

UNICYCLIC GRAPHS AND THE INERTIA OF THE SQUARED DISTANCE MATRIX*

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Abstract. A result of Bapat and Sivasubramanian gives the inertia of the squared distance matrix of a tree. We develop general tools on how pendant vertices and vertices of degree 2 affect the inertia of the squared distance matrix and use these to give an alternative proof of this result. We further use these tools to extend this result to certain families of unicyclic graphs, and we explore how far these results can be extended.

Key words. Squared distance matrix, Inertia, Unicyclic graphs.

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1. Introduction. In spectral graph theory, we study graphs using the spectra of various matrices associated with the graph. Many matrices capture various graph properties, such as the adjacency matrix and the combinatorial Laplacian, which are the most well known and well studied. A matrix that has not received as much attention is the squared distance matrix Δ . For a graph on n vertices, Δ is the $n \times n$ matrix whose entry Δ_{ij} is the square of the distance from vertex i to vertex j in the graph.

The squared distance matrix was studied by Bapat and Sivasubramanian [2] in 2013, where the determinant of the squared distance matrix of a tree was found. The authors later proved a remarkable connection between a tree and the inertia of its squared distance matrix in [3], and Bapat found a formula for the determinant of Δ , as well as a formula for the inverse Δ^{-1} under certain conditions [1]. Mahato and Kannan [7] then extended these results to trees with matrix weights. Recently, Das and Mohanty [5] determined the inertia and energy of the squared distance matrix of a complete multipartite graph.

We will be building upon results from Bapat and Sivasubramanian [3] on the inertia of the squared distance matrix. Recall that the *inertia* of a Hermitian matrix M is defined to be the triple:

$$(i_{+}(M), i_{-}(M), i_{0}(M)),$$

where i_+ , i_- , and i_0 are defined, respectively, to be the number (counting multiplicity) of positive eigenvalues, negative eigenvalues, and the multiplicity of 0 as an eigenvalue of M. In [3], we find the following theorem.

THEOREM 1.1 ([3, Theorem 20]). Let T be a tree with squared distance matrix Δ , let ℓ be the number of vertices of degree 1 in T, and let t be the number of vertices of degree 2 in T. Then

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

and

$$i_{-}(\Delta) = \ell.$$

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Throughout, we will refer to vertices of degree 1 as *leaves* or *pendant vertices* of the graph. While many theorems in spectral graph theory bound some graph parameter in terms of eigenvalues, Theorem 1.1 is striking in that only the inertia of a matrix is needed to get an exact enumeration of certain kinds of vertices in the tree.

The purpose of this paper is to extend Theorem 1.1 to families of graphs other than trees. A natural first step is to consider *unicyclic graphs*, that is, graphs with only one cycle. We will see below that, while there is no single, unifying theorem characterizing the inertia of all unicyclic graphs, there are various families of unicyclic graphs where results analogous to Theorem 1.1 hold.

The remainder of the paper is organized as follows. We begin Section 2 with needed matrix theoretic tools and preliminaries. In Section 3, we prove some technical lemmas about degree 1 and 2 vertices that apply to any graph. We then use these tools in Section 4 to give an alternative, simpler proof to Theorem 1.1. Then, we begin our investigation of unicyclic graphs in Section 5 by giving the complete spectrum (and hence the inertia) of the squared distance matrix of any cycle. Section 6 contains the main result of the paper, which is that if U is a unicyclic graph whose cycle is of even length 2q and whose cycle contains only one vertex of degree three in U, and if Δ is the squared distance matrix of U, then $i_{-}(\Delta) = \ell + q$ and $i_{0}(\Delta) = t$. This is analogous to Theorem 1.1. In Section 7, we study several other families of unicyclic graphs that show that this result cannot be extended to all unicyclic graphs. We end in Section 8 with a discussion of open questions.

2. Preliminaries. Let G be a connected graph with vertex set $V(G) = \{1, ..., n\}$ and edge set E(G). We define the distance d_{ij} between vertices $i, j \in V(G)$, as the minimum number of edges in a path from i to j, and set $d_{ii} = 0$ for i = 1, ..., n. We define the distance matrix D(G) or D of the graph as the matrix whose (i, j)-entry is equal to d_{ij} . We define the squared distance matrix, Δ , as the Hadamard product $D \circ D$. On occasion, we will also use the notation A(i) which refers to the matrix A with the ith column and ith row deleted. Let $\mathbf{1}$ denote the vector whose entries are all equal to 1, and J_n will denote the $n \times n$ matrix whose entries are all 1.

We list here some tools from matrix theory that we will use. We begin with the Cauchy interlacing theorem, which we use extensively.

THEOREM 2.1 (Theorem 4.3.28 of [6]). 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 $\lambda_1 \leq \cdots \leq \lambda_n$ and B has eigenvalues $\beta_1 \leq \cdots \leq \beta_m$. Then

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

If m = n - 1,

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

DEFINITION 2.2. 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 of M, respectively.

We will also use the subadditivity property of inertia.

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Theorem 2.3 (Proposition 3.9 of [4]). Let $A, B \in \mathbb{R}^{n \times n}$ be symmetric. Then we have

$$i_{+}(A+B) \le i_{+}(A) + i_{+}(B),$$

and

$$i_{-}(A+B) \le i_{-}(A) + i_{-}(B),$$

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.

THEOREM 2.4 (Theorem 4.5.8 in [6]). Let A be a symmetric $n \times n$ matrix and let S be a nonsingular $n \times n$ matrix. Then $i(A) = i(S^{\top}AS)$.

We remark that A and $S^{\top}AS$ are called *congruent* matrices, so Sylvester's law of inertia states that congruent matrices have the same inertia. We also have the Haynsworth inertia additivity formula.

Theorem 2.5 (Theorem 4.5.P21 in [6]). 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 take the form:

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_{n-1} & a_n \\ a_n & a_1 & \cdots & a_{n-2} & a_{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_2 & a_3 & \cdots & a_n & a_1 \end{bmatrix}.$$

To abbreviate, we will also express circulant matrices as:

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

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

LEMMA 2.6 (Theorem 2.2.P10 of [6]). Let A be the circulant matrix above. The eigenvectors take the form:

$$\mathbf{v}_j = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & \omega^j & \omega^{2j} & \cdots & \omega^{(n-1)j} \end{bmatrix}^\top \qquad j = 1, 2, \dots, n,$$

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 take the form:

$$\lambda_{j} = a_{1} + a_{2}\omega^{j} + \dots + a_{n}\omega^{(n-1)j}$$
 $j = 1, 2, \dots, n.$

3. Degree 1 and 2 vertices. In this section, we will prove some preliminary results that will apply to general graphs that have multiple degree 1 vertices that are all neighbors, and degree 2 vertices that are part of a 'branch' of the graph.

Let G be any graph obtained by attaching $k \geq 2$ pendant vertices to a vertex w of some graph G' and let Δ be the squared distance matrix of G. We will order the vertices so that vertices 1, ..., k are the pendant vertices. Denote by Δ_k the squared distance matrix of $G \setminus \{1, ..., k\} = G'$ and Δ_{k-1} the squared distance matrix of $G \setminus \{1, ..., k-1\}$.

Proposition 3.1. In the above notation, we have

$$i_{-}(\Delta) = k - 1 + i_{-} \left(\Delta_{k-1} + \left(4 - \frac{4}{k} \right) \mathbf{e}_{k} \mathbf{e}_{k}^{\mathsf{T}} \right),$$

where \mathbf{e}_k denotes the indicator vector for the kth vertex.

Proof. We have

$$\Delta = \begin{bmatrix} 4J_k - 4I_k & X^\top \\ & & \\ X & \Delta_k \end{bmatrix},$$

where Δ_k is the squared distance matrix for $G\setminus\{1,...,k\}$ and X is a $(n-k)\times k$ matrix with all identical columns.

We will proceed by performing row operations and the corresponding column operations to produce a matrix that is congruent to Δ (and hence has the same inertia) whose inertia will be easier to see. Note that performing a row operation and its corresponding column operation corresponds to multiplying the matrix by an elementary matrix on the left and its transpose on the right and is thus a congruence.

First, we subtract row k and column k from each of the first k-1 rows and columns. This will zero out the first k-1 rows of X^{\top} and the first k-1 columns of X and will leave us with $-4I_{k-1}-4J_{k-1}$ in the upper left corner. We then subtract $\frac{1}{k}$ times each of the first k-1 rows from row k and repeat the process for the columns. We then find that Δ is congruent to

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

with Δ_{k-1} being the squared distance matrix for $G\setminus\{1,...,k-1\}$. Notice that $-4I_{k-1}-4J_{k-1}$ is negative definite and so has k-1 negative eigenvalues. Then by Sylvester's law of inertia (Thereom 2.4), $i(\Delta) = i(A)$ and the result follows.

COROLLARY 3.2. In the above setting, we have that either $i_{-}(\Delta) = k - 1 + i_{-}(\Delta_k)$ or $i_{-}(\Delta) = k + i_{-}(\Delta_k)$.

Proof. Since Δ_k results from deleting a row and column of $\Delta_{k-1} + (4 - \frac{4}{k})\mathbf{e}_k\mathbf{e}_k^{\mathsf{T}}$, then the result follows from Proposition 3.1 and interlacing.

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In summary, adding $k \geq 2$ pendant vertices to a single vertex will increase the number of negative eigenvalues of the squared distance matrix by at least k-1, and possibly by k. Examples of both can occur, as we will see, and much of the work in what follows will be to determine if the increase is by k-1 or k in specific kinds of graphs.

LEMMA 3.3. For a graph G with squared distance matrix Δ , let v be a vertex of degree 2 such that its removal disconnects the graph. Let u and w be the neighbors of v, and let x be a vector in \mathbb{R}^n such that

$$x_i = \begin{cases} 1 & \textit{if i corresponds to vertex } u, w \\ -2 & \textit{if i corresponds to vertex } v \\ 0 & \textit{otherwise.} \end{cases}$$

Then $\Delta \mathbf{x} = 2 \cdot \mathbf{1}$.

Proof. Let G be a graph with squared distance matrix Δ . 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 Δ will take the form $[\cdots j^2 (j+1)^2 (j+2)^2 \cdots]$ 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 (note that j itself could be negative). The vector \mathbf{x} will take the form $\begin{bmatrix} \mathbf{0} & 1 & -2 & 1 & \mathbf{0} \end{bmatrix}^{\mathsf{T}}$ 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 Δ with \mathbf{x} gives

$$\begin{bmatrix} \cdots & j^2 & (j+1)^2 & (j+2)^2 & \cdots \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \\ -2 \\ 1 \\ \mathbf{0} \end{bmatrix} = j^2 - 2(j+1)^2 + (j+2)^2$$
$$= j^2 - 2j^2 - 4j - 2 + j^2 + 4j + 4$$
$$= 2$$

This completes the proof of the lemma.

LEMMA 3.4. 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 3.5. If G has $t \geq 2$ vertices of degree 2 whose removal disconnects G, then $i_0(\Delta) \geq t - 1$.

Proof. Let $\{\mathbf{x}_1,...,\mathbf{x}_t\}$ be as in Lemma 3.4. Note that $\{\mathbf{x}_1 - \mathbf{x}_2, \mathbf{x}_1 - \mathbf{x}_3,...,\mathbf{x}_1 - \mathbf{x}_t\}$ is a linearly independent set from the lemma above. Also $\Delta(\mathbf{x}_1 - \mathbf{x}_2) = \Delta\mathbf{x}_1 - \Delta\mathbf{x}_2 = 0$. Thus, each vector is in the null space of Δ and so $i_0(\Delta) \geq t - 1$.

4. Trees. In this section, we will apply the results of the previous section to determine the inertia of the squared distance matrix of a tree. Let T be a tree and Δ be its squared distance matrix.

The following is the main result of this section.

THEOREM 4.1. Let T be a tree of n > 2 vertices and Δ be the squared distance matrix of T. Then

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

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

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

where ℓ is the number of leaves of T.

Proof. We proceed by induction on the number of vertices n. For n=3, we have $T\cong P_3$, 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 diam(T) = 2, then T is a star and

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

where 4J - 4I is $(n-1) \times (n-1)$. We have

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

and

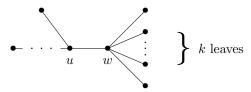
$$i_{+}(4J-4I)=1$$
 (where the eigenvalue equals $4(n-2)$).

Performing similar row and column operations, we subtract from the first row $\frac{1}{4(n-2)}$ times each of the remaining rows of Δ and from the first column $\frac{1}{4(n-2)}$ times each of the remaining columns of Δ . Thus, Δ is congruent to

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

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

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, ..., k. Now let w = k + 1 and u = k + 2.

Case 1: Suppose $k \geq 2$. By Proposition 3.1, we have that $i_{-}(\Delta) = k - 1 + i_{-}(\Delta_{k-1} + (4 - \frac{4}{k}) \mathbf{e}_k \mathbf{e}_k^{\top})$. Let $F = \Delta_{k-1} + (4 - \frac{4}{k}) \mathbf{e}_k \mathbf{e}_k^{\top}$ and notice $F(1) = \Delta_k$. Notice also that Δ_k is the squared distance matrix

for $T\setminus\{1,...,k\}$, which is a tree with $\ell-(k-1)$ leaves and at least 3 vertices. Using our inductive hypothesis on $T \setminus \{1, ..., k\}$ to find $i_{-}(\Delta_k)$, we see that

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

It follows from the Cauchy interlacing theorem that

$$i_{-}(F) \ge \ell - (k-1).$$

Since $F = \Delta_{k-1} + (4 - \frac{4}{k})\mathbf{e}_k\mathbf{e}_k^{\mathsf{T}}$ and $4 - \frac{4}{k} > 0$, the subadditivity of inertia gives us

$$i_{-}(F) \leq i_{-}\left(\left(4 - \frac{4}{k}\right) \mathbf{e}_{k} \mathbf{e}_{k}^{\top}\right) + i_{-}(\Delta_{k-1})$$
$$= 0 + \ell - (k-1)$$
$$= \ell - (k-1),$$

and we conclude that $i_{-}(F) = \ell - (k-1)$. Thus,

$$i_{-}(\Delta) = k - 1 + i_{-}(F)$$

= $k - 1 + \ell - (k - 1)$
= ℓ

Case 2: Suppose k=1. Label the leaf adjacent to w as v. Let $\Delta'=\Delta(1)$. By the inductive hypothesis, $i_{-}(\Delta') = \ell$. 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

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 diam(T)= 4. In any case, using Lemma 3.5, the columns of Δ 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, $rank(\Delta) = rank(\Delta')$ and $i_{-}(\Delta) \leq \ell$.

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

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

$$i_{+}(\Delta') + i_{-}(\Delta') = n - 1,$$

and

$$n > i_{+}(\Delta) + i_{-}(\Delta) > i_{+}(\Delta') + i_{-}(\Delta') + 1 = n.$$

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

If $t \ge 2$, then by Lemma 3.5 we have $i_0(\Delta) \ge t - 1$ and by the inductive hypothesis $i_0(\Delta') = t - 1$. So,

$$n-1 = i_{+}(\Delta') + i_{-}(\Delta') + i_{0}(\Delta'),$$

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and

$$n \ge i_+(\Delta) + i_-(\Delta) + i_0(\Delta) \ge i_+(\Delta') + i_-(\Delta') + 1 + i_0(\Delta') = n.$$

Thus, $i_0(\Delta) = i_0(\Delta') = t - 1$, as desired.

Case 2: Suppose every vertex of T is adjacent to at most one leaf. Since $\operatorname{diam}(T) \geq 3$, 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 one and keeps the number of leaves the same. Note that we have $\operatorname{rank}(\Delta) = \operatorname{rank}(\Delta')$ by arguments similar to the above when we proved $i_{-}(\Delta) = \ell$ in the k = 1 case. By interlacing, $i_{+}(\Delta) \geq i_{+}(\Delta')$ and $i_{-}(\Delta) \geq i_{-}(\Delta')$. Since $i_{+}(\Delta) + i_{-}(\Delta) = \operatorname{rank}(\Delta) = \operatorname{rank}(\Delta') = i_{+}(\Delta') + i_{-}(\Delta')$, we have $i_{+}(\Delta) = i_{+}(\Delta')$ and $i_{-}(\Delta) = i_{-}(\Delta')$. Thus, $i_{0}(\Delta) = i_{0}(\Delta') + 1 = t - 2 + 1 = t - 1$.

Case 3: Suppose T has a vertex which is adjacent to exactly two leaves. We consider the vertex w with 2 adjacent leaves. Then the squared distance matrix has the form:

$$\Delta = \begin{bmatrix} 0 & 4 & \mathbf{x}^{\top} \\ 4 & 0 & \mathbf{x}^{\top} \\ \mathbf{x} & \mathbf{x} & \Delta_2 \end{bmatrix},$$

where Δ_2 is $(n-2) \times (n-2)$ and **x** is a vector of appropriate size. Notice that if we were to remove both leaves, our squared distance matrix would just be Δ_2 . From above, we know that adding one leaf on to the end of the branch would result in a matrix, call it Δ_1 , of the form:

$$\Delta_1 = egin{bmatrix} 0 & \mathbf{x}^ op \ \mathbf{x} & \Delta_2 \end{bmatrix},$$

that has one more zero eigenvalue than Δ_2 . Thus, the vector \mathbf{x} is in the column space of Δ_2 . So the vector \mathbf{x} can be reduced to the all zeros vector without changing the column space of Δ . Hence, $\operatorname{rank}(\Delta_2) = \operatorname{rank}(\Delta) - 2$, since the upper left 2×2 matrix has a rank of 2. Therefore, adding the two leaves onto our vertex w has no effect on the number of zero eigenvalues of Δ and the proof is complete.

5. Cycles. To understand and explore the class of unicyclic graphs, we will now consider cycle graphs. A *cycle* is a connected graph on three or more vertices in which every vertex has degree 2.

We will obtain formulas for the eigenvalues of the squared distance matrix of cycle graphs treating even and odd length cycles separately. The basic squared distance 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, so the eigenvalues will be in the form of $c_1 + c_2\omega_j + \cdots + c_n\omega_j^{n-1}$.

THEOREM 5.1. Let C be a cycle of length n and λ_i be the jth eigenvalue of C. When n is odd, we have

(5.1)
$$\lambda_{j} = 2\cos(\pi j) \left(\cos\left(\frac{(n-2)\pi}{n}j\right) + 4\cos\left(\frac{(n-4)\pi}{n}j\right) + \cdots + \frac{(n-1)^{2}}{4}\cos\left(\frac{\pi}{n}j\right)\right).$$

When n is even, we have

(5.2)
$$\lambda_j = 2\cos(\pi j) \left(\frac{n^2}{8} + \cos\left(\frac{(n-2)\pi}{n}j\right) + 4\cos\left(\frac{(n-4)\pi}{n}j\right) + \cdots + \frac{(n-1)^2}{4}\cos\left(\frac{\pi}{n}j\right)\right).$$

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

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

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 $\frac{n^2}{8}$ in the large quantity of equation 5.1:

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

COROLLARY 5.2. Let C be a cycle graph of length n > 2 and Δ be its squared distance 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 5.1, j is an integer. However, to better understand the inertia, we will examine the expressions in (5.1) and (5.2) allowing j to be any real number. The zeros for equation (5.1) occur when $j = \frac{k}{2}$ 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 $\frac{n}{2}$. Since the equation is

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continuous, this means that none of the eigenvalues will be zero. The derivative with respect to j of this equation is

$$-2\pi \sin(\pi j) \left(\cos\left(\frac{(n-2)\pi}{n}j\right) + 4\cos\left(\frac{(n-4)\pi}{n}j\right) + \cdots\right) + 2\cos(\pi j) \left(-\frac{(n-2)\pi}{n}\sin\left(\frac{(n-2)\pi}{n}j\right) - \frac{4(n-4)\pi}{n}\sin\left(\frac{(n-4)\pi}{n}j\right) - \cdots\right).$$

We will substitute the zeros we found above into the first half of the expression since the second half is 0 at the values of $j = \frac{k}{2}$. The first part of the expression will alternate between positive and negative, starting with negative when $j = \frac{k}{2}$. The second half of the expression will begin positive since the rightmost term will dominate the others until it hits $\frac{n}{2}$, after which it will be negative.

We will now consider the case when $n \equiv 1 \pmod{4}$. When j = 1, λ_j is between two zeros. Since the derivative is negative at $\frac{1}{2}$ and positive at $\frac{3}{2}$, λ_1 will be negative. The eigenvalues will flip between positive and negative until it gets to the integer after $\frac{n}{2}$. Here, there will be another consecutive positive eigenvalue and then the sign will start alternating again. So there will be $\lceil \frac{n}{2} \rceil$ positive eigenvalues and $\lfloor \frac{n}{2} \rfloor$ negative eigenvalues.

The case when $n \equiv 3 \pmod{4}$ will be very similar, except that there will be two consecutive negative eigenvalues instead of two consecutive positive eigenvalues.

Now for the even case, we use equation (5.2). This equation is similar to equation (5.1) 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 $\frac{n}{2}$ positive and $\frac{n}{2}$ negative eigenvalues.

6. 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 6.1. Given an even cycle with p nodes and squared distance matrix Δ , the inverse of Δ is the circulant matrix:

$$\Delta^{-1} = \frac{1}{4\lambda m} \left(2J + \begin{bmatrix} \boldsymbol{0}^\top & -\lambda & 2\lambda & -\lambda & \boldsymbol{0}^\top \\ & \ddots & \ddots & \ddots & \end{bmatrix} \right),$$

where $m = \frac{n}{2}$, λ is the largest eigenvalue of Δ , and the $\boldsymbol{0}$ vectors in the first row are size $\frac{n}{2} - 1$ and $\frac{n}{2} - 2$, respectively, and each row shifting one to the right, forming a circulant matrix.

Proof. For convenience define

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

We have

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

Because Δ is circulent, the sum of each of the rows is the same, that is, λ . So $2\lambda J = 2\Delta J$. Thus,

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

Lemma 6.2. Let Δ be the squared distance matrix of an even cycle with p nodes and a single pendant extending from the cycle. Let $\tilde{\Delta}$ be obtained by deleting the last row and column of Δ , and let \mathbf{x} be the first p elements of the last row of Δ . Then

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

Proof. Using Lemma 6.1, we have

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

We consider each term individually.

Multiplying \mathbf{x}^{\top} 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:

$$2\sum_{j=1}^{m} j^{2} + (m+1)^{2} - 1 = \frac{m(m+1)(2m+1)}{3} + (m+1)^{2} - 1$$
$$= \frac{2m^{3} + 6m^{2} + 7m}{3},$$

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where $m = \frac{p}{2}$. Hence,

$$2\mathbf{x}^{\top} J\mathbf{x} = 2\left(\frac{2m^3 + 6m^2 + 7m}{3}\right) \mathbf{1}^{\top} \mathbf{x}$$
$$= 2\left(\frac{2m^3 + 6m^2 + 7m}{3}\right)^2.$$

Now we consider the second term. Let B be as defined in Lemma 6.1. Letting j denote the index of the element of the vector \mathbf{x} corresponding to the index of the first nonzero 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:

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

Since the index of the first nonzero 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 -6λ as the m+1 term in our vector. Each of the other entries will be given by:

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

$$= -\lambda j^2 + 2\lambda (j^2 + 2j + 1) - \lambda (j^2 + 4j + 4)$$

$$= -2\lambda.$$

Thus, we have

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

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

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

Now, adding the two terms together gives us

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

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

Unicyclic graphs and the inertia of the squared distance matrix

LEMMA 6.3. Let U be a graph which contains exactly one cycle of length p where p is even and a single pendant connected to one of the vertices. Let Δ be the squared distance matrix of U and $m = \frac{p}{2}$. Then $i(\Delta) = (m, m+1, 0)$.

Proof. The squared distance matrix for U has the form:

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

where $\tilde{\Delta}$ and **x** take the same definitions as in Lemma 6.2. By Theorem 2.5, Corollary 5.2, and Lemma 6.2, we'll have that

$$i(\Delta) = i \begin{pmatrix} \begin{bmatrix} \tilde{\Delta} & \mathbf{x} \\ \mathbf{x}^{\top} & 0 \end{bmatrix} \end{pmatrix}$$

$$= i(\tilde{\Delta}) + i(-\mathbf{x}^{\top} \tilde{\Delta}^{-1} \mathbf{x})$$

$$= (m, m, 0) + (0, 1, 0)$$

$$= (m, m + 1, 0).$$

LEMMA 6.4. 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 degree 3 in U and the rest have degree 2 in U. 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 2. 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 2 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:

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

$$0 & \text{otherwise}$$

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

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

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

$$\mathbf{r}^{\top} \mathbf{a} = (m-z)^2 (-1) + z^2 (m+1) + (z+1)^2 (-m)$$

$$= -(m^2 - 2mz + z^2) + z^2 m + z^2 - (z^2 + 2z + 1) m$$

$$= -m^2 + 2mz - z^2 + z^2 m + z^2 - z^2 m - 2mz - m$$

$$= -m^2 - m$$

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and

$$\mathbf{r}^{\top}\mathbf{b} = \frac{(z+u-1)^2 m(m+1)}{2} + (z+u)^2 (-m(m+1)) + \frac{(z+u+1)^2 m(m+1)}{2}$$

$$= \frac{(z^2+u^2+1+2zu-2z-2u)(m^2+m)}{2} - (z^2+2zu+u^2)(m^2+m)$$

$$+ \frac{(z^2+u^2+1+2zu+2z+2u)(m^2+m)}{2}$$

$$= m^2+m$$

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

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

Theorem 6.5. Let U be a graph on n > 2 vertices which has a cycle of p vertices with a tree connected to one of the vertices of the cycle. Assume p is even. Let Δ be the squared distance matrix on U. Then

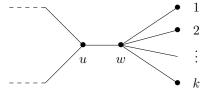
$$i_{-}(\Delta) = \ell + q$$
,

where ℓ is the number of leaves of U and q is the number of negative eigenvalues of the p-cycle. In addition, if U has t vertices of degree 2 whose removal disconnects the graph then

$$i_0(\Delta) = t$$
.

Proof. We will use induction on n. Note that Lemma 6.3 takes care of the case when a single leaf is connected to the cycle. So let U be a unicyclic graph on n vertices with at least two vertices in the tree coming off of one of the vertices in the cycle and assume the conclusion is true for all unicyclic graphs on fewer than n vertices.

As in the proof of Theorem 4.1, 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 $1, \ldots, k$, w is k+1, and u is k+2.

Case 1: Suppose $k \geq 2$. By Proposition 3.1, $i_{-}(\Delta) = k - 1 + i_{-}(\Delta_{k-1} + (4 - \frac{4}{k}) \mathbf{e}_{k} \mathbf{e}_{k}^{\top})$. Let $F = \Delta_{k-1} + (4 - \frac{4}{k}) \mathbf{e}_{k} \mathbf{e}_{k}^{\top}$ and notice $F(1) = \Delta_{k}$. Notice also that Δ_{k} is the squared distance matrix for $U \setminus \{1, \ldots, k\}$, which is a graph with $\ell - (k-1)$ leaves and at least three vertices. By the inductive hypothesis,

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

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

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

$$i_{-}(\Delta) = k - 1 + i_{-}(F)$$

= $(k - 1) + \ell + q - (k - 1)$
= $\ell + q$.

Case 2: Suppose k=1 and w is the only degree 2 vertex in the graph. Let $\Delta' = \Delta(1)$. By our inductive hypothesis, $i_{-}(\Delta') = \ell + q$. 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 6.4 to deduce that the column in Δ corresponding to w is a linear combination of other columns in Δ . Thus, $\operatorname{rank}(\Delta) = \operatorname{rank}(\Delta')$ 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 4.1, we have that $i_{-}(\Delta) = \ell + q$.

We now proceed to prove that $i_0(\Delta) = t$. Note that by Lemmas 3.3, 3.4, and 3.5, we have t-1 linearly independent vectors in the nullspace of Δ , and each of the vectors constructed there are zero on all the vertices of the cycle. Furthermore, from Lemma 6.4, we have another vector in the nullspace of Δ , and the vector constructed in the proof of Lemma 6.4 is linearly independent from these other vectors since it is nonzero on one of the vertices of the cycle. Thus, the nullspace of Δ is at least t dimensional, so $i_0(\Delta) \geq t$.

To show that $i_0(\Delta) \leq t$ we proceed by induction on n. We know the result is true for cycles, and by Lemmas 6.3 and 6.4, we know the result is true for a cycle with a single pendant attached, or a single path of length 2 attached, so suppose that G has more vertices than either of these. Consider the same w as above, adjacent to k leaves. We again consider three cases.

Case 1: Suppose $k \geq 2$. Let U' be the same as U with one of these k leaves deleted and let Δ_U and $\Delta_{U'}$ denote the squared distance matrices on U and U', respectively. Note that deleting a leaf from U does not affect the number of degree 2 vertices in the graph. We have, by interlacing, $i_+(\Delta_U) \geq i_+(\Delta_{U'})$ and from Theorem 4.1 deleting a leaf from U results in $i_-(\Delta_U) = i_-(\Delta_{U'}) + 1$. Thus, $\operatorname{rank}(\Delta_U) = i_+(\Delta_U) + i_-(\Delta_U) = i_+(\Delta_{U'}) + i_-(\Delta_{U'}) + 1$. So the number of zero eigenvalues did not change, and since the number of degree 2 vertices did not change, $i_0(\Delta_U) = t$.

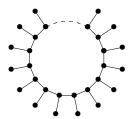
Case 2: Suppose k=1. Deleting the pendant vertex does not change the number of leaves of the graph but decreases the number of degree 2 vertices by 1. Using Lemma 3.5 and the same reasoning in Case 2 of Theorem 4.1, we have $\operatorname{rank}(\Delta_U) = \operatorname{rank}(\Delta_U')$. Because interlacing tells us that $i_+(\Delta_U) \geq i_+(\Delta_U')$ and $i_-(\Delta_U) \geq i_-(\Delta_U')$, we have $i_+(\Delta_U) = i_+(\Delta_U')$ and $i_-(\Delta_U) = i_-(\Delta_U')$. Therefore, $i_0(\Delta_U) \geq i_0(\Delta_U')$. By the inductive hypothesis $i_0(\Delta_U') = t - 1$, so $i_0(\Delta_U) = t$.

Case 3: Suppose k=2. We can call $\Delta_{U''}$ the squared distance matrix for the tree after removing both of its leaves. Then, by similar reasoning to that in Case 3 of Theorem 4.1, we will have $\operatorname{rank}(\Delta_{U''}) = \operatorname{rank}(\Delta_U) - 2$. The squared distance matrix of Δ_U will be identical to that described in Theorem 4.1 except $\Delta_{U''}$ will be different. However, this still leads to the conclusion that adding both of our leaves back onto $\Delta_{U''}$ has no effect on the number of zero eigenvalues of Δ_U , so $i_0(\Delta_U) = t$.

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7. Other families of unicyclic graphs. Theorem 6.5 generalizes Theorem 4.1 from trees to a particular class of unicyclic graphs. It is natural to try to generalize further to the class of all unicyclic graphs. In this section, we will see that the result of Theorem 6.5 does not hold for all unicyclic graphs, but we will see that some information can be given for certain specific families.

7.1. Saturated cycles. Consider the following graph



This graph is a cycle of length p with a pendant extending from each node on the cycle. A squared distance 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 $p \times p$. Here, the first p rows and columns are indexed by the nodes of the main cycle and the last p by the pendant vertices. Since A, B, and C are all $p \times p$ circulant matrices, A, B, and C will all have the same eigenvectors by Lemma 2.6. 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 λ , μ , and ρ are eigenvalues of A, B, and C, respectively, corresponding to the eigenvector \mathbf{x} .

To find the eigenvalues of H, we will assume that an eigenvector of H will take the form $\begin{bmatrix} a\mathbf{x} & b\mathbf{x} \end{bmatrix}^{\top}$. Then an eigenvalue h of H satisfies

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

Thus,

$$\begin{bmatrix} (a\lambda + b\mu)\mathbf{x} \\ (a\mu + b\rho)\mathbf{x} \end{bmatrix} = \begin{bmatrix} (ha)\mathbf{x} \\ (hb)\mathbf{x} \end{bmatrix}.$$

Solving for h gives $h = (a\lambda + b\mu)/a$ and $h = (a\mu + b\rho)/b$. This gives

$$\frac{b}{a} - \frac{a}{b} = \frac{\rho - \lambda}{\mu}.$$

Set b = 1, then solve for a to obtain

$$1 - a^2 = a \left(\frac{\rho - \lambda}{\mu} \right),$$

which yields

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

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

(7.3)
$$h = \frac{\rho}{2} + \frac{\lambda}{2} \pm \sqrt{\frac{(\rho - \lambda)^2}{4} + \mu^2}.$$

So the eigenvalues of H will all correspond to values of the expression above for each combination of λ , μ , ρ corresponding to \mathbf{x} .

Now we need to find expressions for λ , μ , and ρ , which depend on A, B, and C. Since these matrices are circulant, then by Lemma 2.6, the eigenvalues are of the form $c_1 + c_2\omega_j + \cdots + c_p\omega_j^{p-1}$ where c_1, \ldots, 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 $m = \frac{p}{2}$.

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

$$\lambda_j = \omega^j + 4\omega^{2j} + \dots + (m-1)^2 \omega^{(m-1)j} + m^2 \omega^{mj} + (m-1)^2 \omega^{(p-m+1)j} + \dots + 4\omega^{(p-2)j} + \omega^{(p-1)j}$$

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

The first row in B will take the form:

$$\begin{bmatrix} 1 & 4 & 9 & \cdots & m^2 & (m+1)^2 & m^2 & \cdots & 9 & 4 \end{bmatrix}.$$

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

$$\begin{bmatrix} 0 & 9 & 16 & \cdots & (m+1)^2 & (m+2)^2 & (m+1)^2 & \cdots & 16 & 9 \end{bmatrix}$$
.

Again performing similar calculations for each $j \in \{0, ..., p-1\}$, we 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

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

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

$$+ m^{2} \cos(\pi j).$$

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

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

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

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

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

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

Assume j is even and not 0. Then,

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

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

and

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

Now that we have expressions for the eigenvalues of A, B, and C, we will determine the sign of the eigenvalues of the larger matrix H. Equation (7.3) gives the expression for these eigenvalues. Note that it contains a plus-or-minus sign and that for the positive case of (7.3), the output of the square root will always be positive. Adding ρ and λ , 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 nonnegative. Therefore, when j is even, and we are concerned with the positive side case of (7.3), we will only get positive eigenvalues from (7.3).

Now, for the negative case of (7.3), we will show that

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

Manipulating this, we find that

$$\rho\lambda < \mu^2$$
.

Using the definitions of λ , μ , and ρ 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, ℓ will always be positive, so the summations above will evaluate to be positive.

Now assume j is odd. Then

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

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

and

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

So then, once again omitting some calculations,

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

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, 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 $\frac{1}{x^2}$ 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, but we are only concerned with the range from 0 to p. When we apply this restriction, this expression will give two roots in the range from 0 to p.

Since a cycle needs at least three 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 ℓ 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:

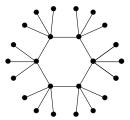
$$\beta = 2 \left| \frac{\lfloor r \rfloor + 1}{2} \right|,\,$$

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

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

7.2. Cycles with a fixed number of pendants per vertex. In this section, we will consider unicyclic graphs consisting of a single even cycle and a fixed number of pendants at least half the length of the cycle coming off of each of its vertices.

Here is an example with a graph that contains a cycle of length six.



THEOREM 7.1. Let U be a unicyclic graph as pictured above with cycle of length 2q where each vertex of the cycle has at least $s \ge q$ pendants attached to it, and ℓ total pendants. Then $i_{-}(\Delta) = \ell$.

Proof. Note that more than one pendant is attached to each vertex of the cycle. A squared distance matrix of this graph can take the form:

$$H = \begin{bmatrix} A & B & X_{13} & X_{14} & \cdots & X_{1,k+1} \\ B & C & X_{23} & X_{24} & \cdots & X_{2,k+1} \\ X_{13} & X_{23} & 4J - 4I & X_{34} & \cdots & X_{3,k+1} \\ X_{14} & X_{24} & X_{34} & 4J - 4I & \cdots & X_{4,k+1} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ X_{1,k+1} & X_{2,k+1} & X_{3,k+1} & X_{4,k+1} & \cdots & 4J - 4I \end{bmatrix},$$

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where A, B, and C have the same definitions as above. Now we will deal with the matrices which take the form X_{ij} . When i=1, X_{ij} is indexed by the connections from the vertices of the cycle and one set of nodes that are connected to a vertex of the cycle except for one node. When i=2, X_{ij} is indexed by the connections from the vertices of a set of p nodes which contains one node from each group of nodes connected to a vertex of the cycle and one set of nodes that are connected to a vertex of the cycle except for one node. The rest of the X_{ij} matrices are of size $(k-1) \times (k-1)$ which contain all the same number and are indexed by groups of nodes (besides one) connected to one vertex of the cycle to other groups of nodes (besides one) connected to another vertex of the cycle.

Using equivalent row and column operations, we can find the following congruent matrix to H.

$$H' = \begin{bmatrix} A & B & 0 & 0 & \cdots & 0 \\ B & C' & 0 & 0 & \cdots & 0 \\ 0 & 0 & -4I - 4J & 0 & \cdots & 0 \\ 0 & 0 & 0 & -4I - 4J & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -4I - 4J \end{bmatrix},$$

where $C' = C + (4 - \frac{4}{k})I$.

Since -4I-4J is negative definite, all of its eigenvalues will be negative. The -4I-4J groups will correspond to the all the pendants on the cycle except for one set. The proof in similar to what is in section 7.1, except that C has been slightly modified. The definitions of λ and ρ will remain the same as the above sections. With C', though, we'll have

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

when j is even and not 0 and

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

when j is odd.

Now we will determine the signs of the rest of the eigenvalues of H. When the index j is even, it will be similar to when j is even in section 7.1. However, things change when j is odd. Using this new definition of ρ which corresponds with j being odd in positive case of equation (7.3), we get

$$\frac{1}{2} \left(-\frac{4}{k} - 2\left(2 + m\right) \csc \left(\frac{\pi j}{2m}\right)^2 + \sqrt{\frac{16}{k^2} + \frac{32}{k}} \csc \left(\frac{\pi j}{2m}\right)^2 + 4\left(8 + m\left(4 + m\right)\right) \csc \left(\frac{\pi j}{2m}\right)^4 \right).$$

Setting this expression equal to zero and solving for k gives

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

Thus, k needs to be at least m to ensure that none of the eigenvalues that come from this will be negative.

Since ρ and λ are negative, the result will be negative in the negative case of equation (7.3).

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Thus, half the eigenvalues returned from (7.3) will be negative and the other half will be nonnegative when j is even and when j is odd. Thus,

$$i_{-}(\Delta) = \ell$$
.

Using various techniques touched on throughout this paper, it should be possible to show that no matter however many trees are attached to the pendants of the particular graph from this section, the number of negative eigenvalues will correspond to its leaves.

7.3. Even cycles with opposite pendants. Let T be a graph on n > 2 vertices which has a cycle of 2k vertices and exactly two pendants. One will be opposite of the other. Let Δ be the squared distance matrix of T. Let the ordering of the vertices go from 0 to 2k around the cycle, then connect the next vertex to the 0th vertex and the next vertex to the kth vertex. Let x, y, z, and z be the columns of Δ which correspond to the 0th, kth, 2kth, and 2k + 1th columns, respectively. Then, we will have

$$\mathbf{x} = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ (k-1)^2 \\ k^2 \\ (k-1)^2 \\ \vdots \\ 4 \\ 1 \\ (k+1)^2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} k^2 \\ (k-1)^2 \\ \vdots \\ 1 \\ 0 \\ 1 \\ \vdots \\ (k-2)^2 \\ (k-1)^2 \\ (k+1)^2 \\ 1 \end{bmatrix}, \quad \mathbf{z} = \begin{bmatrix} 1 \\ 4 \\ \vdots \\ k^2 \\ (k+1)^2 \\ k^2 \\ (k+1)^2 \\ \vdots \\ 9 \\ 4 \\ 0 \\ (k+2)^2 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} (k+1)^2 \\ k \\ \vdots \\ 4 \\ 1 \\ 4 \\ \vdots \\ (k-1)^2 \\ k^2 \\ (k+2)^2 \\ 0 \end{bmatrix}.$$

We can generalize this to k-i for the n-2 vertices.

We want to show $\mathbf{x} - \mathbf{y} - \frac{k}{k+2}(\mathbf{z} - \mathbf{w}) = 0$. Notice that when we take the first entry in these vectors and perform the operation, we get

$$0 - k^{2} - \frac{k}{k+2} (1 - (k+1)^{2}) = -k^{2} - \frac{k}{k+2} (-k^{2} - 2k)$$
$$= -k^{2} + \frac{k}{k+2} (k(k+2))$$
$$= -k^{2} + k^{2}$$
$$= 0$$

We can do a similar operation to all other entries. Thus, it is possible to find a linear combination of three of the vectors above to get the other. Therefore, Δ will have at least one 0 eigenvalue.

7.4. Triangle with one tree.

Theorem 7.2. Let U be a graph on n > 2 vertices which has a cycle of three vertices and a tree connected to one of the vertices of the cycle. Let Δ be the squared distance matrix of U. Then

$$i_{-}(\Delta) = \ell + 2.$$

Proof. Use induction on n. For n=3, we know from Corollary 5.2 that there will be two negative eigenvalues of Δ , which satisfies the conclusion of the theorem.

When n = 4, we have a cycle of three vertices, one of which is connected to exactly one other vertex not contained in the cycle. The squared distance 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 $i_{-}(\Delta) = 3 = \ell + 2$.

Let U be a unicyclic graph on n > 4 and observe $\operatorname{diam}(T) \geq 2$. If $\operatorname{diam}(T) = 2$, then

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

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)). Δ is equivalent (performing similar row and column operations) to

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

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

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

As n > 4, the lower right 3×3 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 $\operatorname{diam}(U) \geq 3$. 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 $1, \ldots, k, w$ is k+1, and u is k+2.

Case 1: Let $k \geq 2$. By the proof of Proposition 3.1,

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

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Notice that $-4I_{k-1} - 4J_{k-1}$ is negative definite and so has k-1 negative eigenvalues. Let $F = \Delta_k + (4 - \frac{4}{k}) \mathbf{e}_k \mathbf{e}_k^{\mathsf{T}}$ and notice $F(1) = \Delta_k$ where Δ_k is the squared distance matrix for the unicyclic graph $U \setminus \{1, \ldots, k\}$ with $\ell - (k-1)$ leaves and at least four vertices. By our inductive hypothesis, we have $i_-(\Delta_k) = \ell - (k-1) + 2$. By interlacing, we see that $i_-(F) \ge \ell - (k-1) + 2$. Since $F = (4 - \frac{4}{k}) \mathbf{e}_k \mathbf{e}_k^{\mathsf{T}} + \Delta_{k-1}$ and $4 - \frac{4}{k} > 0$, we have

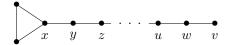
$$i_{-}(F) \le i_{-}\left(\left(4 - \frac{4}{k}\right)\mathbf{e}_{k}\mathbf{e}_{k}^{\top}\right) + i_{-}(\Delta_{k})$$

= $0 + \ell - (k - 1) + 2$
= $\ell - (k - 1) + 2$.

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

$$i_{-}(A) = i_{-}(-4I_{k-1} - 4J_{k-1}) + i_{-}(F)$$
$$= k - 1 + \ell - (k - 1) + 2$$
$$= \ell + 2.$$

Case 2: Let k = 1. Because $diam(U) \ge 3$, 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 $\operatorname{diam}(U) \geq 4$. We let $\Delta' = \Delta(1)$. Now using our inductive hypothesis, we have $i_{-}(\Delta') = \ell + 2$. So, by interlacing, we get $i_{-}(\Delta) \geq \ell + 2$. Then, once again making use of Lemma 3.3, we see that the columns of Δ corresponding to x, y, z with weights 1, -2, 1 form the all 2s vector. Thus $\operatorname{rank}(\Delta) = \operatorname{rank}(\Delta')$ and, therefore, $i_{-}(\Delta) = \ell + 2$.

Case 2b: Suppose 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.

8. Conclusion and further research. We have shown that some specific information about the inertia of the squared distance matrix can be given when there are pendant vertices or vertices of degree 2 whose removal disconnects the graph. From this fact, we gave an alternate proof to the theorem of [3] which determines the inertia of the squared distance matrix of a tree. We were able to further use these tools to prove an analogous theorem for unicyclic graphs whose cycle is even and have one tree coming off of a single vertex. We have also used these tools for a few other specific families of unicyclic graphs.

Unicyclic graphs and the inertia of the squared distance matrix

Examples in Section 7 show us that our main theorem cannot generalize to arbitrary unicyclic graphs. However, it is possible that general bounds could be proven. Based on results from Section 7.2, we see the $i_{-}(\Delta)$ can be as small as ℓ , the number of leaves, and the largest $i_{-}(\Delta)$ we have seen is $\ell + q$ where q is the number of negative eigenvalues coming from the cycle itself. Thus, we could conjecture that

$$\ell \le i_{-}(\Delta) \le \ell + q$$
.

Possible directions for further research could include proving these bounds for general unicyclic graphs or finding explicit values for other specific families of unicyclic graphs. Section 7.3 shows that the question of finding $i_0(\Delta)$ can have many subtleties that could make a general theorem difficult. This is another possible avenue for future research.

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