Note on the Spectra of Steiner Distance Hypermatrices

Joshua Cooper[a] Zhibin Du[b]

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Abstract

The Steiner distance of a set of vertices in a graph is the fewest number of edges in any connected subgraph containing those vertices. The order-k Steiner distance hypermatrix of a graph is the n-dimensional array indexed by vertices, whose entries are the Steiner distances of their corresponding indices. In the case of $k = 2$, this reduces to the classical distance matrix of a graph. Graham and Pollak showed in 1971 that the determinant of the distance matrix of a tree only depends on its number n of vertices. Here, we show that the hyperdeterminant of the Steiner distance hypermatrix of a tree vanishes if and only if (a) $n \geqslant 3$ and k is odd, (b) $n = 1$, or (c) $n = 2$ and $k \equiv 1 \pmod 6$. Two proofs are presented of the $n = 2$ case – the other situations were handled previously – and we use the argument further to show that the distance spectral radius for $n = 2$ is equal to $2^{k-1} - 1$. Some related open questions are also discussed.

Mathematics Subject Classifications: 05C50, 05C12

1 Introduction

Distance matrices are a natural object of study in graph theory. An influential paper of Graham and Pollak ([7]) showed, among other things, the surprising result that determinants of distance matrices of trees only depend on the number n of vertices: $(1-n)(-2)^{n-2}$. This led to a tremendous amount of scholarship concerning these matrices' spectral properties. Interested readers are directed to [1] for a thorough history.

Steiner distance, a generalization of pairwise distance to any set of vertices, was introduced by [2]; an extensive survey can be found in [10]. Let $V(G)$ be the vertex set of G. The Steiner distance $d(S)$ of a set $S \subseteq V(G)$ of vertices in a graph G is the fewest number of edges in any connected subgraph of G containing S. A straightforward generalization of distance matrices is then the order-k "Steiner distance hypermatrix" of a

[a]Department of Mathematics, University of South Carolina, 1523 Greene St, Columbia, SC, 29208, U.S.A. (cooper@math.sc.edu).
[b]School of Software, South China Normal University, Foshan 528225, P.R. China (zhibindu@126.com).

graph G on n vertices, the order-k dimension-n array $D_k(G)$ whose $(v_1,\dots,v_k)\in V(G)^k$ entry is $d(\{v_1,\dots,v_k\})$.

Since Qi ([12]) defined the symmetric hyperdeterminants of a symmetric tensor and provided tools for studying spectra, it is natural to ask for multilinear generalizations of the Graham-Pollak Tree Theorem. In general, hyperdeterminants are computationally intensive to compute and conceptually difficult to study. However, [5] showed that, for trees T on $n \geqslant 3$ vertices, $\det(D_k(T))$ is zero when k is odd; and [4] showed that it is nonzero for k even. It is trivial that $\det(D_k(T))$ is 0 when $n=1$, so – as far as the vanishing of this quantity is concerned – the only remaining case to resolve is $n=2$, which is the main result of this note.

Theorem 1. *The Steiner distance hyperdeterminant* $\det(D_k(T))$ *of a tree* T *on* n *vertices vanishes iff one of the following three conditions holds (1)* $n=1$*, (2)* $n=2$ *and* $k\equiv 1 \pmod 6$*, (3)* $n>2$ *and* k *is odd.*

We present two short proofs: one of which is an application of Qi's version of Sylvester's formula, and another of which uses a description of the characteristic polynomial of the all-ones hypermatrix. An interesting aspect of our formula for the hyperdeterminant is that, up to sign, it equals "Wendt's determinant" (see [8]) (see also [11, OEIS A048954]) with well-known connections to Fermat's Last Theorem ([9]). We also use our computations to describe exactly the spectral radius of $D_k(T)$, and present a few open questions in this area.

2 Proofs

An order-k hypermatrix M with index set S is "symmetric" if, for each permutation σ of $[k]$, the $(i_1,\dots,i_k)\in S^k$ entry of M equals the $(i_{\sigma(1)},\dots,i_{\sigma(k)})$ entry. Of course, if $S=\{0,1\}$, then the entries of a symmetric hypermatrix depend only on the number of their indices which equal 0 or 1. In this special case, Qi gives the following version of Sylvester's formula in [12] for the hyperdeterminant:

Proposition 2. *Let* M *be an order-*k*, dimension-*2 *symmetric hypermatrix with the* $(i_1,\dots,i_k)$ *entry equal to* a_t*,* $0\leqslant t\leqslant k$*, where* t *is the number of coordinates in* $(i_1,\dots,i_k)$ *that are equal to* 1*. Then* $\det(M)$ *is given by the following determinant of order* $2(k-1)$*:*

$$\begin{vmatrix}
a_0 & \binom{k-1}{1}a_1 & \binom{k-1}{2}a_2 & \cdots & a_{k-1} & 0 & \cdots & 0 & 0\\
0 & a_0 & \binom{k-1}{1}a_1 & \cdots & \binom{k-1}{k-2}a_{k-2} & a_{k-1} & \cdots & 0 & 0\\
\vdots & & & & \vdots & & & & \vdots\\
0 & 0 & 0 & \cdots & \binom{k-1}{1}a_1 & \binom{k-1}{2}a_2 & \cdots & \binom{k-1}{k-2}a_{k-2} & a_{k-1}\\
a_1 & \binom{k-1}{1}a_2 & \binom{k-1}{2}a_3 & \cdots & a_k & 0 & \cdots & 0 & 0\\
0 & a_1 & \binom{k-1}{1}a_2 & \cdots & \binom{k-1}{k-2}a_{k-1} & a_k & \cdots & 0 & 0\\
\vdots & & & & \vdots & & & & \vdots\\
0 & 0 & 0 & \cdots & \binom{k-1}{1}a_2 & \binom{k-1}{2}a_3 & \cdots & \binom{k-1}{k-2}a_{k-1} & a_k
\end{vmatrix}.$$

Let $D := D_k(K_2)$ throughout this note, where K_2 is the single-edge graph. For the hypermatrix D, we have $a_0 = 0$, $a_k = 0$, $a_t = 1$ for all $0 < t < k$. Therefore,

$$\det(D) = \begin{vmatrix} 0 & \binom{k-1}{1} & \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} & \binom{k-1}{k-2} & 1 & \cdots & 0 & 0 \\ & & & & \vdots & & & & & \\ 0 & 0 & 0 & \cdots & \binom{k-1}{1} & \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} & \binom{k-1}{k-2} & 1 \\ 1 & \binom{k-1}{1} & \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} & \binom{k-1}{k-2} & 0 & \cdots & 0 & 0 \\ & & & & \vdots & & & & & \\ 0 & 0 & 0 & \cdots & \binom{k-1}{1} & \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} & \binom{k-1}{k-2} & 0 \end{vmatrix}.$$

Let

$$A = \begin{bmatrix} 0 & \binom{k-1}{1} & \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} \\ 0 & 0 & \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \binom{k-1}{1} \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

and

$$B = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ \binom{k-1}{k-2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \binom{k-1}{2} & \cdots & \binom{k-1}{k-2} & 0 & 0 \\ \binom{k-1}{1} & \cdots & \binom{k-1}{k-3} & \binom{k-1}{k-2} & 0 \end{bmatrix}.$$

As usual, we use I_k and O_k to represent an identity matrix and a zero matrix of order k, respectively.

It is easy to see that $A + B + I_{k-1}$ is a circulant matrix, generated by the row $(\binom{k-1}{0}, \binom{k-1}{1}, \dots, \binom{k-1}{k-2})$, thus the eigenvalues of $A + B + I_{k-1}$ are

$$\sum_{r=0}^{k-2} \binom{k-1}{r} \left(e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^r = \left(1 + e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1} - 1,$$

where $\mathbf{i}$ is the imaginary unit, $j = 0, \dots, k-2$.

Next, we would like to obtain all the eigenvalues of the matrix

$$\begin{bmatrix} A & B + I_{k-1} \\ A + I_{k-1} & B \end{bmatrix},$$

whose determinant equals to $\det(D)$ by virtue of Proposition 2. From

$$\begin{bmatrix} I_{k-1} & O_{k-1} \\ I_{k-1} & I_{k-1} \end{bmatrix}^{-1} \begin{bmatrix} A & B + I_{k-1} \\ A + I_{k-1} & B \end{bmatrix} \begin{bmatrix} I_{k-1} & O_{k-1} \\ I_{k-1} & I_{k-1} \end{bmatrix}$$

$$= \begin{bmatrix} A+B+I_{k-1} & B+I_{k-1} \\ O_{k-1} & -I_{k-1} \end{bmatrix},$$

we may conclude that the eigenvalues of

$$\begin{bmatrix} A & B+I_{k-1} \\ A+I_{k-1} & B \end{bmatrix}$$

are the eigenvalues of $A+B+I_{k-1}$, and -1 of multiplicity $k-1$. Thus,

$$\det(D) = (-1)^{k-1} \prod_{j=0}^{k-2} \left(\left(1 + e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1} - 1 \right).$$

It is worth mentioning that

$$(-1)^{k-1} \det(D) = \prod_{j=0}^{k-2} \left(\left(1 + e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1} - 1 \right)$$

is Wendt's determinant W_{k-1} ([11, A048954]); see [8] for example. Lehmer showed ([9]) that W_m is 0 iff $6|m$, from which Theorem 1 follows.

Now, we reprove this identity using characteristic polynomial of D. The following theorem appears in [3]. Denote by J_n^k the all-ones, dimension-n, order-k hypermatrix, and I the dimension-n, order-k identity hypermatrix.

We would use $\binom{n}{r_1,\ldots,r_{k-1}}$ to represent the multinomial coefficient in the subsequent theorem, which is the coefficient of $x_1^{r_1}x_2^{r_2}\ldots x_{k-1}^{r_{k-1}}$ in $(x_1+x_2+\cdots+x_{k-1})^n$.

Theorem 3. *Let $\phi_n(\lambda)$ denote the characteristic polynomial of J_n^k, $n \geqslant 2$. Then*

$$\phi_n(\lambda) = \lambda^{(n-1)(k-1)^{n-1}} \prod_{\substack{r_1,\ldots,r_{k-1}\in\mathbb{N} \\ r_1+\cdots+r_{k-1}=n}} \left(\lambda - \left(\sum_{j=1}^{k-1} r_j e^{\frac{2\pi j}{k-1}\mathbf{i}} \right)^{k-1} \right)^{\frac{\binom{n}{r_1,\ldots,r_{k-1}}}{k-1}}.$$

If we take the $n=2$ case of this expression, the result is

$$\begin{aligned} \phi_n(\lambda) &= \lambda^{k-1} \prod_{\substack{r_1,\ldots,r_{k-1}\in\mathbb{N} \\ r_1+\cdots+r_{k-1}=2}} \left(\lambda - \left(\sum_{j=1}^{k-1} r_j e^{\frac{2\pi j}{k-1}\mathbf{i}} \right)^{k-1} \right)^{\frac{\binom{2}{r_1,\ldots,r_{k-1}}}{k-1}} \\ &= \lambda^{k-1} \prod_{j_1,j_2=1}^{k-1} \left(\lambda - \left(e^{\frac{2\pi j_1}{k-1}\mathbf{i}} + e^{\frac{2\pi j_2}{k-1}\mathbf{i}} \right)^{k-1} \right)^{\frac{1}{k-1}}. \end{aligned}$$

Note that $D = J_2^k - I$, so the characteristic polynomial $\phi_D(\lambda)$ of D is given by

$$\phi_D(\lambda) = \phi_n(\lambda+1) = (\lambda+1)^{k-1} \prod_{j_1,j_2=1}^{k-1} \left(\lambda - \left(e^{\frac{2\pi j_1}{k-1}\mathbf{i}} + e^{\frac{2\pi j_2}{k-1}\mathbf{i}} \right)^{k-1} + 1 \right)^{\frac{1}{k-1}}.$$

We claim that

$$\prod_{j_1,j_2=1}^{k-1}\left(\lambda-\left(e^{\frac{2\pi j_1}{k-1}\mathbf{i}}+e^{\frac{2\pi j_2}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{1}{k-1}}=\prod_{j=0}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right). \tag{1}$$

As a consequence, the constant term of $\phi_D(\lambda)$ is

$$\det(D)=\prod_{j=0}^{k-2}\left(-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)=(-1)^{k-1}\prod_{j=0}^{k-2}\left(\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}-1\right).$$

It is left to confirm (1). First, for any $1\leqslant j_1,j_2\leqslant k-1$, based on

$$\left(e^{\frac{2\pi j_1}{k-1}\mathbf{i}}+e^{\frac{2\pi j_2}{k-1}\mathbf{i}}\right)^{k-1}=\left(e^{\frac{2\pi\min\{j_1,j_2\}}{k-1}\mathbf{i}}\right)^{k-1}\left(e^{\frac{2\pi|j_1-j_2|}{k-1}\mathbf{i}}+1\right)^{k-1}=\left(e^{\frac{2\pi|j_1-j_2|}{k-1}\mathbf{i}}+1\right)^{k-1},$$

and there are exactly $k-1$ pairs (j_1,j_2) such that $|j_1-j_2|=0$, and $2(k-1-|j_1-j_2|)$ ordered pairs (j_1,j_2) such that $1\leqslant|j_1-j_2|\leqslant k-2$, we have

$$\begin{aligned}
&\prod_{j_1,j_2=1}^{k-1}\left(\lambda-\left(e^{\frac{2\pi j_1}{k-1}\mathbf{i}}+e^{\frac{2\pi j_2}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{1}{k-1}}\\
=&\prod_{j_1,j_2=1}^{k-1}\left(\lambda-\left(e^{\frac{2\pi|j_1-j_2|}{k-1}\mathbf{i}}+1\right)^{k-1}+1\right)^{\frac{1}{k-1}}\\
=&\prod_{j=0}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{k-1-2j}{k-1}}.
\end{aligned}\tag{2}$$

Further, we can get

$$\begin{aligned}
&\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{2j}{k-1}}\\
=&\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{j}{k-1}}\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{j}{k-1}}\\
=&\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{j}{k-1}}\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi(k-1-j)}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{k-1-j}{k-1}}\\
=&\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{j}{k-1}}\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{-2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{k-1-j}{k-1}}\\
=&\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{j}{k-1}}\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{k-1-j}{k-1}}
\end{aligned}$$

$$=\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right),$$

or equivalently,

$$\prod_{j=1}^{k-2}\left(\lambda-\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}+1\right)^{\frac{k-1-2j}{k-1}}=1. \tag{3}$$

Finally, (1) follows by combining (2) and (3).

We may now take advantage of the above analysis to compute the spectral radius of D.

Corollary 4. *The Steiner distance hypermatrix of order k with $n = 2$ has spectral radius $2^{k-1} - 1$.*

Proof. Recall from both proofs of Theorem 1 that the eigenvalues of D are -1 with multiplicity $k-1$, and $\left(1+e^{\frac{2\pi j}{k-1}\mathbf{i}}\right)^{k-1}-1$ once for each $0 \leqslant j \leqslant k-2$. Since the point on the unit circle farthest from $z = -1$ is 1, the maximum eigenvalue is achieved by taking $j = 0$, i.e., $2^{k-1} - 1$. □

3 Conclusion

We present a few open questions that arose in the present context. First, we conjecture that the Graham-Pollak Tree Theorem has a full generalization to Steiner distance:

Conjecture 5. The quantity $\det(D_k(T))$ is a function only of n and k for trees T on n vertices.

The above is trivially true for $n \leqslant 3$ or k odd, and [4] checked it computationally for $(k, n) = (4, 4)$, $(4, 5)$, and $(6, 4)$ (even if there are two trees of order $n = 4, 5$). We also venture the following conjecture, supported by all available evidences (as well as the Graham-Pollak results).

Conjecture 6. Whenever it is nonzero, the sign of the quantity $\det(D_k(T))$ for trees T on n vertices is $(-1)^{n-1}$.

Next, since [6] showed that the Perron-Frobenius Theorem generalizes to hypermatrices like $D_k(G)$, and distance spectral radii have been studied extensively, we ask,

Question 7. Provide bounds for the spectral radii of Steiner distance hypermatrices for trees and general connected graphs, in terms of their degree sequence and other statistics.

Although the spectral radius of ordinary distance matrices is a rather active topic in spectral graph theory, until now, to the best of our knowledge, nothing is known about the spectral radius of Steiner distance hypermatrices (a preliminary result can refer to Corollary 4). Along this line, we wonder whether the extremal spectral radius is achieved by the path, as [13] showed holds for ordinary distance matrices:

Question 8. Is the largest spectral radius of the order-k Steiner distance hypermatrix among all n-vertex connected graphs achieved by the path P_n?

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