of each of the entries of the row multiplied by their respective cofactor element [8].

The main theorem gives us a formula for the determinant of a distance matrix of a tree. This formula is a function of the number of vertices, and is otherwise completely

independent of the structure of the tree. For a tree on *n* vertices, the determinant will be $-(n-1)(-2)^{n-2}$.

Therefore, according to the theorem, the distance matrices of the following two trees should have the same determinant. Let us use co-factor expansion to see.

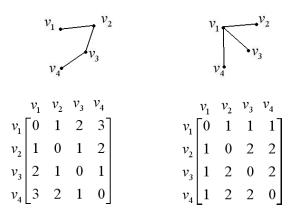


Figure 5

These are clearly different matrices—the matrix on the left has 3 as an entry twice while the matrix on the right does not. Let us compute the determinants using cofactor expansion.

$$\begin{aligned} & -1 \begin{vmatrix} 1 & 1 & 2 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{vmatrix} + 2 \begin{vmatrix} 1 & 0 & 2 \\ 2 & 1 & 1 \\ 3 & 2 & 0 \end{vmatrix} - 3 \begin{vmatrix} 1 & 0 & 1 \\ 2 & 1 & 0 \\ 3 & 2 & 1 \end{vmatrix} \\ = -(-1-(-3)+2(2))+2((-2)+2)-3(1+1) \\ = -6+-6 \\ = -12 \\ & -\begin{vmatrix} 1 & 2 & 2 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{vmatrix} + \begin{vmatrix} 1 & 0 & 2 \\ 1 & 2 & 2 \\ 1 & 2 & 0 \end{vmatrix} - \begin{vmatrix} 1 & 0 & 2 \\ 1 & 2 & 0 \\ 1 & 2 & 0 \end{vmatrix} \\ = -(-4-2(-2)+2(2))+(-4)-(4) \\ = -4-4-4 \\ = -12 \end{aligned}$$

Although the previous calculations were not very tedious, to carry out the process for the matrix in figure 4 would be nightmarish. The first step would be the sum of 8

determinants of 8x8 matrices. The next step would be up to 8 summands of determinants of 7x7 matrices For matrices this large, there is an alternative way (besides technology) to find the determinant. Dodgson's method for evaluating determinants is called Condensation, because it "condenses" a matrix step by step until the determinant is left at the end. The process can be outlined by the following steps:

1) Use elementary row operations so that no zeros occur as an "interior"

entry. $\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & [zero - free] & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix}$

2) Compute the determinant of each minor of 4 adjacent terms to form a new $n-1 \times n-1$ matrix:

$ \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ \vdots \end{bmatrix} $	$egin{aligned} a_{12} \ a_{22} \end{aligned}$	$\begin{vmatrix} a_{13} \\ a_{23} \end{vmatrix}$		
	$egin{aligned} a_{n-2,n-1}\ a_{n,n-2} \end{aligned}$	$\left. egin{array}{c} a_{n-1,n-1} \ a_{n,n-1} \end{array} ight $	$egin{aligned} a_{n-1,n-1} \ a_{n,n-1} \end{aligned}$	$\left. \begin{array}{c} a_{n-1,n} \\ a_{nn} \end{array} \right $

- 3) Repeat step 2) for the $n-1 \times n-1$ matrix, except now divide the new entry by the corresponding interior entry of the $n \times n$. This division is the reason why we did not want zeros in the interior.
- 4) If a zero appears in the interior of any subsequent matrix, then repeat step 3. In general, for the $n-t \times n-t$ matrix obtained by the 2x2 determinants of the $n-(t-1)\times n-(t-1)$ matrix, divide each entry by the interior of the $n-(t-2)\times n-(t-2)$ matrix. Repeat until a single value is reached.
- 5) If a zero occurs in the interior of any resultant matrix, the process cannot continue. Dodgson did develop a solution to this problem but it is itself tedious. It will be omitted in this discussion, but for the curious reader, the explanation of the method can be found in the article: Condensation of Determinants, Being a New and Brief Method for Computing their Arithmetical Values [4].

Dodgson developed this method in response to the time consumption that ensues when trying to apply cofactor expansion to a large matrix, such as our 9x9 matrix for instance.[4] Although the Condensation method would require around 9 steps (or more if zeros occur), the method of cofactor expansion could require up to 9!=362,880 steps. Condensation is overall a good resort for finding the determinant of very large matrices.

Below is the calculation of the determinant of the matrix from Figure 5 using Condensation.

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{bmatrix}$$

Since zeros are in the interior of this matrix, we must perform elementary row operations on it to remedy this problem. We arrive at the matrix:

$$\begin{bmatrix} 1 & 1 & 3 & 5 \\ 6 & 3 & 2 & 3 \\ 3 & 2 & 3 & 6 \\ 5 & 3 & 1 & 1 \end{bmatrix}$$

The first step of condensation yields:

$$\begin{bmatrix} -3 & -7 & -1 \\ 3 & 5 & 3 \\ -1 & -7 & -3 \end{bmatrix}$$

The next step requires us to consult the interior of our starting matrix. After condensing and dividing by the appropriate interior entry, we arrive at:

$$\begin{bmatrix} (-15 - (-21))/3 & (-21 - (-5))/2 \\ (-21 - (-5))/2 & (-15 - (-21))/3 \end{bmatrix} = \begin{bmatrix} 2 & -8 \\ -8 & 2 \end{bmatrix}$$

Finally, we take step 3 again to obtain with a determinant of $\frac{4-64}{5} = -12$.

Now using the formula given by our main theorem, we obtain

$$-(4-1)(-2)^{4-2} = -3 \cdot 4 = -12.$$

The theorem Dodgson used to develop this method is known as the Desnanot-Jacobi Adjoint Matrix Theorem, but is also referred to as Dodgson's Determinant Evaluation Rule,

$$\det(A)\det(A_2) = \det(A_{11})\det(A_{nn}) - \det(A_{1n})\det(A_{n1})$$

where A is an $n \times n$ matrix, A_2 is the minor obtained by deleting both the first and last rows and columns, A_{ij} is the minor obtained by deleting the ith row and jth column [6]. This identity will come in very handy when proving the main theorem.

4. PROOF OF THE MAIN THEOREM

Theorem. (Graham Pollack) Suppose *T* is a tree with vertex set $V(T) = \{v_1, v_2, ..., v_n\}$. Let $D = (d_{i,j})_{n \times n}$ be the $n \times n$ distance matrix of *T*, where $d_{i,j}$ is the distance between the vertices v_i and v_j .

Then the determinant of the matrix is

$$\det(D) = -(n-1)(-2)^{n-2}$$

which is independent of the structure of T [6].

Proof. (by induction on *n*)

Base case: n = 3



Figure 5

There is only one tree on 3 vertices (see Figure 5).

The distance matrix for this tree is:

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

For the sake of simplicity in calculations, from here on out we will denote the determinant of D as |D|.

Using cofactor expansion along the first row, we find

$$|D| = 0 \begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix} - 1 \begin{vmatrix} 1 & 1 \\ 2 & 0 \end{vmatrix} + 2 \begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix} = 0 + 2 + 2 = 4$$

Using the formula in the hypothesis, we have that

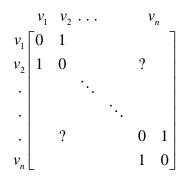
 $|D| = -(3-1)(-2)^{3-2} = -(2)(-2) = 4$

Induction Step: Suppose the hypothesis holds for trees on less than n vertices.

Suppose T is a tree on $n \ge 4$ vertices. Every tree has a least two leaves, so find two leaves of T and call them v_1 and v_n .

Leaves have unique neighbors, so call the unique neighbors of v_1 and v_n , v_2 and v_{n-1} respectively. So the distance between v_1 and v_2 is 1, and so is the distance between v_n and v_{n-1} .

Consider the distance matrix of T:



Now, let d_i denote the ith column of D. Note that any entry in d_1 is the distance of some vertex to v_1 , while any entry in d_2 is the distance of some vertex to v_2 . Since v_1 is a pendant adjacent to v_2 , any vertex of distance t from v_2 will be distance t+1 from v_1 . Therefore the entry $d_{1i} = d_{2i}+1$ for all $2 \le i \le n-2$. Similar for the columns d_{n-1} and d_n .

Keeping this in mind, we can compute the following:

$$(d_1 - d_2)^T = \langle -1 \ 1 \ 1 \ \dots \ 1 \rangle$$

 $(d_n - d_{n-1})^T = \langle 1 \ 1 \ \dots \ 1 \ -1 \rangle$

Recall that adding multiples of columns to other columns does not change the determinant of the matrix.

So use the column $(d_1 - d_2)^T + (d_n - d_{n-1})^T = \langle -2 \quad 0 \quad \dots \quad 0 \quad 2 \rangle$ in place of the column d_1 and rename it d_t .

Therefore the matrix below has the same determinant as D but is easier to compute:

$$\begin{bmatrix} -2 & d_{12} & \dots & \dots & d_{1n} \\ 0 & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 2 & d_{n2} & \dots & d_{n,n-1} & 0 \end{bmatrix}$$

Use cofactor expansion along the first column to compute the determinant,

$$|D| = -2|D_1^1| + 2(-1)^{n+1}|D_1^n|$$

where D_j^i is the matrix obtained by deleting the ith row and jth column of D.

Note that D_1^1 is the distance matrix of $T - v_1$, which is a tree on less than *n* vertices, so the hypothesis holds for it.

So we have that

$$D| = -2|D_1^1| + 2(-1)^{n+1}|D_1^n|$$

= -2(-(n-2)(-2)^{n-3}) + 2(-1)^{n+1}|D_1^n| (1)

To get another expression for the determinant of D, we turn to the following lemma.

Lemma. (Desnanot-Jacobi). M_j^i is a matrix obtained by deleting the ith row and jth column of an $n \times n$ matrix M, and M_{jl}^{ik} is a matrix obtained by deleting the ith and kth rows and jth and lth rows of a matrix M, then

$$|M||M_{1n}^{1n}| = |M_1^1||M_n^n| - |M_1^1||M_1^n|.$$

Proof.

Form the cofactor matrix, M^{c} , whose entry in the ith row and jth column is $(-1)^{i+j} |M_{j}^{i}|$ where M_{j}^{i} is as defined above. Then

$$M^{C} = \begin{bmatrix} |M_{1}^{1}| & -|M_{1}^{2}| & \dots & (-1)^{n+1} |M_{1}^{n}| \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{n+1} |M_{n}^{1}| & \dots & \dots & |M_{n}^{n}| \end{bmatrix}$$

Consider the matrix $M = \begin{bmatrix} m_{11} & m_{12} & \dots & m_{1n} \\ m_{21} & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ m_{n1} & m_{n2} & \dots & m_{nn} \end{bmatrix}$ and the dot product of the ith row of

M and the ith row of M^{C} :

$$\langle m_{i1} \ m_{i2} \ \dots \ m_{in} \rangle \bullet \langle (-1)^{i+1} | M_1^i | + (-1)^{i+2} | M_2^i | \dots \ (-1)^{i+n} | M_n^i | \rangle$$

which simplifies to:

$$(-1)^{i+1} \left(m_{i1} \left| M_1^i \right| - m_{i2} \left| M_2^i \right| + \dots + (-1)^{n-1} m_{in} \left| M_n^i \right| \right)$$

Note that using the cofactor expansion formula along the i^{th} row of M would yield the same expression for the determinant of M.

Also, note the expression

$$(-1)^{i+1} \left(m_{i1} \left| M_1^{j} \right| - m_{i2} \left| M_2^{j} \right| + \dots + (-1)^{n-1} m_{in} \left| M_n^{j} \right| \right)$$

with $j \neq i$ is the determinant of the matrix in which row *i* is replaced with a copy of row j. Such a matrix has determinant 0, so we have that

$$(-1)^{i+1} \left(m_{i1} \left| M_1^{j} \right| - m_{i2} \left| M_2^{j} \right| + \dots + (-1)^{n-1} m_{in} \left| M_n^{j} \right| \right) = \begin{cases} |M| & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Define a new matrix M^* . This matrix has the same 1^{st} and n^{th} column as M^{C} , but for $2 \leq i, j \leq n-1$,

$$m_{ij}^* = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

$$M^{*} = \begin{bmatrix} |M_{1}^{1}| & 0 & \dots & 0 & (-1)^{n+1} |M_{1}^{n}| \\ -|M_{2}^{1}| & 1 & 0 & (-1)^{n+2} |M_{2}^{n}| \\ \vdots & & \vdots \\ \vdots & 0 & 1 & \vdots \\ (-1)^{n+1} |M_{n}^{1}| & 0 & \dots & 0 & |M_{n}^{n}| \end{bmatrix}$$

Note that by construction of M^* , the matrix product MM^* gives

$$MM * = \begin{bmatrix} |M| & m_{12} & m_{13} & \dots & 0 \\ 0 & m_{22} & . & & 0 \\ 0 & \vdots & . & . & 0 \\ \vdots & . & . & . & \vdots \\ 0 & m_{n2} & m_{n3} & \dots & |M| \end{bmatrix}$$

Using cofactor expansion along the first column of MM *, the determinant of MM * is given by

$$|MM *| = |M| | (MM *)_1^1 |.$$

Then, expanding along the last column of MM_{1}^{*1} this expression simplifies to:

$$\left|MM *\right| = \left|M\right| \left|M\right| \left|M_{1n}^{1n}\right|$$
.

Since $|MM^*| = |M| |M^*|$, we have

$$|M^*| = |M| |M_{1n}^{1n}|$$
 (2)

Now compute the determinant of M^* a second way. Expanding along the first row, we get:

$$|M^*| = |M_1^1| \cdot |M^{*1}| + (-1)^{n+1} (-1)^{n+1} \cdot |M_1^n| \cdot |M^{*1}_n|$$
$$= |M^*| = |M_1^1| \cdot |M^{*1}_1| - (-1)^{n+1} \cdot |M_1^n| \cdot |M^{*1}_n|$$

To simplify this, continue with cofactor expansion exploiting the many zeros in the first and last rows, to obtain $|M_1^{*1}| = |M_n^n|$ and $|M_n^{*1}| = (-1)^n (-1)^{n+1} |M_n^1| \cdot 1$, so that

$$|M^{*}| = |M_{1}^{1}| \cdot |M_{n}^{n}| - |M_{n}^{1}| \cdot |M_{1}^{n}|.$$
(3)

Equating the two expressions (2) and (3) we have for $|M^*|$ we have the statement of the lemma.

Returning to the proof of the main theorem, we make use of the identity. By the lemma, we have that

$$|D||D_{1n}^{1n}| = |D_1^1||D_n^n| - |D_n^1||D_1^n|.$$

By the definition of the distance matrix of T, $|D_1^n| = |D_n^1|$, since T is symmetric. Recalling that D_{1n}^{1n} , D_1^1 , and D_n^n are the distance matrices of $T - v_1 - v_n$, $T - v_1$, and $T - v_n$ respectively, we can apply the induction hypothesis and obtain:

$$|D||D_{1n}^{1n}| = |D_1^1||D_n^n| - |D_n^1||D_1^n|,$$

which, upon substitution, yields

$$|D|(-(n-3)(-2)^{n-4}) = [-(n-2)(-2)^{n-3}]^2 - |D_n^1|^2.$$
(4)

We now have, in (1) and (4), a system of two equations in two unknowns:

$$\begin{cases} |D|(-(n-3)(-2)^{n-4}) = [-(n-2)(-2)^{n-3}]^2 - |D_n^1|^2 \\ |D| = -2(-(n-2)(-2)^{n-3}) + 2(-1)^{n+1} |D_1^n| \end{cases}$$

For simplicity, let $x = |D_1^n|$. Simplifying the above equations and using the method of substitution to eliminate the variable |D|, we obtain:

$$x^{2} + (n-3)2^{n-3}x - (n-2)2^{2n-6} = 0$$

This is a quadratic, and factors into

$$(x-2^{n-3})(x+(n-2)2^{n-3})=0$$

which has solutions

$$x = 2^{n-3}$$
 or $x = 2^{n-3}(2-n)$

Using the solution $x = 2^{n-3}(2-n)$ in either of the original equations gives that the determinant of any distance matrix is 0. This is clearly a contradiction to the base case of the induction proof. So our solution must be $x = 2^{n-3}$. We now have that

$$|D| = -2(-(n-2)(-2)^{n-3}) + 2(-1)^{n+1} 2^{n-3}$$

= -(n-1)(-2)^{n-2}

Remark: As a corollary, we have that $|D_j^i| = 2^{n-3}$ where *i*, *j* are leaves vertices of *T*.

5. CONCLUSION

The need to find the determinant of a distance matrix of a tree arose in an application problem involving telephone call routing. It was discovered by Ron Graham in his work on this application that the determinant of a distance matrix of a tree is in fact independent of the structure of the tree itself. It depends only upon the number of vertices in the tree, and can be expressed by a simple formula. This result is so simple yet so intriguing, that it has led to many different proofs of the formula over the last few decades. Through examples we explored the method of condensation and learned co-factor expansion, since these were needed to understand the proof of the formula. We also experienced the fascinating formula at work in different trees of the same number of vertices. We then looked in detail at the proof given by Weigen Yan and Yeong-Nan Yeh.

6. QUESTIONS

Although it is not immediately or intuitively clear why the determinant has no regard for the tree's structure, it may help to recall that a tree of n vertices always has n-1 edges. Edges are directly related to distance, and the term n-1 appears in the formula.

In my discussions with others and research in other articles, still nowhere have I found a satisfying intuitive explanation for why the determinant is expressed by such a formula. The formula $-(n-1)(-2)^{n-2}$ seems to be a counting problem. Ignoring sign, it could be counting the number of ways to first pick an edge in the tree, then whether to include or exclude each remaining edge. The sign of the determinant depends on the number of vertices in the tree. An even number of vertices will yield a negative determinant while an odd number gives a positive. How does the determinant relate geometrically to the number of edges in a tree?

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