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## Finding Patterns in the Inertia of the Distance Squared Matrix of Unicyclic Graphs

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Honors Thesis

FINDING PATTERNS IN THE INERTIA OF THE  
DISTANCE SQUARED MATRIX OF UNICYCLIC GRAPHS

by  
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Submitted to Brigham Young University in partial fulfillment  
of graduation requirements for University Honors

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## ABSTRACT

### FINDING PATTERNS IN THE INERTIA OF THE DISTANCE SQUARED MATRIX OF UNICYCLIC GRAPHS

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Bachelor of Science

We analyze the spectrum of the distance squared matrix of a tree and give a relation between the inertia of the distance squared matrix and the structure of the tree. We take the result one step further and consider the addition of exactly one cycle in the tree. We obtain an expression for the inertia of the distance squared matrix of a cycle graph. We obtain a bound on the inertia of the distance squared matrix of an arbitrary unicyclic graph.



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# 1 Introduction

In the field of spectral graph theory, matrices are used to convey information about a graph. For example, the Laplacian of a graph can be used to calculate the number of spanning trees in a graph and the distance matrix is useful in different algorithms like  $k$ -nearest neighbors or clustering. The eigenvalues of these associated matrices can be used to glean information about different characteristics of the graph.

Throughout this paper, we will be focusing on the inertia of a particular matrix called the distance squared matrix. The inertia is a tuple which consists of the number of positive, negative, and zero eigenvalues. The inertia can be used to determine different features of certain graphs without explicitly examining these graphs. One use for this could be instances where the graph is so large that computing the inertia could be easier than analyzing the graph.

Let  $G$  be a connected graph with vertex set  $V(G) = \{1, \dots, n\}$  and edge set  $E(G)$ . We define the distance between vertices  $i, j \in V(G)$ ,  $d_{ij}$ , as the minimum number of edges in a path from  $i$  to  $j$ . We will set  $d_{ii} = 0$  for  $i = 1, \dots, n$ . We will define the distance matrix  $D(G)$  or  $D$  of the graph as the matrix where each  $(i, j)$ -entry is equal to  $d_{ij}$ . Throughout this paper we will be mainly using the distance squared matrix,  $\Delta$ , which we will define as the Hadamard product  $D \circ D$  so that  $\Delta_{ij} = d_{ij}^2$ . On occasion, we will also use the notation  $A(i)$  which refers to some matrix  $A$  with the  $i$ th column and  $i$ th row deleted. We will also use the word pendant to refer to a vertex with exactly one edge connected to it.

In [1], the authors show how the inertia of the distance squared matrix of a tree corresponds with the structure of the tree. We will give an alternate proof of their result in this paper. We then build upon the result by adding a cycle into a tree which we call a unicyclic graph. A unicyclic graph is a graph which contains exactly one cycle.

We list here some tools from matrix theory that we will use. We will use the Cauchy Interlacing Theorem extensively which is the following result.

**Theorem 1.1** (Theorem 4.3.28 of [3]). *Suppose  $A \in \mathbb{R}^{n \times n}$  is symmetric. Let  $B \in \mathbb{R}^{m \times m}$  with  $m < n$  be a principal submatrix (obtained by deleting both the  $i$ -th row and  $i$ -th column for some values of  $i$ ). Suppose  $A$  has eigenvalues  $\lambda_1 \leq \dots \leq \lambda_n$  and  $B$  has eigenvalues  $\beta_1 \leq \dots \leq \beta_m$ . Then*

$$\lambda_k \leq \beta_k \leq \lambda_{k+n-m} \quad \text{for} \quad k = 1, \dots, m.$$

If  $m = n - 1$ ,

$$\lambda_1 \leq \beta_1 \leq \lambda_2 \leq \beta_2 \leq \dots \leq \beta_{n-1} \leq \lambda_n.$$

The following definition contains a shorthand for expressing inertia for the remainder of the paper.

**Definition 1.2.** *The inertia,  $i(M)$ , of a matrix  $M$  is the triple*

$$i(M) = (i_+(M), i_-(M), i_0(M))$$

where  $i_+$ ,  $i_-$ , and  $i_0$  represent the number of positive, negative, and zero eigenvalues respectively.

We will also use the subadditivity property of inertia which is described by the following theorem.

**Theorem 1.3** (Proposition 3.9 of [2]). *Let  $A, B \in \mathbb{R}^{n \times n}$  be symmetric. Then we have*

$$i_+(A + B) \leq i_+(A) + i_+(B)$$

and

$$i_-(A + B) \leq i_-(A) + i_-(B),$$

where  $i_+$  and  $i_-$  denote the number of positive and negative eigenvalues respectively.

We will use Sylvester's law of inertia in many of the row and column operations we perform which is the following.

**Theorem 1.4** (Theorem 4.5.8 in [3]). *Let  $A \in \mathbb{R}^{n \times n}$  be symmetric and let  $S$  be a nonsingular  $n \times n$  matrix. Then  $i(A) = i(S^T A S)$ .*

Finally, we have the Haynsworth inertia additivity formula.

**Theorem 1.5** (Theorem 4.5.P21 in [3]). *Let  $H$  be a Hermitian matrix given by*

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix},$$

where  $H_{11}$  is nonsingular and  $H_{12}^*$  is the conjugate transpose of  $H_{12}$ . Then

$$i(H) = i(H_{11}) + i(H_{22} - H_{12}^* H_{11}^{-1} H_{12}).$$

When we deal with cycles, we will often use circulant matrices which are matrices in which the first row is repeated for each row of the matrix except shifted one entry to the right. They will take the form

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_{n-1} & a_n \\ a_n & a_1 & \cdots & a_{n-2} & a_{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_2 & a_3 & \cdots & a_n & a_1 \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

To abbreviate, we will also express circulant matrices as

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_{n-1} & a_n \\ & \ddots & \ddots & \ddots & \\ & & & & \end{bmatrix}$$

throughout the paper. The following lemma gives the eigenvalues and eigenvectors of circulant matrices.

**Lemma 1.6** (Theorem 2.2.P10 of [3]). *Let  $A$  be the circulant matrix above. The eigenvectors will take the form*

$$v_j = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & \omega^j & \omega^{2j} & \dots & \omega^{(n-1)j} \end{bmatrix}^\top \quad j = 1, 2, \dots, n,$$

where  $\omega = \exp\left(\frac{2\pi i}{n}\right)$  is a primitive  $n$ -th root of unity and  $i$  is the imaginary unit.

*The eigenvalues will take the form*

$$\lambda_j = a_1 + a_2\omega^j + \dots + a_n\omega^{(n-1)j} \quad j = 1, 2, \dots, n.$$

## 2 Trees

In this section we find the inertia of a matrix corresponding to a noncyclical graph or tree. We let  $T$  be a tree and  $\Delta$  be its distance squared matrix. The following result is a generalization of Lemma 17 from [1].

**Lemma 2.1.** *For a graph  $G$  with distance squared matrix  $\Delta$ , let  $v$  be a vertex of degree 2 with neighbors  $u$  and  $w$ , and let  $\mathbf{x}$  be a vector in  $\mathbb{R}^n$  such that*

$$x_i = \begin{cases} 1 & \text{if } i = u \text{ or } i = w \\ -2 & \text{if } i = v \\ 0 & \text{otherwise.} \end{cases}$$

*If the graph can be disconnected by removing edge  $(u, v)$  or  $(v, w)$ , then  $\Delta\mathbf{x}$  is the all 2's vector.*

*Proof.* Let  $G$  be a graph with distance squared matrix  $\Delta$ . Suppose that  $v$  is vertex

of degree 2 with neighbors  $u$  and  $w$ . Let  $\mathbf{x}$  be a vector in  $\mathbb{R}^n$  defined as above. Suppose also that  $G$  can be disconnected by removing  $(u, v)$  or  $(v, w)$ . Each row of  $\Delta$  will take the form  $\left[ \dots \quad j^2 \quad (j+1)^2 \quad (j+2)^2 \quad \dots \right]$  where  $j$  depends on the location of the vertex in the graph with which the row corresponds and the positions of  $j^2$ ,  $(j+1)^2$ , and  $(j+2)^2$  correspond with the positions of  $u$ ,  $v$ , and  $w$  in  $G$  respectively. The vector  $\mathbf{x}$  will take the form  $\left[ \mathbf{0} \quad 1 \quad -2 \quad 1 \quad \mathbf{0} \right]^\top$  where the 1, -2, and 1 appear in the same position as  $j^2$ ,  $(j+1)^2$ , and  $(j+2)^2$  respectively. Multiplying an arbitrary row of  $\Delta$  with  $\mathbf{x}$  gives

$$\begin{aligned} \left[ \dots \quad j^2 \quad (j+1)^2 \quad (j+2)^2 \quad \dots \right] \begin{bmatrix} \mathbf{0} \\ 1 \\ -2 \\ 1 \\ \mathbf{0} \end{bmatrix} &= j^2 - 2(j+1)^2 + (j+2)^2 \\ &= j^2 - 2j^2 - 4j - 2 + j^2 + 4j + 4 \\ &= 2. \end{aligned}$$

Thus  $\Delta \mathbf{x} = \mathbf{2}$ . □

**Lemma 2.2.** *Define a vector  $\mathbf{x}_i$  for each vertex of degree 2 in the same fashion as the lemma above. Then  $\{\mathbf{x}_i\}$  is a linearly independent set.*

**Lemma 2.3.** *Let  $T$  be a tree of  $n > 2$  vertices and  $\Delta$  be the distance squared matrix of  $T$ . If  $T$  has  $d \geq 2$  vertices of degree 2, then  $i_0(\Delta) \geq d - 1$ .*

*Proof.* Let  $\{\mathbf{x}_1, \dots, \mathbf{x}_d\}$  be as in Lemma 2.2. Note that  $\{\mathbf{x}_1 - \mathbf{x}_2, \mathbf{x}_1 - \mathbf{x}_3, \dots, \mathbf{x}_1 - \mathbf{x}_d\}$  is a linearly independent set from the lemma above. Also  $\Delta(\mathbf{x}_1 - \mathbf{x}_2) = \Delta \mathbf{x}_1 - \Delta \mathbf{x}_2 = \mathbf{0}$ . Thus each vector is in the null space of  $\Delta$  and so  $i_0(\Delta) \geq d - 1$ . □

The following is the main result of this section.

**Theorem 2.4.** *Let  $T$  be a tree of  $n > 2$  vertices and  $\Delta$  be the distance squared matrix of  $T$ . Then*

$$i_0(\Delta) = \begin{cases} 0 & \text{if } t = 0, 1 \\ t - 1 & \text{if } t \geq 2, \end{cases}$$

where  $t$  is the number of degree 2 vertices of  $T$  and

$$i_-(\Delta) = \ell,$$

where  $\ell$  is the number of leaves (vertices of degree one) of  $T$ .

*Proof.* We proceed by induction on the number of vertices  $n$ . For  $n = 3$ ,  $T \cong P_3$ , and

$$\Delta = \begin{bmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{bmatrix},$$

with eigenvalues of  $2 + \sqrt{6}$ ,  $-4$ ,  $2 - \sqrt{6}$ , satisfying the conclusion of the theorem.

Now, let  $T$  be a tree of  $n > 3$  vertices and assume the conclusion is true for all trees of fewer than  $n$  vertices (but at least 3 vertices). If  $\text{diam}(T) = 2$ , then  $T$  is a star and

$$\Delta = \begin{bmatrix} 0 & \mathbf{1}^T \\ \mathbf{1} & 4J - 4I \end{bmatrix},$$

where  $4J - 4I$  is  $(n - 1) \times (n - 1)$ , and  $J$  is the all ones matrix. We have

$$i_-(4J - 4I) = n - 2 \text{ (where the eigenvalue equals } -4 \text{ with multiplicity of } n - 2\text{),}$$

$$i_+(4J - 4I) = 1 \text{ (where the eigenvalue equals } 4(n - 2)\text{).}$$

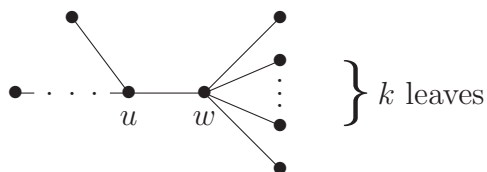
Performing similar row and column operations we subtract from the first row

$1/(4(n-2))$  times each of the remaining rows of  $\Delta$  and from the first column  $1/(4(n-2))$  times each of the remaining columns of  $\Delta$ . Thus,  $\Delta$  is congruent to

$$\begin{bmatrix} \frac{n-1}{4(n-2)} & \mathbf{0}^T \\ \mathbf{0} & 4J - 4I \end{bmatrix}.$$

Therefore, by Sylvester's law of inertia,  $i_-(\Delta) = n - 1$  and  $i_0(\Delta) = 0$ . Hence, from here we assume  $\text{diam}(T) \geq 3$ .

Consider a diametrical path in  $T$ . There exists a vertex  $w$  such that  $w$  has exactly one non-leaf neighbor  $u$ .



Let  $w$  be adjacent to  $k$  leaves, and label leaves  $1, \dots, k$ . Now let  $w = k + 1$  and  $u = k + 2$ .

**Case 1:**  $k \geq 2$ . Then we have

$$\Delta = \begin{bmatrix} 4J_k - 4I_k & X^T \\ X & \Delta_{k+1} \end{bmatrix},$$

where  $\Delta_{k+1}$  is the square distance matrix for  $T \setminus \{1, \dots, k\}$  and  $X$  is a  $(n - k) \times k$  matrix with all identical columns.

We can use row and column  $k$  to zero out the first  $k - 1$  rows or columns of the upper right and lower left blocks of  $\Delta$  ( $X$  and  $X^T$ ). Continuing with similar row and column operations, we find that  $\Delta$  is equivalent to



$$A = \begin{bmatrix} -4I_{k-1} - 4J_{k-1} & 0 \\ 0 & (4 - 4/k)\mathbf{e}_k\mathbf{e}_k^T + \Delta_k \end{bmatrix},$$

with  $\Delta_k$  being the square distance matrix for  $T \setminus \{1, \dots, k-1\}$ . Notice that  $-4I_{k-1} - 4J_{k-1}$  is negative definite and so has  $k-1$  negative eigenvalues.

Let  $F = (4 - 4/k)\mathbf{e}_k\mathbf{e}_k^T + \Delta_k$  and notice  $F(1) = \Delta_{k+1}$  where  $\Delta_{k+1}$  is the distance squared matrix for  $T \setminus \{1, \dots, k\}$ . Notice that  $T \setminus \{1, \dots, k\}$  is a tree with  $\ell - (k-1)$  leaves and at least 3 vertices. Using our inductive hypothesis on  $T \setminus \{1, \dots, k\}$  to find  $i_-(\Delta_k)$ , we see that

$$i_-(\Delta_{k+1}) = \ell - (k-1).$$

It follows from the Cauchy interlacing theorem that

$$i_-(F) \geq \ell - (k-1).$$

Since  $F = (4 - 4/k)\mathbf{e}_k\mathbf{e}_k^T + \Delta_k$  and  $4 - 4/k > 0$ , the subadditivity of inertia gives us

$$\begin{aligned} i_-(F) &\leq i_-((4 - 4/k)\mathbf{e}_k\mathbf{e}_k^T) + i_-(\Delta_k) \\ &= 0 + \ell - (k-1) \\ &= \ell - (k-1). \end{aligned}$$

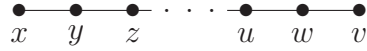
Thus

$$i_-(F) = \ell - (k-1).$$

Further,

$$\begin{aligned}
i_-(\Delta) &= i_-(-4I_{k-1} - 4J_{k-1}) + i_-(F) \\
&= k - 1 + \ell - (k - 1) \\
&= \ell.
\end{aligned}$$

**Case 2:**  $k = 1$ . Label the leaf adjacent to  $w$  as  $v$ . Let  $\Delta_2 = \Delta(1)$ . By the inductive hypothesis,  $i_-(\Delta_2) = \ell$ . Thus, by interlacing,  $i_-(\Delta) \geq \ell$ . As there are two ends in a diametrical path, we may assume that there exists a vertex  $y$  such that  $y$  is adjacent to exactly one leaf  $x$  and exactly one non-leaf  $z$ . If this were not the case we would be able to apply the argument from Case 1.



It is possible that  $u = y$  and  $z = w$  in the case that  $T \cong P_4$  or that  $u = z$  in the case that  $\text{diam}(T) = 4$ . In any case, using Lemma 2.3, the columns of  $\Delta$  corresponding to  $x, y, z$  with weights  $1, -2, 1$  form the all 2's vector. Thus the column corresponding to  $v$  is a linear combination of the columns corresponding to  $x, y, z, u, w$ . Thus  $\text{rank}(\Delta) = \text{rank}(\Delta_2)$  and  $i_-(\Delta) \leq \ell$ .

Now we continue to show that  $i_0(\Delta) = t - 1$ , where  $t \geq 2$  is the number of vertices of degree 2, or, in the case that  $t = 0, 1$ , that  $\Delta$  is invertible. Recall from the beginning of the proof that  $n \geq 4$  and  $\text{diam}(T) \geq 3$ .

**Case 1:**  $T$  has a vertex which is adjacent to more than two leaves. Then deleting a leaf from  $T$  yields  $\Delta_2$ , which is a principal submatrix of  $\Delta$ . Note that the number of degree 2 vertices has not changed. By interlacing,  $i_+(\Delta) \geq i_+(\Delta_2)$ , and by the first part of the theorem  $i_-(\Delta) = i_-(\Delta_2) + 1$ . If  $t = 0$  or 1 then, by our inductive hypothesis,  $\Delta_2$  is invertible. Thus  $i_0(\Delta_2) = 0$ . So

$$i_+(\Delta_2) + i_-(\Delta_2) = n - 1$$

and

$$n \geq i_+(\Delta) + i_-(\Delta) \geq i_+(\Delta_2) + i_-(\Delta_2) + 1 = n.$$

Thus  $i_0(\Delta) = 0$ , as desired.

If  $t \geq 2$ , then by Lemma 2.3 we have  $i_0(\Delta) \geq t - 1$  and by the inductive hypothesis  $i_0(\Delta_2) = t - 1$ . So

$$n - 1 = i_+(\Delta_2) + i_-(\Delta_2) + i_0(\Delta_2)$$

and

$$n \geq i_+(\Delta) + i_-(\Delta) + i_0(\Delta) \geq i_+(\Delta_2) + i_-(\Delta_2) + 1 + i_0(\Delta_2) = n.$$

Thus  $i_0(\Delta) = i_0(\Delta_2) = t - 1$ , as desired.

**Case 2:**  $T$  has a vertex which is adjacent to exactly two leaves. We consider the vertex  $w$  with 2 adjacent leaves. Then the distance squared matrix has the form

$$\Delta = \begin{bmatrix} 0 & 4 & \mathbf{x}^T \\ 4 & 0 & \mathbf{x}^T \\ \mathbf{x} & \mathbf{x} & \Delta' \end{bmatrix},$$

where  $\Delta'$  is  $(n-2) \times (n-2)$  and  $\mathbf{x}$  is a vector of appropriate size. We notice that the vector  $\mathbf{x}$  can be reduced to the all zeros vector without changing the column space of  $\Delta$  because  $\mathbf{x}$  is in the column space of  $\Delta'$ . Hence  $\text{rank}\Delta' = \text{rank}\Delta - 2$ , since the upper left  $2 \times 2$  matrix has a rank of 2. Therefore, adding a leaf onto our vertex  $w$  has no effect on the number of negative eigenvalues of  $\Delta$ .

**Case 3:** Every vertex of  $T$  is adjacent to at most one leaf. Since  $\text{diam}(T) \geq 3$ , there exists at least two vertices of degree 2, each adjacent to a leaf (consider a diametrical path). Deleting such a pendant vertex decreases the number of vertices of degree 2 by 1 and keeps the number of leaves the same. Note that we have  $\text{rank}(\Delta) = \text{rank}(\Delta_2)$  by arguments similar to the above when we proved  $i_-(\Delta) = \ell$

in the  $k = 1$  case above. By interlacing,  $i_+(\Delta) \geq i_+(\Delta_2)$  and  $i_-(\Delta) \geq i_-(\Delta_2)$ . Since  $i_+(\Delta) + i_-(\Delta) = \text{rank}(\Delta) = \text{rank}(\Delta_2) = i_+(\Delta_2) + i_-(\Delta_2)$ , we have  $i_+(\Delta) = i_+(\Delta_2)$  and  $i_-(\Delta) = i_-(\Delta_2)$ . Thus  $i_0(\Delta) = i_0(\Delta_2) + 1 = t - 2 + 1 = t - 1$  and the proof is complete.

□

### 3 Cycles

To continue our journey to understanding unicyclic graphs, we will now consider cycle graphs.

**Definition 3.1.** *Let  $C$  be a graph containing three or more nodes. We call  $C$  a cycle graph if every node has exactly two edges connected to it.*

We will obtain formulas for the eigenvalues of the distance squared matrix of cycle graphs. We will treat even and odd length cycles separately. The basic distance squared matrices of these graphs take the form

$$\begin{bmatrix} c_1 & c_2 & \cdots & c_{n-1} & c_n \\ c_n & c_1 & \cdots & c_{n-2} & c_{n-1} \\ \vdots & \vdots & & \vdots & \vdots \\ c_2 & c_3 & \cdots & c_n & c_1 \end{bmatrix}$$

where  $c_1 = 0$  and  $c_i = c_{n+2-i} = (i - 1)^2$  for  $i > 1$ . This is an example of a circulant matrix. Thus, the eigenvalues will be in the form of  $c_1 + c_2\omega_j + \cdots + c_n\omega_j^{n-1}$  by Lemma 1.6.

**Theorem 3.2.** *Let  $C$  be a cycle graph of length  $n$  and  $\lambda_j$  be the  $j$ th eigenvalue of  $C$*

where the eigenvalues are ordered as  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ . When  $n$  is odd, we have

$$\lambda_j = 2 \cos(\pi j) \left( \cos \left( \frac{(n-2)\pi j}{n} \right) + 4 \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots + \frac{(n-1)^2}{4} \cos \left( \frac{\pi j}{n} \right) \right). \quad (1)$$

When  $n$  is even, we have

$$\lambda_j = 2 \cos(\pi j) \left( \frac{n^2}{8} + \cos \left( \frac{(n-2)\pi j}{n} \right) + 4 \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots + \frac{(n-1)^2}{4} \cos \left( \frac{\pi j}{n} \right) \right). \quad (2)$$

*Proof.* We consider the case where  $n$  is odd. When we substitute our  $c_i$ 's into the eigenvalue equation, we will get

$$\begin{aligned} \lambda_j &= \omega_j + 4\omega_j^2 + \dots + 4\omega_j^{n-2} + \omega_j^{n-1} \\ &= e^{i\frac{2\pi}{n}j} + 4e^{i\frac{4\pi}{n}j} + \dots + 4e^{i\frac{(2n-4)\pi}{n}j} + e^{i\frac{(2n-2)\pi}{n}j} \\ &= \cos \left( \frac{2\pi j}{n} \right) + i \sin \left( \frac{2\pi j}{n} \right) + 4 \cos \left( \frac{4\pi j}{n} \right) + i4 \sin \left( \frac{4\pi j}{n} \right) + \dots + 4 \cos \left( \frac{(2n-4)\pi j}{n} \right) \\ &\quad + i4 \sin \left( \frac{(2n-4)\pi j}{n} \right) + \cos \left( \frac{(2n-2)\pi j}{n} \right) + i \sin \left( \frac{(2n-2)\pi j}{n} \right) \\ &= \cos \left( \frac{2\pi j}{n} \right) + 4 \cos \left( \frac{4\pi j}{n} \right) + \dots + 4 \cos \left( \frac{(2n-4)\pi j}{n} \right) + \cos \left( \frac{(2n-2)\pi j}{n} \right) \\ &= 2 \cos \left( \left( \frac{2\pi j}{n} + \frac{(2n-2)\pi j}{n} \right) \frac{1}{2} \right) \cos \left( \left( \frac{2\pi j}{n} - \frac{(2n-2)\pi j}{n} \right) \frac{1}{2} \right) \\ &\quad + 8 \cos \left( \left( \frac{4\pi j}{n} + \frac{(2n-4)\pi j}{n} \right) \frac{1}{2} \right) \cos \left( \left( \frac{4\pi j}{n} - \frac{(2n-4)\pi j}{n} \right) \frac{1}{2} \right) + \dots \\ &\quad + \frac{(n-1)^2}{2} \cos \left( \left( \frac{(n-1)\pi j}{n} + \frac{(n+1)\pi j}{n} \right) \frac{1}{2} \right) \cos \left( \left( \frac{(n-1)\pi j}{n} - \frac{(n+1)\pi j}{n} \right) \frac{1}{2} \right) \\ &= 2 \cos(\pi j) \cos \left( \frac{(n-2)\pi j}{n} \right) + 8 \cos(\pi j) \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots \\ &\quad + \frac{(n-1)^2}{2} \cos(\pi j) \cos \left( \frac{\pi j}{n} \right) \\ &= 2 \cos(\pi j) \left( \cos \left( \frac{(n-2)\pi j}{n} \right) + 4 \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots + \frac{(n-1)^2}{4} \cos \left( \frac{\pi j}{n} \right) \right). \end{aligned}$$

Now we will consider the case of an even cycle. In this case, the above derivation

will be very similar except there will be a  $n^2/8$  in the large quantity of equation 1:

$$\lambda_j = 2 \cos(\pi j) \left( \frac{n^2}{8} + \cos \left( \frac{(n-2)\pi j}{n} \right) + 4 \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots + \frac{(n-1)^2}{4} \cos \left( \frac{\pi j}{n} \right) \right).$$

□

**Corollary 3.3.** *Let  $C$  be a cycle graph of length  $n > 2$  and  $\Delta$  be its distance squared matrix. If  $n \equiv 1 \pmod{4}$ , then  $i_+(\Delta) = \frac{n-1}{2} + 1$  and  $i_-(\Delta) = \frac{n-1}{2}$ . If  $n \equiv 3 \pmod{4}$ , then  $i_+(\Delta) = \frac{n-1}{2}$  and  $i_-(\Delta) = \frac{n-1}{2} + 1$ . If  $n$  is even, then  $i_+(\Delta) = \frac{n}{2}$  and  $i_-(\Delta) = \frac{n}{2}$ .*

*Proof.* In Theorem 3.2,  $j$  is an integer. However, by thinking of it as a real number, we can glean information about how the values of the eigenvalues of the matrix are connected. So we will now think of (1) as an equation on the real numbers. The zeros for this equation will appear when  $j = k/2$  for some  $k \in \mathbb{Z}$ . These will be the only zeros for this equation since the second half only becomes zero when all of the individual components are in sync and that happens only at  $n/2$ . Since the equation is continuous, this means that none of the eigenvalues will be zero. Now we'll use the first derivative test to find the quantity of positive eigenvalues and negative eigenvalues. The derivative with respect to  $j$  of this equation is

$$\begin{aligned} & -2\pi \sin(\pi j) \left( \cos \left( \frac{(n-2)\pi j}{n} \right) + 4 \cos \left( \frac{(n-4)\pi j}{n} \right) + \dots \right) \\ & + 2 \cos(\pi j) \left( -\frac{(n-2)\pi}{n} \sin \left( \frac{(n-2)\pi j}{n} \right) - \frac{4(n-4)\pi}{n} \sin \left( \frac{(n-4)\pi j}{n} \right) - \dots \right). \end{aligned}$$

We will only focus on substituting the zeros we found above into the first half of the expression since the second half is 0 at the values of  $j = k/2$  for reasons stated above. The  $-2\pi \sin(\pi j)$  part of the expression will alternate between positive and negative starting with negative when  $j = k/2$ . The other half of the expression will be positive at first since the rightmost term will dominate the others until it hits

$n/2$  where it will be 0 for reasons stated above. After that it will be negative.

We will now deal with the case when the number of vertices mod 4 equals 1. When  $j = 1$ ,  $\lambda_j$  is between two zeros. Since the derivative is negative at .5 and positive at 1.5,  $\lambda_1$  will be negative. The eigenvalues will flip between positive and negative until it gets to the integer after  $n/2$ . Here there will be another positive eigenvalue in a row and then start alternating again. So there will be  $\lceil n/2 \rceil$  positive eigenvalues and  $\lfloor n/2 \rfloor$  negative eigenvalues.

It will be very similar to the case when the number of vertices mod 4 equals 3. Only in this case there will be a subsequent negative eigenvalue instead of a positive eigenvalue.

Now for the even case, we'll focus on equation (2). This equation is similar to equation (1) except it has an extra term. This will cause the derivative to strictly alternate between positive and negative values on the roots of the equation. Therefore, there will be  $n/2$  positive and  $n/2$  negative eigenvalues.  $\square$

## 4 An even length cycle with exactly one tree connected to a vertex

In the previous section, we examined the eigenvalues of a graph which was a single cycle. In this section, we will build upon the previous result and observe what occurs when we attach a tree to one node of the cycle graph. We will build up to this with a few lemmas.

**Lemma 4.1.** *Given an even cycle with  $p$  nodes and distance squared matrix  $\Delta$ , the inverse of this matrix can be expressed as the circulant matrix*

$$\Delta^{-1} = \frac{1}{4\lambda m} \left( 2J + \begin{bmatrix} \theta^T & -\lambda & 2\lambda & -\lambda & \theta^T \\ & \ddots & \ddots & \ddots & \\ & & & & \end{bmatrix} \right),$$

where  $m = n/2$ ,  $\lambda$  is the largest eigenvalue of  $\Delta$ , and the  $\mathbf{0}$  vectors in the first row are size  $(n/2) - 1$  and  $(n/2) - 2$ , respectively, and each row shifting one to the right, forming a circulant matrix.

*Proof.* For convenience define

$$B = \begin{bmatrix} \mathbf{0}^T & -\lambda & 2\lambda & -\lambda & \mathbf{0}^T \\ & \ddots & \ddots & \ddots & \\ & & & & \end{bmatrix}.$$

We have

$$\begin{aligned} I &= \frac{1}{4\lambda m} \left( \lambda \begin{bmatrix} 4m-2 & -2 & -2 & \dots & -2 \\ -2 & 4m-2 & -2 & \dots & -2 \\ \vdots & \vdots & \ddots & & \vdots \\ -2 & -2 & -2 & \dots & 4m-2 \end{bmatrix} + 2\lambda J \right) \\ &= \frac{1}{4\lambda m} \left( \lambda \begin{bmatrix} -2m^2 + 4m - 2 + 2m^2 & -2 & \dots & -2 \\ \vdots & \ddots & & \vdots \\ -2 & \dots & -2 & -2m^2 + 4m - 2 + 2m^2 \end{bmatrix} + 2\lambda J \right) \\ &= \frac{1}{4\lambda m} \left( \lambda \begin{bmatrix} -(m-1)^2 + 2m^2 - (m-1)^2 & -2 & \dots & -2 \\ \vdots & \ddots & & \vdots \\ -2 & \dots & -2 & -(m-1)^2 + 2m^2 - (m-1)^2 \end{bmatrix} + 2\lambda J \right) \\ &= \frac{1}{4\lambda m} (\Delta B + 2\lambda J). \end{aligned}$$

Because  $\Delta$  is circulant, the sum of each of the rows is the same, i.e.  $\lambda$ . So  $2\lambda J = 2\Delta J$ . Thus

$$\begin{aligned} \frac{1}{4\lambda m} (\Delta B + 2\lambda J) &= \frac{1}{4\lambda m} (\Delta B + 2\Delta J) \\ &= \frac{1}{4\lambda m} \Delta (B + 2J). \end{aligned}$$



□

**Lemma 4.2.** *Let  $\Delta$  be the distance squared matrix of an even cycle with  $p$  nodes and a single pendant extending from the cycle. Let the first  $p$  columns and rows be indexed by the nodes of the cycle and the last column and row be indexed by the node attached to the pendant we added. Let  $\tilde{\Delta} = \Delta(p+1)$ , and let  $\mathbf{x}$  be the first  $p$  elements of the last row of  $\Delta$ .*

$$\mathbf{x}^T \tilde{\Delta}^{-1} \mathbf{x} > 0.$$

*Proof.* Using Lemma 4.1 we have

$$\mathbf{x}^T \tilde{\Delta}^{-1} \mathbf{x} = \frac{1}{4\lambda m} \left( 2\mathbf{x}^T J \mathbf{x} + \mathbf{x}^T \begin{bmatrix} \mathbf{0}^T & -\lambda & 2\lambda & -\lambda & \mathbf{0}^T \\ & \ddots & \ddots & \ddots & \\ & & & & \end{bmatrix} \mathbf{x} \right).$$

We consider each term individually.

Multiplying  $\mathbf{x}^T$  by  $J$  results in a vector whose entries are all equal to the sum of the entries of  $\mathbf{x}$ . The sum of the elements of  $\mathbf{x}$  can be written as

$$\begin{aligned} 2 \sum_{j=1}^m j^2 + (m+1)^2 - 1 &= \frac{m(m+1)(2m+1)}{3} + (m+1)^2 - 1 \\ &= \frac{2m^3 + 6m^2 + 7m}{3} \end{aligned}$$

where  $m = p/2$ . Hence

$$\begin{aligned} 2\mathbf{x}^T J \mathbf{x} &= 2 \left( \frac{2m^3 + 6m^2 + 7m}{3} \right) \mathbf{1}^T \mathbf{x} \\ &= 2 \left( \frac{2m^3 + 6m^2 + 7m}{3} \right)^2. \end{aligned}$$

Now we consider the second term. Let  $B$  be as defined in Lemma 4.1. Letting  $j$  denote the index of the element of the vector  $\mathbf{x}$  corresponding to the index of the first non-zero entry of the row of the matrix  $B$  by which we are multiplying  $\mathbf{x}$ , we

see that the first entry of  $B\mathbf{x}$  is given by

$$\begin{aligned} \begin{bmatrix} -\lambda & 2\lambda & -\lambda \end{bmatrix} \begin{bmatrix} j^2 \\ (j+1)^2 \\ j^2 \end{bmatrix} &= -\lambda j^2 + 2\lambda(j+1)^2 - \lambda j^2 \\ &= -2\lambda j^2 + 2\lambda(j^2 + 2j + 1) \\ &= 4\lambda j + 2\lambda. \end{aligned}$$

Since the index of the first non-zero term will be  $m+1$ , the first entry of our resultant matrix will be  $4\lambda(m+1) + 2\lambda$ . The  $m+1$  entry of our resultant matrix will be given similarly, replacing  $m+1$  with 1. This gives us  $-6\lambda$  as the  $m+1$  term in our vector. Each of the other entries will be given by

$$\begin{aligned} \begin{bmatrix} -\lambda & 2\lambda & -\lambda \end{bmatrix} \begin{bmatrix} j^2 \\ (j+1)^2 \\ (j+2)^2 \end{bmatrix} &= -\lambda j^2 + 2\lambda(j+1)^2 - \lambda(j+2)^2 \\ &= -\lambda j^2 + 2\lambda(j^2 + 2j + 1) - \lambda(j^2 + 4j + 4) \\ &= -2\lambda. \end{aligned}$$

Thus, we have

$$B\mathbf{x} = \begin{bmatrix} 4\lambda(m+1) + 2\lambda & -2\lambda & \cdots & -2\lambda & -6\lambda & -2\lambda & \cdots & -2\lambda \end{bmatrix}^T.$$

Left-multiplying by  $\mathbf{x}^T$  gives us

$$\begin{aligned}\mathbf{x}^T B \mathbf{x} &= \mathbf{x}^T \begin{bmatrix} 4\lambda(m+1) + 2\lambda & -2\lambda & \cdots & -2\lambda & -6\lambda & -2\lambda & \cdots & -2\lambda \end{bmatrix}^T \\ &= 4\lambda(m+1) + 2\lambda - 6\lambda(m+1)^2 - 2\lambda \left( 2 \sum_{j=1}^m (j^2) - 2 \right) \\ &= -\frac{4}{3}\lambda m^3 - 8\lambda m^2 - \frac{26}{3}\lambda m + 4\lambda.\end{aligned}$$

Now, adding the two terms together gives us

$$\begin{aligned}\mathbf{x}^T \tilde{\Delta}^{-1} \mathbf{x} &= \frac{1}{4\lambda m} \left( 2 \left( \frac{2m^3 + 6m^2 + 7m}{3} \right)^2 - \frac{4}{3}\lambda m^3 - 8\lambda m^2 - \frac{26}{3}\lambda m + 4\lambda \right) \\ &= \frac{1}{4\lambda m} \left( \frac{8}{9}m^6 + \frac{16}{3}m^5 + \frac{128}{9}m^4 + \frac{56}{3}m^3 + \frac{98}{9}m^2 - \frac{4}{3}\lambda m^3 - 8\lambda m^2 - \frac{26}{3}\lambda m + 4\lambda \right).\end{aligned}$$

Because  $\lambda$  is the column sum of  $\tilde{\Delta}$ , it is given by  $m(2m^2 + 1)/3$ . The previous expression is greater than 0 for any integer  $m$ .

□

**Lemma 4.3.** *Let  $U$  be a graph which contains exactly one cycle of length  $p$  where  $p$  is even and one pendant connected to one of the vertices. Let  $\Delta$  be the distance squared matrix of  $U$  and  $m = p/2$ . Then  $i(\Delta) = (m, m + 1, 0)$ .*

*Proof.* The distance squared matrix for  $U$  will take the form

$$\begin{bmatrix} \tilde{\Delta} & \mathbf{x} \\ \mathbf{x}^T & 0 \end{bmatrix},$$

where  $\tilde{\Delta}$  and  $\mathbf{x}$  take the same definitions as in Lemma 4.2. By Theorem 1.5, Corol-

lary 3.3, and Lemma 4.2, we'll have that

$$\begin{aligned}
i(\Delta) &= i\left(\begin{bmatrix} \tilde{\Delta} & \mathbf{x} \\ \mathbf{x}^\top & 0 \end{bmatrix}\right) \\
&= i(\tilde{\Delta}) + i(-\mathbf{x}^\top \tilde{\Delta}^{-1} \mathbf{x}) \\
&= (m, m, 0) + (0, 1, 0) \\
&= (m, m + 1, 0).
\end{aligned}$$

□

**Lemma 4.4.** *Let  $U$  be a graph which contains exactly one cycle and assume that the cycle contains an even number of vertices. Also assume that of the vertices of the cycle, only one has exactly three edges connected to it and the rest only have two edges connected to each vertex. If  $U$  has at least one vertex of degree 2 not part of the cycle, then  $i_0(\Delta) \geq 1$ .*

*Proof.* Let  $m$  be the length of the cycle divided by two. Let the vertices in the cycle be numbered from 1 to  $2m$ . Let  $2m + 1$  be the number of the vertex connected to  $2m$ , but not part of the cycle. Let  $u$  be a degree two vertex not in the cycle.

Let  $n$  be the number of vertices in  $U$ . Let the entries of  $\mathbf{a} \in \mathbb{R}^n$  be defined by

$$a_j = \begin{cases} -1 & \text{if } j = m \\ m + 1 & \text{if } j = 2m \\ -m & \text{if } j = 2m + 1 \\ 0 & \text{otherwise} \end{cases}$$

and the entries of  $\mathbf{b} \in \mathbb{R}^n$  be defined by

$$b_j = \begin{cases} m(m+1)/2 & \text{if } j = u-1 \text{ or } j = u+1 \\ -m(m+1) & \text{if } j = u \\ 0 & \text{otherwise.} \end{cases}$$

Let  $\Delta$  be the distance squared matrix of  $U$  and  $\mathbf{r}$  be an arbitrary row in  $\Delta$ . With the assumptions of the lemma, observe that

$$\begin{aligned} \mathbf{r}^\top \mathbf{a} &= (m-z)^2(-1) + z^2(m+1) + (z+1)^2(-m) \\ &= -(m^2 - 2mz + z^2) + z^2m + z^2 - (z^2 + 2z + 1)m \\ &= -m^2 + 2mz - z^2 + z^2m + z^2 - z^2m - 2mz - m \\ &= -m^2 - m \end{aligned}$$

and

$$\begin{aligned} \mathbf{r}^\top \mathbf{b} &= \frac{(z+u-1)^2m(m+1)}{2} + (z+u)^2(-m(m+1)) + \frac{(z+u+1)^2m(m+1)}{2} \\ &= \frac{(z^2 + u^2 + 1 + 2zu - 2z - 2u)(m^2 + m)}{2} - (z^2 + 2zu + u^2)(m^2 + m) \\ &\quad + \frac{(z^2 + u^2 + 1 + 2zu + 2z + 2u)(m^2 + m)}{2} \\ &= m^2 + m \end{aligned}$$

where  $z$  corresponds to the location of  $\mathbf{r}$  in  $\Delta$ . Combining these together, we have  $\mathbf{r}^\top(\mathbf{a} + \mathbf{b}) = 0$ , and so  $\Delta(\mathbf{a} + \mathbf{b}) = 0$ . Hence,  $i_0(\Delta) > 0$  by the Invertible Matrix Theorem.  $\square$

We are now ready for the main result of this section.

**Theorem 4.5.** *Let  $U$  be a graph on  $n > 2$  vertices which has a single cycle of  $p$*

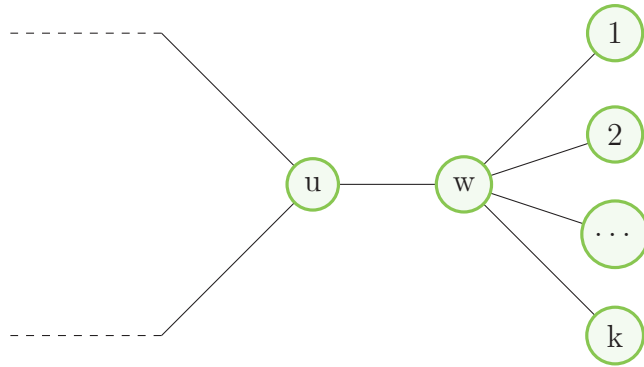
vertices with a tree connected to one of the vertices of the cycle. Assume  $p$  is even. Let  $\Delta$  be the distance squared matrix on  $U$ . Then

$$i_-(\Delta) = \ell + q,$$

where  $\ell$  is the number of leaves of  $U$  and  $q$  is the number of negative eigenvalues of the  $p$ -cycle.

*Proof.* We will use induction on  $n$ . Note that Lemma 4.3 takes care of the case when a single leaf is connected to the cycle. So let  $U$  be a unicyclic graph on  $n \geq 4$  vertices and assume the conclusion is true for all unicyclic graphs on fewer than  $n$  vertices.

Consider a diametrical path in  $U$ . There exists a vertex  $w$  such that  $w$  has exactly one non-leaf neighbor  $u$ .



Let  $w$  be adjacent to  $k$  leaves, and label leaves  $1, \dots, k$ ,  $w$  is  $k+1$ , and  $u$  is  $k+2$ .

**Case 1:** Suppose  $k \geq 2$ . Then the distance squared matrix is

$$\Delta = \begin{bmatrix} 4J_k - 4I_k & X \\ X^T & \Delta_{k+1} \end{bmatrix},$$

where  $J_n$  is the  $n \times n$  matrix of ones,  $X$  is a matrix which has the distances from the leaves  $1, \dots, k$  to the rest of the graph, and  $\Delta_n$  is the distance squared

matrix for  $U \setminus 1, \dots, n-1$ . Using corresponding row and column operations,  $\Delta$  can be written as

$$\Delta = \begin{bmatrix} -4I_{k-1} - 4J_{k-1} & 0 \\ 0 & \frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^\top + \Delta_k \end{bmatrix}.$$

Notice that  $-4I_{k-1} - 4J_{k-1}$  is negative definite, so it will have  $k-1$  negative eigenvalues. Let  $\frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^\top + \Delta_k = F$  and notice  $F(1) = \Delta_{k+1}$ . Notice that  $U \setminus 1, \dots, k$  is a tree with  $\ell - (k-1)$  leaves and at least three vertices. By the inductive hypothesis,

$$i_-(\Delta_{k+1}) = \ell + q - (k-1).$$

By interlacing,  $i_-(F) \geq \ell + q - (k-1)$ . Since  $F = \frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^\top + \Delta_k$  and  $\frac{4(k-1)}{k} > 0$ ,

$$\begin{aligned} i_-(F) &\leq i_-\left(\frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^\top\right) + i_-(\Delta_k) \\ &\leq 0 + \ell + q - (k-1) \\ &= \ell + q - (k-1). \end{aligned}$$

Thus,  $i_-(F) = \ell + q - (k-1)$ . Now notice

$$\begin{aligned} i_-(\Delta) &= i_-(-4I_{k-1} - 4J_{k-1}) + i_-(F) \\ &= (k-1) + \ell + q - (k-1) \\ &= \ell + q. \end{aligned}$$

**Case 2:** Suppose  $k = 1$  and  $w$  is the only degree 2 vertex in the graph. Let  $\Delta_2 = \Delta(1)$ . By our inductive hypothesis,  $i_-(\Delta_2) = \ell + q$ . By interlacing,  $i_-(\Delta) \geq$

$\ell + q$ . Since  $p$  is even and  $w$  is a degree 2 vertex not in the cycle, we can use Lemma 4.4 to deduce that the column in  $\Delta$  corresponding to  $w$  is a linear combination of other columns in  $\Delta$ . Thus,  $\text{rank}(\Delta) = \text{rank}(\Delta_2)$  and  $i_-(\Delta) \leq \ell + q$ .

**Case 3:** Suppose  $k = 1$  and there is some other degree 2 vertex in the graph besides  $w$ . By an argument similar to the first Case 2 of Theorem 2.4, we'll have that  $i_-(\Delta) = \ell + q$ .

□

## 5 General Unicyclic Graphs

For general unicyclic graphs we weren't able to get a formula as precise as the last sections, but we were able to get a bound on the number of negative eigenvalues in certain more general situations.

**Theorem 5.1.** *Let  $U$  be a unicyclic graph on  $n > 2$  vertices which has a single cycle of  $p$  vertices. Assume  $p$  is even. Let  $\Delta$  be the distance squared matrix of  $U$ ,  $\ell$  be the number of leaves of  $U$ ,  $q$  be the number of negative eigenvalues of the  $p$ -cycle, and let*

$$\beta = 2 \left\lfloor \frac{\lfloor \sin^{-1} \left( 1/\sqrt{p/2} \right) \frac{p}{\pi} \rfloor + 1}{2} \right\rfloor.$$

*Then*

$$\ell + q - \beta \leq i_-(\Delta) \leq \ell + q$$

*if there are no degree 2 vertices in the graph besides the degree 2 vertices of the cycle. Otherwise,*

$$\ell + q - \beta \leq i_-(\Delta) \leq \ell + q + 1$$

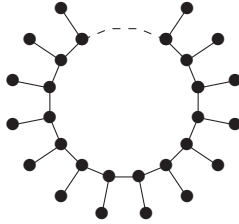


if there is at least one degree 2 vertex in the graph besides the degree 2 vertices of the cycle.

The remainder of this section will be devoted to proving this.

## 5.1 Base case

Consider the following graph



This graph is a cycle with a pendant extending from each node on the cycle. A distanced squared matrix for this graph can take the form

$$H = \begin{bmatrix} A & B \\ B & C \end{bmatrix},$$

where  $A$ ,  $B$ , and  $C$  are circulant matrices of size  $p \times p$ .  $A$  is indexed by the nodes of the main cycle.  $B$  is indexed by the nodes of the main cycle and the pendant nodes.  $C$  is indexed by the pendant nodes. Since  $A$ ,  $B$ , and  $C$  are all  $p \times p$  circulant matrices,  $A$ ,  $B$ , and  $C$  will all have the same eigenvectors. Thus, if  $\mathbf{x}$  is an eigenvector of  $A$  then  $A\mathbf{x} = \lambda\mathbf{x}$ ,  $B\mathbf{x} = \mu\mathbf{x}$ , and  $C\mathbf{x} = \rho\mathbf{x}$ , where  $\lambda$ ,  $\mu$ , and  $\rho$  are eigenvalues of  $A$ ,  $B$ , and  $C$  respectively corresponding to the eigenvector  $\mathbf{x}$ .

Assume that an eigenvector of  $H$  will take the form  $\begin{bmatrix} a\mathbf{x} & b\mathbf{x} \end{bmatrix}^T$ . Then we need to find values of  $h$  such that

$$\begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} a\mathbf{x} \\ b\mathbf{x} \end{bmatrix} = h \begin{bmatrix} a\mathbf{x} \\ b\mathbf{x} \end{bmatrix}.$$

Using the eigenvalues corresponding to  $\mathbf{x}$  above, notice that

$$\begin{aligned}
 \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} a\mathbf{x} \\ b\mathbf{x} \end{bmatrix} &= h \begin{bmatrix} a\mathbf{x} \\ b\mathbf{x} \end{bmatrix} \\
 \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} a\mathbf{x} \\ b\mathbf{x} \end{bmatrix} &= \begin{bmatrix} ha\mathbf{x} \\ hb\mathbf{x} \end{bmatrix} \\
 \begin{bmatrix} Aa\mathbf{x} + Bb\mathbf{x} \\ Ba\mathbf{x} + Cb\mathbf{x} \end{bmatrix} &= \begin{bmatrix} ha\mathbf{x} \\ hb\mathbf{x} \end{bmatrix} \\
 \begin{bmatrix} a\lambda\mathbf{x} + b\mu\mathbf{x} \\ a\mu\mathbf{x} + b\rho\mathbf{x} \end{bmatrix} &= \begin{bmatrix} ha\mathbf{x} \\ hb\mathbf{x} \end{bmatrix} \\
 \begin{bmatrix} (a\lambda + b\mu)\mathbf{x} \\ (a\mu + b\rho)\mathbf{x} \end{bmatrix} &= \begin{bmatrix} (ha)\mathbf{x} \\ (hb)\mathbf{x} \end{bmatrix}.
 \end{aligned}$$

So  $a\lambda + b\mu = ha$  and  $a\mu + b\rho = hb$ . Solving for  $h$  gives  $h = (a\lambda + b\mu)/a$  and  $h = (a\mu + b\rho)/b$ . Therefore,

$$\begin{aligned}
 \frac{a\lambda + b\mu}{a} &= \frac{a\mu + b\rho}{b} \\
 ab\lambda + b^2\mu &= a^2\mu + ab\rho \\
 b^2\mu - a^2\mu &= ab\rho - ab\lambda \\
 \frac{b^2 - a^2}{ab} &= \frac{\rho - \lambda}{\mu} \\
 \frac{b}{a} - \frac{a}{b} &= \frac{\rho - \lambda}{\mu}.
 \end{aligned}$$

Now the eigenvalue  $h$  will have many multiples of  $\begin{bmatrix} a\mathbf{x} & b\mathbf{x} \end{bmatrix}^T$  as eigenvectors. So let

$b = 1$ . Now we'll solve for  $a$ .

$$\begin{aligned}\frac{b}{a} - \frac{a}{b} &= \frac{\rho - \lambda}{\mu} \\ \frac{1}{a} - a &= \frac{\rho - \lambda}{\mu} \\ 1 - a^2 &= a \left( \frac{\rho - \lambda}{\mu} \right) \\ a^2 + a \left( \frac{\rho - \lambda}{\mu} \right) - 1 &= 0.\end{aligned}$$

Using the quadratic formula we get

$$a = \frac{-\left(\frac{\rho - \lambda}{\mu}\right) \pm \sqrt{\left(\frac{\rho - \lambda}{\mu}\right)^2 + 4}}{2}$$

Then we can solve for  $h$  using  $a\mu + b\rho = hb$ . Since  $b = 1$ , we have  $a\mu + \rho = h$ . Hence,

$$\begin{aligned}h &= a\mu + \rho \\ &= \left( \frac{-\left(\frac{\rho - \lambda}{\mu}\right) \pm \sqrt{\left(\frac{\rho - \lambda}{\mu}\right)^2 + 4}}{2} \right) \mu + \rho \\ &= -\frac{(\rho - \lambda)}{2} \pm \frac{\mu}{2} \sqrt{\left(\frac{\rho - \lambda}{\mu}\right)^2 + 4} + \rho \\ &= \frac{\rho}{2} + \frac{\lambda}{2} \pm \sqrt{\frac{(\rho - \lambda)^2}{4} + \mu^2}.\end{aligned}\tag{3}$$

So the eigenvalues of  $H$  will all correspond to values of the expression above for each combination of  $\lambda$ ,  $\mu$ ,  $\rho$  corresponding to  $\mathbf{x}$ .

Now we need to find expressions for  $\lambda$ ,  $\mu$ , and  $\rho$ . These will depend on  $A$ ,  $B$ , and  $C$ . Since these matrices are circulant, all information will be contained in the first row of each matrix. Recall that the eigenvalues are of the form  $c_1 + c_2\omega_j + \dots + c_p\omega_j^{p-1}$  where  $c_1, \dots, c_p$  are the entries of the first row and  $\omega = e^{2\pi i/p}$ .

We are going to consider an even cycle now. The first row of  $A$  will take the form

$$\begin{bmatrix} 0 & 1 & 4 & \cdots & (m-1)^2 & m^2 & (m-1)^2 & \cdots & 4 & 1 \end{bmatrix},$$

where  $m = p/2$ .

So for every index  $j \in \{0, \dots, p-1\}$ , we'll have

$$\begin{aligned} \lambda_j &= \omega^j + 4\omega^{2j} + \cdots + (m-1)^2\omega^{(m-1)j} + m^2\omega^{mj} + (m-1)^2\omega^{(p-m+1)j} + \cdots \\ &\quad + 4\omega^{(p-2)j} + \omega^{(p-1)j} \\ &= \omega^j + \omega^{(p-1)j} + 4\omega^{2j} + 4\omega^{(p-2)j} + \cdots + (m-1)^2\omega^{(m-1)j} \\ &\quad + (m-1)^2\omega^{(p-(m-1))j} + m^2\omega^{mj} \\ &= \exp\left(\frac{2\pi i}{p}j\right) + \exp\left(\frac{2\pi i}{p}(p-1)j\right) + 4\exp\left(\frac{2\pi i}{p}2j\right) + 4\exp\left(\frac{2\pi i}{p}(p-2)j\right) + \cdots \\ &\quad + (m-1)^2\exp\left(\frac{2\pi i}{p}(m-1)j\right) + (m-1)^2\exp\left(\frac{2\pi i}{p}(p-(m-1))j\right) \\ &\quad + m^2\exp\left(\frac{2\pi i}{p}mj\right) \\ &= \exp\left(\frac{2\pi i}{p}j\right) + \exp\left(-\frac{2\pi i}{p}j\right) + 4\exp\left(\frac{2\pi i}{p}2j\right) + 4\exp\left(-\frac{2\pi i}{p}2j\right) + \cdots \\ &\quad + (m-1)^2\exp\left(\frac{2\pi i}{p}(m-1)j\right) + (m-1)^2\exp\left(-\frac{2\pi i}{p}(m-1)j\right) + m^2\exp\left(\frac{2\pi i}{p}mj\right) \\ &= \cos\left(\frac{2\pi}{p}j\right) + i\sin\left(\frac{2\pi}{p}j\right) + \cos\left(-\frac{2\pi}{p}j\right) + i\sin\left(-\frac{2\pi}{p}j\right) \\ &\quad + 4\cos\left(\frac{2\pi}{p}2j\right) + 4i\sin\left(\frac{2\pi}{p}2j\right) + 4\cos\left(-\frac{2\pi}{p}2j\right) + 4i\sin\left(-\frac{2\pi}{p}2j\right) + \cdots \\ &\quad + (m-1)^2\cos\left(\frac{2\pi}{p}(m-1)j\right) + (m-1)^2i\sin\left(\frac{2\pi}{p}(m-1)j\right) \\ &\quad + (m-1)^2\cos\left(-\frac{2\pi}{p}(m-1)j\right) + (m-1)^2i\sin\left(-\frac{2\pi}{p}(m-1)j\right) + m^2\cos\left(\frac{2\pi}{p}mj\right) \\ &\quad + m^2\sin\left(\frac{2\pi}{p}mj\right) \end{aligned}$$

$$\begin{aligned}
&= \cos\left(\frac{2\pi}{p}j\right) + i \sin\left(\frac{2\pi}{p}j\right) + \cos\left(\frac{2\pi}{p}j\right) - i \sin\left(\frac{2\pi}{p}j\right) + 4 \cos\left(\frac{2\pi}{p}2j\right) + 4i \sin\left(\frac{2\pi}{p}2j\right) \\
&\quad + 4 \cos\left(\frac{2\pi}{p}2j\right) - 4i \sin\left(\frac{2\pi}{p}2j\right) + \cdots + (m-1)^2 \cos\left(\frac{2\pi}{p}(m-1)j\right) \\
&\quad + (m-1)^2 i \sin\left(\frac{2\pi}{p}(m-1)j\right) + (m-1)^2 \cos\left(\frac{2\pi}{p}(m-1)j\right) \\
&\quad - (m-1)^2 i \sin\left(\frac{2\pi}{p}(m-1)j\right) + m^2 \cos(\pi j) + m^2 \sin(\pi j) \\
&= 2 \cos\left(\frac{2\pi}{p}j\right) + 8 \cos\left(\frac{2\pi}{p}2j\right) + \cdots + 2(m-1)^2 \cos\left(\frac{2\pi}{p}(m-1)j\right) + m^2 \cos(\pi j) \\
&= 2 \sum_{\ell=1}^{m-1} \ell^2 \cos\left(\frac{2\pi}{p}\ell j\right) + m^2 \cos(\pi j).
\end{aligned}$$

The first row in  $B$  will take the form

$$\left[ 1 \quad 4 \quad 9 \quad \cdots \quad m^2 \quad (m+1)^2 \quad m^2 \quad \cdots \quad 9 \quad 4 \right].$$

We can do a similar calculation above for every  $j \in \{0, \dots, p-1\}$  to find

$$\mu_j = 2 \sum_{\ell=1}^{m-1} (\ell+1)^2 \cos\left(\frac{2\pi}{p}\ell j\right) + (m+1)^2 \cos(\pi j) + 1.$$

The first row in  $C$  will take the form

$$\left[ 0 \quad 9 \quad 16 \quad \cdots \quad (m+1)^2 \quad (m+2)^2 \quad (m+1)^2 \quad \cdots \quad 16 \quad 9 \right].$$

We can do a similar calculation above for every  $j \in \{0, \dots, p-1\}$  to find

$$\rho_j = 2 \sum_{\ell=1}^{m-1} (\ell+2)^2 \cos\left(\frac{2\pi}{p}\ell j\right) + (m+2)^2 \cos(\pi j).$$

Using algebraic and trigonometric manipulations, we can find that

$$\begin{aligned}
\lambda_j &= 2 \sum_{\ell=1}^{m-1} \ell^2 \cos\left(\frac{2\pi}{p}\ell j\right) + m^2 \cos(\pi j) \\
&= m \cos(\pi j) \left( -m + \csc\left(\frac{\pi}{2m}j\right)^2 \right) + \frac{1}{4} \left( 4m^2 \cot\left(\frac{\pi}{2m}j\right) - \csc\left(\frac{\pi}{2m}j\right)^4 \sin\left(\frac{\pi}{2m}j\right) \right) \sin(\pi j) \\
&\quad + m^2 \cos(\pi j).
\end{aligned}$$

Since  $j$  is an integer, the  $\sin(\pi j)$  will always evaluate to 0. Therefore, we'll have

$$\begin{aligned}\lambda_j &= m \cos(\pi j) \left( -m + \csc \left( \frac{\pi}{2m} j \right)^2 \right) + m^2 \cos(\pi j) \\ &= m \cos(\pi j) \csc \left( \frac{\pi}{2m} j \right)^2 \\ &= (-1)^j m \csc \left( \frac{\pi}{2m} j \right)^2.\end{aligned}$$

Using similar manipulations and the fact that  $j$  is an integer, we can find that

$$\mu_j = (-1 + (1 + m)(-1)^j) \csc \left( \frac{\pi}{2m} j \right)^2$$

and

$$\rho_j = -4 + (-2 + (2 + m)(-1)^j) \csc \left( \frac{\pi}{2m} j \right)^2.$$

We will now determine the amount of eigenvalues in the saturated cycle with the  $\lambda_j$ 's,  $\mu_j$ 's, and  $\rho_j$ 's.

Assume  $j$  is even and not 0. Then

$$\lambda = m \csc \left( \frac{\pi j}{2m} \right)^2$$

and

$$\mu = m \csc \left( \frac{\pi j}{2m} \right)^2$$

and

$$\rho = -4 + m \csc \left( \frac{\pi j}{2m} \right)^2.$$

Now that we have expressions for the eigenvalues of  $A$ ,  $B$ ,  $C$ , we will determine the sign of the eigenvalues of the larger matrix  $H$ . Equation (3) gives the expression of these eigenvalues. Note that it contains a plus-or-minus sign. Notice that for the positive case of (3), the output of the square root will always be positive. When we

add  $\rho$  and  $\lambda$ , we get

$$-4 + 2m \csc \left( \frac{\pi j}{2m} \right)^2.$$

Observe that the cosecant squared term will have a minimum value of 1. Since  $m > 1$ , this expression must be 0 or greater. Therefore, when  $j$  is even, and we are concerned with the positive side case of (3), we will only get positive eigenvalues from (3).

Now to deal with the negative case of (3), we will show that it less than zero. Or in other words,

$$\begin{aligned} \frac{\rho}{2} + \frac{\lambda}{2} - \sqrt{\frac{(\rho - \lambda)^2}{4} + \mu^2} &< 0 \\ \frac{\rho}{2} + \frac{\lambda}{2} &< \sqrt{\frac{(\rho - \lambda)^2}{4} + \mu^2} \\ \frac{\rho^2 + 2\rho\lambda + \lambda^2}{4} &< \frac{\rho^2 - 2\rho\lambda + \lambda^2}{4} + \frac{4\mu^2}{4} \\ \rho\lambda &< \mu^2. \end{aligned}$$

Using the definitions of  $\lambda$ ,  $\mu$ , and  $\rho$  above and letting  $a = \csc \left( \frac{\pi j}{2m} \right)$ , notice that

$$\rho\lambda = -4ma^2 + m^2a^2 < m^2a^2 = \mu^2.$$

So all the eigenvalues that are produced under those conditions will be negative. This corresponds to the number of negative eigenvalues of the cycle or  $q$  in the above theorem.

When  $j$  is zero, the summations above will evaluate to a positive number since  $\ell$  will always be positive.

Now assume  $j$  is odd. Then

$$\lambda_j = -m \csc \left( \frac{\pi}{2m} j \right)^2$$

and

$$\mu_j = (-2 - m) \csc\left(\frac{\pi}{2m}j\right)^2$$

and

$$\rho_j = -4 + (-4 - m) \csc\left(\frac{\pi}{2m}j\right)^2.$$

So then

$$\begin{aligned} & \frac{\rho_j}{2} + \frac{\lambda_j}{2} \pm \sqrt{\frac{(\rho_j - \lambda_j)^2}{4} + \mu_j^2} \\ &= \frac{1}{2} \left( -4 + (-4 - m) \csc\left(\frac{\pi}{2m}j\right)^2 - m \csc\left(\frac{\pi}{2m}j\right)^2 \right) \\ & \pm \sqrt{\frac{1}{4} \left( -4 + (-4 - m) \csc\left(\frac{\pi}{2m}j\right)^2 + m \csc\left(\frac{\pi}{2m}j\right)^2 \right)^2 + \left( (-2 - m) \csc\left(\frac{\pi}{2m}j\right)^2 \right)^2} \\ &= -2 - (2 + m) \csc\left(\frac{\pi}{2m}j\right)^2 \pm \sqrt{\frac{1}{4} \left( -4 + -4 \csc\left(\frac{\pi}{2m}j\right)^2 \right)^2 + (2 + m)^2 \csc\left(\frac{\pi}{2m}j\right)^4} \\ &= -2 - (2 + m) \csc\left(\frac{\pi}{2m}j\right)^2 \pm \sqrt{4 + 8 \csc\left(\frac{\pi}{2m}j\right)^2 + (m^2 + 4m + 8) \csc\left(\frac{\pi}{2m}j\right)^4}. \end{aligned}$$

Essentially, this equation will give pairs of eigenvalues for the saturated graph. Notice that for the negative case, the square root function is defined to give positive values,  $m$  is positive, and the cosecant squared term will also be positive, so the above expression must be negative no matter which value of  $j$  we choose.

For the positive case, it's a bit more uncertain, so we need to set the equation to zero and find where the roots are so we can see which values of  $j$  produce positive or negative eigenvalues. We will be using the continuity of the sine function and the  $1/x^2$  function in the range  $(0, p)$ . Setting the equation to 0 and simplifying gives

$$\frac{1}{\sin\left(\frac{\pi}{2m}j\right)^2} = m$$

or

$$\frac{1}{\sin\left(\frac{\pi}{2m}j\right)^2} = 0.$$



The second equation is impossible, so we will proceed with solving for  $j$  in the first equation. This gives the roots

$$\sin^{-1}\left(\frac{1}{\sqrt{m}}\right) \frac{2m}{\pi}$$

for a given  $m$ . The inverse sine can output multiple values. We are only concerned with the range from 0 to  $p$ , though. When we apply this restriction, this expression will give two roots in the range from 0 to  $p$ .

Since a cycle needs at least 3 vertices,  $m$  must be greater than 1. When we substitute  $m$  for  $j$  in the equation above, we get  $-4 - m + \sqrt{m^2 + 4m + 20}$ . By inspection, we can see that  $m$  will always be between the two roots. We will now show that this resulting expression is always negative. We need to show  $0 > -4 - m + \sqrt{m^2 + 4m + 20}$ . This is equivalent to showing

$$m^2 + 8m + 16 > m^2 + 4m + 20.$$

Since  $m > 1$ , this expression is true. Therefore, by continuity we'll have that all the eigenvalues produced between the two roots will be negative and the eigenvalues produced above and below the roots, but within the range  $(0, p)$  will be positive.

Now note that if all the eigenvalues were negative in the case that  $j$  is odd, the number of those negative eigenvalues would correspond with the  $\ell$  term in the above theorem. However as shown above, there are a few eigenvalues that are positive in this case. So let  $r$  be the lower root. When we apply the function

$$2 \left\lfloor \frac{\lfloor r \rfloor + 1}{2} \right\rfloor$$

this will give us the number of positive eigenvalues that we need to subtract off to get the lower bound,  $\ell + q - \beta$ , of the theorem. Overall in the case when the cycle is

saturated in the unicyclic graph, we will have

$$i_-(\Delta) = \ell + q - \beta.$$

## 5.2 Generalizing to unsaturated graphs

Now we need to consider what happens when each vertex of the cycle part of the graph has either 0 or 1 pendants. In each possible graph, the respective distance squared matrix is a principal submatrix of the distance squared matrix of the saturated graph. By interlacing, we can place a lower bound on the negative eigenvalues of each possible principal submatrix that is created. Let

$$\lambda_1 \leq \dots \leq \lambda_k \leq \lambda_{\ell} \leq \dots \leq \lambda_n$$

be the eigenvalues of the distance squared matrix of the saturated graph where  $\lambda_1, \dots, \lambda_k$  are the negative eigenvalues and the rest are positive. When one pendant is removed, interlacing dictates that the eigenvalues of the resulting matrix must occur between each consecutive pair of eigenvalues of the original matrix. Thus, the amount of resulting negative eigenvalues must be at least  $k - 1$ . This corresponds with Theorem 5.1 which says that  $i_-(\Delta) \geq \ell + q - \beta$ .

When we remove another pendant, then the range for which the resulting eigenvalues could appear increases by the interlacing theorem. So there will be an eigenvalue between  $\lambda_1$  and  $\lambda_3$  and another between  $\lambda_2$  and  $\lambda_4$  and so on. Thus, we will only know for certain that  $k - 2$  eigenvalues are negative.

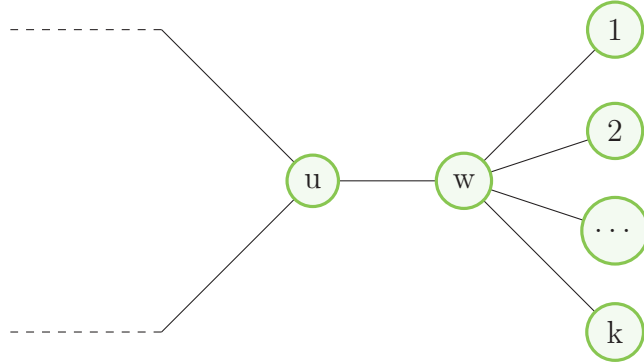
As we remove more pendants, the number of negative eigenvalues that we know must be present from the resulting distance squared matrix decreases by one with each leaf removed since the range between the eigenvalues with interlacing increases as rows and columns are removed from the distances squared matrix. This corre-

sponds to the lower bound of Theorem 5.1,  $i_-(\Delta) \geq \ell + q - \beta$ .

The result from Theorem 4.5 is what we arrive at when we remove pendants until one remains. Luckily, Theorem 4.5 gives an equality for this situation. When we add pendants on from here by interlacing, we'll know that the negative eigenvalues from the cycle plus the negative eigenvalue from the pendant will remain negative, but we won't know the signs of the eigenvalues between the border from negative to positive eigenvalues. However, the signs of the unknown eigenvalues will correlate with the number of pendants added on. Thus, we'll get the upper bound of Theorem 5.1,  $i_-(\Delta) \leq \ell + q$ .

### 5.3 Inductive step

Consider a diametrical path in  $U$ . There exists a vertex  $w$  such that  $w$  has exactly one non-leaf neighbor  $u$ .



Let  $w$  be adjacent to  $k$  leaves, and label leaves  $1, \dots, k$ ,  $w$  is  $k+1$ , and  $u = k+2$ .

**Case 1:** Suppose  $k \geq 2$ . Then the distance squared matrix is

$$\Delta = \begin{bmatrix} 4J_k - 4I_k & B \\ B^T & \Delta_{k+1} \end{bmatrix},$$

where  $J_n$  is the  $n \times n$  matrix of ones,  $B$  is a matrix which has the distances from the leaves  $1, \dots, k$  to the rest of the graph, and  $\Delta_n$  is the distance squared

matrix for  $U \setminus \{1, \dots, n-1\}$ . Using corresponding row and column operations,  $\Delta$  can be written as

$$\Delta = \begin{bmatrix} -4I_{k-1} - 4J_{k-1} & 0 \\ 0 & \frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^T + \Delta_k \end{bmatrix}.$$

Notice that  $-4I_{k-1} - 4J_{k-1}$  is negative definite, so it will have  $k-1$  negative eigenvalues. Let  $K = -4I_{k-1} - 4J_{k-1} \frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^T + \Delta_k = C$  and notice  $C(1) = \Delta_{k+1}$ . Notice that  $U \setminus \{1, \dots, k\}$  is a tree with  $\ell - (k-1)$  leaves and at least 3 vertices. By the inductive hypothesis,

$$\ell + q - \beta - (k-1) \leq i_-(\Delta_{k+1}) \leq \ell + q + 1 - (k-1).$$

By interlacing,  $i_-(C) \geq \ell + q - \beta - (k-1)$ . Since  $C = \frac{4(k-1)}{k} \mathbf{e}_k \mathbf{e}_k^T + \Delta_k$  and  $\frac{4(k-1)}{k} > 0$ , we have

$$\begin{aligned} i_-(C) &\leq i_- \left( \left( \frac{4(k-1)}{k} \right) \mathbf{e}_k \mathbf{e}_k^T \right) + i_-(\Delta_k) \\ &\leq 0 + \ell + q - (k-1) \\ &= \ell + q + 1 - (k-1). \end{aligned}$$

Notice that  $i_-(\Delta) = i_-(K) + i_-(C)$  and

$$\begin{aligned} \ell + q - \beta - (k-1) &\leq i_-(C) \leq \ell + q + 1 - (k-1) \\ i_-(K) + \ell + q - \beta - (k-1) &\leq i_-(K) + i_-(C) \leq i_-(K) + \ell + q + 1 - (k-1) \\ (k-1) + \ell + q - \beta - (k-1) &\leq i_-(\Delta) \leq (k-1) + \ell + q + 1 - (k-1) \\ \ell + q - \beta &\leq i_-(\Delta) \leq \ell + q + 1. \end{aligned}$$

**Case 2:** Suppose  $k = 1$ . Let  $\Delta_2 = \Delta(1)$ .

Suppose  $w$  is the only degree 2 vertex in the graph besides the degree 2 vertices of the cycle. By our inductive hypothesis,  $\ell + q - \beta \leq i_-(\Delta_2) \leq \ell + q$ . By interlacing,  $\ell + q - \beta \leq i_-(\Delta) \leq \ell + q + 1$ .

Now suppose the another degree 2 vertex  $y$  exists in the graph which is not part of the cycle and not  $w$ . Let  $x$  be the vertex before  $y$  and  $z$  be the vertex after  $y$ . Then by Lemma 2.3, the columns of  $\Delta$  corresponding  $x, y, z$  with weights 1,  $-2$ , 1 form the all two's vector. Thus the column corresponding to  $v$  is a linear combination of the columns corresponding to  $x, y, z, u, w$ . Thus  $\text{rank}(\Delta) = \text{rank}(\Delta_2)$  and  $\ell + q - \beta \leq i_-(\Delta) \leq \ell + q$ .

## 6 Conclusion and Further Research

By the end of the derivations, we were able to get a bound on the number of negative eigenvalues of the distance squared matrix of a special type of unicyclic graph. There are three main avenues of further research that could make the result more general. One of the most obvious ones is allowing the cycle length to be odd in a unicyclic graph. From my research, the results look promising that the bound we derived still holds in this case. Here is an example theorem for a unicyclic graph which has an internal cycle length of 3.

**Theorem 6.1.** *Let  $U$  be a graph on  $n > 2$  vertices which has a cycle of 3 vertices and a tree connected to one of the vertices of the cycle. Let  $\Delta$  be the distance squared matrix of  $U$ . Then*

$$i_-(\Delta) = \ell + 2,$$

where  $\ell$  is the number of leaves of  $U$ .

*Proof.* Use induction on  $n$ . For  $n = 3$ , we know from Corollary 3.3 that there will

be 2 negative eigenvalues of  $\Delta$  which satisfies the conclusion of the theorem.

When  $n = 4$ , we have a cycle of 3 vertices, one of which is connected to exactly one other vertex not contained in the cycle. The distance squared matrix of this graph is then

$$\Delta = \begin{bmatrix} 0 & 1 & 4 & 4 \\ 1 & 0 & 1 & 1 \\ 4 & 1 & 0 & 1 \\ 4 & 1 & 1 & 0 \end{bmatrix},$$

resulting in  $i_-(\Delta) = 3 = \ell + 2$ . We now look at unicyclic graphs of  $n > 4$  vertices.

Let  $U$  be a unicyclic graph on  $n > 4$  and assume the conclusion is true for all trees on fewer than  $n$  vertices (but at least 3 vertices). If  $\text{diam}(T) = 2$  (there isn't a case where  $\text{diam}(T) = 1$ ), then

$$\Delta = \begin{bmatrix} 4J - 4I & \mathbf{1} & \mathbf{41} & \mathbf{41} \\ \mathbf{1}^T & 0 & 1 & 1 \\ \mathbf{4}^T & 1 & 0 & 1 \\ \mathbf{4}^T & 1 & 1 & 0 \end{bmatrix},$$

where  $4J - 4I$  is  $(n - 3) \times (n - 3)$ . We will have that  $i_-(4J - 4I) = n - 4$  (-4 with a multiplicity of  $n - 4$ ) and  $i_+(4J - 4I) = 1$  ( $4(n - 2)$ ).  $\Delta$  is equivalent (performing similar row and column operations) to

$$\begin{bmatrix} 4J - 4I & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & -\frac{n-3}{4(n-4)} & 1 & 1 \\ \mathbf{0}^T & 1 & -8 & -7 \\ \mathbf{0}^T & 1 & -7 & -8 \end{bmatrix}.$$

Continuing to perform similar row and column operations, we can diagonalize the upper left  $3 \times 3$  matrix, giving us

$$\begin{bmatrix} 4J - 4I & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & -\frac{7n - 13}{60(n - 4)} & 0 & 0 \\ \mathbf{0}^T & 0 & -15/8 & 0 \\ \mathbf{0}^T & 0 & 0 & -8 \end{bmatrix}.$$

As  $n > 4$ , the lower right  $3 \times 3$  matrix only has negative eigenvalues, so we have that  $i_-(\Delta) = 3 + (n - 4) = n - 1 = \ell + 2$  and  $i_0(\Delta) = 0$ .

Thus from here we assume  $\text{diam}(U) \geq 3$ . Consider a diametrical path in  $U$ . There exists a vertex  $w$  such that  $w$  has exactly one non-leaf neighbor  $u$ . Let  $w$  be adjacent to  $k$  leaves, and label leaves  $1, \dots, k$ ,  $w$  is  $k + 1$ , and  $u$  is  $k + 2$ .

**Case 1:** Assume  $k \geq 2$ . Looking at the distance squared matrix of  $U$ , we see that the columns in the lower left  $(n - k) \times k$  submatrix are all identical, so using row and column  $k$ , we can zero out the top right and lower left corners (like in section 1). Continuing performing similar row and column operations, we see that  $\Delta$  is equivalent to

$$A = \begin{bmatrix} -4I_{k-1} - 4J_{k-1} & 0 \\ 0 & (4 - 4/k) e_k e_k^T + \Delta_k \end{bmatrix},$$

where  $\Delta_k$  is the square distance matrix for  $U \setminus \{1, \dots, k - 1\}$ . Notice that  $-4I_{k-1} - 4J_{k-1}$  is negative definite and so has  $k - 1$  negative eigenvalues. Let  $(4 - 4/k) e_k e_k^T + \Delta_k = B$  and notice  $B(1) = \Delta_{k+1}$  where  $\Delta_{k+1}$  is the distance squared matrix for  $U \setminus \{1, \dots, k\}$ . Notice that  $U \setminus \{1, \dots, k\}$  is a unicyclic graph with  $\ell - (k - 1)$  leaves

and at least 4 vertices. By our inductive hypothesis, we have

$$i_-(\Delta_{k+1}) = \ell - (k - 1) + 2.$$

By interlacing,

$$i_-(B) \geq \ell - (k - 1) + 2.$$

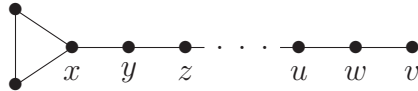
Since  $B = \left(4 - \frac{4}{k}\right) e_k e_k^T + \Delta_k$  and  $4 - \frac{4}{k} > 0$ , we have

$$\begin{aligned} i_-(B) &\leq i_-\left(\left(4 - \frac{4}{k}\right) e_k e_k^T\right) + i_-(\Delta_k) \\ &= 0 + \ell - (k - 1) + 2 \\ &= \ell - (k - 1) + 2. \end{aligned}$$

(We used the inductive hypothesis on  $U \setminus \{1, \dots, k - 1\}$  to find  $i_-(\Delta_k)$ .) Thus  $i_-(B) = \ell - (k - 1) + 2$ . Furthermore,

$$\begin{aligned} i_-(A) &= i_-(-4I_{k-1} - 4J_{k-1}) + i_-(B) \\ &= k - 1 + \ell - (k - 1) + 2 \\ &= \ell + 2. \end{aligned}$$

**Case 2:** Assume  $k = 1$ . Because  $\text{diam}(U) \geq 3$ , we know that there exists some vertex  $y$  that is adjacent to a vertex in the cycle (call this vertex  $x$ ) and has at least one other neighbor  $z$ .



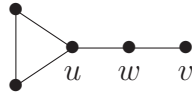
We again consider two distinct cases.

**Case 2a:** Suppose  $x \neq u$ . Then  $\text{diam}(U) \geq 4$ . We let  $\Delta_2 = \Delta(1)$ . Now using our inductive hypothesis, we have  $i_-(\Delta_2) = \ell + 2$ . So, by interlacing, we get  $i_-(\Delta) \geq$



$\ell + 2$ . Then, once again making use of Lemma 2.1, we see that the columns of  $\Delta$  corresponding to  $x, y, z$  with weights  $1, -2, 1$  form the all 2s vector. Thus  $\text{rank}\Delta = \text{rank}\Delta_2$  and, therefore,  $i_-(\Delta) = \ell + 2$ .

**Case 2b:** Suppose  $\text{diam}(U) = 3$ , with  $u = x$  a part of the cycle,  $w$  its neighbor, and  $v$  the only leaf adjacent to  $w$ .



By direct computation, we have that  $i_-(\Delta) = 3 = \ell + 2$  as desired.

□

Note that unicyclic graphs with an internal cycle length of 3 or 4 often exhibit special behavior, so we were able to get equality on the number of negative eigenvalues above. However, when the internal cycle length is at least 5, it is more complicated. It should be possible to get a bound though.

Another addition that could make the result more general is allowing multiple trees to be attached to one vertex of the cycle. This should also be possible to prove, but the bound may become wider.

Finally, throughout the proof we had to make the bound relatively wide to account for many cases. There may be techniques that could tighten the bound we determined.

## References

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