The Distance Matrix of a Graph

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Abstract

The distance matrix of a graph is defined in a similar way as the adjacency matrix: the entry in the i^{th} row, j^{th} column is the distance (length of a shortest path) between the i^{th} and j^{th} vertex. The study of the distance matrix started in the 1970s with the seminal work of Graham, Lovász, Pollak and others. There are many nice results on these matrices, their characteristic polynomials, spectra, etc., similar to those for the adjacency matrix, some of which will be treated in this project. To give an example, a classical result of Graham and Pollak states that the determinant of the distance matrix of a tree only depends on the order of the tree, not its precise structure.

Declaration

I, the undersigned, hereby declare that the work contained in this research project is my original work, and that any work done by others or by myself previously has been acknowledged and referenced accordingly.

Kenneth Dadedzi, 22 May 2014.

Contents

Abstract **i**

1 Introduction **1**
1.1 General results about the distance matrix 2

2 The Determinant of the Distance Matrix **5**
2.1 Schur Complement 5
2.2 Sum of Cofactors of a Matrix 5
2.3 Blocks of Graphs 7
2.4 Determinant of the Distance Matrix of a Tree 11

3 The Eigenvalues and Spectral Radius of the Distance Matrix of a Tree **13**

4 The Characteristic Polynomial of the Distance Matrix of Trees **15**

5 Explicit Formulas for some Special Classes of Graphs **20**
5.1 The Complete Graph 20
5.2 Complete Bipartite Graphs 22

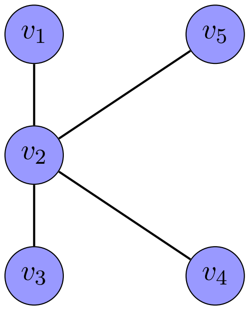
6 Conclusion **28**

References **30**

1. Introduction

The distance matrix is one of the matrix representations of graphs in algebraic graph theory. It is defined in a similar way as the adjacency matrix.

Suppose G is a connected graph with set of vertices $V(G) = \{v_1, v_2, \ldots, v_n\}$ and d_{ij} represent the shortest path length between vertices v_i and v_j. Then we define the distance matrix of G, denoted by $D(G)$, as an $n \times n$ matrix whose $(i, j)^{\text{th}}$ entry is d_{ij}. It is real, symmetric and also has trace equal to zero. An example of the distance matrix $D(G)$ of a graph G is shown in Figure 1.1;



(a) The graph G

$$D(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & v_4 & v_5 \end{array} \\ \begin{pmatrix} 0 & 1 & 2 & 2 & 2 \\ 1 & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 \\ 2 & 1 & 2 & 0 & 2 \\ 2 & 1 & 2 & 2 & 0 \end{pmatrix} \end{array}.$$

(b) Distance matrix $D(G)$

Figure 1.1: A graph and its distance matrix.

The study of the distance matrix started in the 1970s with the seminal work of Graham, Lovász, Pollak and others. Graham and Pollak studied the loop switching problem that determines which sequence of loops a message in a communication network will follow. The problem was to come up with a suitable routing strategy which would allow messages to use the shortest possible path to their destination. To resolve this, the authors represented the network of loops as a connected graph with each loop a vertex. An address, which is an m-tuple with binary coordinates (0's, 1's or d's) of size m, was assigned to each loop (vertex). Therefore, if two vertices vary by one position in the address, then they are adjacent. The number of positions that differ between the addresses of any two vertices is the Hamming distance between them (Graham and Pollak, 1971).

Graham and Pollak proposed that in order to find the shortest path between vertices v_i and v_j, the Hamming distance between the vertices, denoted by $H(v_i, v_j)$, must be equal to d_{ij}, the shortest path length between vertices v_i and v_j in the graph. The next problem was to determine the appropriate length m of m-tuples for the addresses in order to achieve this shortest routing strategy. They suggested that the length should not be greater than $s(n-1)$, where s is the maximum distance between any two loops and n the number of loops. The authors wanted to determine a suitable m for specific networks of loops so they studied their distance matrices. For instance, they found that if the loop network is a complete graph or a tree or a cycle with odd number of vertices, the best m for an address is $n - 1$ (Graham and Pollak, 1971).

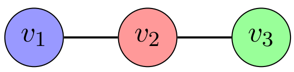
The distance matrix has several applications not only in telecommunication, but also in chemistry. Several topological indices, which characterise the molecular graph of chemical compounds, have been derived from the study of the distance matrix. For instance, Wiener in his paper (Wiener, 1947) used the Wiener index, which he called the path number w, and other structural properties of paraffins (alkanes) to approximately calculate their boiling points. The value that results from summing all the d_{ij} over all unordered pairs of vertices $\{v_i, v_j\}$ in a graph is the Wiener index of the graph (Gutman and Furtula, 2012b, p. 22). The Wiener index of any graph is therefore half the sum of all the entries of its distance matrix. Wiener himself defined the path number w as the sum of the distances between pairs of carbon to carbon bonds in the molecular structure of alkanes. He explained that a smaller path number implies larger compactness of atoms in the molecular structure and hence a lower boiling point. With this and other properties of paraffins, he derived a linear equation to approximately calculate their boiling points (Wiener, 1947). These results and their variety of applications motivated the study of the properties of the distance matrices of various types of graphs.

In this project, we investigate the properties of the distance matrices of simple, connected and undirected graphs. We then discuss and prove some of the intrinsic results that have come up from the study of the determinant, eigenvalues and characteristic polynomials of the distance matrices of such graphs. For example, the determinant of a tree can be calculated using a formula, derived by Graham and Pollak (Graham and Pollak, 1971), which is independent of the structure of the tree. Also, the eigenvalues of the distance matrix of a tree consist of one positive eigenvalue and $n-1$ negative eigenvalues, where n is the number of vertices of the graph. We also go further to explicitly determine formulas for special types of graphs.

1.1 General results about the distance matrix

The determinant and the characteristic polynomial of the distance matrix do not depend on the order of the vertices. This is because reordering the vertices results in interchanging the same number of rows and columns corresponding to the reordered vertices to give a similar matrix. If two matrices are similar then they have the same determinant and characteristic polynomial (Beezer, 2012, p. 335-337).

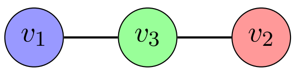
1.1.1 Example. Suppose we relabel vertices v_2 and v_3 in G_1 to get G_2, then $D(G_2)$ is the matrix obtained from $D(G_1)$ by interchanging row 2 and 3 and also column 2 and 3 of $D(G_1)$, see the figure below:



(a) Graph G_1

$$D(G_1) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \end{array} \begin{array}{c} \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix} \end{array}$$

(b) Distance matrix $D(G_1)$



(a) Graph G_2

$$D(G_2) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \end{array} \begin{array}{c} \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{pmatrix} 0 & 2 & 1 \\ 2 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{array}$$

(b) Distance matrix $D(G_2)$

In order to interchange the rows and columns of $D(G_1)$ to get $D(G_2)$, we multiply $D(G_1)$ by a permutation matrix P and its inverse P^{-1} as follows:

$$P^{-1} \cdot D(G_1) \cdot P = D(G_2)$$
$$\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1 & 2\\ 1 & 0 & 1\\ 2 & 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} = \begin{pmatrix}0 & 2 & 1\\ 2 & 0 & 1\\ 1 & 1 & 0\end{pmatrix}.$$

This implies that $D(G_1)$ and $D(G_2)$ are similar matrices, hence they have the same determinant and characteristic polynomial.

$$\begin{aligned}
\det D(G_1) &= -1\begin{vmatrix}1 & 2\\ 1 & 0\end{vmatrix} + 2\begin{vmatrix}1 & 2\\ 0 & 1\end{vmatrix}\\
&= 2+2 = 4.\\
\Delta_{D_{G_1}}(\lambda) &= \det(I\lambda - D(G_1)) = \lambda\begin{vmatrix}\lambda & -1\\ -1 & \lambda\end{vmatrix} + 1\begin{vmatrix}-1 & -2\\ -1 & \lambda\end{vmatrix} - 2\begin{vmatrix}-1 & -2\\ \lambda & -1\end{vmatrix}\\
&= \lambda^3 - 6\lambda - 4.\\
\det D(G_2) &= -2\begin{vmatrix}2 & 1\\ 1 & 0\end{vmatrix} + 1\begin{vmatrix}2 & 1\\ 0 & 1\end{vmatrix}\\
&= 2+2 = 4.\\
\Delta_{D_{G_2}}(\lambda) &= \det(I\lambda - D(G_2)) = \lambda\begin{vmatrix}\lambda & -1\\ -1 & \lambda\end{vmatrix} + 2\begin{vmatrix}-2 & -1\\ -1 & \lambda\end{vmatrix} - 1\begin{vmatrix}-2 & -1\\ \lambda & -1\end{vmatrix}\\
&= \lambda^3 - 6\lambda - 4.
\end{aligned}$$

Compared to other matrix representations of graphs, like the adjacency matrix, incidence matrix, etc., the distance matrix is denser since it has zeros only on its diagonal. It is therefore harder to determine the characteristic polynomials of the distance matrix of a graph with a large number of vertices. From our knowledge in linear algebra, we know that these coefficients can be expressed in terms of the principal minors. This leads us to a proposition about the coefficients of the characteristic polynomial of the distance matrix.

Before we state the proposition, we state a lemma which will aid us in the proof of the proposition.

Let a $(n-k)^{\text{th}}$ order principal minor be the determinant of the submatrix obtained from $D(G)$ by deleting k rows and columns with the same indices. For each $k \in \{1, 2, \ldots, n\}$, let $(-1)^k\delta_k(G)$ be the sum of all $(n-k)^{\text{th}}$ order principal minors of $D(G)$ (Biggs, 1993, p. 8).

1.1.2 Lemma. Let G be a graph with n vertices and $D(G)$ its distance matrix. The characteristic polynomial of $D(G)$ is given by

$$\Delta_G(\lambda) = \det(D(G) - \lambda I) = \sum_{k=0}^{n} \delta_k(G)\lambda^k.$$

1.1.3 Proposition. The coefficient $\delta_{n-1}(G)$ of the characteristic polynomial of $D(G)$ is equal to zero.

Proof. The first order principal minors, for which $k = n - 1$, are the diagonal entries of $D(G)$. Since all the diagonal entries are zeros, then

$$(-1)^{n-1}\delta_{n-1}(G) = 0,$$
$$\delta_{n-1}(G) = 0.$$

□

In addition, the distance matrix is real and symmetric implying that it is equal to its conjugate transpose. Hence the distance matrix is Hermitian. Therefore, it has real eigenvalues (Beezer, 2012, p. 331).

1.1.4 Example. The eigenvalues of $D(G_1)$ are given by

$$\Delta_D(\lambda) = 0,$$
$$\Leftrightarrow \lambda^3 - 6\lambda - 4 = 0,$$
$$\Leftrightarrow (\lambda + 2)(\lambda^2 - 2\lambda - 2) = 0,$$
$$\text{thus} \quad \lambda = -2 \quad \text{or} \quad \lambda = 1 \pm \sqrt{3}.$$

The eigenvalues of $D(G_1)$, $-2, 1 - \sqrt{3}$ and $1 + \sqrt{3}$, are all real numbers.

2. The Determinant of the Distance Matrix

In this section, we shall prove a theorem which will enable us to find the determinant of the distance matrix using the determinant and the sum of cofactors of the distance matrices of blocks in the graph.

Furthermore, we shall use the theorem to prove the result about the determinant of the distance matrix of a tree by Graham and Pollak.

Before we prove the theorem, we state some definitions and prove some lemmas which will help us in the proof of the theorem.

2.1 Schur Complement

2.1.1 Definition. (Bapat, 2010, p. 3,4) Let M be a square matrix partitioned into submatrices as

$$\underset{(m+n)\times(m+n)}{M} = \begin{pmatrix} \underset{n\times n}{A} & \underset{n\times m}{B} \\ \underset{m\times n}{C} & \underset{m\times m}{D} \end{pmatrix}.$$

For the square submatrix A, if it is non-singular, its Schur complement in M is defined to be the matrix $D - CA^{-1}B$ and similarly for D it is $A - BD^{-1}C$.

Let I be the identity matrix. Then we have

$$\begin{pmatrix} I & 0 \\ -CA^{-1} & I \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} I & -A^{-1}B \\ 0 & I \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix}. \tag{2.1.1}$$

Computing the determinant on both sides of equation (2.1.1), we get

$$\det(I) \cdot \det(M) \cdot \det(I) = \det[A \cdot (D - CA^{-1}B)],$$
$$\det(M) = \det(A) \cdot \det(D - CA^{-1}B). \tag{2.1.2}$$

Equation (2.1.2) is the Schur complement formula for the determinant.

2.2 Sum of Cofactors of a Matrix

Let M be an $n \times n$ matrix and $M_{(i|j)}$ be a submatrix obtained from M by deleting the i^{th} row and the j^{th} column. We define the cofactor of m_{ij} as $(-1)^{i+j} \det M_{(i|j)}$.

Let C be an $n \times n$ matrix whose entries are the cofactors of M. The transpose of C, denoted by C^T, is the adjoint of M. We recall from the properties of non-singular matrices that

$$M^{-1} = \frac{C^T}{\det M},$$
$$C^T = M^{-1} \cdot \det M.$$

In order to sum all the entries of C^T, we compute $\mathbf{1}^{\boldsymbol{T}} C^T \mathbf{1}$, where $\mathbf{1}$ is an $n \times 1$ vector with all entries equal to one.

Therefore, the sum of all the cofactors of M, denoted by Cof M, is given by

$$\begin{aligned} \mathbf{1}^{\boldsymbol{T}} C^T \mathbf{1} &= \det M \cdot \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1}, \\ \text{Cof } M &= \det M \cdot \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1}. \end{aligned} \tag{2.2.1}$$

2.2.1 Lemma. (Bapat, 2010, p. 97) Suppose M and J are $n \times n$ matrices and the entries of J are all equal to one. Then

$$\det(M + J) = \det M + \text{Cof } M.$$

Proof. Suppose P is a matrix partitioned as

$$P = \begin{pmatrix} 1 & -\mathbf{1}^{\boldsymbol{T}} \\ \mathbf{1} & M \end{pmatrix},$$

then applying the Schur complement formula we get

$$\begin{aligned} \det P &= \det(1) \det[M - \mathbf{1}\, 1^{-1}(-\mathbf{1}^{\boldsymbol{T}})] \\ &= \det(M + \mathbf{1}\mathbf{1}^{\boldsymbol{T}}) \\ &= \det(M + J). \end{aligned} \tag{2.2.2}$$

Also,

$$\det P = \det(M) \cdot \det(1 + \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1}). \tag{2.2.3}$$

Since $(1 + \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1})$ results in a simple constant value, this means we can rewrite equation (2.2.3) as

$$\det P = \det(M) \cdot (1 + \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1}). \tag{2.2.4}$$

Now, comparing equations (2.2.2) and (2.2.4), we obtain

$$\det(M + J) = \det(M) \cdot (1 + \mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1}). \tag{2.2.5}$$

But from equation (2.2.1), we get

$$\mathbf{1}^{\boldsymbol{T}} M^{-1} \mathbf{1} = \frac{\text{Cof } M}{\det M},$$

hence equation (2.2.5) becomes

$$\begin{aligned} \det(M + J) &= \det(M) \left[1 + \frac{\text{Cof } M}{\det M}\right] \\ &= \det(M) + \text{Cof } (M). \end{aligned} \tag{2.2.6}$$

□

2.2.2 Lemma. (Bapat, 2010, p. 97) Suppose M is an $n \times n$ matrix and D is obtained from M by subtracting the first row from all the other rows and similarly subtracting the first column from all the other columns. Let $D_{(1|1)}$ be a submatrix obtained from D by deleting row 1 and column 1. Then

$$\text{Cof } M = \det D_{(1|1)}.$$

Proof. Suppose K is obtained from $(M + J)$ by subtracting the first row and the first column from all other rows and columns respectively. Let d_{ij} denote the ij^{th} entry of D. Then

$$K = \begin{pmatrix} d_{11}+1 & d_{12}+0 & \dots & d_{1n}+0 \\ d_{21}+0 & d_{22}+0 & \dots & d_{2n}+0 \\ \vdots & \vdots & \vdots & \vdots \\ d_{n1}+0 & d_{n2}+0 & \dots & d_{nn}+0 \end{pmatrix},$$

$$\begin{aligned} \det(K) &= \begin{vmatrix} d_{11} & d_{12} & \dots & d_{1n} \\ d_{21} & d_{22} & \dots & d_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ d_{n1} & d_{n2} & \dots & d_{nn} \end{vmatrix} + \begin{vmatrix} 1 & 0 & \dots & 0 \\ d_{21} & d_{22} & \dots & d_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ d_{n1} & d_{n2} & \dots & d_{nn} \end{vmatrix} \\ &= \det(D) + \det D_{(1|1)}. \end{aligned} \tag{2.2.7}$$

Lemma 2.2.1 implies

$$\begin{aligned} \det(K) &= \det(M + J) \\ &= \det(M) + \text{Cof } (M), \\ \text{but} \quad \det(M) &= \det(D), \\ \text{therefore,} \quad \det(K) &= \det(D) + \text{Cof } (M). \end{aligned} \tag{2.2.8}$$

Now, comparing equations (2.2.7) and (2.2.8), we obtain

$$\text{Cof } (M) = \det D_{(1|1)}. \tag{2.2.9}$$

□

2.3 Blocks of Graphs

2.3.1 Definition. A block is a maximal connected subgraph which has no cut vertex. A cut vertex of a connected graph is a vertex whose removal causes the graph to become disconnected while a bridge is an edge whose removal also disconnects the graph. A block is either a complete graph with two vertices, thus K_2, or a graph that contains a cycle.

Now, the theorem about the determinant of the distance matrix is as follows:
2.3.2 Theorem. *(Bapat, 2010, p. 98) Suppose G is a graph with vertex set $v(G) = \{v_1, v_2, \dots, v_n\}$ and blocks $B_1, B_2, \dots, B_k$. Then*

(i)

$$\textit{Cof}\, D(G) = \prod_{i=1}^{k} \textit{Cof}\, D(B_i),$$

and

(ii)

$$\det D(G) = \sum_{i=1}^{k} \det D(B_i) \prod_{j \neq i} \textit{Cof}\, D(B_j),$$

where $D(G)$ and $D(B_i)$ are respectively the distance matrices of the graph G and the block B_i in G.

Proof. We make the following assumptions:

- Let B_1 be an end block of the graph G, so that it contains only one cut-vertex of G, which we call v_1.
- We remove B_1 from G without the cut-vertex to obtain $G \setminus (B_1 \setminus \{v_1\})$, the remaining subgraph will be denoted by G_1. This is illustrated in Figure 2.1.

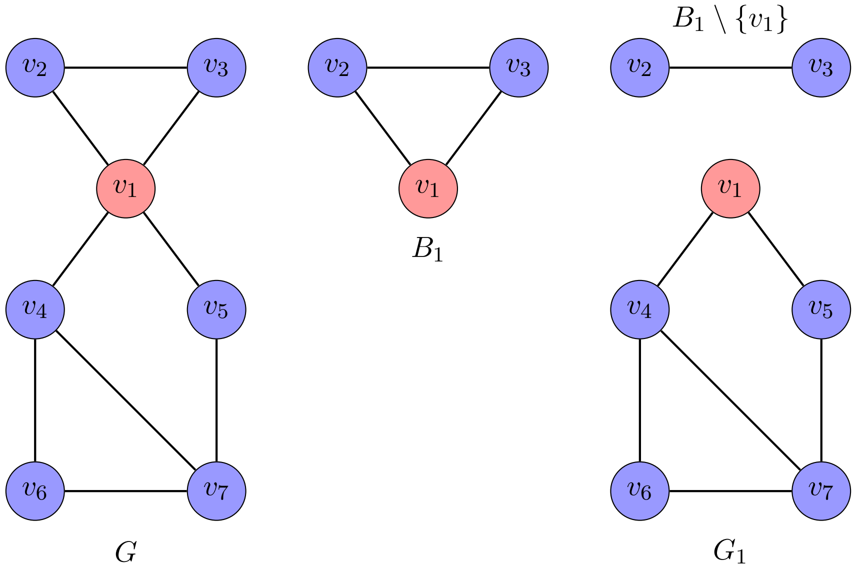


Figure 2.1: The graph G, the block B_1 and the subgraph G_1.

From the above illustration, it is obvious that G_1 still contains all the remaining blocks and the cut vertex v_1. Therefore, $V(B_1) = \{v_1, \ldots, v_m\}$ and $V(G_1) = \{v_1, v_{m+1}, \ldots, v_n\}$.

Let

$$D(B_1) = \begin{array}{c} \\ v_1 \\ v_{2,m} \end{array} \begin{array}{c} \begin{array}{cc} v_1 & v_{2,m} \end{array} \\ \begin{pmatrix} 0 & b^T \\ b & A \end{pmatrix} \end{array},$$

where $v_{2,m} = \{v_2, \ldots, v_m\}$ and

$$D(G_1) = \begin{array}{c} \\ v_1 \\ v_{m+1,n} \end{array} \begin{array}{c} \begin{array}{cc} v_1 & v_{m+1,n} \end{array} \\ \begin{pmatrix} 0 & g^T \\ g & H \end{pmatrix} \end{array},$$

where $v_{m+1,n} = \{v_{m+1}, \ldots, v_n\}$.

Therefore, we can write

$$D(G) = \begin{array}{c} \\ v_1 \\ v_{2,m} \\ v_{m+1,n} \end{array} \begin{array}{c} \begin{array}{ccc} v_1 & v_{2,m} & v_{m+1,n} \end{array} \\ \begin{pmatrix} 0 & b^T & g^T \\ b & A & b\boldsymbol{1^T} + \boldsymbol{1}g^T \\ g & g\boldsymbol{1^T} + \boldsymbol{1}b^T & H \end{pmatrix} \end{array}. \tag{2.3.1}$$

Note here that, in order to get the shortest distance from a vertex in the block B_1 to a vertex in the subgraph G_1 we sum the shortest distance from each vertex to the cut-vertex v_1. This is because the path from any vertex in B_1 to any vertex in G_1 contains the cut-vertex v_1. That is, if b_i and g_j are the shortest distances from v_i to v_1 in B_1 and v_1 to v_j in G_1 respectively, then $b_i + g_j$ is the shortest distance from v_i to v_j in G. Thus the matrix $b\boldsymbol{1^T} + \boldsymbol{1}g^T$ contains all the shortest distances from every v_i in B_1 to every v_j in G_1:

$$\begin{aligned} b\boldsymbol{1^T} + \boldsymbol{1}g^T &= \begin{pmatrix} b_2 \\ b_3 \\ \vdots \\ b_m \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \begin{pmatrix} g_{m+1} & g_{m+2} & \cdots & g_n \end{pmatrix} \\ &= \begin{pmatrix} b_2 + g_{m+1} & b_2 + g_{m+2} & \ldots & b_2 + g_n \\ b_3 + g_{m+1} & b_3 + g_{m+2} & \ldots & b_3 + g_n \\ \vdots & \vdots & \vdots & \vdots \\ b_m + g_{m+1} & b_m + g_{m+2} & \ldots & b_m + g_n \end{pmatrix}. \end{aligned}$$

By symmetry, we find the transpose of $(b\boldsymbol{1^T} + \boldsymbol{1}g^T)$ to be $(g\boldsymbol{1^T} + \boldsymbol{1}b^T)$.

Now, let K be a matrix obtained from $D(G)$ by subtracting the first row and the first column from all the other rows and columns respectively. This implies $\det K = \det D(G)$. Therefore,

$$
\begin{aligned}
\det D(G) = \det K &= \begin{vmatrix} 0 & b^T & g^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ g & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} \\
&= \begin{vmatrix} 0 & b^T & g^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ 0 & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} + \begin{vmatrix} 0 & b^T & g^T \\ 0 & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ g & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} \\
&= \begin{vmatrix} 0 & b^T & g^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ 0 & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} + \begin{vmatrix} 0 & 0 & g^T \\ 0 & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ g & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} \\
&+ \begin{vmatrix} 0 & b^T & 0 \\ 0 & A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ g & 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{vmatrix} \\
&= \det(H - g\mathbf{1^T} - \mathbf{1}g^T) \det \begin{pmatrix} 0 & b^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T \end{pmatrix} \\
&+ \det(A - b\mathbf{1^T} - \mathbf{1}b^T) \det \begin{pmatrix} 0 & g^T \\ g & H - g\mathbf{1^T} - \mathbf{1}g^T \end{pmatrix} \\
&+ \det(H - g\mathbf{1^T} - \mathbf{1}g^T) \det \begin{pmatrix} 0 & b^T \\ 0 & A - b\mathbf{1^T} - \mathbf{1}b^T \end{pmatrix} \\
&= \det(H - g\mathbf{1^T} - \mathbf{1}g^T) \det \begin{pmatrix} 0 & b^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T \end{pmatrix} \\
&+ \det(A - b\mathbf{1^T} - \mathbf{1}b^T) \det \begin{pmatrix} 0 & g^T \\ g & H - g\mathbf{1^T} - \mathbf{1}g^T \end{pmatrix}. \qquad (2.3.2)
\end{aligned}
$$

But we know that

$$
\det D(B_1) = \det \begin{pmatrix} 0 & b^T \\ b & A \end{pmatrix} = \det \begin{pmatrix} 0 & b^T \\ b & A - b\mathbf{1^T} - \mathbf{1}b^T \end{pmatrix}
$$

and

$$
\det D(G_1) = \det \begin{pmatrix} 0 & g^T \\ g & H \end{pmatrix} = \det \begin{pmatrix} 0 & g^T \\ g & H - g\mathbf{1^T} - \mathbf{1}g^T \end{pmatrix}.
$$

By Lemma 2.2.2, we can write

$$
\begin{aligned}
\text{Cof } D(B_1) &= \det(A - b\mathbf{1^T} - \mathbf{1}b^T), \qquad (2.3.3) \\
\text{Cof } D(G_1) &= \det(H - g\mathbf{1^T} - \mathbf{1}g^T), \qquad (2.3.4) \\
\text{Cof } D(G) &= \det \begin{pmatrix} A - b\mathbf{1^T} - \mathbf{1}b^T & 0 \\ 0 & H - g\mathbf{1^T} - \mathbf{1}g^T \end{pmatrix} \\
&= \det(A - b\mathbf{1^T} - \mathbf{1}b^T) \cdot \det(H - g\mathbf{1^T} - \mathbf{1}g^T) \\
&= \text{Cof } D(B_1) \cdot \text{Cof } D(G_1). \qquad (2.3.5)
\end{aligned}
$$

Hence equation (2.3.2) becomes

$$\det D(G) = \det D(B_1)\text{Cof } D(G_1) + \det D(G_1)\text{Cof } D(B_1). \tag{2.3.6}$$

Now, when G has only two blocks, we have

$$\text{Cof } D(G) = \text{Cof } D(B_1) \cdot \text{Cof } D(B_2).$$

This proves the statement for two blocks and we proceed by induction on the number of blocks in G_1. We recall that G_1 has all the remaining blocks $B_2, B_3, \ldots, B_k$ in G, therefore

$$\text{Cof } D(G_1) = \prod_{i=2}^{k} \text{Cof } D(B_i) \tag{2.3.7}$$

and

$$\det D(G_1) = \sum_{i=2}^{k} \det D(B_i) \prod_{j \neq i} \text{Cof } D(B_j). \tag{2.3.8}$$

Substituting equation (2.3.7) into equation (2.3.5) we get

$$\begin{aligned} \text{Cof } D(G) &= \text{Cof } D(B_1) \cdot \prod_{i=2}^{k} \text{Cof } D(B_i) \\ &= \prod_{i=1}^{k} \text{Cof } D(B_i). \end{aligned}$$

Also, when we substitute equations (2.3.7) and (2.3.8) into equation (2.3.6), we get

$$\begin{aligned} \det D(G) &= \det D(B_1) \cdot \prod_{i=2}^{k} \text{Cof } D(B_i) + \sum_{i=2}^{k} \det D(B_i) \prod_{j \neq i} \text{Cof } D(B_j) \cdot \text{Cof } D(B_1) \\ &= \sum_{i=1}^{k} \det D(B_i) \prod_{j \neq i} \text{Cof } D(B_j). \end{aligned}$$

□

2.4 Determinant of the Distance Matrix of a Tree

2.4.1 Definition. A connected graph with no cycles is called a tree. For a tree with n vertices, the number of edges is given by $n-1$. Each edge of a tree is a bridge and since it has no cycles, every block in a tree is a K_2.

Let T be a tree with vertex set $V(T) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(T) = \{e_1, e_2, \ldots, e_{n-1}\}$. By definition, we know that every edge forms a block and hence the tree has $n-1$ blocks. Therefore, the distance matrix of each block will be of the form $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ with determinant -1 and cofactor sum -2.

We therefore find an explicit formula for the determinant of the distance matrix of a tree using Theorem 2.3.2.

$$\begin{aligned}
\det D(T) &= \sum_{i=1}^{k} \det D(B_i) \prod_{j \neq i} \text{Cof } D(B_j) \\
&= \sum_{i=1}^{k} (-1) \prod_{j \neq i} (-2).
\end{aligned}$$

We have $k = n-1$ (number of blocks), so

$$\det D(T) = \sum_{i=1}^{n-1} (-1) \prod_{j \neq i} (-2).$$

Since $k = n-1$, for every j there exist $n-2$ indices i such that $j \neq i$. Therefore,

$$\begin{aligned}
\det D(T) &= \sum_{i=1}^{n-1} (-1) \cdot (-2)^{n-2} \\
&= \sum_{i=1}^{n-1} (-1) \cdot (-1)^{n-2} \cdot 2^{n-2} \\
&= \sum_{i=1}^{n-1} (-1)^{n-1} \cdot 2^{n-2} \\
&= (n-1)(-1)^{n-1} \cdot 2^{n-2}. \qquad (2.4.1)
\end{aligned}$$

From equation (2.4.1), it can be observed that the determinant of the distance matrix of a tree depends only on the number of vertices of the tree, but not its structure.

3. The Eigenvalues and Spectral Radius of the Distance Matrix of a Tree

Following from the result about the determinant of the distance matrix of a tree, we obtain a theorem about its eigenvalues.

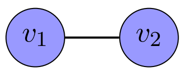
Before we state and prove the theorem, we state Cauchy's interlacing theorem which will help us in the proof of the theorem.

3.0.1 Theorem. *(Bapat, 2010, p. 7) Let A be an $n \times n$ Hermitian matrix and B be an $(n-1) \times (n-1)$ submatrix obtained from A by deleting a row and a column with the same index. Suppose that $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$ are the eigenvalues of A and $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_{n-1}$ are the eigenvalues of B, then $\alpha_1 \geq \beta_1 \geq \alpha_2 \geq \beta_2 \geq \cdots \geq \alpha_{n-1} \geq \beta_{n-1} \geq \alpha_n$.*

Now, the theorem about the eigenvalues of the distance matrix of a tree is as follows.

3.0.2 Theorem. *(Bapat, 2010, p. 104) Suppose T is a tree with $n \geq 2$ vertices and $D(T)$ is the distance matrix of the tree. Then $D(T)$ has one positive eigenvalue and $n-1$ negative eigenvalues.*

Proof. We will prove this by the method of induction on the number of vertices n. We begin with $n = 2$: there is only one tree with two vertices.



(a) Tree T

$$D(T) = \begin{array}{c} \\ v_1 \\ v_2 \end{array} \begin{array}{c} \begin{matrix} v_1 & v_2 \end{matrix} \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{array}$$

(b) Distance Matrix $D(T)$

We determine the eigenvalues of $D(T)$, and for the purpose of simplicity we denote $D(T)$ by D. Then we solve

$$\begin{aligned} \det(D - \lambda I) &= 0, \\ \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} &= 0, \\ \lambda^2 - 1 &= 0, \\ (\lambda + 1)(\lambda - 1) &= 0. \end{aligned}$$

Thus, we have one positive eigenvalue, namely $\lambda = 1$, and one negative eigenvalue, namely $\lambda = -1$.

Now we consider $n > 2$, and make the assumption that the theorem is true for trees with $n-1$ vertices. We form a subgraph (which is again a tree) with $n-1$ vertices from T by deleting a pendant vertex (leaf), which we call v_p; that is, a vertex with degree one. The distance matrix for the resulting subgraph is denoted by D_{v_p}.

Note that, since v_p is pendant, its removal does not affect the distances among the other vertices. This means that D_{v_p} is a submatrix of D obtained by deleting the row and the column corresponding to the pendant vertex v_p.

Based on our assumption, we let the eigenvalues of D_{v_p} be $\mu_1, \mu_2, \cdots, \mu_{n-1}$ such that μ_1 is positive and the rest negative.

Now, let the eigenvalues of D be given as $\lambda_1, \lambda_2, \cdots, \lambda_n$. We can use the idea of Cauchy's Interlacing theorem for the eigenvalues of Hermitian matrix.

We know from the introduction that D is Hermitian. Then applying the interlacing theorem, we get $\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n$. We observe that λ_2 can be either positive or negative. If positive, then D will have two positive eigenvalues, but when it is negative, then D has only one positive eigenvalue. To justify the sign of λ_2, we use the fact that the product of the eigenvalues is equal to the determinant of the matrix. Thus

$$\frac{\det D}{\det D_{v_p}} = \frac{\lambda_1 \cdot \lambda_2 \cdot \cdots \cdot \lambda_n}{\mu_1 \cdot \mu_2 \cdot \cdots \cdot \mu_{n-1}}.$$

Since λ_1, μ_1 are positive, μ_2 is negative and $\mu_2 \geq \lambda_3 \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n$, so the sign of $\frac{\det D}{\det D_{v_p}}$ depends on the sign of λ_2.

Using the formula for the determinant of a tree we get

$$\begin{aligned}\frac{\det D}{\det D_{v_p}} &= \frac{(-1)^{n-1}(n-1)2^{n-2}}{(-1)^{n-1-1}(n-1-1)2^{n-1-2}} \\ &= \frac{(n-1)}{(-1)(n-2)2^{-1}} \\ &= \frac{-2(n-1)}{(n-2)} < 0.\end{aligned}$$

This implies that λ_2 is negative and hence D has only one positive eigenvalue. □

The spectral radius is the absolute value of the largest eigenvalue of a matrix. From Theorem 3.0.2, we can conclude that the spectral radius of the distance matrix of a tree is the only positive eigenvalue.

4. The Characteristic Polynomial of the Distance Matrix of Trees

The study of the relationship between the coefficients of the characteristic polynomial of the adjacency matrix and the frequency of certain subgraphs was begun by Collatz and Singowitz (Collatz and Singowitz, 1957). Several authors discovered independently (the first of them being Sachs (Cvetković et al., 2010, p. 36)) how the coefficients of the characteristic polynomial can be determined exactly by counting so-called elementary subgraphs. For trees, the characteristic polynomial reduces to the matching polynomial, which means that the coefficients are given by the number of subgraphs consisting of disjoint edges only (Mowshowitz, 1972). Graham and Pollak (Graham and Pollak, 1971) had also shown that the determinant of the distance matrix of a tree, which is the constant term in its characteristic polynomial, is independent of the structure of the tree as we have seen in the previous section. All these results motivated Graham, Garey and Edelberg (Edelberg et al., 1976) to study the dependence of other coefficients of the characteristic polynomial of the distance matrix of a tree on the structure of the tree. Following these results, a remarkable result that explicitly determines the coefficients of the characteristic polynomial of the distance matrix of a tree was found by Graham and Lovász (Graham and Lovász, 1978). They also showed that the coefficients depend on the occurrence of certain subgraphs (forests with no isolated vertices) of the tree. We shall state the theorem of Graham and Lovasz and use it to solve an example. Before that, we shall define the following terms in the theorem.

- A forest F is a graph consisting of a disjoint union of trees. Let $N_F(T)$ denote the number of occurrences of a forest F in a tree T. That is, the number of subgraphs of T which are isomorphic to F. If F is an empty graph, then we set $N_F(T) = 1$.
- Suppose F is a forest with connected components $T_1, T_2, \ldots, T_t$ (trees). Then

$$\begin{aligned} |F| &= \text{the number of vertices of } F, \\ ||F|| &= \text{the number of edges of } F, \\ \pi(F) &= \prod_{i=1}^{t} |T_i|. \end{aligned}$$

  For an empty forest, $\pi(F) = 1$.
- Let $\mathcal{F}_k$ denote the set of all forests having no isolated vertices and exactly k edges.

4.0.1 Theorem. *(Graham and Lovász, 1978) Let T be a tree with $n \geq 2$ vertices and distance matrix $D(T)$. If we write*

$$\Delta_T(\lambda) = \det(D(T) - \lambda I) = \sum_{k=0}^{n} \delta_k(T)\lambda^k$$

then

$$\delta_k(T) = (-1)^{n-1}2^{n-k-2} \times \left[\sum_{F \in \mathcal{F}_{k+1}} a_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_k} b_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_{k-1}} c_F \pi(F) N_F(T) \right],$$

where a_F, b_F, c_F are defined as follows:

(i) For the empty forest F^*, $a_{F^*} = b_{F^*} = 0, c_{F^*} = -4$.

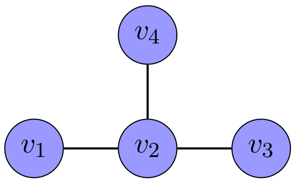
(ii) If F is a tree T with $n \geq 2$ vertices and distance matrix (d_{ij}), then

$$a_F = \frac{1}{n}\sum_{i<j} d_{ij}(2-d_{ij}),$$
$$b_F = \frac{4}{n}\sum_{i<j}(2-d_{ij}),$$
$$c_F = -\frac{4}{n}.$$

(iii) If F is the disjoint union of forests F_1 and F_2 then

$$a_F = a_{F_1} + a_{F_2},$$
$$b_F = b_{F_1} + b_{F_2},$$
$$c_F = c_{F_1} + c_{F_2} + 4.$$

4.0.2 Example. For the tree T below, we want to calculate the characteristic polynomial of its distance matrix $D(T)$.



(a) Tree T

$$D(T) = \begin{array}{c c} & \begin{matrix} v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 1 & 2 & 2 \\ 1 & 0 & 1 & 1 \\ 2 & 1 & 0 & 2 \\ 2 & 1 & 2 & 0 \end{pmatrix} \end{array}.$$

(b) Distance matrix $D(T)$

Figure 4.1: A tree T and its distance matrix $D(T)$

The characteristic polynomial of $D(T)$ is given by

$$\Delta_T(\lambda) = \det(D(T) - \lambda I) = \sum_{k=0}^{4} \delta_k(T)\lambda^k,$$

where

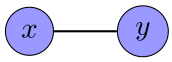
$$\delta_k(T) = (-1)^{4-1}2^{4-k-2} \times \left[\sum_{F\in\mathcal{F}_{k+1}} a_F\pi(F)N_F(T) + \sum_{F\in\mathcal{F}_k} b_F\pi(F)N_F(T) + \sum_{F\in\mathcal{F}_{k-1}} c_F\pi(F)N_F(T)\right].$$

For each k, we shall consider all forests $F \in \mathcal{F}_k$ with no isolated vertices that are isomorphic to a subgraph of T.

For $k = 0$, thus $\mathcal{F}_0$, we have an empty forest F_0, for which

$$N_{F_0}(T) = 1, \quad \pi(F_0) = 1, \quad a_{F_0} = b_{F_0} = 0, \quad c_{F_0} = -4.$$

For $k = 1$, thus $\mathcal{F}_1$, we have only one forest:



(a) Forest F_1

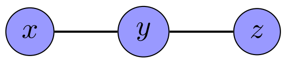
$$D(F_1) = \begin{array}{c} \\ x \\ y \end{array} \begin{array}{c} \begin{matrix} x & y \end{matrix} \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{array}.$$

(b) Distance matrix $D(F_1)$

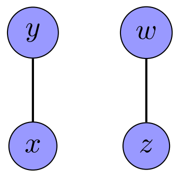
Figure 4.2: A forest F_1 and its distance matrix $D(F_1)$.

$$\begin{aligned} N_{F_1}(T) &= 3, \quad \pi(F_1) = 2, \\ a_{F_1} &= \frac{1}{2}1(2-1) = \frac{1}{2}, \\ b_{F_1} &= \frac{4}{2}(2-1) = 2, \\ c_{F_1} &= -\frac{4}{2} = -2. \end{aligned}$$

For $k = 2$, thus $\mathcal{F}_2$, we have only two possible forests:



(a) Forest F_{21}



(b) Forest F_{22}

Figure 4.3: The forests F_{21} and F_{22}.

Since the forest F_{22} is not isomorphic to any subgraph of T, it will not be considered. The distance matrix of the forest F_{21} is

$$D(F_{21}) = \begin{array}{c} \\ x \\ y \\ z \end{array} \begin{array}{c} \begin{matrix} x & y & z \end{matrix} \\ \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix} \end{array}.$$

Therefore,

$$\begin{aligned} N_{F_{21}}(T) &= 3, \quad \pi(F_{21}) = 3, \\ a_{F_{21}} &= \frac{1}{3}[1(2-1) + 1(2-1)] = \frac{2}{3}, \\ b_{F_{21}} &= \frac{4}{3}[(2-1) + (2-1)] = \frac{8}{3}, \\ c_{F_{21}} &= -\frac{4}{3}. \end{aligned}$$

For $k = 3$, thus $\mathcal{F}_3$, we only have the forest F_3 which is isomorphic to T. Hence, we let $D(T) = D(F_3)$. Then

$$
\begin{aligned}
N_{F_3}(T) = 1, \quad \pi(F_3) = 4,& \\
a_{F_3} &= \frac{1}{4}[1(2-1) + 1(2-1) + 1(2-1)] = \frac{3}{4}, \\
b_{F_3} &= \frac{4}{4}[(2-1) + (2-1) + (2-1)] = 3, \\
c_{F_3} &= -\frac{4}{4} = -1.
\end{aligned}
$$

For $k = 4$, thus $\mathcal{F}_4$, there are no forests with k edges that are subgraphs of T since the number of edges exceeds that of T. Therefore we take the sum to be zero.

Now, we can calculate the coefficients of $\Delta_T(\lambda)$:

$$
\begin{aligned}
\delta_0(T) &= (-1)^3 2^2 \times \left[\sum_{F \in \mathcal{F}_1} a_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_0} b_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_{-1}} c_F \pi(F) N_F(T) \right] \\
&= (-1)^3 2^2 \times [a_{F_1} \pi(F_1) N_{F_1}(T) + b_{F_0} \pi(F_0) N_{F_0}(T) + 0] \\
&= (-1)^3 2^2 \times \left[\frac{1}{2} \cdot 3 \cdot 2 \right] \\
&= -12.
\end{aligned}
$$

$$
\begin{aligned}
\delta_1(T) &= (-1)^3 2 \times \left[\sum_{F \in \mathcal{F}_2} a_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_1} b_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_0} c_F \pi(F) N_F(T) \right] \\
&= (-1)^3 2 \times [a_{F_{21}} \pi(F_{21}) N_{F_{21}}(T) + b_{F_1} \pi(F_1) N_{F_1}(T) + c_{F_0} \pi(F_0) N_{F_0}(T)] \\
&= (-1)^3 2 \times \left[\frac{2}{3} \cdot 3 \cdot 3 + 2 \cdot 3 \cdot 2 - 4 \cdot 1 \cdot 1 \right] \\
&= -28.
\end{aligned}
$$

$$
\begin{aligned}
\delta_2(T) &= (-1)^3 \times \left[\sum_{F \in \mathcal{F}_3} a_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_2} b_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_1} c_F \pi(F) N_F(T) \right] \\
&= (-1)^3 \times [a_{F_3} \pi(F_3) N_{F_3}(T) + b_{F_{21}} \pi(F_{21}) N_{F_{21}}(T) + c_{F_1} \pi(F_1) N_{F_1}(T)] \\
&= (-1)^3 \times \left[\frac{3}{4} \cdot 4 \cdot 1 + \frac{8}{3} \cdot 3 \cdot 3 - 2 \cdot 3 \cdot 2 \right] \\
&= -15.
\end{aligned}
$$

By Proposition 1.1.3, we know that $\delta_3(T) = 0$.

$$
\begin{aligned}
\delta_4(T) &= (-1)^3 2^{-2} \times \left[\sum_{F \in \mathcal{F}_5} a_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_4} b_F \pi(F) N_F(T) + \sum_{F \in \mathcal{F}_3} c_F \pi(F) N_F(T) \right] \\
&= (-1)^3 2^{-2} \times [0 + 0 + c_{F_3} \pi(F_3) N_{F_3}(T)] \\
&= (-1)^3 2^{-2} \times [-1 \cdot 4 \cdot 1] \\
&= 1.
\end{aligned}
$$

Therefore,

$$\Delta_T(\lambda) = \det(D(T) - \lambda I) = \lambda^4 - 15\lambda^2 - 28\lambda - 12.$$

5. Explicit Formulas for some Special Classes of Graphs

In this section, we shall discuss and prove some results about the eigenvalues, the characteristic polynomial and the determinant of the distance matrix of some special graphs.

5.1 The Complete Graph

5.1.1 Definition. A complete graph K_n is a simple graph with each vertex having degree $n-1$, where n is the number of vertices of the graph. That is, each vertex is adjacent to all other vertices of the graph.
5.1.2 Example. Examples of complete graphs are shown in Figure 5.1.

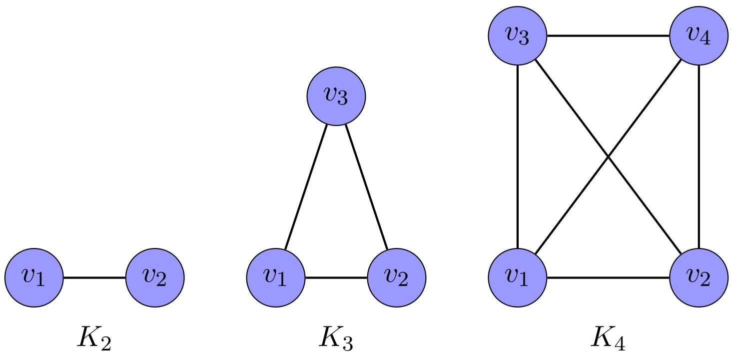


Figure 5.1: Complete graphs K_n.

Let D denote the distance matrix of K_n. Then by the definition of K_n, D has entries given by

$$d_{ij} = \begin{cases} 1 & i \neq j, \\ 0 & i = j. \end{cases}$$

5.1.3 Theorem. *Let K_n be a complete graph with n vertices and D its distance matrix. Then the eigenvalues of D are $n-1$ and -1 with algebraic multiplicity of $n-1$.*

Proof. Firstly, we show that -1 is an eigenvalue of D by considering

$$(D-(-1)I_n) = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix}.$$

The rank of $(D-(-1)I_n)$ is 1 implying that $\det(D-(-1)I_n) = 0$ and that -1 is an eigenvalue of D with algebraic multiplicity of $n-1$.

The second part of the proof finds the other eigenvalue. We know that the sum of the eigenvalues is equal to the trace. Therefore, we let e be the other eigenvalue, so that

$$
\begin{aligned}
e + \sum_{i=1}^{n-1}(-1) &= 0 \\
e - (n-1) &= 0 \\
e &= (n-1).
\end{aligned}
$$

□

5.1.4 Theorem. *The determinant of the distance matrix D for a complete graph K_n is given by*

$$(-1)^{n-1}(n-1).$$

Proof. We shall use the property of matrices that the determinant of a matrix is equal to the product of its eigenvalues. Therefore,

$$\det(D) = (-1)^{n-1}(n-1). \tag{5.1.1}$$

□

5.1.5 Theorem. *Let K_n be a complete graph with n vertices and D its distance matrix. Then the characteristic polynomial of D is given by*

$$\Delta_{K_n}(\lambda) = \det(D - \lambda I) = \sum_{k=0}^{n} \delta_k \lambda^k,$$

where

$$
\begin{aligned}
&\delta_0 = -(n-1), \\
&\delta_k = \left[\binom{n-1}{k-1} - (n-1)\binom{n-1}{k}\right] \quad k \in \{1, 2, \ldots, n-1\}, \\
\text{and} \quad &\delta_n = 1.
\end{aligned}
$$

Proof. We will use the eigenvalues of D to prove the formula for the characteristic polynomial. Thus

$$\Delta_{K_n}(\lambda) = (\lambda+1)^{n-1}(\lambda - (n-1)). \tag{5.1.2}$$

We expand (5.1.2) using the binomial theorem and obtain

$$
\begin{aligned}
\Delta_{K_n}(\lambda) &= \left[\sum_{k=0}^{n-1}\binom{n-1}{k}\lambda^k\right][\lambda - (n-1)] \\
&= \sum_{k=0}^{n-1}\binom{n-1}{k}\lambda^{k+1} - (n-1)\sum_{k=0}^{n-1}\binom{n-1}{k}\lambda^k \\
&= \left[\binom{n-1}{0}\lambda + \binom{n-1}{1}\lambda^2 + \ldots + \lambda^n\right] - (n-1)\left[\binom{n-1}{0} + \binom{n-1}{1}\lambda + \ldots + \lambda^{n-1}\right] \\
&= -(n-1) + \left[\binom{n-1}{0} - (n-1)\binom{n-1}{1}\right]\lambda + \left[\binom{n-1}{1} - (n-1)\binom{n-1}{2}\right]\lambda^2 + \ldots + \lambda^n \\
&= -(n-1) + \sum_{k=1}^{n-1}\left[\binom{n-1}{k-1} - (n-1)\binom{n-1}{k}\right]\lambda^k + \lambda^n.
\end{aligned}
$$

□

5.2 Complete Bipartite Graphs

5.2.1 Definition. A complete bipartite graph is a graph whose set of vertices can be grouped into two disjoint subsets, say V_m and V_n, such that each vertex in V_m is adjacent to every vertex in V_n. That is, it contains precisely the edges of the form $e = \{p, q\}$ with $p \in V_m$ and $q \in V_n$. Suppose V_m and V_n have respectively m and n vertices. Then we denote the complete bipartite graph by $K_{m,n}$ or $K_{n,m}$.

$K_{m,n}$ has $m+n$ vertices. Every vertex in V_m has degree n and every vertex in V_n has degree m implying that $K_{m,n}$ has $m \times n$ edges. Examples of complete bipartite graphs are shown in Figure 5.2.

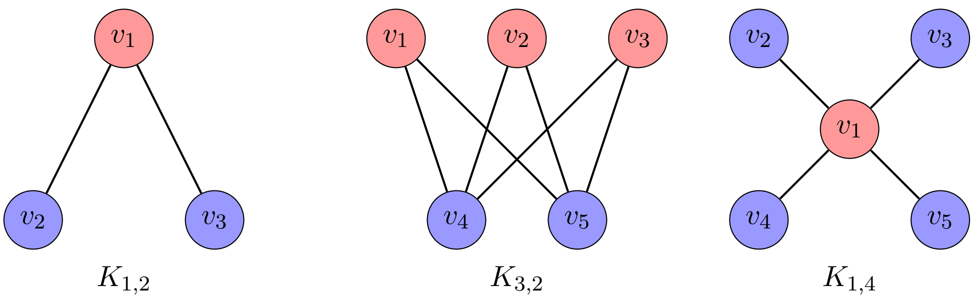


Figure 5.2: Complete bipartite graphs $K_{m,n}$.

In this section, we shall discuss the determinant, characteristic polynomial, and the eigenvalues of the distance matrix of $K_{m,n}$ for all $n \geq 1$ and $m \geq 1$.

Let the vertices of $K_{m,n}$ be partitioned into $V_m = \{v_1, v_2, \ldots, v_m\}$ and $V_n = \{v_{m+1}, v_{m+2}, \ldots, v_{m+n}\}$. Then the distance matrix of $K_{m,n}$, denoted by D, is given by

$$D = \begin{array}{c} \\ v_1 \\ v_2 \\ \vdots \\ v_m \\ v_{m+1} \\ v_{m+2} \\ \vdots \\ v_{m+n} \end{array} \begin{array}{c} \begin{array}{cccccccc} v_1 & v_2 & \cdots & v_m & v_{m+1} & v_{m+2} & \cdots & v_{m+n} \end{array} \\ \left(\begin{array}{cccccccc} 0 & 2 & \cdots & 2 & 1 & 1 & \cdots & 1 \\ 2 & 0 & \ddots & \vdots & 1 & 1 & \cdots & 1 \\ \vdots & \ddots & \ddots & 2 & \vdots & \vdots & \vdots & \vdots \\ 2 & \cdots & 2 & 0 & 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 & 0 & 2 & \cdots & 2 \\ 1 & 1 & \cdots & 1 & 2 & 0 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 2 \\ 1 & 1 & \cdots & 1 & 2 & \cdots & 2 & 0 \end{array} \right) \end{array}.$$

5.2.2 Theorem. *Let $K_{m,n}$ be a complete bipartite graph and D its distance matrix. Then the determinant of D is given by*

$$\det(D) = (-2)^{m+n-2}[4(m-1)(n-1) - mn].$$

Proof. Let r_i represent the i^{th} row of D and $r = \sum_{k=1}^{m} \frac{1}{2(m-1)} r_k$. Then we let D' be the matrix obtained from D by subtracting r from the rows $r_{m+1}, r_{m+2}, \ldots, r_{m+n}$. We obtain

$$D' = \begin{array}{c} \\ v_1 \\ v_2 \\ \vdots \\ v_m \\ v_{m+1} \\ v_{m+2} \\ \vdots \\ v_{m+n} \end{array} \begin{array}{c} \begin{array}{cccccccc} v_1 & v_2 & \cdots & v_m & v_{m+1} & v_{m+2} & \cdots & v_{m+n} \end{array} \\ \begin{pmatrix} 0 & 2 & \cdots & 2 & 1 & 1 & \cdots & 1 \\ 2 & 0 & \ddots & \vdots & 1 & 1 & \cdots & 1 \\ \vdots & \ddots & \ddots & 2 & \vdots & \vdots & \vdots & \vdots \\ 2 & \cdots & 2 & 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & \frac{-m}{2(m-1)} & 2-\frac{m}{2(m-1)} & \cdots & 2-\frac{m}{2(m-1)} \\ 0 & 0 & \cdots & 0 & 2-\frac{m}{2(m-1)} & \frac{-m}{2(m-1)} & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 2-\frac{m}{2(m-1)} \\ 0 & 0 & \cdots & 0 & 2-\frac{m}{2(m-1)} & \cdots & 2-\frac{m}{2(m-1)} & \frac{-m}{2(m-1)} \end{pmatrix} \end{array}.$$

We decompose D' as follows:

$$\underset{(m+n)\times(m+n)}{D'} = \begin{pmatrix} \underset{m\times m}{P} & \underset{m\times n}{Q} \\ \underset{n\times m}{R} & \underset{n\times n}{S} \end{pmatrix}.$$

Since the submatrix R of D' consists entirely of zeros, we obtain

$$\begin{aligned} \det(D) &= \det(D') \\ &= \det(P)\cdot\det(S). \end{aligned} \tag{5.2.1}$$

We first consider

$$\det(P) = \begin{vmatrix} 0 & 2 & \cdots & 2 \\ 2 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 2 \\ 2 & \cdots & 2 & 0 \end{vmatrix} = 2^m \begin{vmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 1 & \cdots & 1 & 0 \end{vmatrix} = 2^m \det(P_1). \tag{5.2.2}$$

P_1 is the distance matrix of a complete graph with m vertices. From Theorem 5.1.4 we obtain $\det(P_1) = (-1)^{m-1}(m-1)$. Therefore equation (5.2.2) becomes

$$\det(P) = 2^m(-1)^{m-1}(m-1). \tag{5.2.3}$$

The matrix S has -2 as an eigenvalue with algebraic multiplicity $n-1$: consider

$$S-(-2)I_n = \begin{pmatrix} 2-\frac{m}{2(m-1)} & \cdots & 2-\frac{m}{2(m-1)} \\ \vdots & \cdots & \vdots \\ 2-\frac{m}{2(m-1)} & \cdots & 2-\frac{m}{2(m-1)} \end{pmatrix}.$$

The matrix $(S-(-2)I_n)$ has rank of 1 implying that $\det(S-(-2)I_n)=0$ and that -2 is an eigenvalue with algebraic multiplicity of $n-1$.

We know that the sum of the eigenvalues of S is equal to its trace, by that we find the other eigenvalue, denoted by e.

$$\begin{aligned}(-2)(n-1)+e &= \sum_{k=1}^{n} -\frac{m}{2(m-1)} \\ e &= 2(n-1)-\frac{mn}{2(m-1)}.\end{aligned}$$

We use the product of the eigenvalues to find the determinant of S.

$$\begin{aligned}\det(S) &= (-2)^{n-1}\cdot\left[2(n-1)-\frac{mn}{2(m-1)}\right] \\ &= (-1)^{n-1}2^n(n-1)-\frac{(-1)^{n-1}2^{n-2}mn}{(m-1)}. \qquad (5.2.4)\end{aligned}$$

We substitute equations (5.2.4) and (5.2.3) into (5.2.1) to get

$$\begin{aligned}\det(D) &= \left[2^m(-1)^{m-1}(m-1)\right]\left[(-1)^{n-1}2^n(n-1)-\frac{(-1)^{n-1}2^{n-2}mn}{(m-1)}\right] \\ &= (-1)^{m+n-2}2^{m+n}(m-1)(n-1)-(-1)^{m+n-2}2^{m+n-2}mn \\ &= (-1)^{m+n-2}2^{m+n-2}[4(m-1)(n-1)-mn] \\ &= (-2)^{m+n-2}[4(m-1)(n-1)-mn]. \qquad (5.2.5)\end{aligned}$$

□

5.2.3 Theorem. *Let $K_{m,n}$ be a complete bipartite graph and D its distance matrix. Then the eigenvalues of D are -2 with algebraic multiplicity of $m+n-2$, $(m+n-2)-\sqrt{(m+n)^2-3mn}$ and $(m+n-2)+\sqrt{(m+n)^2-3mn}$.*

Proof. In the first part of the proof, we will show that -2 is an eigenvalue and also determine its algebraic multiplicity. We consider

$$(D-(-2)I_{n+m}) = \begin{pmatrix} 2 & \cdots & 2 & 1 & \cdots & 1 \\ 2 & \cdots & 2 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 2 & \cdots & 2 & 1 & \cdots & 1 \\ 1 & \cdots & 1 & 2 & \cdots & 2 \\ 1 & \cdots & 1 & 2 & \cdots & 2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \cdots & 1 & 2 & \cdots & 2 \end{pmatrix}.$$

The rank of $(D-(-2)I_{n+m})$ is 2 implying that $\det(D-(-2)I_{n+m})=0$ and that -2 is an eigenvalue with algebraic multiplicity $m+n-2$.

Now, the second part of the proof is to find the other two eigenvalues. Let the other two eigenvalues be a and b. The determinant of D is known from equation (5.2.5), and the trace of D is zero. Using the property that the sum of the eigenvalues is equal to the trace, we get

$$(-2)(m+n-2)+a+b=0, \tag{5.2.6}$$

and from the fact that the product of the eigenvalues is equal to the determinant, we get

$$\begin{aligned}(-2)^{m+n-2}ab &= (-2)^{m+n-2}[4(m-1)(n-1)-mn]\\ b &= \frac{4(m-1)(n-1)-mn}{a}.\end{aligned} \tag{5.2.7}$$

Substituting (5.2.7) into (5.2.6), we get

$$\begin{aligned}(-2)(m+n-2)+a+\frac{4(m-1)(n-1)-mn}{a} &= 0\\ (-2)(m+n-2)a+a^2+4(m-1)(n-1)-mn &= 0.\end{aligned} \tag{5.2.8}$$

Using the quadratic formula, we obtain a from equation (5.2.8):

$$\begin{aligned}a &= \frac{2(m+n-2)\pm\sqrt{4(m+n-2)^2-16(m-1)(n-1)+4mn}}{2}\\ &= (m+n-2)\pm\sqrt{(m+n-2)^2-4(m-1)(n-1)+mn}\\ &= (m+n-2)\pm\sqrt{(m+n)^2-3mn}.\end{aligned} \tag{5.2.9}$$

Let $a=(m+n-2)+\sqrt{(m+n)^2-3mn}$ and substitute it into equation (5.2.6) to get

$$(-2)(m+n-2)+(m+n-2)+\sqrt{(m+n)^2-3mn}+b=0$$
$$b=(m+n-2)-\sqrt{(m+n)^2-3mn}.$$

Also, we let $a=(m+n-2)-\sqrt{(m+n)^2-3mn}$ and substitute it into equation (5.2.6) to get

$$(-2)(m+n-2)+(m+n-2)-\sqrt{(m+n)^2-3mn}+b=0$$
$$b=(m+n-2)+\sqrt{(m+n)^2-3mn}.$$

Therefore the eigenvalues for D are -2 with algebraic multiplicity of $(m+n-2)$, $(m+n-2)-\sqrt{(m+n)^2-3mn}$ and $(m+n-2)+\sqrt{(m+n)^2-3mn}$. □

5.2.4 Theorem. *Let $K_{m,n}$ be a complete bipartite graph and D its distance matrix. Then the characteristic polynomial of D is given by*

$$\Delta_{K_{m,n}}(\lambda)=\det(D-\lambda I)=\sum_{k=0}^{m+n}\delta_k\lambda^k$$

where

$$\delta_0 = (3mn - 4(m+n-1))2^{m+n-2}, \quad \delta_1 = (m+n-2)(3mn-4(m+n))2^{m+n-3},$$
$$\delta_k = 2^{m+n-k-2}\left[4\binom{m+n-2}{k-2} - 4(m+n-2)\binom{m+n-2}{k-1}\right.$$
$$\left.+(3mn-4(m+n-1))\binom{m+n-2}{k}\right] \quad k \in \{2,\dots,m+n-2\},$$
$$\delta_{m+n-1} = 0 \quad \textit{and} \quad \delta_{m+n} = 1.$$

Proof. We will use the eigenvalues of D to prove the formula for the characteristic polynomial. Thus

$$\Delta_{K_{m,n}}(\lambda) = (\lambda+2)^{m+n-2}\left[\lambda - ((m+n-2)+\sqrt{(m+n)^2-3mn})\right] \tag{5.2.10}$$
$$\times\left[\lambda - ((m+n-2)-\sqrt{(m+n)^2-3mn})\right]$$
$$= (\lambda+2)^{m+n-2}\left[\lambda^2 - 2(m+n-2)\lambda + 3mn - 4(m+n-1)\right]. \tag{5.2.11}$$

We expand equation (5.2.11) using the binomial theorem to get

$$\Delta_{K_{m,n}}(\lambda) = \left[\sum_{k=0}^{m+n-2}\binom{m+n-2}{k}2^{m+n-2-k}\lambda^k\right]\left[\lambda^2 - 2(m+n-2)\lambda + 3mn - 4(m+n-1)\right]$$
$$= \sum_{k=0}^{m+n-2}\binom{m+n-2}{k}2^{m+n-2-k}\lambda^{k+2} - (m+n-2)\sum_{k=0}^{m+n-2}\binom{m+n-2}{k}2^{m+n-k-1}\lambda^{k+1}$$
$$+ (3mn-4(m+n-1))\sum_{k=0}^{m+n-2}\binom{m+n-2}{k}2^{m+n-2-k}\lambda^k.$$

Expanding each summation we get

$$\Delta_{K_{m,n}}(\lambda) = \left[\binom{m+n-2}{0}2^{m+n-2}\lambda^2 + \dots + 2\binom{m+n-2}{m+n-3}\lambda^{m+n-1} + \lambda^{m+n}\right]$$
$$- (m+n-2)\left[\binom{m+n-2}{0}2^{m+n-1}\lambda + \binom{m+n-2}{1}2^{m+n-2}\lambda^2 + \dots + 2\lambda^{m+n-1}\right]$$
$$+ (3mn-4(m+n-1))\left[\binom{m+n-2}{0}2^{m+n-2} + \dots + 2\lambda^{m+n-2}\right].$$

Grouping terms with the same exponent and simplifying we get

$$
\begin{aligned}
\Delta_{K_{m,n}}(\lambda) &= (3mn - 4(m+n-1))2^{m+n-2} \\
&+ \left[-(m+n-2)2^{m+n-1} + (3mn-4(m+n-1))(m+n-2)2^{m+n-3}\right]\lambda \\
&+ \sum_{k=2}^{m+n-2} 2^{m+n-k-2}\left[4\binom{m+n-2}{k-2} - 4(m+n-2)\binom{m+n-2}{k-1}\right. \\
&\left. +(3mn-4(m+n-1))\binom{m+n-2}{k}\right]\lambda^k \\
&+ \left[2\binom{m+n-2}{m+n-3} - 2(m+n-2))\right]\lambda^{m+n-1} + \lambda^{m+n} \\
\Delta_{K_{m,n}}(\lambda) &= (3mn - 4(m+n-1))2^{m+n-2} \\
&+ \left[(m+n-2)(3mn-4(m+n))2^{m+n-3}\right]\lambda \\
&+ \sum_{k=2}^{m+n-2} 2^{m+n-k-2}\left[4\binom{m+n-2}{k-2} - 4(m+n-2)\binom{m+n-2}{k-1}\right. \\
&\left. +(3mn-4(m+n-1))\binom{m+n-2}{k}\right]\lambda^k + \lambda^{m+n}.
\end{aligned}
$$

□

5.2.5 Corollary. A star graph S_v is a tree with $v-1$ pendant vertices (leaves), where v is the number of vertices of the tree. It is also a special case of the complete bipartite graph $K_{m,n}$ for which $m=1$ and $n=v-1$. An example of a star graph is the graph $K_{1,4}$ in Figure 5.2.

Let D be the distance matrix of a star graph S_v. Then by Theorem 5.2.2, the determinant of D is given by

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

In addition, the eigenvalues of D, by Theorem 5.2.3, are -2 with algebraic multiplicity of $v-2$, $v-2+\sqrt{v^2-3v+3}$ and $v-2-\sqrt{v^2-3v+3}$.

Furthermore, by Theorem 5.2.4, the characteristic polynomial of D is given by

$$\Delta_{S_v}(\lambda) = \det(D-\lambda I) = \sum_{k=0}^{v}\delta_k\lambda^k$$

where

$$
\begin{aligned}
&\delta_0 = -(v-1)2^{v-2}, \quad \delta_1 = -(v-2)(v+3)2^{v-3}, \\
&\delta_k = 2^{v-2-k}\left[4\binom{v-2}{k-2} - 4(v-2)\binom{v-2}{k-1} - (v-1)\binom{v-2}{k}\right] \quad k \in \{2,\dots,v-2\}, \\
&\delta_{v-1} = 0 \quad \text{and} \quad \delta_v = 1.
\end{aligned}
$$

6. Conclusion

In this project, we investigated the determinant, eigenvalues and the characteristic polynomial of the distance matrices of simple, connected and undirected graphs. We began by showing that the determinants and the characteristic polynomials of the distance matrices do not depend on the order of the vertices and its eigenvalues are real. We also proved that the determinant of the distance matrix of a graph can be calculated by computing the determinants and cofactors of the distance matrices of blocks in the graph. Using this result, we proved the determinant formula of Graham and Pollak for the distance matrix of a tree. This formula depends only on the number of vertices of the tree, not on its structure.

We showed that for trees with n vertices, their distance matrices have one positive eigenvalue and $n-1$ negative eigenvalues. We then stated the theorem of Graham and Lovász about the coefficients of the characteristic polynomial of the distance matrix of a tree. This theorem reveals that these coefficients depend on the frequency of certain forests occurring as subgraphs of the tree. This was illustrated with an example.

We then proceeded to find the eigenvalues and formulas to calculate the determinant and the characteristic polynomial for the complete graph, the complete bipartite graph and the star graph. We found that knowing the number of vertices only, we can find all the eigenvalues, the determinant and the characteristic polynomial of the distance matrix of such graphs.

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