DISTANCE MATRICES OF A TREE: TWO MORE INVARIANTS, AND IN A UNIFIED FRAMEWORK

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To Ravindra B. Bapat with admiration and thanks, for introducing us to distance matrices

Abstract. A classical result of Graham and Pollak [*Bell Sys. Tech. J.* 1971] states that the determinant of the distance matrix D_T of any tree T depends only on the number of edges of T. This and several other variants of D_T have since been studied – including a q-version, a multiplicative version, and directed versions of these – and in all cases, $\det(D_T)$ depends only on the edge-data.

In this paper, we introduce a more general framework for bi-directed weighted trees that has not been studied to date; our work is significant for three reasons. First, our setting strictly generalizes – and unifies – all variants of D_T studied to date (with coefficients in an arbitrary unital commutative ring) – including in [*Bell Sys. Tech. J.* 1971] above, as well as [*Adv. Math.* 1978], [*J. Combin. Theory Ser. A* 2006], [*Adv. Appl. Math.* 2007], [*Electron. J. Combin.* 2010], and others.

Second, our results strictly improve on state-of-the-art for every variant of the distance matrix studied to date, even in the classical Graham–Pollak case. Here are three results for trees: (1) We compute the minors obtained by deleting arbitrary equinumerous sets of pendant nodes (in fact, more general sub-forests) from the rows and columns of D_T, and show these minors depend only on the edge-data and not the tree-structure. (2) We compute a second function of the distance matrix D_T: the sum of all its cofactors, termed $\operatorname{cof}(D_T)$. We do so in our general setting *and* in stronger form, after deleting equinumerous pendant nodes (and more generally) as above – and show these quantities also depend only on the edge-data. (3) We compute in closed form the inverse of D_T, extending a result of Graham and Lovász [*Adv. Math.* 1978] and answering an open question of Bapat–Lal–Pati [*Linear Algebra Appl.* 2006] in greater generality.

Third, a new technique is to crucially use commutative algebra arguments – specifically, Zariski density – which to our knowledge are hitherto unused for such matrices/invariants, but are richly rewarding. We also explain why our setting is "most general", in that for more general edgeweights, $\det(D_T), \operatorname{cof}(D_T)$ depend on the tree structure. In a sense, this completes the study of the invariants $\det(D_T), \operatorname{cof}(D_T)$ for distance matrices of trees T with edge-data in a commutative ring.

Our proofs use novel results for arbitrary bi-directed strongly connected graphs G: we prove a multiplicative analogue of an additive result by Graham–Hoffman–Hosoya [*J. Graph Theory* 1977], as well as a novel q-version thereof. In particular, we provide closed-form expressions for $\det(D_G)$, $\operatorname{cof}(D_G)$, and D_G^{-1} in terms of their strong blocks. We then show how this subsumes the classical 1977 result, and provide sample applications to adding pendant trees and to cycle-clique graphs (including cactus/polycyclic graphs and hypertrees), subsuming variants in the literature. The final section introduces and computes a third – and novel – invariant for trees, as well as a parallel Graham–Hoffman–Hosoya type result for our "most general" distance matrix D_T.

Contents

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We work over an arbitrary unital commutative ground ring R, unless otherwise specified. For a fixed integer $n \geqslant 1$, we define $[n] := \{1, \dots, n\}$, $\mathbf{e} = \mathbf{e}(n) := (1, \dots, 1)^T \in R^n$, and $J_{n\times n} := \mathbf{e}\mathbf{e}^T$. The standard basis of R^n will be denoted by $\mathbf{e}_1, \dots, \mathbf{e}_n$. Also, given a matrix $A = (a_{ij}) \in R^{n\times n}$ with cofactors $c_{ij} = (-1)^{i+j} \det A_{ij}$, its adjugate matrix is $\operatorname{adj}(A) := (c_{ji})_{i,j=1}^n$.

Recall that a tree is a finite connected graph $T = (V, E)$ with $|E| = |V| - 1$, or equivalently, with a unique path between any two vertices. We write $i \sim j$ to mean that $i \neq j$ and i, j are adjacent in T: $\{i, j\} \in E$. Given a pendant node $i \in V$, we denote the unique node adjacent to it by $p(i)$.

1. General framework and main results

This paper contributes to the study of matrices associated to a graph G – see e.g. [2, 9, 10] for a rich history and detailed information. Specifically, we work with distance matrices. Given an unweighted, undirected tree T with node set V, and nodes $v, w \in V$, let $d(v, w)$ denote the integer length of the unique path from v to w; thus $d(v, v) := 0$. Now define the *distance matrix* D_T to be the $V \times V$ matrix with (v, w) entry $d(v, w)$. Such matrices and their variants have connections to communication networks, network flow algorithms, quantum chemistry and molecular stability, and graph embeddings. For more information, see e.g. [13, 24] and the references therein.

We begin with a well-known and striking result from fifty years ago, by Graham and Pollak in [15]. Namely, if D_T denotes the $n \times n$ path-distance matrix (with entries in $\mathbb{Z}^{\geqslant 0}$) for a tree T with node set $[n]$ and edge-set E, then $\det(D_T)$ does not depend on the tree-structure of T:

$$\det(D_T) = (-1)^{|E|}|E|2^{|E|-1}, \tag{1.1}$$

This has since been extended in several ways. For instance, Bapat–Kirkland–Neumann [3] and Yan–Yeh [24] consider weighted and undirected trees, in which case the distance $d(v, w)$ is taken as the sum of the edgeweights along the unique path from v to w. This further extends to using the unique directed path if one considers the more general case of a directed weighted tree with directed edgeweights a_e, a'_e between the vertices of e. Even in this generality, a result similar to (1.1) holds:

Theorem 1.1 (Bapat–Lal–Pati [5]). *Given a tree $T = (V, E)$ with edgeweights $\{a_e, a'_e : e \in E\}$,*

$$\det(D_T) = (-1)^{|E|} \sum_{e\in E} a_e a'_e \prod_{f\in E,\ f\neq e} (a_f + a'_f).$$

Note that $\det(D_T)$ is "doubly symmetric" in its edgeweights, in that (a) it is independent of the tree structure $e \mapsto \{a_e, a'_e\}$, in the flavor of (1.1); and (b) it is also independent of the "orientation assignment" (a_e, a'_e) or (a'_e, a_e) for a pair of oppositely directed edges.

As may be expected, these results soon led to q-versions; now one replaces a_e by $[a_e] := \frac{q^{a_e}-1}{q-1}$ (and also for a'_e) either for a parameter q (by Yan–Yeh [24]) or for q real, e.g. $q \neq 1$ (by Bapat–Lal–Pati [4]) or $q \neq \pm 1$ (by Bapat–Rekhi [6]). These works considered the undirected case, which was subsequently extended to bi-directed trees:

Theorem 1.2 (Li–Su–Zhang [19]). *Given a tree $T = (V, E)$ with edgeweights $\{a_e, a'_e : e \in E\}$, let its q-distance matrix $D_q(T)$ have (v, w) entry $[d(v, w)] := \frac{q^{d(v,w)}-1}{q-1}$ if $q \neq 1$, and $d(v, w)$ otherwise, where the original distance matrix $(d(v, w))_{v,w\in V}$ is as in Theorem 1.1. Then*

$$\det(D_q(T)) = (-1)^{|E|} \sum_{e\in E} [a_e][a'_e] \prod_{f\in E,\ f\neq e} [a_f + a'_f].$$

Notice again the doubly symmetric formula; also, this generalizes Theorem 1.1, hence all other "additive" variants mentioned above.

In a different vein, Bapat–Lal–Pati [4], Bapat–Rekhi [6], and Yan–Yeh [24] studied the "q-exponential distance matrix" $(q^{d(v,w)})_{v,w\in V}$. This was extended by Bapat–Sivasubramanian [7] to arbitrary multiplicative edgeweights $\{m_e, m'_e : e \in E\}$, and separately by Zhou–Ding [25]:

Theorem 1.3. *Given a directed tree with weighted edge-data* $\{m_e, m'_e : e \in E\}$*, let* D^*_T *denote the* $V \times V$ *matrix with diagonal entries* 1*, and the* (v,w)*-entry (for* $v \neq w$*) the product of the multiplicative edgeweights along the unique directed path* $: v \to w$*. Then* $\det(D^*_T) = \prod_{e \in E}(1 - m_e m'_e)$.

1.1. **Novel, general framework.** In this paper we introduce a more general class of weighted trees which strictly encompass all of the variants studied to date; and for each such tree (including in the aforementioned settings), we will prove the above independence result, but in a stronger form. More precisely, we work with trees with edgeweights in a unital commutative ring R, and so our results hold for all such R. In the most general such version, each edge $\{i,j\}$ is also *bi-directed*, and the weights are pairs of labels. Thus, each edge $\{i,j\}$ comes with two pairs of elements

$$(a_{i\to j}, m_{i\to j}) \qquad \text{and} \qquad (a_{j\to i}, m_{j\to i}), \tag{1.2}$$

where a and m are to be thought of as "additive" and "multiplicative", respectively.

Definition-Notation 1.4. We work with a tree $T = (V,E)$ where $V = [n]$, and over an arbitrary unital commutative ring R. In the sequel, we will omit the arrows in (1.2) and merely write a_{ij}, m_{ij} for vertices $i,j \in V = [n]$. The corresponding **tree-data** or set of **edgeweights** is denoted by

$$\mathcal{T} = \mathcal{T}(T) := \{(i,j; a_{ij}, m_{ij}; a_{ji}, m_{ji}) : i \sim j,\ i < j\}. \tag{1.3}$$

As we explain below, all variants in the literature (and in this paper) involve using $a_{ij} = a_{ji}\ \forall i,j$. Thus, for an edge $e = \{i,j\}$ we will denote symmetric functions in m_{ij}, m_{ji} using the symbols m_e, m'_e. We will then also write $a_e = a_{ij} = a_{ji}$, and call the *triple* (a_e, m_e, m'_e) as the **edgeweight** for $e \in E$. (As we see below, this is a mild abuse of notation for $(a_e, \{m_e, m'_e\})$.)

With this notation, the **directed distance matrix** associated to $\mathcal{T}$ is the matrix $D_{\mathcal{T}}$, with (i,j) entry $w_{i\to j}$ defined as follows: let the unique directed path from i to j be given by

$$i =: i_0 \longrightarrow i_1 \longrightarrow \cdots \longrightarrow i_k := j, \qquad k \geqslant 0.$$

Now define $D_{\mathcal{T}} := (w_{i\to j})_{i,j=1}^n$, where $w_{i\to i} := 0$; and for $i \neq j$,

$$w_{i\to j} := a_{i_0 i_1}(m_{i_0 i_1} - 1) + a_{i_1 i_2}(m_{i_0 i_1} m_{i_1 i_2} - m_{i_0 i_1}) + \cdots = \sum_{l=0}^{k-1} a_{i_l i_{l+1}}(m_{i_l i_{l+1}} - 1) \prod_{u=0}^{l-1} m_{i_u i_{u+1}}. \tag{1.4}$$

Example 1.5 (The tree on 3 nodes)**.** For the tree in Figure 1, the corresponding matrix $D_{\mathcal{T}}$ is

$$\begin{pmatrix} 0 & a_{12}(m_{12}-1) & a_{12}(m_{12}-1) + a_{23}m_{12}(m_{23}-1) \\ a_{12}(m_{21}-1) & 0 & a_{23}(m_{23}-1) \\ a_{23}(m_{32}-1) + a_{12}m_{32}(m_{21}-1) & a_{23}(m_{32}-1) & 0 \end{pmatrix}. \tag{1.5}$$

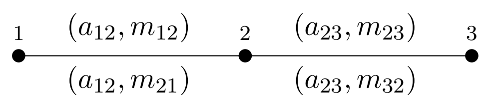

FIGURE 1. The tree $T = P_3$, with general edge-data $\mathcal{T}$.

Notice (e.g. in the above example) that $D_{\mathcal{T}}$ need not be symmetric in our model. Indeed, this is the case in several previous papers, see e.g. [4, 5, 7, 13, 17, 25, 26].

Remark 1.6. To our knowledge, the above "additive-multiplicative" setting encompasses all previous variants in the literature. For example, the setting of Theorem 1.2 with $q \neq 1$ involves setting all additive edgeweights to be $1/(q-1)$, and $m_e = q^{a_e}$, $m'_e = q^{a'_e}$ (with a mild abuse of notation). Thus, a formula for $\det(D_{\mathcal{T}})$ in our setting would extend the one in Theorem 1.2, hence all prior variants. Note, such a formula would naively work only for q^{a_e} with $a_e \in \mathbb{Z}$, and so the $q \to 1$ case provides formulas for $\det(D_\mathcal{T})$ that work only for $a_e \in \mathbb{Z}$. However, we show that the same formula will work for a_e in any unital commutative ring, using the power of Zariski density – a novel technique in this context, which we introduce and explain in multiple proofs. Thus, our general framework subsumes all "additive" variants of $D_\mathcal{T}$ considered in the literature.

Similarly, the multiplicative setting of Theorem 1.3 is recovered by setting $a_e = 1$. Then the "multiplicative distance matrix" is given by $D_\mathcal{T} + J$, where J is the all-ones matrix.

Our first main result implies as a special case that all of the above distance matrices have determinants independent of the tree structure, and depending only on the edge-data. As the preceding remark shows, we will require a formula for $\det(D + xJ)$, where x is a scalar. This necessitates recalling a notion studied by Graham–Hoffman–Hosoya [13]:

Definition 1.7. Given a square matrix A, its **cofactor-sum** $\operatorname{cof}(A)$ is defined to be the sum of all cofactors of A, namely, the sum over all $i, j \in [n]$ of $(-1)^{i+j} \det(A_{i|j})$. Here, $A_{i|j}$ is the submatrix of A obtained by deleting the ith row and jth column.

We immediately record – and use below, occasionally without further reference – the following straightforward facts from linear algebra. See e.g. [2, 13] for a proof of these or of close variants:

Lemma 1.8. *Let R be any unital commutative ring, $A \in R^{n\times n}$ any square matrix (for $n \geqslant 1$), and x an indeterminate that commutes with R. Then $\det(A + xJ) = \det(A) + x \operatorname{cof}(A)$. Moreover,*

$$\operatorname{cof}(A) = \mathbf{e}^T \operatorname{adj}(A)\mathbf{e} = \operatorname{cof}(A + xJ),$$

and $\operatorname{adj}(A + xJ)\mathbf{e}$ does not depend on x.

The quantity $\operatorname{cof}(D_\mathcal{T})$ was first studied by Graham, Hoffman, and Hosoya in [13] for arbitrary graphs G, in the special case of additive edgeweights a_e, a'_e.

1.2. **Main results and novel features.** In this section, we describe the various novel features of the paper. In a nutshell: (a) We prove formulas in our general setting for trees, which specialize to novel identities for every single variant – even in the original Graham–Pollak case of integer-valued unweighted distance matrices. To our knowledge, such a unification has not been achieved to date. (b) As a consequence, the invariance of $\det(D_\mathcal{T}), \operatorname{cof}(D_\mathcal{T})$ holds in our general setting, implying the same in all previous cases. (c) We compute the inverse of $D_\mathcal{T}$ in our general setting, resolving an open question of Bapat et al [4] in greater generality (and recovering all such formulas for trees in the literature, over arbitrary unital commutative rings). (d) These results use in part, strengthenings of state-of-the-art for *arbitrary* strongly connected graphs, which will be the subject of Section 2. (e) In Section 4 we introduce a novel, edge-multiplicative invariant for trees, which we term $\kappa(D_\mathcal{T})$. We then formulate and prove identities relating $\det, \operatorname{cof}$, and κ.

A satisfying feature: further generalizing our setting leads to both $\det(D_\mathcal{T}), \operatorname{cof}(D_\mathcal{T})$ depending on the tree structure. Thus, in a sense, our framework is "*most general*"; see Example 1.13.

Before proceeding to the results, we also stress on a **novel technique** that we adopt from commutative algebra: *Zariski density*. This is immensely rewarding and helps bypass various artificial technical restrictions; it also can be applied more broadly; and to our knowledge, it has not been used in this context previously. See also Remark 3.4 for additional details.

We next state our main results: two for trees, and one for general graphs (which has a host of applications that strengthen the existing results in the literature – see the next section). Our first result computes in closed-form both $\det(D_\mathcal{T})$ and $\operatorname{cof}(D_\mathcal{T})$ for "additive-multiplicative edge-data" for trees in our general setting above. In fact, we will compute these quantities for the submatrices of $D_\mathcal{T}$ corresponding to removing equal-sized sets of pendant nodes (and more generally):

Theorem A. *Suppose a tree $T = (V = [n], E)$ is equipped with edge-data $\mathcal{T} = \{(a_{ij} = a_{ji}, m_{ij}, m_{ji}) : \{i,j\} \in E\}$ as above. (We write (a_e, m_e, m'_e) for the weights for edges $e \in E$.) Let $I, J' \subset V$ satisfy: (a) $|I| = |J'| \leqslant n-3$; (b) $|I \cup J'| \leqslant n-1$; (c) $T \setminus I$, $T \setminus J'$, $T \setminus (I \cap J')$ are connected. Now let $E_\circ := E_{(I\cap J')^c}$ denote the edges in E not among the common edges adjacent to $I \cap J'$.*

As an additional notation, given a $V \times V$ matrix D, let $D_{I|J'}$ denote the submatrix formed by removing the rows and columns labelled by I, J' respectively. Then $\det(D_\mathcal{T} + xJ)_{I|J'}$ depends on the edge-data but not on the tree structure:

$$\det(D_\mathcal{T} + xJ)_{I|J'} \tag{1.6}$$
$$= \begin{cases} \displaystyle\prod_{e \in E_\circ} (a_e(1 - m_e m'_e)) \left[x + \sum_{e \in E_\circ} \frac{(a_e - x)(m_e - 1)(m'_e - 1)}{m_e m'_e - 1} \right], & \text{if } |I \Delta J'| = 0, \\ \displaystyle\prod_{e \in E_\circ \setminus \{(p(i_0), i_0), (j_0, p(j_0))\}} (a_e(m_e m'_e - 1)) \cdot a_{(p(i_0),i_0)} (a_{(j_0,p(j_0))} - x)(m_{(p(i_0),i_0)} - 1)(m_{(j_0,p(j_0))} - 1), & \\ & \text{if } |I \Delta J'| = 2, \\ 0, & \text{if } |I \Delta J'| > 2, \end{cases}$$

where the denominators (for $I = J'$) are placeholders that cancel with a factor in $\prod_e (1 - m_e m'_e)$. We also assume that if $|I \Delta J'| = 2$, then the nodes i_0, j_0 are given by $I \setminus J' = \{i_0\}$, $J' \setminus I = \{j_0\}$.

Theorem A says more precisely that $\det(D_\mathcal{T} + xJ)_{I|J'}$ depends only on the edge-data of the edges in $I \setminus J'$, $J' \setminus I$, $I \cap J'$, and $E \setminus (I \cap J')$. A curious feature is that $\mathrm{cof}(\cdot)$ for $|I \Delta J'| = 2$ is asymmetric in the additive edge-data for i_0, j_0. Also, the (possibly non-optimal) choice of notation for the index set $J' \subset [n]$ is to avoid conflict with the all-ones matrix J.

We now make several clarifying remarks:

Remark 1.9. Equation (1.6) computes principal as well as non-principal minors of $D_\mathcal{T}$. The case when $I \neq J'$ (and both are non-singleton) of non-principal minors reveals new information about $D_\mathcal{T}$ even in the original setting of Graham–Pollak, hence for every other variant studied.

Remark 1.10. Theorem A includes the originally sought-for case of $I = J' = \emptyset$:

$$\begin{aligned} \det(D_\mathcal{T}) &= \prod_{e \in E} (a_e(1 - m_e m'_e)) \sum_{e \in E} \frac{a_e(m_e - 1)(m'_e - 1)}{m_e m'_e - 1}, \\ \mathrm{cof}(D_\mathcal{T}) &= \prod_{e \in E} (a_e(1 - m_e m'_e)) \left[1 + \sum_{e \in E} \frac{(a_e - 1)(m_e - 1)(m'_e - 1)}{m_e m'_e - 1} \right]. \end{aligned} \tag{1.7}$$

Note, the invariant $\det(D_\mathcal{T})$ depends only on $(a_e, \{m_e, m'_e\})_{e \in E}$, while $\mathrm{cof}(D_\mathcal{T})$ depends on even less: on $\{a_e : e \in E\}$ and $\{\{m_e, m'_e\} : e \in E\}$ – and so this holds for every variant studied to date.

Remark 1.11. By Theorem 1.2, the formulas for $\det(\cdot), \mathrm{cof}(\cdot)$ for the classical distance matrix follow from from their q-versions. We observe in Remark 1.12 that these q-versions follow themselves from the multiplicative versions where $a_e = a'_e = 1/(q-1)$, but using $D_\mathcal{T} = D^*_T - J$ instead of the multiplicative matrix D^*_T. Thus by Lemma 1.8, using $\det(\cdot)$ alone does not help unify the host of previously studied variants; one crucially has to also use $\mathrm{cof}(\cdot)$. To our knowledge, such a unification (and its generalization) had not previously been achieved in the literature.

Remark 1.12. As anticipated in Remark 1.6: Theorem 1.1 (where $a_e \neq a'_e$) can be deduced from the $a_e = a'_e$ formula (1.6) as follows: First work over $\mathbb{Q}(q)$ for a parameter q, and set all additive edgeweights to be $1/(q-1)$, and $m_e = q^{a_e}, m'_e = q^{a'_e}$. For integer values of a_e, a'_e, one can use (1.6) for $I = J = \emptyset$ to deduce Theorem 1.2. Now evaluate at $q = 1$ to obtain Theorem 1.1. This works for weights $a_e, a'_e \in \mathbb{Z}$; the extension to a_e, a'_e in a commutative ring R follows by Zariski density.

Our next contribution (after Theorem A) shows that our setting is the "most general" possible:

Example 1.13. Theorem A and its special case (by Remark 1.12) Theorem 1.1 say that in the two cases when (a) m_{ij}, m_{ji} need not coincide, while $a_e = a_{ij} = a_{ji}$; and (b) a_{ij}, a_{ji} need not coincide, while $m_e = m_{ij} = m_{ji} = q$ and $q \to 1$ – the terms $\det(D_{\mathcal{T}}), \operatorname{cof}(D_{\mathcal{T}})$ depend only on the edge-data, but not on the tree structure. It is natural to ask if this holds for the remaining variant of weighted bi-directed trees: where $a_{ij} \neq a_{ji}$ and $m_{ij} = m_{ji} \neq 1$ (or even more generally, $m_{ij} \neq m_{ji}$). The following example shows that this does not happen in the (perhaps) simplest imaginable such situation: suppose a_{ij} and a_{ji} are allowed to be unequal, and set $m_e = m_{ij} = m_{ji} = q,\ \forall e \in E$.

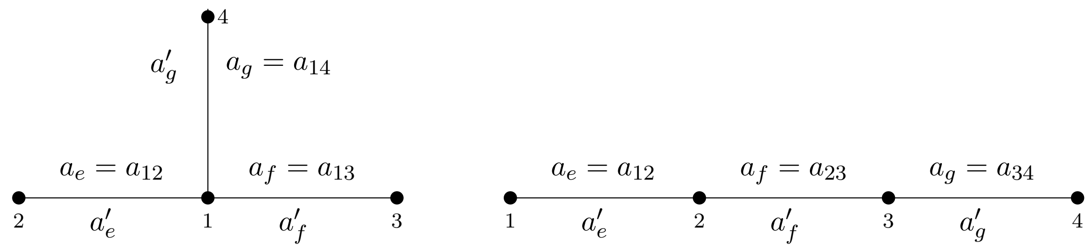

FIGURE 2. The trees $K_{1,3}$ and P_4, with all $m_e = m_{ij} = m_{ji} = q$.

Then a straightforward computation shows that even for the two non-isomorphic graphs with four nodes with edge-data as above, neither $\det(D_{\mathcal{T}})$ nor $\operatorname{cof}(D_{\mathcal{T}})$ agree (unless $q = 1$). ☐

Our next main result for trees provides a closed-form expression for $D_{\mathcal{T}}^{-1}$ in our general setting, thereby subsuming the special cases worked out in [3]–[7], [14, 25, 26].

Theorem B. *Suppose $T = (V = [n], E)$ is equipped with edge-data $\mathcal{T} = \{(a_{ij} = a_{ji}, m_{ij}, m_{ji}) : \{i,j\} \in E\}$, such that $a_{ij}, m_{ij}m_{ji} - 1$, and $\det(D_{\mathcal{T}})$ are invertible in R. Define the vectors $\boldsymbol{\tau}_{\rm in}, \boldsymbol{\tau}_{\rm out} \in R^V$ to have ith coordinates:*

$$\boldsymbol{\tau}_{\rm in}(i) := 1 - \sum_{j : j \sim i} \frac{m_{ji}(m_{ij} - 1)}{m_{ij}m_{ji} - 1}, \qquad \boldsymbol{\tau}_{\rm out}(i) := 1 - \sum_{j : j \sim i} \frac{m_{ij}(m_{ji} - 1)}{m_{ij}m_{ji} - 1}, \tag{1.8}$$

and also define the Laplacian matrix $L_{\mathcal{T}} \in R^{|V| \times |V|}$ *via:*

$$(L_{\mathcal{T}})_{ij} = \begin{cases} \dfrac{-m_{ij}}{a_{ij}(m_{ij}m_{ji} - 1)}, & \text{if } i \sim j; \\ \displaystyle\sum_{k \sim i} \frac{m_{ki}}{a_{ik}(m_{ik}m_{ki} - 1)}, & \text{if } i = j; \\ 0, & \text{otherwise.} \end{cases} \tag{1.9}$$

Then there exists a matrix $C_{\mathcal{T}} \in R^{|V| \times |V|}$ (see (3.3) below) such that

$$D_{\mathcal{T}}^{-1} = \left(\sum_{e \in E} \frac{a_e(m_e - 1)(m_e' - 1)}{m_e m_e' - 1} \right)^{-1} \boldsymbol{\tau}_{\rm out} \boldsymbol{\tau}_{\rm in}^T - L_{\mathcal{T}} + C_{\mathcal{T}} \operatorname{diag}(\boldsymbol{\tau}_{\rm in}). \tag{1.10}$$

This result is proved in Section 3, and in a sense is the strongest result in the paper, since as we explain, it – and its proof – implies most of Theorem A, and hence all preceding results.

Having dealt with trees, our final (until the last section) main result concerns distance matrices of arbitrary finite directed, strongly connected, weighted graphs. We mention some definitions for completeness, referring the reader to e.g. [16] for the basics of graph theory.

Definition 1.14. Let G be a directed or undirected graph with node-set V.

(1) A node $v \in V$ is said to be a *cut-vertex* if its removal increases the number of (undirected) graph components of G. Denote the set of cut-vertices by V^{cut}.
(2) The maximal induced subgraphs of G with no cut-vertices are called the *strong blocks*.
(3) If G is undirected (directed), we say G is *(strongly) connected* if for all $v \neq w \in V$ there exists a (directed) path from v to w.

Now suppose G is a finite directed, strongly connected, weighted graph. Distance matrices D_G with trivial multiplicative edgeweights – i.e. $m_e = m'_e = q \ \forall e \in E(G)$ and $q \to 1$ as in the setting of Theorem 1.1 – were studied by Graham–Hoffman–Hosoya [13], and they obtained beautiful formulas for $\det(D_G), \operatorname{cof}(D_G)$ in terms of the strong blocks of G:

$$\begin{aligned} \operatorname{cof}(D_G) &= \prod_j \operatorname{cof}(D_{G_j}), \\ \det(D_G) &= \sum_j \det(D_{G_j}) \prod_{i \neq j} \operatorname{cof}(D_{G_i}). \end{aligned} \tag{1.11}$$

Here G_j (and G_i) run over the strong blocks of G. In particular when $\operatorname{cof}(D_G) \neq 0$, one has:

$$\frac{\det(D_G)}{\operatorname{cof}(D_G)} = \sum_j \frac{\det(D_{G_j})}{\operatorname{cof}(D_{G_j})}.$$

We next present similar formulas for $\operatorname{cof}(D_G)$ and $\det(D_G)$ in the parallel multiplicative setting. More generally, we now work with distance matrices whose (i, j) entries are themselves matrices:

Definition 1.15. Fix a unital commutative ring R and a directed, strongly connected graph G with vertex set $V = [n]$. For us, a *product distance* on G is a choice of integers $k_1, \dots, k_n \geqslant 1$ and matrices $\eta(i, j) \in R^{k_i \times k_j}$ such that (a) $\eta(v, v) := \operatorname{Id}_{k_v}$ for all cut-vertices v, and (b) for $i, j \in [n]$, if every directed path from $i \to j$ passes through the cut-vertex v, then $\eta(i, j) = \eta(i, v)\eta(v, j)$. Here the *product distance matrix* is the $K \times K$ block matrix with (i, j) block $\eta(i, j)$, where $K := \sum_{v \in V} k_v$.

Product distance matrices have been previously studied – mostly for trees [24, 25], but also in [7] for general graphs, with $k_i = 1 \ \forall i$. The above definition simultaneously extends the settings in all of these works. Now in this overarching setting – and for arbitrary graphs – we will show:

Theorem C. *Suppose $G = (V, E)$ is a finite directed, strongly connected, weighted graph, with additive edgeweights $a_e = a'_e = 1 \ \forall e \in E$. Suppose G has strong blocks G_j, and D^*_G denotes any product distance matrix for G, with principal submatrices $D^*_{G_j}$ corresponding to G_j. Then,*

$$\begin{aligned} \det(D^*_G) &= \prod_j \det(D^*_{G_j}), \\ \operatorname{cof}(D^*_G) &= \sum_j \operatorname{cof}(D^*_{G_j}) \prod_{i \neq j} \det(D^*_{G_i}) - \det(D^*_G) \sum_{v \in V} k_v(\#\{j : v \in G_j\} - 1), \end{aligned} \tag{1.12}$$

where the final sum may be taken over only the subset of cut-vertices. In particular, and parallel to the setting of [13], *if D^*_G is invertible, and the integers $k_v = k \ \forall v \in V^{cut}$ are all equal, then*

$$\frac{\operatorname{cof}(D^*_G)}{\det(D^*_G)} - k = \sum_j \left(\frac{\operatorname{cof}(D^*_{G_j})}{\det(D^*_{G_j})} - k \right). \tag{1.13}$$

Also: if $D^*_{G_j}$ is invertible for all j, then

$$(D^*_G)^{-1} = \sum_j \left[(D^*_{G_j})^{-1} \right]_j - \sum_{v \in V} (\#\{j : v \in G_j\} - 1) \cdot [\operatorname{Id}_{k_v}]_v, \tag{1.14}$$

where $[A]_j$ denotes the $K \times K$ matrix with the matrix A occurring in the rows and columns corresponding to the nodes of G_j, and zeros in the other entries (and similarly for $[\operatorname{Id}_{k_v}]_v$).

In the special case $k_v = 1\ \forall v$, the formulas here for $\det, \mathrm{cof}$ resemble those in (1.11). In fact our results strengthen the classical Graham–Hoffman–Hosoya identities (1.11) in multiple ways: first, we show in the next section how our multiplicative formulas imply the additive ones in (1.11). Second, in the final Section 4 we propose (and prove) similar formulas to Theorem C in our current, general setting – with scalar entries; and then show how these too specialize to the identities (1.11). This uses a third, novel invariant $\kappa(D_{\mathcal{T}})$.

Remark 1.16. For example, Theorem C implies explicit formulas for $\det(D^*_T)$, $\mathrm{cof}(D^*_T)$, $(D^*_T)^{-1}$ for $G = T$ an arbitrary tree, as in [6, 24, 25]. This is because the strong blocks of T are precisely its edges, and it is easy to compute the above quantities for 2×2 block matrices – in fact of the form $\begin{pmatrix} \mathrm{Id}_{k_1} & M_{12} \\ M_{21} & \mathrm{Id}_{k_2} \end{pmatrix}$. Note, the explicit formulas for $\det(D^*_T), (D^*_T)^{-1}$ for trees in [6, 24, 25] – for distance matrices D^*_T with matrix weights as above – are stated in a different form.

Remark 1.17. In this paper, we mainly focus on advancing the state-of-the-art (e.g. non-principal minors) for matrices $D_{\mathcal{T}}$ over arbitrary unital commutative rings R. Indeed, the commutative case is the far better-studied and mathematically active framework for distance matrices and their variants. That said, there are also results in the literature over non-commutative rings R'. See e.g. [8, 25, 26], several of which work in fact with $R' = R^{k \times k}$ – precisely the setting in our Theorem C.

For completeness, we conclude by mentioning a generalization of the formula (1.13) for invertible D^*_G. Namely, fix a cut-vertex v. Then every block G_j has a unique cut-vertex $v(j)$ which is closest to v. Now (1.13) extends to the case of possibly unequal k_v as follows:

$$\frac{\mathrm{cof}(D^*_G)}{\det(D^*_G)} - k_v = \sum_j \left(\frac{\mathrm{cof}(D^*_{G_j})}{\det(D^*_{G_j})} - k_{v(j)} \right), \qquad \forall v \in V^{cut}. \tag{1.15}$$

Organization of the paper. In Section 2 we prove Theorem C, followed by several applications:

- The classical Graham–Hoffman–Hosoya formulas (1.11) – more generally, a novel q-variant.
- Attaching finitely many pendant trees to G, and showing the independence of $\det, \mathrm{cof}$ from the locations where these are attached;
- Computing these invariants for the classical and q-weighted cycle-clique graphs, thereby recovering known results for unicyclic, bicyclic, and cactus graphs, as well as hypertrees.

In Section 3 we prove Theorem B, and use it to show Theorem A. We add that one can provide other proofs of Theorem A or its special cases that are not in the literature, but we omit these for brevity. Also remark that the multiplicative special case of $a_e = a'_e = 1$ (proved in Section 2) is required in order to prove Theorem A via a novel technique that we introduce in this field: applying Zariski density to distance matrices; to our knowledge, this is new to the area. Namely:

- we note that $\det(D_{\mathcal{T}})_{I|J'}, \mathrm{cof}(D_{\mathcal{T}})_{I|J'}$, and also our stated formulas for them in Theorem A are *polynomial functions* of the matrix entries in $(D_{\mathcal{T}})_{I|J'}$;
- hence we first work with variable edgeweights and use Zariski density – since $\det(D_{\mathcal{T}}), 1 - m_e m'_e \not\equiv 0$ from the multiplicative case, proved independently. This shows the result over $\mathbb{Z}[\{a_e, m_e, m'_e : e \in E\}]$; we then specialize to an arbitrary unital commutative ring R.

This technique is immensely useful in our proofs – see also Remark 3.4 for some of the advantages.

In the final Section 4, we introduce a *third*, novel invariant $\kappa(D_{\mathcal{T}})$ for the above "general" distance matrices $D_{\mathcal{T}}$ for trees (1.4). We show that κ is also independent of the tree structure, and is multiplicative across edges; and for general graphs we prove Graham–Hoffman–Hosoya type identities for $\det(D_G), \mathrm{cof}(D_G), \kappa(D_G)$ in terms of the strong blocks of G – see Theorem D. This provides an alternate, short proof of the formulas for $\det(D_{\mathcal{T}}), \mathrm{cof}(D_{\mathcal{T}})$ in the general setting of Theorem A – from which all known formulas for $\det(D_{\mathcal{T}}), \mathrm{cof}(D_{\mathcal{T}})$ for trees can be deduced.

2. The multiplicative GHH Theorem C for digraphs, and its applications

In this section we prove Theorem C for product distance matrices over arbitrary weighted strongly connected graphs, and provide several applications to graphs that are not trees. The final two sections will focus on weighted bi-directed trees.

Proof of Theorem C. Inducting on the number of cut-vertices, it suffices to show the result for G having a cut-vertex $v \in V = [n]$ and consisting of strongly connected subgraphs G_1 and G_2 separated by v, with node sets $\{1, \dots, v\}$ and $\{v, \dots, n\}$ respectively. Thus G has distance matrix

$$D^*_G = \begin{pmatrix} D_1 & A & AB \\ A' & \mathrm{Id}_{k_v} & B \\ B'A' & B' & D_2 \end{pmatrix}, \tag{2.1}$$

where the leading (resp. trailing) principal 2×2 block submatrix equals $D^*_{G_1}$ (resp. $D^*_{G_2}$).

We first quickly sketch the argument for computing $\det(D^*_G)$, since it is similar to the one for various special cases shown in [7, 24, 25]. By elementary linear algebra it is clear that

$$\det D^*_G = \det \begin{pmatrix} D_1 & A & 0 \\ A' & \mathrm{Id}_{k_v} & 0 \\ B'A' & B' & D_2 - B'B \end{pmatrix} = \det D^*_{G_1} \cdot \det(D_2 - B' \, \mathrm{Id}_{k_v}^{-1} B) = \det D^*_{G_1} \cdot \det D^*_{G_2},$$

where the final equality uses Schur complements. This proves the assertion.

Next, if D^*_G is invertible (i.e., $\det(D^*_{G_j}) \in R^\times$ for all j) then an explicit computation shows the claimed formula for its inverse. Once again, it suffices by induction to work with G having one cut-vertex $v \in [n]$ as above, in which case if D^*_G is of the form (2.1), then

$$D^*_G \cdot \begin{pmatrix} (D^*_{G_1})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + D^*_G \cdot \begin{pmatrix} 0 & 0 \\ 0 & (D^*_{G_2})^{-1} \end{pmatrix} - D^*_G \cdot \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathrm{Id}_{k_v} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \mathrm{Id}_{|V(G_1)|} & 0 \\ B'(0 \quad \mathrm{Id}_{k_v}) & 0 \end{pmatrix} + \begin{pmatrix} 0 & A(\mathrm{Id}_{k_v} \quad 0) \\ 0 & \mathrm{Id}_{|V(G_2)|} \end{pmatrix} - \begin{pmatrix} 0 & A & 0 \\ 0 & \mathrm{Id}_{k_v} & 0 \\ 0 & B' & 0 \end{pmatrix} = \mathrm{Id}_{|V(G)|}.$$

Finally, if D^*_G is invertible (equivalently, all $D^*_{G_j}$ are thus), then pre- and post- multiplying (1.14) by $\mathbf{e}^T, \mathbf{e}$ respectively yields via Lemma 1.8:

$$\frac{\mathrm{cof}(D^*_G)}{\det(D^*_G)} = \sum_j \frac{\mathrm{cof}(D^*_{G_j})}{\det(D^*_{G_j})} - \sum_{v \in V^{cut}} (\#\{j : v \in G_j\} - 1) \cdot k_v.$$

Now the claimed identity for $\mathrm{cof}(D^*_G)$ follows from the one for $\det(D^*_G)$ – note this holds whenever $\det(D^*_G)$ is invertible. To prove this holds uniformly, we use a Zariski density argument (or Weyl's "principle of irrelevance of algebraic inequalities" [22]). More precisely, we first work over the field $R_0 := \mathbb{Q}(\{a_{i,i'}\})$ of rational functions, where i, i' together index rows (or columns) of the block matrix D^*_G which belong to the block-entries of unequal nodes in a common block $D^*_{G_j}$.

Now in the field R_0, $\det(D^*_G)$ is a nonzero polynomial (hence invertible), since specializing to $\eta(i,j) = 0 \ \forall i \neq j$ yields $D^*_G = \mathrm{Id}$. In particular, it follows that

$$p := \mathrm{cof}(D^*_G) - \sum_j \mathrm{cof}(D^*_{G_j}) \prod_{i \neq j} \det(D^*_{G_i}) + \det(D^*_G) \sum_{v \in V} k_v (\#\{j : v \in G_j\} - 1)$$

is a polynomial in $\mathbb{Z}[\{a_{i,i'}\}] \subset R_0$, which vanishes on the set $U := D(\det(D^*_G))$ of non-roots of $\det(D^*_G)$. Now invoke Lemma 2.1, stated and proved below: U is Zariski dense in the affine space $\mathbb{A}^N_{\mathbb{Q}}$, where $N := \mathrm{tr}\deg_{\mathbb{Q}}(R_0)$ denotes the number of variables $a_{i,i'}$ in R_0. Thus p vanishes on all of $\mathbb{A}^N_{\mathbb{Q}}$, and the formula for $\mathrm{cof}(D^*_G)$ holds uniformly for all values of $(a_{i,i'}) \in \mathbb{Q}^N$. Again using Lemma 2.1 shows $p = 0$ in $\mathbb{Z}[\{a_{i,i'}\}]$, so one can specialize the variables $a_{i,i'}$ to any unital commutative ring R, to prove the formula for $\operatorname{cof}(D^*_G)$ over R. Now (1.13) follows from (1.14). $\square$

Notice that modulo a Zariski density lemma, the final two paragraphs of our proof of Theorem C spelled out the "Zariski density" part of the proof in great detail; this was because we will use similar arguments in what follows. The remaining piece is a basic and well-known lemma on polynomials:

Lemma 2.1. *Suppose $\mathbb{F}$ is an infinite field and $k > 0$ an integer.*

1. *If a polynomial $p \in \mathbb{F}[T_1, \dots, T_k]$ vanishes on $\mathbb{F}^k$, then $p = 0$.*
2. *For a polynomial $0 \neq f \in \mathbb{F}[T_1, \dots, T_k]$, let $D(f) := \{(a_1, \dots, a_k) \in \mathbb{A}^k_{\mathbb{F}} \cong \mathbb{F}^k : f(a_1, \dots, a_k) \neq 0\}$. Then $D(f)$ – in fact, every nonempty Zariski open set – is Zariski dense in $\mathbb{F}^k$. (Recall, $U \subseteq \mathbb{F}^k$ is Zariski dense if $p|_{\mathbb{F}^k} \equiv 0$ whenever $p \in \mathbb{F}[T_1, \dots, T_k]$ vanishes on U.)*
3. *Consider the following inductively indexed family of sets, each of which is infinite in size: (a) $S \subseteq \mathbb{F}$ is an infinite subset; (b) for each $j \in [k-1]$, given $s_1 \in S, s_2 \in S_{s_1}, \dots, s_j \in S_{s_1,\dots,s_{j-1}}$, let $S_{s_1,\dots,s_j} \subseteq \mathbb{F}$ be an infinite subset. Then the set of tuples*
$$\mathcal{S}(k) := \{\mathbf{s} = (s_1, \dots, s_k) \in \mathbb{F}^k : s_1 \in S,\ s_{j+1} \in S_{s_1,\dots,s_j}\ \forall j \in [k-1]\}$$
is Zariski dense in $\mathbb{A}^k_{\mathbb{F}} \cong \mathbb{F}^k$.

For instance in part (3), one can choose $S_{s_1,\dots,s_j} = S\ \forall j,\ s_1, \dots, s_{j-1}$, in which case $\mathcal{S}(k) := S^k$. Also note that a strengthening of part (3) is well-known, e.g. see [1, Lemma 2.1] in Alon's famous work. Moreover, part (2) is a (weaker) version of Weyl's principle of irrelevance of algebraic inequalities [22].

Remark 2.2. For completeness, we discuss various special cases of Theorem C in the literature. The formula for $\det(D^*_G)$ was recently obtained for matrices with all $k_i \equiv 1$ in [7] in the spirit of previous results in [24, 25]. Also, with Lemma 1.8 in hand, it is not hard to observe that the multiplicative "q-results" – analogous to the classical Graham–Hoffman–Hosoya identities (1.11) – which were obtained recently in [19, 21] can be derived from Theorem C, by specializing to $m_e = m_{ij} = m_{ji} = q$ and $a_e = a_{ij} = a_{ji} = 1/(q-1)$. In these works [19, 21], the authors consider $\det(D^*_G - J) = (\det - \operatorname{cof})(D^*_G)$ and $\xi(D^*_G - J) = \det(D^*_G)$ (up to a power of $q-1$).

Also notice, Theorem C immediately implies the independence of $\operatorname{cof}(D^*_T)$ from the tree structure (for G a tree), since now the strong blocks are precisely the edges of G. Moreover, the entries $\eta(i,j)$ of the distance matrix D^*_G can be matrices and we allow $\eta(i,j) \neq \eta(j,i)$, extending the scalar-entries case in the works [7, 19, 21] cited above.

2.1. **Application 1: the q- and classical Graham–Hoffman–Hosoya identities.** Before focussing on trees below, we discuss some applications of Theorem C. Our first application shows that Theorem C implies analogous identities for the *q-distance matrix* that (we believe) were not yet written down. Consider a weighted bi-directed graph G with $d(u,v) = \alpha_{uv} \in \mathbb{Z}$, say; now set

$$(D_q(G))_{u,v} = [\alpha_{uv}] := \frac{q^{\alpha_{uv}} - 1}{q - 1} = 1 + q + \cdots + q^{\alpha_{uv}-1}, \tag{2.2}$$

where q is a formal parameter. Thus we work over the field $\mathbb{Q}(q)$. Notice that

$$D_q(G) = (q-1)^{-1}(D^*_q(G) - J), \tag{2.3}$$

where $D^*_q(G)$ is the "q-multiplicative" $V \times V$ matrix with (u,v) entry $q^{d(u,v)}$; now specializing $q \to 1$ (for integer entries $d(u,v)$) yields precisely the classical distance matrix $(d(u,v))_{u,v}$. Thus, $D_q(G)$ is an "intermediate" matrix used to pass from $D^*_q(G)$ (or more generally, the multiplicative variant D^*_G) to $D_G = D_1(G)$, and we have Graham–Hoffman–Hosoya type formulas (1.11) and (1.12) for the two "endpoints" of this procedure:

$$\begin{aligned}
\det(D^*_G) &= \prod_j \det(D^*_{G_j}),\\
\operatorname{cof}(D^*_G) &= \prod_j \det(D^*_{G_j}) + \sum_j (\operatorname{cof}(D^*_{G_j}) - \det(D^*_{G_j})) \prod_{i\neq j} \det(D^*_{G_i}),\\
\det(D_G) &= \sum_j \det(D_{G_j}) \prod_{i\neq j} \operatorname{cof}(D_{G_i}),\\
\operatorname{cof}(D_G) &= \prod_j \operatorname{cof}(D_{G_j}).
\end{aligned}$$

The following result presents the corresponding formulas for the intermediate matrices $D_q(G)$:

Proposition 2.3 (q-GHH identities)**.** *Say G is a directed strongly connected graph with node set V, and $D \in \mathbb{Z}^{V\times V}$ is any matrix such that $d(v,v) = 0\ \forall v \in V$, and if every directed path from $u \to v$ passes through the cut vertex v_0, then $d(u,v) = d(u,v_0) + d(v_0,v)$. Now let the $V \times V$ matrix $D_q(G)$ have (u,v) entry $[d(u,v)] = (q-1)^{-1}(q^{d(u,v)} - 1)$. If G has strong blocks G_j with corresponding principal submatrices $D_q(G_j)$, then defining $d^*_j := (q-1)\det(D_q(G_j)) + \operatorname{cof}(D_q(G_j))$, we have:*

$$\begin{aligned}
\det(D_q(G)) &= \sum_j \det(D_q(G_j)) \prod_{i\neq j} d^*_i,\\
\operatorname{cof}(D_q(G)) &= \prod_j d^*_j - (q-1)\sum_j \det(D_q(G_j)) \prod_{i\neq j} d^*_i.
\end{aligned} \tag{2.4}$$

The proof is omitted, as it is merely a computation using Theorem C (and Lemma 1.8), via (2.3).

Remark 2.4. The restriction that $d(u,v) \in \mathbb{Z}$ in $D_q(G)$ was merely in order to work in a familiar setting. However, Proposition 2.3 allows $d(u,v)$ to take values in an arbitrary abelian group Γ; it would then hold in the group algebra $\mathbb{Z}[q^\Gamma] \cong \mathbb{Z}[\Gamma]$. Once again, these formulas can be shown using the polynomiality of $\det(D_q(G))$ and $\operatorname{cof}(D_q(G))$ in the matrix entries.

Remark 2.5. In addition to implying the additive Graham–Hoffman–Hosoya identities (1.11), our q-variant also implies that $\det(D_q(G)), \operatorname{cof}(D_q(G))$, and $\operatorname{cof}(D_q(G))/\det(D_q(G)) = \mathbf{e}^T D_q(G)^{-1}\mathbf{e}$ depend only on the corresponding quantities for the strong blocks G_j of G, and not on the block/tree structure of G. This immediately proves all such observations made in the literature, see e.g. [20], and has perhaps an advantage over the variants in the literature that use q-cofsum$(D_q(G))$ or $\xi(D_q(G))$, since deducing from the latter the invariance of $\mathbf{e}D_q(G)^{-1}\mathbf{e}$ is not as immediate.

In turn, Proposition 2.3 leads to (a novel proof of) the original additive GHH-identities:

Proposition 2.6. *Notation as in Proposition 2.3, except that now D has entries $d(u,v)$ in a general unital commutative ring R. If G_j denote the strong blocks of G, with corresponding principal submatrices D_{G_j}, then the identities* (1.11) *follow from Theorem C (via Proposition 2.3):*

$$\operatorname{cof}(D_G) = \prod_j \operatorname{cof}(D_{G_j}), \qquad \det(D_G) = \sum_j \det(D_{G_j}) \prod_{k\neq j} \operatorname{cof}(D_{G_k}).$$

Proof. The result for integer values of $d(u,v)$ is immediate by setting $q = 1$ in Proposition 2.3, since then $d^*_j = \operatorname{cof}(D_{G_j})$. Now to go from such matrices with integer entries to arbitrary unital commutative rings uses a Zariski density argument, given that $\det(D_G), \operatorname{cof}(D_G)$ are polynomials in the matrix entries in $E := \bigsqcup_k \overrightarrow{E}(G_k)$, where $\overrightarrow{E}(G_k)$ runs over the directed edges of the strong block G_k of G. We work over the ring $R_0 := \mathbb{Q}(E)$, and denote by $p_d, p_c \in \mathbb{Z}[E]$ the polynomials

$$p_d := \det(D_G) - \sum_j \det(D_{G_j}) \prod_{i\neq j} \operatorname{cof}(D_{G_i}), \qquad p_c := \operatorname{cof}(D_G) - \prod_j \operatorname{cof}(D_{G_j}).$$

Since p_d, p_c vanish on $\mathbb{Z}^E_{>0}$, which is Zariski dense in $\mathbb{Q}^E$ by Lemma 2.1(3), it follows that $p_d = p_c = 0$ in $\mathbb{Z}[E]$. The proof concludes by specializing to an arbitrary unital commutative ring. $\square$

Remark 2.7. Suppose $d(u,v) \in \mathbb{Z}\ \forall u,v \in V$, and define the matrix $D^*_q(G)$ to have (u,v) entry $q^{d(u,v)}$, where q is a parameter as above. Then it is possible to jump directly from $D^*_q(G)$ to D_G:

$$\begin{aligned}\lim_{q\to 1}(q-1)^{-|V|}(\det - \operatorname{cof})(D^*_q(G)) =&\ \det(D_G),\\ \lim_{q\to 1}(q-1)^{1-|V|}\det(D^*_q(G)) =&\ \operatorname{cof}(D_G),\end{aligned} \tag{2.5}$$

where $q \to 1$ stands for setting $q=1$ after dividing by the relevant power of $q-1$. Notice that while the first of these formulas can be anticipated from previous papers (see Remark 2.2), the latter formula is new, or at least not immediately clear. Also, the specializations in (2.5) mean that Theorem C is more general than its classical, additive version in [13].

To show (2.5), we again appeal to $D_q(G)$. The first of the identities (2.5) follows immediately from Lemma 1.8, since $D^*_q(G) = (q-1)D_q(G) + J$. This last equality also implies

$$(q-1)^{|V|}\det(D_q(G)) + (q-1)^{|V|-1}\operatorname{cof}(D_q(G)) = \det(D^*_q(G)),$$

via Lemma 1.8. Subtracting from this the first of the formulas (2.5) (times $(q-1)^{|V|}$) yields:

$$(q-1)^{|V|-1}\operatorname{cof}(D_q(G)) = \operatorname{cof}(D^*_q(G)),$$

so that $\operatorname{cof}(D_G) = \lim_{q\to 1}(q-1)^{1-|V|}\operatorname{cof}(D^*_q(G))$. Now the first identity in (2.5) implies the claim:

$$\lim_{q\to 1}(q-1)^{1-|V|}\operatorname{cof}(D^*_q(G)) = \lim_{q\to 1}(q-1)^{1-|V|}\det(D^*_q(G)).$$

2.2. **Application 2: inverse identities.** In several papers in the literature (see the remarks prior to Theorem B for trees; but also e.g. [17, 18]), the inverse of distance matrices of graphs is computed. These are additive matrices of specific graphs G, and we now discuss a recipe to obtain such formulas for general strongly connected G.

Recall that the previous subsection discussed formulas for $\det(\cdot)$ and $\operatorname{cof}(\cdot)$ for strongly connected graphs in terms of their strong blocks – for both the q- and classical distance matrices. These formulas were obtained as consequences of Theorem C – which contains identities for $\det(D^*_G)$ and $\operatorname{cof}(D^*_G)$, but also for $(D^*_G)^{-1}$. In that spirit, we now record the analogous identity for $D_q(G)^{-1}$ in terms of the matrices $D_q(G_j)^{-1}$. (This is done for completeness, and in slightly greater generality; we leave to the interested reader the explicit such identity, as well as its specialization to $q=1$.)

Proposition 2.8. *Notation as in Theorem C; assume $k_v = 1\ \forall v \in V$. Let*

$$\mathbf{u}_j := [(D^*_{G_j})^{-1}]_j[\mathbf{e}(|V(G_j)|)]_j \in R^V,$$

where $[\mathbf{v}]_j$ denotes the $|V|\times 1$ vector in which the entries of $\mathbf{v} \in R^{|V(G_j)|}$ occur in the rows corresponding to the nodes of G_j, with all other entries zero; and similarly, $[A]_j$ denotes the $|V|\times|V|$ matrix with the matrix $A \in R^{|V(G_j)|\times|V(G_j)|}$ occurring in the rows and columns corresponding to the nodes of G_j, with all other entries zero. Also let $\mathbf{e}_{cut} \in R^V$ denote the $\{0,1\}$-vector with ones in precisely the coordinates corresponding to V^{cut}. Then for x an indeterminate over R,

$$\begin{aligned}(D^*_G + xJ)^{-1} =&\ \sum_j \left(\left[(D^*_{G_j} + xJ)^{-1} \right]_j + \frac{x\det(D^*_{G_j})}{\det(D^*_{G_j} + xJ)}\mathbf{u}_j\mathbf{u}_j^T \right) - \sum_{v\in V^{cut}} E_{v,v}\\ &- \frac{x\det(D^*_G)}{\det(D^*_G + xJ)}\left(-\mathbf{e}_{cut} + \sum_j \mathbf{u}_j\right)\left(-\mathbf{e}_{cut} + \sum_j \mathbf{u}_j\right)^T.\end{aligned} \tag{2.6}$$

Here $E_{v,v}$ is the elementary matrix with (i,j) entry $\delta_{i,v}\delta_{v,j}$. The proof involves carefully applying the above results as well as the Sherman–Morrison formula for the inverse of a rank-one update.

The point is that this result provides a closed-form expression for the inverse of $\widetilde{D}_G := D^*_G + xJ$ in terms of the inverse and invariants for $\widetilde{D}_{G_j} := D^*_{G_j} + xJ$. Indeed, one now writes $D^*_{G_j} = \widetilde{D}_{G_j} - xJ$, and using Theorem C, one also writes $\det(D^*_G), \det(D^*_G + xJ)$ in terms of $\det(\widetilde{D}_{G_j}), \operatorname{cof}(\widetilde{D}_{G_j})$. Moreover, by the final assertion in Lemma 1.8, $\mathbf{u}_j$ can also be written purely in terms of $\widetilde{D}_{G_j}$:

$$\mathbf{u}_j = \frac{\det(\widetilde{D}_{G_j})}{\det(\widetilde{D}_{G_j} - xJ)}[(\widetilde{D}_{G_j} - xJ)^{-1}]_j[\mathbf{e}(|V(G_j)|)]_j.$$

Now if $D_q(G)$ denotes the usual q-distance matrix for G, and $D^*_G = D^*_q(G)$, then $D_q(G) = (q-1)^{-1}\widetilde{D}_G|_{x=-1}$. This and the above result allow one to compute $D_q(G)^{-1}$. Specializing to $q = 1$ yields a formula for D_G^{-1} that subsumes special cases in [3]–[7], [14, 17, 18, 25, 26].

Remark 2.9. Proposition 2.8 can be further generalized to the setting of Theorem C, in which D^*_G is no longer $|V| \times |V|$. We leave to the interested reader the similar formulation and proof.

2.3. **Application 3: adding pendant trees.** The next application of our above results generalizes several results in the literature for graphs outside of trees. We provide detailed references below; in all of them, the classical or q-distance matrix is what has been studied.

As a first step, the (multiplicative and q-) Graham–Hoffman–Hosoya identities in Theorem C and Proposition 2.3 immediately give that the changes in the determinant and cofactor that occur due to "attaching trees to graphs", depend only on the set of additional nodes/edges:

Corollary 2.10. *If G is as in Theorem C, and G' is obtained by attaching finitely many pendant trees T_j to the nodes of G, with a total of m additional bi-directed edges, then*

$$\det(D^*_{G'}), \quad \operatorname{cof}(D^*_{G'}), \quad \det(D_q(G')), \quad \operatorname{cof}(D_q(G'))$$

are independent of the structure or location of the T_j, and depend only on G and the m edge-data.

Consider the special case $k_v = 1$ for all nodes v of G. Then we are dealing with the q-distance matrix, and one can use Proposition 2.3 and $\det(D_q(T)), \operatorname{cof}(D_q(T))$ for T each attached edge:

Proposition 2.11. *Let $k \geqslant 1$ be an integer, and for each $j \in [k]$ let G_j be a weighted bi-directed graph on p_j nodes, with q-distance matrix $D_q(G_j)$ that satisfies:*

$$D_q(G_j)\mathbf{e}(p_j) = d_j\mathbf{e}(p_j), \qquad \forall j \in [k],$$

where $d_j \in R$ are scalars. Now let G be any strongly connected graph with strong blocks $G_1, \dots, G_k$, and let G' be obtained from G by further attaching finitely many pendant trees to the nodes of G, with a total of m new vertices and hence m new bi-directed edges E with weights $\{(\alpha_e, \alpha'_e) : e \in E\}$.

Then $\det(D_q(G')), \operatorname{cof}(D_q(G'))$ depend not on the structure and location of the attached trees, but only on their edge-data, and as follows:

$$\begin{aligned}\det(D_q(G') + xJ) = &\prod_{j=1}^k \det(D_q(G_j)) \prod_{j=1}^k (q - 1 + (p_j/d_j)) \prod_{e\in E}(-[\alpha_e + \alpha'_e])\times \\ &\times \left[x + (1-(q-1)x)\left(\sum_{j=1}^k \frac{1}{q-1+(p_j/d_j)} + \sum_{e\in E}\frac{[\alpha_e][\alpha'_e]}{[\alpha_e + \alpha'_e]}\right)\right].\end{aligned} \tag{2.7}$$

We omit the proof as it is a straightforward consequence of Proposition 2.3 and Lemma 1.8.

Remark 2.12. Proposition 2.11 simultaneously generalizes a host of results in the literature. First, it subsumes all undirected q-weighted trees – by letting G have two nodes and one edge – hence all undirected additively weighted trees as well (setting $q=1$). Next, it also extends [19, Theorem 7] (which addressed the special case $\alpha_e = \alpha'_e\ \forall e$ and $x=0$), as well as [3, Theorem 2.3], which dealt with the special case $\alpha_e = \alpha'_e\ \forall e$ and $q=1$ (so $[\alpha]=\alpha$). Finally, Proposition 2.11 specialized to $G_1 = \cdots = G_m$ and adding *no* extra trees, recovers certain results of Sivasubramanian [20].

2.4. **Application 4: cycle-clique graphs and special cases.** As a final application of Theorem C and its applications above, we study *cycle-clique graphs*. These are unweighted graphs G whose strong blocks are cycles and complete graphs. Special cases include unicyclic, bicyclic, and cactus graphs – where each of the complete subgraphs is an edge, and the number of cycle-blocks is one, two, or greater, respectively. For G a unicyclic or bicyclic graph, $\det(D_q(G))$ has been computed in e.g. [3, 12, 19]; and moreover, $\det(D_G)$ for an arbitrary cycle-clique graph G was computed in [18]. Another special case is the family of *regular hypertrees* – see [20] – whose distance matrices precisely coincide with those of graphs whose strong blocks are isomorphic cliques.

In our final application, we extend all of these formulas to arbitrary cycle-clique graphs, in two ways. First, we allow for weighted edges; and second, we explain how our results above help compute $\det(D_q(G)+xJ)$. In other words, we also compute $\operatorname{cof}(D_q(G))$, and not only for $q=1$.

Our setting is as follows: G is a weighted strongly connected graph with strong blocks

$$C_{r_1},\ \ldots,\ C_{r_k}, \quad K_{p_1},\ \ldots,\ K_{p_m}, \qquad (r_j, p_i \geqslant 1)$$

where C_r, K_p denote the cycle and complete graphs with node sets $[r],[p]$ respectively. Notice that under a suitable labelling of the nodes of C_r, if all edges have weight β, then $D_q(C_r)$ is a symmetric Toeplitz circulant matrix, with super/sub diagonal entries $[\beta] = (q-1)^{-1}(q^\beta - 1)$. Denote this matrix by $D_q(C_r;\beta)$. Then all rows and columns of $D_q(C_r;\beta)$ have the same sum.

Lemma 2.13. *With the above notation, if $d_{r,\beta}$ is the common row/column sum of $D_q(C_r;\beta)$, then $\operatorname{cof}(D_q(C_r;\beta)) = \frac{r}{d_{r,\beta}} \det(D_q(C_r;\beta))$ for $r \geqslant 1$, where for $r=1$ we define $\det(D_q(C_1;\beta))/d_{1,\beta} := 1$.*

Since $D_q(C_r;\beta)$ is a circulant matrix for each $r \geqslant 1$, its determinant has a well-known closed-form expression using roots of unity (say working over some extension of our ground ring R).

Proof. Apply Proposition 2.11 to $G = C_r$ (with edgeweights $[\beta]$), with $m=0$ new edges added. ☐

The other kind of blocks are the cliques (complete subgraphs) in G. We first study the q-distance matrix of each such graph K_p, again under a suitable labelling of the nodes. The following model generalizes the $p=2$ case of bi-directed edges with weights a_e, a'_e:

Definition 2.14. Given an integer $p \geqslant 1$ and elements a, a' in a unital commutative ring, let $D(K_p;a,a')$ denote the matrix with (i,j) entry $a,\ 0,\ a'$ for $i<j,\ i=j,\ i>j$ respectively. Then $D(K_p;a,a')$ is a Toeplitz matrix, which we will denote using its entries in the first column (bottom to top) and then the first row (left to right):

$$D(K_p;a,a') = \operatorname{Toep}(a',\ldots,a';\ 0;\ a,\ldots,a).$$

Lemma 2.15. *With the above notation,*

$$\begin{aligned}
\det D(K_p;a,a') &= (-1)^{p-1} a a' \, \frac{a^{p-1} - (a')^{p-1}}{a - a'}, \\
\operatorname{cof} D(K_p;a,a') &= (-1)^{p-1} \, \frac{a^p - (a')^p}{a-a'}, \\
\operatorname{adj} D(K_p;a,a') &= (-1)^{p-1} \operatorname{Toep}((a')^{p-1}, (a')^{p-2}a, \ldots, a' a^{p-2};\ \alpha;\ (a')^{p-2}a, \ldots, a^{p-1}),
\end{aligned} \tag{2.8}$$

where $\alpha = -aa' \, \dfrac{a^{p-2} - (a')^{p-2}}{a-a'}$ and $p \geqslant 2$ in the last equation; while for $p=1$ we have

$$\operatorname{adj}(D(K_1;a,a')) = \operatorname{cof}(D(K_1;a,a')) = 1.$$

Proof. First compute $\det D(K_p; a, a')$ by induction on p. Next, work over the field $R_0 = \mathbb{Q}(a, a')$, and assume by a Zariski density argument using Lemma 2.1 that $D(K_p; a, a')$ is invertible; indeed, this is so whenever $a = a' \neq 0$, since $\det D(K_p; a, a) = \det a(J - \mathrm{Id}) = (-1)^{p-1} a^p (p-1)$. This yields the expression for $\mathrm{adj}(\cdot)$ via an easy verification. This shows the result over R_0; now Zariski density arguments as above imply the result over any unital commutative ring R. Finally, the assertion for $\mathrm{cof}(\cdot)$ is shown via another computation that uses Lemma 1.8 and the formula for $\mathrm{adj}(\cdot)$. ☐

With these results in hand, one can show:

Theorem 2.16. *Let G be a connected cycle-clique graph whose strong blocks are cycles $C_{r_1}, \dots, C_{r_k}$ and complete subgraphs $K_{p_1}, \dots, K_{p_m}$, with all $r_j, p_i \geqslant 1$. Also assume there exist scalars*

$$\beta_1, \ \dots, \ \beta_k; \quad \alpha_1, \alpha'_1, \ \dots, \ \alpha_m, \alpha'_m$$

and a labelling of the nodes of G such that the q-distance matrices of the blocks are of the form

$$D_q(C_{r_j}; \beta_j), \ j \in [k] \qquad \text{and} \qquad D(K_{p_i}; [\alpha_i], [\alpha'_i]), \ i \in [m].$$

1. *Then $\det(D_q(G)), \mathrm{cof}(D_q(G))$ have closed-form expressions which can be derived using Lemmas 2.13 and 2.15 and Proposition 2.3.*
2. *A sample special case: say $\beta_j = 1 \ \forall j$, and $d_{r,1}$ is as in Lemma 2.13. Also say $p_i = 2 \ \forall i$ and denote these 2-cliques/edges $i \in [m]$ by $e \in E$. Then the formulas in part (1) specialize to:*

$$\begin{aligned} \det(D_q(G) + xJ) = & \prod_{j=1}^{k} \left((q-1) \det D_q(C_{r_j}) + r_j \frac{\det D_q(C_{r_j})}{d_{r_j,1}} \right) \prod_{e \in E} (-[\alpha_e + \alpha'_e]) \times \\ & \times \left[x + (1 - (q-1)x) \left(\sum_{j=1}^{k} \frac{d_{r_j,1}}{(q-1) d_{r_j,1} + r_j} + \sum_{e \in E} \frac{[\alpha_e][\alpha'_e]}{[\alpha_e + \alpha'_e]} \right) \right]. \end{aligned} \tag{2.9}$$

3. *Another special case: suppose the strong blocks of G are cliques of sizes $p_1, \dots, p_m$. Then,*

$$\det(D_q(G) + xJ) = (-1)^{\sum_i (p_i - 1)} \prod_{i=1}^{m} (p_i q - q + 1) \left[x + (1 - (q-1)x) \sum_{i=1}^{p} \frac{p_i - 1}{p_i q - q + 1} \right], \tag{2.10}$$

where the denominators are again placeholders, cancelled by factors in the numerators.

We omit the proof as it involves straightforward computations using the results shown above.

As mentioned above, Theorem 2.16 subsumes the corresponding results in [3, 12, 18, 19, 20]. For instance, (2.10) is a twofold generalization of a result in [20], where it was shown in the special case $p_i = 3 \ \forall i, \ x = 0$. As another special case, the determinant of the classical additive distance matrix over such a cycle-clique graph is now stated:

Corollary 2.17. *In the setting of Theorem 2.16, specialize to $q = 1$, $\alpha_i = \alpha'_i = 1 \ \forall i \in [m]$, $\beta_j = 1 \ \forall j \in [r]$. Then $\det(D(G) + xJ)$ vanishes if any cycle (i.e. r_j) is even, else*

$$\det(D(G) + xJ) = \prod_{j=1}^{k} r_j \prod_{i=1}^{m} ((-1)^{p_i - 1} p_i) \left(x + \sum_{i=1}^{m} \frac{p_i - 1}{p_i} + \sum_{j=1}^{k} \frac{1}{r_j} \lfloor r_j/2 \rfloor \lceil r_j/2 \rceil \right). \tag{2.11}$$

In the further special case $x = 0$, this formula subsumes various results in the literature – see prior to Corollary 2.17. Note that it is another sample special case of Theorem 2.16(1), and again follows from Lemmas 2.13 and 2.15 and Proposition 2.3. The proof of (2.11) uses the fact that $\det D(C_r)$ is zero if r is even, and equals $d_{r,1} = \lfloor r/2 \rfloor \lceil r/2 \rceil$ otherwise (see e.g. [3, Theorem 3.4]).

3. Inverse, determinant, cofactor-sum of the general distance matrix: Theorems A, B

We now return to trees. A natural question – pursued for all variants of $D_{\mathcal{T}}$ studied to date – is to compute $D_{\mathcal{T}}^{-1}$. This was first carried out by Graham and Lovász in [14]; in this case and subsequent variants, $D_{\mathcal{T}}^{-1}$ is usually a rank-one update of a related "Laplacian" matrix or a q-version thereof. Later in [4], Bapat–Lal–Pati worked with $m_e = m'_e = q$ and $a_e = a'_e \ \forall e \in E$, and wrote: "*... it appears that such a formula [for $D_{\mathcal{T}}^{-1}$] will be very complicated and we leave it as an open problem.*"

We now prove Theorem B, which provides a closed-form expression for $D_{\mathcal{T}}^{-1}$ in our general framework, hence resolves the open question in [4] in greater generality and also extends the Graham–Lovász result. As a by-product of our proof, we will obtain closed-form expressions for $\det(D_{\mathcal{T}}), \operatorname{cof}(D_{\mathcal{T}})$, and will then prove the rest of Theorem A.

We begin by explaining the matrix $C_{\mathcal{T}}$ in Theorem B, via some notation:

Definition 3.1. Setting as in Theorem A. In other words, $T = (V, E)$ is a tree on n nodes with edge-data $\mathcal{T} = \{(a_e = a'_e, m_e, m'_e) : e \in E\}$.

(1) Define the scalar

$$\alpha_{\mathcal{T}} := \sum_{e \in E} \frac{a_e(m_e - 1)(m'_e - 1)}{m_e m'_e - 1}. \tag{3.1}$$

In working with $\alpha_{\mathcal{T}}$ in the proof below, we will assume that $m_e m'_e - 1$ is invertible in R, as is (the numerator of the rational function) $\alpha_{\mathcal{T}}$, via a Zariski density argument.

(2) Given adjacent nodes $i \sim j$, define $T_{i \to j}$ to be the sub-tree induced on i, j, and all nodes $v \in V$ such that the path from i to v passes through j. Note this partitions the edge-set:

$$E = \bigsqcup_{j : j \sim i} E(T_{i \to j}), \qquad \forall i \in V.$$

(3) Finally, define for $i \in V$ the scalar

$$\beta_i := \frac{1}{\alpha_{\mathcal{T}}} \sum_{j : j \sim i} \frac{1}{a_{ij}} \sum_{e \in E(T_{i \to j})} \frac{a_e(m_e - 1)(m'_e - 1)}{m_e m'_e - 1}, \tag{3.2}$$

where we assume by Zariski density that $a_e, m_e m'_e - 1$ are invertible for all e, as is $\alpha_{\mathcal{T}}$.

With this notation in hand, we finally define $C_{\mathcal{T}}$ to have entries

$$(C_{\mathcal{T}})_{ij} := \begin{cases} \beta_i, & \text{if } j = i; \\ \beta_i - \frac{1}{a_{ik}}, & \text{if } j \neq i, \ j \in T_{i \to k}. \end{cases} \tag{3.3}$$

Remark 3.2. If $i \in V$ is pendant with neighbor $p(i)$, then $\beta_i = \frac{1}{a_{i,p(i)}}$ and $C_{\mathcal{T}}$ has ith row $\frac{1}{a_{i,p(i)}} \mathbf{e}_i^T$.

Now we are ready to compute the inverse of $D_{\mathcal{T}}$, as asserted in Theorem B:

$$D_{\mathcal{T}}^{-1} = \frac{1}{\alpha_{\mathcal{T}}} \boldsymbol{\tau}_{\text{out}} \boldsymbol{\tau}_{\text{in}}^T - L_{\mathcal{T}} + C_{\mathcal{T}} \operatorname{diag}(\boldsymbol{\tau}_{\text{in}}),$$

where the vectors $\boldsymbol{\tau}_{\text{in}}, \boldsymbol{\tau}_{\text{out}} \in R^V$ and the Laplacian matrix $L_{\mathcal{T}} \in R^{V \times V}$ were defined in Theorem B. Note for this Laplacian that $\mathbf{e}^T L_{\mathcal{T}} = 0$.

Proof of Theorem B. This proof is self-contained, modulo one fact which was shown in the "multiplicative" special case above: the nonvanishing of $\det(D_{\mathcal{T}})$. Hence we may assume via Zariski density that $\det(D_{\mathcal{T}}) \in R^\times$. In particular, we work throughout this proof over the ring $R = R_0 := \mathbb{Q}(\{a_e, m_e, m'_e : e \in E\})$, and then observe that all of the results proved hold (by Zariski density) over $\mathbb{Z}[\{a_e, m_e, m'_e : e \in E\}]$, hence in any unital commutative ring by specialization.

In addition to $\det(D_{\mathcal{T}})$, we also use via Zariski density that the quantities $a_e,\ m_e m'_e - 1,\ m_e - 1,\ m'_e - 1, \alpha_{\mathcal{T}}$ are invertible in $R = R_0$. We use the following notation without further reference: for nodes $i \neq j$ let m_{ij} denote the product of the edgeweights over the unique directed path in T from i to j. Also set $m_{ii} = 1$. Let the vector $\mathbf{m}_{\bullet \to j} \in R^{V \times 1}$ have ith coordinate m_{ij}; here $i, j \in V$.

We now prove the result; the proof is split into steps for ease of exposition.

Step 1. We begin by showing the following identities:

$$\boldsymbol{\tau}_{\text{in}}^T \mathbf{m}_{\bullet \to l} = 1, \qquad \forall l \in V; \tag{3.4}$$

$$\boldsymbol{\tau}_{\text{in}}^T \mathbf{e} = \mathbf{e}^T \boldsymbol{\tau}_{\text{out}} = 1 - \sum_{e \in E} \frac{(m_e - 1)(m'_e - 1)}{m_e m'_e - 1}; \tag{3.5}$$

$$\mathbf{e}^T C_{\mathcal{T}} = \frac{1}{\alpha_{\mathcal{T}}} \sum_{e \in E} \frac{(m_e - 1)(m'_e - 1)}{m_e m'_e - 1} \cdot \mathbf{e}^T; \tag{3.6}$$

To prove (3.4), first convert the sum over nodes into a sum over edges. For each edge $e = \{i, j\} \in E$, if j lies on the path between i and l, then the terms in $(\boldsymbol{\tau}_{\text{in}}^T - \mathbf{e}^T)\mathbf{m}_{\bullet \to l}$ on the left-hand side of (3.4) corresponding to $e = \{i, j\}$ contribute precisely

$$(1 - m_e m'_e)^{-1} \left(m_{ji}(m_{ij} - 1) m_{il} + m_{ij}(m_{ji} - 1) m_{jl} \right) = -m_{il},$$

where the positions of i, j, l imply: $m_{il} = m_{ij} m_{jl}$. Therefore,

$$\boldsymbol{\tau}_{\text{in}}^T \mathbf{m}_{\bullet \to l} = \sum_{i \in V} m_{il} - \sum_{e \in E} m_{i_l(e) l}, \tag{3.7}$$

where $i_l(e)$ is the vertex of $e \in E$ that is farther away from l. Now the map $i_l : E \to V \setminus \{l\}$ is a bijection, since T is a tree. Hence the above computation yields precisely $m_{ll} = 1$, proving (3.4).

We next show (3.5). The first equality is easily shown by converting sums over nodes to ones over edges. For the second equality, by summing the components of $\boldsymbol{\tau}_{\text{out}}$ and again converting the sum over nodes to one over edges, one obtains

$$1 + \sum_{e \in E} \left(1 - \frac{m_e(m'_e - 1)}{m_e m'_e - 1} - \frac{m'_e(m_e - 1)}{m_e m'_e - 1} \right) = 1 + \sum_{e \in E} \frac{-(m_e - 1)(m'_e - 1)}{m_e m'_e - 1},$$

as desired. We next turn to (3.6). For each $j \in V$, note that

$$(\mathbf{e}^T C_{\mathcal{T}})_j = \sum_{i \in V} \beta_i - \sum_{i \in V \setminus \{j\}} \frac{1}{a_{ik}},$$

where the k in the final summand is such that $j \in T_{i \to k}$ – in other words, k is the neighbor of i that is closest to j. Now by the reasoning following (3.7), the latter sum can be converted into a sum over edges to yield precisely $\displaystyle\sum_{e \in E} \frac{1}{a_e}$. As for the former sum, first write for convenience:

$$\varphi_e := \frac{a_e(m_e - 1)(m'_e - 1)}{m_e m'_e - 1};$$

thus e.g. $\alpha_{\mathcal{T}} = \displaystyle\sum_{e \in E} \varphi_e$. Now convert $\sum_i \beta_i$, which is a sum over nodes, into one over edges:

$$\sum_i \beta_i = \frac{1}{\alpha_{\mathcal{T}}} \sum_i \sum_{k \sim i} \frac{1}{a_{ik}} \sum_{e \in E(T_{i \to k})} \varphi_e = \frac{1}{\alpha_{\mathcal{T}}} \sum_{e = \{i,j\} \in E} \frac{1}{a_e} \left(\sum_{f \in E(T_{i \to j})} \varphi_f + \sum_{f \in E(T_{j \to i})} \varphi_f \right).$$

The summand in the outer sum on the right is $\dfrac{1}{a_e}\,(\alpha_{\mathcal{T}} + \varphi_e)$. Combining these shows (3.6):

$$(\mathbf{e}^T C_{\mathcal{T}})_j = \frac{1}{\alpha_{\mathcal{T}}} \sum_{e \in E} \frac{\alpha_{\mathcal{T}} + \varphi_e}{a_e} - \sum_{e \in E} \frac{1}{a_e} = \frac{1}{\alpha_{\mathcal{T}}} \sum_{e \in E} \frac{\varphi_e}{a_e},$$

Step 2. We claim the following identity also holds for each fixed node $l \in V$:

$$C_{\mathcal{T}} \mathbf{e}_l = (-L_{\mathcal{T}} + C_{\mathcal{T}} \operatorname{diag}(\boldsymbol{\tau}_{\text{in}}))\mathbf{m}_{\bullet \to l}, \quad l \in V. \tag{3.8}$$

We will show the equality of the ith components, for all $i, l \in V$. First note that the ith component of the left-hand side is β_i for $i = l$, else it is $\beta_i - \frac{1}{a_{ik_0}}$, where $k_0 \sim i$ is between i and l.

We claim the ith component of the right-hand side is the same. Let $\mathbf{r}_i$ denote the ith row of $-L_{\mathcal{T}} + C_{\mathcal{T}} \operatorname{diag}(\boldsymbol{\tau}_{\text{in}})$. To show $\mathbf{r}_i \cdot \mathbf{m}_{\bullet \to l}$ equals β_i or $\beta_i - \frac{1}{a_{ik_0}}$, we will partition the dot-product

$$\mathbf{r}_i \cdot \mathbf{m}_{\bullet \to l} = \sum_{v \in V} (\mathbf{r}_i)_v m_{vl} \tag{3.9}$$

into sub-summations over $V(T_{i \to k}) \setminus \{i\}$, running over $k \sim i$ – and to each such sum, we will add a component of the ith summand of (3.9). (Recall that the sets $V(T_{i \to k}) \setminus \{i\}$ partition $V \setminus \{i\}$.)

First write out the ith summand of (3.9):

$$\sum_{k \sim i} \frac{-m_{ki}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{il} + (\boldsymbol{\tau}_{\text{in}})_i \beta_i m_{il}. \tag{3.10}$$

Consider only the sum of the terms in (3.9) that contain the β_i's that come from $C_{\mathcal{T}}$ (i.e. from $(\mathbf{r}_i)_v$). Each entry of the ith row of $C_{\mathcal{T}}$ contains a β_i term, and by (3.4) these contribute

$$\beta_i\, \mathbf{e}^T \operatorname{diag}(\boldsymbol{\tau}_{\text{in}}) \cdot \mathbf{m}_{\bullet \to l} = \beta_i \cdot \boldsymbol{\tau}_{\text{in}}^T \mathbf{m}_{\bullet \to l} = \beta_i.$$

With these preliminaries, we proceed. Given a node $k \sim i$, let G_k denote the sub-tree induced on $T_{i \to k} \setminus \{i\}$; thus $V(G_k) = V(T_{i \to k}) \setminus \{i\}$. Using the above observations, the sum (3.9) equals

$$\mathbf{r}_i \cdot \mathbf{m}_{\bullet \to l} = \sum_{v \in V} (\mathbf{r}_i)_v m_{vl} = \beta_i + \sum_{k \sim i} \Psi_k, \tag{3.11}$$

where

$$\Psi_k := \frac{-m_{ki}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{il} + \frac{m_{ik}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{kl} + \frac{-1}{a_{ik}} \sum_{v \in V(G_k)} (\boldsymbol{\tau}_{\text{in}})_v m_{vl}. \tag{3.12}$$

We now claim that $\Psi_k = 0$ if $l \notin V(G_k)$. Indeed, $m_{vl} = m_{vk} m_{kl}$ for $v \in V(G_k)$, and taking m_{kl} common outside of the latter sum yields an expression analogous to (3.4), but for G_k. There is but one extra component in this sum in the $v = k$ term:

$$\begin{aligned}
\Psi_k &= \frac{-m_{ki}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{il} + \frac{m_{ik}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{kl} + \frac{-m_{kl}}{a_{ik}} \left((\boldsymbol{\tau}_{\text{in}}^{(G_k)})^T \mathbf{m}_{\bullet \to k}^{(G_k)} - \frac{m_{ik}(m_{ki} - 1)}{m_{ik} m_{ki} - 1} \right) \\
&= \frac{-m_{ki}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{il} + \frac{m_{kl}}{a_{ik}(m_{ik} m_{ki} - 1)} \left(m_{ik} - (m_{ik} m_{ki} - 1) + m_{ik}(m_{ki} - 1) \right) \\
&= \frac{-m_{ki}}{a_{ik}(m_{ik} m_{ki} - 1)} \cdot m_{il} + \frac{m_{kl}}{a_{ik}(m_{ik} m_{ki} - 1)}.
\end{aligned}$$

(Here, $\boldsymbol{\tau}_{\text{in}}^{(G_k)}, \mathbf{m}_{\bullet \to k}^{(G_k)}$ are clear from context.) But this vanishes as $m_{kl} = m_{ki} m_{il}$. Hence $\Psi_k = 0$.

This already concludes the verification if $i = l$, by (3.11). Thus we suppose now that $i \neq l$, in which case there is a unique $k_0 \sim i$ such that $l \in T_{i \to k_0}$. Again by (3.11), it suffices to show that $\Psi_{k_0} = -1/a_{ik_0}$. But this essentially is a repetition of the above computation, where now we *do not* take an m_{kl} common. We leave the relevant details to the reader.

Step 3. We now prove our formula for the inverse of $D_{\mathcal{T}}$ by induction on n (or on $|E|$). The base case of $n = 2$ is a straightforward verification. For the induction step, we assume the formula for the inverse of $D = D_{\mathcal{T}}$ for a tree on k nodes:

$$D^{-1} = \frac{1}{\alpha}\boldsymbol{\tau}_{\text{out}}\boldsymbol{\tau}_{\text{in}}^T - L + C\operatorname{diag}(\boldsymbol{\tau}_{\text{in}}).$$

Here and below, $\alpha = \alpha_{\mathcal{T}}$, $L = L_{\mathcal{T}}$, and $C = C_{\mathcal{T}}$. Now using the identities (3.4)–(3.8) from Step 1,

$$\mathbf{e}^T D^{-1} = \frac{1}{\alpha}\boldsymbol{\tau}_{\text{in}}^T, \qquad D^{-1}\mathbf{m}_{\bullet\to k} = \frac{1}{\alpha}\boldsymbol{\tau}_{\text{out}} + C\mathbf{e}_k. \tag{3.13}$$

Write $D_{\mathcal{T}}$ over $k+1$ vertices as a block-matrix, assuming that node $k+1$ is pendant and $k+1 \sim k$:

$$\begin{aligned} \overline{D} &:= D_{\mathcal{T}_{k+1}} = \begin{pmatrix} D & \mathbf{u} \\ \mathbf{v}^T & 0 \end{pmatrix}, \\ \text{where } \mathbf{u} &:= D\mathbf{e}_k + a_{k,k+1}(m_{k,k+1} - 1)\mathbf{m}_{\bullet\to k}, \\ \text{and } \mathbf{v}^T &:= a_{k,k+1}(m_{k+1,k} - 1)\mathbf{e}(k)^T + m_{k+1,k}\mathbf{e}_k^T D. \end{aligned} \tag{3.14}$$

We write $\overline{D}, \overline{\alpha}, \overline{L}, \overline{\boldsymbol{\tau}_{\text{in}}}, \overline{\boldsymbol{\tau}_{\text{out}}}$ for the larger distance matrix (i.e., on $k+1$ nodes). Thus,

$$\overline{L} := \begin{pmatrix} L + \dfrac{m_{k+1,k}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k} - 1)}\mathbf{e}_k\mathbf{e}_k^T & \dfrac{-m_{k,k+1}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k} - 1)}\mathbf{e}_k \\ \dfrac{-m_{k+1,k}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k} - 1)}\mathbf{e}_k^T & \dfrac{m_{k,k+1}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k} - 1)} \end{pmatrix}, \tag{3.15}$$

$$\overline{\boldsymbol{\tau}_{\text{in}}} := \begin{pmatrix} \boldsymbol{\tau}_{\text{in}} - \dfrac{m_{k+1,k}(m_{k,k+1} - 1)}{m_{k,k+1}m_{k+1,k} - 1}\mathbf{e}_k \\ \dfrac{m_{k,k+1} - 1}{m_{k,k+1}m_{k+1,k} - 1} \end{pmatrix}, \tag{3.16}$$

$$\overline{\boldsymbol{\tau}_{\text{out}}} := \begin{pmatrix} \boldsymbol{\tau}_{\text{out}} - \dfrac{m_{k,k+1}(m_{k+1,k} - 1)}{m_{k,k+1}m_{k+1,k} - 1}\mathbf{e}_k \\ \dfrac{m_{k+1,k} - 1}{m_{k,k+1}m_{k+1,k} - 1} \end{pmatrix}, \tag{3.17}$$

$$\overline{\alpha} := \alpha + \frac{a_{k,k+1}(m_{k,k+1} - 1)(m_{k+1,k} - 1)}{m_{k,k+1}m_{k+1,k} - 1}. \tag{3.18}$$

Now recall the formula for the inverse of a block matrix – via Schur complements – and apply this to the distance matrix (3.14). The following assumes by Zariski density that $D, \overline{D}$ are invertible:

$$\overline{D}^{-1} = \begin{pmatrix} D^{-1} + \psi^{-1}D^{-1}\mathbf{u}\mathbf{v}^T D^{-1} & -\psi^{-1}D^{-1}\mathbf{u} \\ -\psi^{-1}\mathbf{v}^T D^{-1} & \psi^{-1} \end{pmatrix}, \qquad \text{where } \psi := -\mathbf{v}^T D^{-1}\mathbf{u} = \frac{\det \overline{D}}{\det D}. \tag{3.19}$$

In this step we compute ψ and show that ψ^{-1} equals the corresponding $(2,2)$-block of our claimed formula for the inverse:

$$\frac{1}{\overline{\alpha}}\overline{\boldsymbol{\tau}_{\text{out}}}\,\overline{\boldsymbol{\tau}_{\text{in}}}^T - \overline{L} + \overline{C}\operatorname{diag}(\overline{\boldsymbol{\tau}_{\text{in}}}), \tag{3.20}$$

where this matrix is partitioned in the same manner as (3.19). The other three components of the matrix (3.19) will then be computed in subsequent steps, together with showing that they equal the corresponding blocks of the matrix (3.20). This will conclude the proof. We begin by computing:

$$\begin{aligned} -\psi = \mathbf{v}^T D^{-1}\mathbf{u} &= (a_{k,k+1}(m_{k+1,k} - 1)\mathbf{e}(k)^T + m_{k+1,k}\mathbf{e}_k^T D)D^{-1}(D\mathbf{e}_k + a_{k,k+1}(m_{k,k+1} - 1)\mathbf{m}_{\bullet\to k}^{(k)}) \\ &= a_{k,k+1}(m_{k+1,k} - 1)\mathbf{e}(k)^T\mathbf{e}_k + a_{k,k+1}^2(m_{k+1,k} - 1)(m_{k,k+1} - 1)\mathbf{e}(k)^T \cdot D^{-1} \cdot \mathbf{m}_{\bullet\to k}^{(k)} \\ &\quad + m_{k+1,k}\mathbf{e}_k^T D\mathbf{e}_k + a_{k,k+1}m_{k+1,k}(m_{k,k+1} - 1)\mathbf{e}_k^T \cdot \mathbf{m}_{\bullet\to k}^{(k)}. \end{aligned}$$

The third term is zero; the first and fourth terms add up to $a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)$. Hence,

$$\psi = a_{k,k+1}(1-m_{k,k+1}m_{k+1,k}) - \frac{a_{k,k+1}^2}{\alpha}(m_{k,k+1}-1)(m_{k+1,k}-1) = \frac{a_{k,k+1}(1-m_{k,k+1}m_{k+1,k})\overline{\alpha}}{\alpha}, \tag{3.21}$$

where the first equality follows from (3.13) and (3.4).

As discussed following (3.19), we now show that ψ^{-1} equals the $(2,2)$-block of (3.20), to complete this step of the proof of Theorem B. The latter $(2,2)$-block equals the scalar

$$\frac{1}{\overline{\alpha}}\frac{m_{k,k+1}-1}{m_{k,k+1}m_{k+1,k}-1}\frac{m_{k+1,k}-1}{m_{k,k+1}m_{k+1,k}-1} - \frac{m_{k,k+1}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)} + \frac{1}{a_{k,k+1}}\frac{m_{k,k+1}-1}{m_{k,k+1}m_{k+1,k}-1},$$

where the final term comes from Remark 3.2. Now an easy computation simplifies this to (by (3.21))

$$\frac{\alpha}{a_{k,k+1}(1-m_{k,k+1}m_{k+1,k})\overline{\alpha}} = \psi^{-1}.$$

Step 4. Next, we show the $(2,1)$-blocks of the expressions (3.19) and (3.20) agree. The former is

$$-\psi^{-1}\mathbf{v}^T D^{-1} = \frac{m_{k+1,k}-1}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}\boldsymbol{\tau}_{\text{in}}^T + \frac{\alpha\, m_{k+1,k}}{\overline{\alpha}\, a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k^T,$$

using (3.13) and (3.21). By the definition of $\alpha, \overline{\alpha}$, a straightforward computation shows this equals

$$\frac{m_{k+1,k}-1}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\left(\boldsymbol{\tau}_{\text{in}}^T - \frac{m_{k+1,k}(m_{k,k+1}-1)}{m_{k,k+1}m_{k+1,k}-1}\mathbf{e}_k^T\right) + \frac{m_{k+1,k}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k^T,$$

which equals the $(2,1)$-block of (3.20) via Remark 3.2 for $i = k+1$.

We now consider the $(1,2)$-blocks in (3.19) and (3.20). We begin with the former; using (3.13),

$$\begin{aligned} &-\psi^{-1}D^{-1}\mathbf{u} \\ &= \frac{m_{k,k+1}-1}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}\boldsymbol{\tau}_{\text{out}} + \frac{\alpha(m_{k,k+1}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k + \frac{\alpha}{\overline{\alpha}\, a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k. \end{aligned}$$

Now add-and-subtract two terms to get:

$$\begin{aligned} = {} & \frac{m_{k,k+1}-1}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}\left(\boldsymbol{\tau}_{\text{out}} - \frac{m_{k,k+1}(m_{k+1,k}-1)}{m_{k,k+1}m_{k+1,k}-1}\mathbf{e}_k\right) \\ & + \frac{m_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)^2}\mathbf{e}_k + \frac{\alpha\, m_{k,k+1}}{\overline{\alpha}\, a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k \\ & - \frac{\alpha\, m_{k,k+1}}{\overline{\alpha}\, a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k + \frac{\alpha}{\overline{\alpha}\, a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k + \frac{\alpha(m_{k,k+1}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k. \end{aligned}$$

The terms on the first line (resp. second line) in the right-hand side here add up to yield the $(1,2)$-block of $\frac{1}{\overline{\alpha}}\overline{\boldsymbol{\tau}_{\text{out}}}\,\overline{\boldsymbol{\tau}_{\text{in}}}^T$ (resp. of $-\overline{L}$). The terms in the third line add up to yield

$$\frac{\alpha(m_{k,k+1}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}\left(C\mathbf{e}_k - \frac{1}{a_{k,k+1}}\mathbf{e}_k\right),$$

and a straightforward but careful calculation shows this equals the $(1,2)$-block of $\overline{C}\operatorname{diag}(\overline{\boldsymbol{\tau}_{\text{in}}})$. This concludes the verification for the $(1,2)$-blocks of (3.19) and (3.20).

Step 5. In this final step, we handle the most involved of the computations: the equality of the $(1,1)$-blocks of (3.19) and (3.20). As the computations are fairly involved, we begin by outlining the strategy. We expand out the expression

$$D^{-1} + \psi^{-1}\cdot(D^{-1}\mathbf{u})\cdot(\mathbf{v}^T D^{-1}),$$

substituting $D^{-1} = \frac{1}{\alpha}\boldsymbol{\tau}_{\text{out}}\boldsymbol{\tau}_{\text{in}}^T - L + C\operatorname{diag}(\boldsymbol{\tau}_{\text{in}})$ in the first term, and computing $D^{-1}\mathbf{u}$, $\mathbf{v}^T D^{-1}$ using the intermediate identities proved above. Then we rearrange terms to obtain expressions for the $(1,1)$-blocks of $\frac{1}{\overline{\alpha}}\overline{\boldsymbol{\tau}_{\rm out}}\,\overline{\boldsymbol{\tau}_{\rm in}}^T$ and $-\overline{L}$, plus some extra terms. Finally, these extra terms will be shown to add up to the $(1,1)$-block of $\overline{C}\,{\rm diag}(\overline{\boldsymbol{\tau}_{\rm in}})$.

Thus, we begin with

$$\begin{aligned}
&D^{-1}+\psi^{-1}\cdot(D^{-1}\mathbf{u})\cdot(\mathbf{v}^TD^{-1}) \qquad (3.22)\\
={}&\frac{1}{\alpha}\boldsymbol{\tau}_{\rm out}\boldsymbol{\tau}_{\rm in}^T-\frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\alpha\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\boldsymbol{\tau}_{\rm out}\boldsymbol{\tau}_{\rm in}^T-\frac{m_{k+1,k}(m_{k,k+1}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\boldsymbol{\tau}_{\rm out}\mathbf{e}_k^T\\
&-L-\frac{\alpha\, m_{k+1,k}}{\overline{\alpha}\,a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\mathbf{e}_k^T\\
&+C\,{\rm diag}(\boldsymbol{\tau}_{\rm in})-\frac{m_{k+1,k}-1}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\boldsymbol{\tau}_{\rm in}^T-\frac{\alpha\, m_{k+1,k}(m_{k,k+1}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k\mathbf{e}_k^T\\
&-\frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k\boldsymbol{\tau}_{\rm in}^T.
\end{aligned}$$

Now the first three terms (on the first line on the right-hand side of Equation (3.22)) add up to

$$\begin{aligned}
&\frac{1}{\overline{\alpha}}\left(\boldsymbol{\tau}_{\rm out}-\frac{m_{k,k+1}(m_{k+1,k}-1)}{m_{k,k+1}m_{k+1,k}-1}\mathbf{e}_k\right)\left(\boldsymbol{\tau}_{\rm in}-\frac{m_{k+1,k}(m_{k,k+1}-1)}{m_{k,k+1}m_{k+1,k}-1}\mathbf{e}_k\right)^T\\
+{}&\frac{m_{k,k+1}(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\boldsymbol{\tau}_{\rm in}^T-\frac{m_{k,k+1}m_{k+1,k}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)^2}\mathbf{e}_k\mathbf{e}_k^T.
\end{aligned}\qquad (3.23)$$

Similarly, the next two terms (on the second line on the right-hand side of (3.22)) add up to

$$\left(-L-\frac{m_{k+1,k}}{a_{k,k+1}(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\mathbf{e}_k^T\right)+\frac{m_{k+1,k}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)^2}\mathbf{e}_k\mathbf{e}_k^T. \qquad (3.24)$$

Notice by (3.15), (3.16), (3.17) that the first expression in (3.23) (resp. (3.24)) equals the $(1,1)$-block of $\frac{1}{\overline{\alpha}}\overline{\boldsymbol{\tau}_{\rm out}}\,\overline{\boldsymbol{\tau}_{\rm in}}^T$ (resp. $-\overline{L}$). Thus, it remains to show that the $(1,1)$-block of $\overline{C}\,{\rm diag}(\overline{\boldsymbol{\tau}_{\rm in}})$ equals the sum of the remaining seven terms in (3.22), (3.23), (3.24), which we now collect together:

$$\begin{aligned}
&C\,{\rm diag}(\boldsymbol{\tau}_{\rm in})-\frac{\alpha\, m_{k+1,k}(m_{k,k+1}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k\mathbf{e}_k^T-\frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k\boldsymbol{\tau}_{\rm in}^T\\
+{}&\frac{(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\boldsymbol{\tau}_{\rm in}^T-\frac{m_{k+1,k}(m_{k,k+1}-1)^2(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)^2}\mathbf{e}_k\mathbf{e}_k^T.
\end{aligned}\qquad (3.25)$$

In (3.25), the two expressions on the last line are each obtained by combining two of the "remaining seven terms" above. Now define the vector

$$\boldsymbol{\tau}'_{\rm in}:=\boldsymbol{\tau}_{\rm in}-\frac{m_{k+1,k}(m_{k,k+1}-1)}{m_{k,k+1}m_{k+1,k}-1}\mathbf{e}_k \qquad (3.26)$$

and notice this precisely equals the $(1,1)$-block of $\overline{\boldsymbol{\tau}_{\rm in}}$ by (3.16). Then the last two terms – all on the second line – of (3.25) add up to yield

$$\frac{(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k(\boldsymbol{\tau}'_{\rm in})^T.$$

Similarly, the first three terms – all on the first line – of (3.25) add up to give

$$C\,{\rm diag}(\boldsymbol{\tau}'_{\rm in})-\frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}C\mathbf{e}_k(\boldsymbol{\tau}'_{\rm in})^T.$$

Indeed, break up the second term in (3.25) via $\alpha=\overline{\alpha}-\frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{m_{k,k+1}m_{k+1,k}-1}$, and add these components to the first and third terms respectively, using ${\rm diag}(\boldsymbol{\tau}_{\rm in})+\gamma\mathbf{e}_k\mathbf{e}_k^T={\rm diag}(\boldsymbol{\tau}_{\rm in}+\gamma\mathbf{e}_k)$.

Now since $\mathbf{e}_k(\boldsymbol{\tau}'_{\rm in})^T = \mathbf{e}_k\mathbf{e}^T\operatorname{diag}(\boldsymbol{\tau}'_{\rm in})$, the terms in (3.25) all add up to

$$\left(C - \frac{a_{k,k+1}(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}(m_{k,k+1}m_{k+1,k}-1)}(C\mathbf{e}_k)\mathbf{e}^T + \frac{(m_{k,k+1}-1)(m_{k+1,k}-1)}{\overline{\alpha}\,(m_{k,k+1}m_{k+1,k}-1)}\mathbf{e}_k\mathbf{e}^T\right)\operatorname{diag}(\boldsymbol{\tau}'_{\rm in}).$$

Notice the final summand only updates the final row of the first term. Now another careful computation shows that the preceding expression indeed equals the $(1,1)$-block of $\overline{C}\operatorname{diag}(\overline{\boldsymbol{\tau}_{\rm in}})$. This concludes the proof of the inverse-formula, by induction. $\square$

As a by-product of the above proof, we can now show the remaining main theorem above:

Proof of Theorem A. The formula (1.7) (with $x=0$) for $\det(D_{\mathcal{T}})$ easily follows by induction on $|E|$ and (3.19), (3.21). Moreover, the formula for $\operatorname{cof}(D_{\mathcal{T}}) = \det(D_{\mathcal{T}})\cdot(\mathbf{e}^T D_{\mathcal{T}}^{-1}\mathbf{e})$ follows from (3.13), (3.5), and the formulas for $D_{\mathcal{T}}^{-1}, \det(D_{\mathcal{T}})$. This shows (1.6) for $|I\Delta J'|=0$. (Here, we assume $D_{\mathcal{T}}$ is invertible by Zariski density, since $\operatorname{cof}(D_{\mathcal{T}})$ is also a polynomial in the entries.)

Next using Cramer's rule, Theorem B provides a proof of (1.7) for $|I\Delta J'|=2$; we also provide an alternate proof below. First, we show that $(D_{\mathcal{T}}+xJ)_{I|J'}$ is singular if $|I\Delta J'|>2$. Let $\mathbf{d}_v^T$ denote the J'-truncated vth row for $v\in V(G)\setminus I$. There are now two cases:

Case 1: First suppose $J'\setminus I$ contains an edge $\{j_1,j_2\}\in E$. Then there exists a unique node $p\in T\setminus J'$ that is closest to j_2. Without loss of generality, interchange the labels j_1,j_2 such that p is closer to j_2 than j_1; then the path from j_1 to p has length at least 2. Denote this path by

$$j_1 \longleftrightarrow j_2 \longleftrightarrow \cdots \longleftrightarrow a \longleftrightarrow b \longleftrightarrow p.$$

Then $a,b\in J'$ by the assumptions, and we re-set $j_1:=a, j_2:=b$, so that $p\sim j_2$ and $j_2\sim j_1$. Now p cannot lie in I, else the maximum sub-tree containing $p\notin J'$ but not $j_2\notin J'$ (resp. j_2 but not p) would completely lie in I (resp. J'), in which case $V=I\cup J'$, a contradiction. We now have:

$$\mathbf{d}_{j_1}^T - m_{j_1j_2}\mathbf{d}_{j_2}^T = (a_{j_1j_2}-x)(m_{j_1j_2}-1)\mathbf{e}^T, \qquad \mathbf{d}_{j_2}^T - m_{j_2p}\mathbf{d}_p^T = (a_{j_2p}-x)(m_{j_2p}-1)\mathbf{e}^T,$$

and so the determinant of $\det(D_{\mathcal{T}}+xJ)_{I|J'}$ vanishes, as claimed.

Case 2: If the previous case does not hold, then $J'\setminus I = J'$ contains only pendant vertices. Choose $j_1,j_2\in J'$ with neighbors $p(j_1),p(j_2)$ respectively. Now it is clear from the hypotheses that $p(j_l)\notin I\cup J'$ for $l=1,2$; and with the same notation as in the previous case, we have

$$\mathbf{d}_{j_l}^T - m_{j_lp(j_l)}\mathbf{d}_{p(j_l)}^T = (a_{j_lp(j_l)}-x)(m_{j_lp(j_l)}-1)\mathbf{e}^T, \qquad l=1,2.$$

Once again, it follows that $\det(D_{\mathcal{T}}+xJ)_{I|J'}$ vanishes.

It remains to show (1.6) when $|I\Delta J'|=2$, and we prove it by induction on $n\geqslant |I|+2$. The assertion is not hard to verify for $n=3,4$, so we will assume henceforth that $\mathcal{T}$ has at least $n+1\geqslant 5$ nodes, and that (1.6) holds for all trees with at most n nodes. Without loss of generality we set $I=\{1\}$ and $J'=\{n+1\}$, with both $1,n+1$ pendant vertices. Since every tree on at least 3 nodes has at least two pendant nodes and these are necessarily non-adjacent, we also relabel the nodes such that if one deletes the node 1 (respectively, $n+1$) then the node 2 (respectively, n) is pendant to the deleted portion of the tree. We may also assume the nodes $2,n$ are not adjacent, since $n\geqslant 5$.

Let $D:=(D_{\mathcal{T}}+xJ)_{1|n+1}$; we compute $\det(D)$ using Dodgson condensation [11], which says:

$$\det D\cdot\det D_{1n|1n} = \det D_{1|1}\cdot\det D_{n|n} - \det D_{1|n}\cdot\det D_{n|1}. \tag{3.27}$$

Note that

$$\begin{aligned} D_{1|1} &= (D_{\mathcal{T}}+xJ)_{12|1(n+1)}, \qquad & D_{n|n} &= (D_{\mathcal{T}}+xJ)_{1(n+1)|n(n+1)},\\ D_{1|n} &= (D_{\mathcal{T}}+xJ)_{12|n(n+1)}, \qquad & D_{n|1} &= (D_{\mathcal{T}}+xJ)_{1(n+1)|1(n+1)},\\ D_{1n|1n} &= (D_{\mathcal{T}}+xJ)_{12(n+1)|1n(n+1)}. \end{aligned}$$

Since $n+1 \geqslant 5$, it follows by the preceding case of $|I\Delta J'| > 2$ that $\det D_{1|n} = 0$. Hence by (3.27),

$$\begin{aligned}\det D &= (\det D_{1n|1n})^{-1}(\det D_{1|1})(\det D_{n|n})\\ &= (\det(D_{\mathcal{T}} + xJ)_{12(n+1)|1n(n+1)})^{-1}(\det(D_{\mathcal{T}} + xJ)_{12|1(n+1)})(\det(D_{\mathcal{T}} + xJ)_{1(n+1)|n(n+1)}).\end{aligned}$$

But all three terms on the right are computable by the induction hypothesis; and we may assume by Zariski density (i.e. a suitable application of Lemma 2.1) that the factors of $\det D_{1n|1n}$ and all a_e and $m_e m'_e - 1$ are invertible, namely:

$$a_e, \quad m_e m'_e - 1, \ (e \in E); \qquad a_{p(n),n} - x, \quad m_{p(2),2} - 1, \quad m_{p(n),n} - 1.$$

Now the induction step follows by a straightforward cancellation, completing the proof. $\square$

Remark 3.3. The above proof for $|I\Delta J'| > 2$ also goes through verbatim for arbitrary I of size $|J'|$, which do not contain the two nodes a, b, p in case 1, or $j_1, j_2, p(j_1), p(j_2)$ in case 2. Alternately, one can work with the transpose of $D_{\mathcal{T}} + xJ$, and hence with J' as specified but more general I.

Remark 3.4 (New technique: Zariski density arguments)**.** We now make some remarks on our – to our knowledge, novel – use of Zariski density in this paper. There are at least three advantages:

1. As cited in the introduction, various papers work with e.g. q-distance matrices, under the assumption that q is a real number and $q \neq \pm 1$; or that q is a parameter (see e.g. [4, 6, 24]). Zariski density enables working over any unital commutative ring, and immediately eliminates such restrictions.
2. Using Zariski density allows one to assume nonzero expressions such as $\det(D_{\mathcal{T}})$ or $1 - m_e m'_e$ or $1 - m_e$ to then be invertible, hence $D_{\mathcal{T}}$. This provides stronger tools to prove results.
3. Zariski density can help clarify arguments. E.g. in [23], the authors tackle the original case $a_e = a'_e = 1$ and $m_e = m'_e = q$, $q \to 1$, and show that $(\det D_T)^2 = -(\det D_T)|E|(-2)^{|E|-1}$. Here one cannot *a priori* cancel $\det D_T$, unless one assumes somehow that $\det D_T \not\equiv 0$. In our case, this can be done using Zariski density, because specializing to $a_e = a'_e = 1\ \forall e$, it follows by Theorem C that $\det(D_{\mathcal{T}}) \not\equiv 0$. This point seems not to have been made in [23], where the authors cancel $\det D_T$ in the above equation – in effect showing in the special case $x = 0$, $a_e = a'_e = 1$, and $m_e = m'_e = 1$, $q \to 1$ that $\det(D_{\mathcal{T}}) = -|E|(-2)^{|E|-1}$ assuming $\det(D_{\mathcal{T}}) \neq 0$.[1] Zariski density helps fill such gaps.

Thus, we hope that the present work leads to Zariski density being used in this area – not just for distance matrices – and also leads to the removal of various superfluous/unnecessary mathematical restrictions, as well as enabling one to use stronger tools, e.g. the invertibility of various matrices or the nonvanishing of certain polynomials.

We end this section by briefly discussing instances of how Theorem B specializes to known formulas in the literature [3]–[7], [14, 25, 26]. First, for every q-distance matrix, i.e. with $a_e = \frac{1}{q-1}$, $m_e = q^{\alpha_e}$, $m'_e = q^{\alpha'_e}$, one verifies that

$$C = (q-1)\mathrm{Id}_V, \qquad \alpha_{\mathcal{T}} = \sum_{e \in E} \frac{[\alpha_e][\alpha'_e]}{[\alpha_e + \alpha'_e]}.$$

In particular, if one specializes to $q = 1$ then $C = 0$; if moreover the tree is unweighted, we get

$$\alpha_{\mathcal{T}} = \frac{|E|}{2}, \qquad \boldsymbol{\tau}_{\text{in}} = \boldsymbol{\tau}_{\text{out}} = \mathbf{e} - \mathbf{d}/2,$$

where $\mathbf{d}$ is the vector of node-degrees. These are precisely the expressions that appear in the Graham–Lovász formula for $D_{\mathcal{T}}^{-1}$ in the original unweighted and undirected setting [14].

[1]The authors have since mentioned to us (personal communication) that they prove $\det(D_{\mathcal{T}}) \neq 0$ in other papers and hence can cancel it away. These other papers are not cited in the proof in [23].

A parallel setting involves the product distance matrix $D^*_T = D_{\mathcal{T}} + J$ studied in [25]. Here $a_e = 1\ \forall e$. Now one verifies that $C = \mathrm{Id}_V$; moreover, $(D^*_T)^{-1}$ can be computed alternately (to the argument in Section 2) by using the Sherman–Morrison formula for $(D_{\mathcal{T}} + J)^{-1}$. Carrying out the computations using the formula for $D_{\mathcal{T}}^{-1}$ and the identities shown above yields precisely:

$$(D^*_T)^{-1} = -L + \mathrm{diag}(\boldsymbol{\tau}_{\mathrm{in}}).$$

This specializes to several of the formulas in the literature cited in the above discussion. Notice also that when $a_e = 1\ \forall e$, we have $(D^*_T)^{-1}\mathbf{e} = \boldsymbol{\tau}_{\mathrm{out}},\ \mathbf{e}^T(D^*_T)^{-1} = \boldsymbol{\tau}_{\mathrm{in}}^T$; this in particular reveals the presence of $\boldsymbol{\tau}_{\mathrm{out}}, \boldsymbol{\tau}_{\mathrm{in}}^T$ in a formula for $D_{\mathcal{T}}^{-1} = (D^*_T - J)^{-1}$, when going the reverse way via the Sherman–Morrison formula.

Remark 3.5. Theorem B in particular answers an open question of Bapat–Lal–Pati [4], where they ask for the explicit form of $D_{\mathcal{T}}^{-1}$ in the special case $a_e = \frac{w_e}{q-1},\ m_e = m'_e = q,\ e \in E$ with $q \neq \pm 1, w_e \neq 0$ scalars. For completeness we spell out the specialization of Theorem B to this setting, assuming all denominators below are invertible:

$$D_{\mathcal{T}}^{-1} = \frac{q+1}{\sum_{e\in E} w_e}\boldsymbol{\tau}\boldsymbol{\tau}^T - \frac{q}{q+1}L_w + C_{\mathcal{T}}\,\mathrm{diag}(\boldsymbol{\tau}),$$

where $\boldsymbol{\tau} := \mathbf{e} - \frac{q}{q+1}\mathbf{d}$ for $\mathbf{d}$ the vector of node-degrees, L_w is the (symmetric) weighted Laplacian matrix of Bapat–Kirkland–Neumann [3] given by

$$(L_w)_{ij} = \begin{cases} \frac{-1}{w_{ij}}, & \text{if } i \sim j; \\ \sum_{k\sim i} \frac{1}{w_{ik}}, & \text{if } i = j; \\ 0, & \text{otherwise;} \end{cases}$$

and $C_{\mathcal{T}}$ is the $V \times V$ matrix with entries given by

$$(C_{\mathcal{T}})_{ij} := \beta_i - \mathbf{1}_{i\neq j} \cdot \frac{q-1}{w_{ik}} \quad \text{where} \quad j \in T_{i\to k} \quad \text{and} \quad \beta_i := \frac{q-1}{\sum_{e\in E} w_e} \sum_{k:k\sim i} \frac{1}{w_{ik}} \sum_{e\in E(T_{i\to k})} w_e.$$

4. A novel, third invariant for trees, and its Graham–Hoffman–Hosoya Theorem D

In this paper, we have studied three variants of the distance matrix for trees: (a) the most general version $D_{\mathcal{T}}$ with entries given by (1.4); (b) the "product" distance matrix D^*_G; and (c) the q-matrix $D_q(G)$ (and its $q = 1$ specialization, $D_1(G)$). In Section 2 we stated and proved Graham–Hoffman–Hosoya type identities in settings (b) and (c) – see Proposition 2.3 and the preceding equations. The latter of these identities specialized to the classical Graham–Hoffman–Hosoya identities (1.11).

It is natural to ask if there exist similar identities in the "most general" setting (a) of the present paper – and also whether or not these specialize to the original results (1.11) of [13]. In this final section, we affirmatively answer both questions, and in particular, provide a third proof of the formula (1.7) for $\det(D_{\mathcal{T}}), \mathrm{cof}(D_{\mathcal{T}})$. Our new identities below will use $\det(\cdot)$ but not $\mathrm{cof}(\cdot)$, and in its place we now introduce a novel, third invariant:

Definition 4.1. Suppose G is a finite directed, strongly connected graph with node set V, a distinguished cut-vertex $v_0 \in V$, and R-valued maps $d, m : V \times V \to R$ that satisfy:

$$d(v, w) = d(v, v_0) + m(v, v_0)d(v_0, w), \quad d(v_0, v_0) = 0, \tag{4.1}$$

whenever v, w lie in adjacent strong blocks, both containing v_0. Given a subgraph G' induced on the subset of nodes V' which contains v_0, write

$$D_{G'} := (d(v, w))_{v,w\in V'} = \begin{pmatrix} D|_{V'\setminus\{v_0\}} & \mathbf{u}_1 \\ \mathbf{w}_1^T & 0 \end{pmatrix},$$

by relabelling the nodes, and define the invariant

$$\kappa(D_{G'}, v_0) := \det\left(D|_{V' \setminus \{v_0\}} - \mathbf{u}_1 \mathbf{e}^T - \mathbf{m}(V' \setminus \{v_0\}, v_0)\mathbf{w}_1^T\right). \tag{4.2}$$

Note here that $\mathbf{u}_1 = \mathbf{d}(V' \setminus \{v_0\}, v_0)$ and $\mathbf{w}_1 = \mathbf{d}(v_0, V' \setminus \{v_0\})$.

Remark 4.2. For arbitrary graphs G, the notion of distance matrix in Definition 4.1 is a general one. When one works with $G = T$ a tree, this data is precisely that of our setting in (1.4), via: $d_e \leftrightarrow a_e(m_e - 1)$, $d'_e \leftrightarrow a_e(m'_e - 1)$, since m_e, m'_e are parameters (hence unequal in general to 1). In this case, one has (4.1) for any two nodes v, w and any intermediate node v_0.

With this terminology in hand, we state three results on the invariant κ, deferring the proofs to a later subsection. These results compute $\kappa(D_G, v_0)$ for graphs G with a cut-vertex v_0, as well as $\kappa(D_{\mathcal{T}})$ for arbitrary trees. We will then mention a few corollaries, and end with Example 4.9 which shows that our results are, once again, "best possible" in a sense.

Our first – and final main – result presents GHH-type identities for the three invariants:

Theorem D. *Notation as in Definition 4.1. Let $G_1, \dots, G_k$ be strongly connected subgraphs of G containing $v_0 \in V$ such that the sets $V(G_j) \setminus \{v_0\}$ are pairwise disjoint. Then,*

$$\begin{aligned}
\kappa(D_G, v_0) &= \prod_{j=1}^{k} \kappa(D_{G_j}, v_0), \\
\det(D_G) &= \sum_{j=1}^{k} \det(D_{G_j}) \prod_{i \neq j} \kappa(D_{G_i}, v_0), \\
\operatorname{cof}(D_G) &= \kappa(D_G, v_0) + \sum_{j=1}^{k} (\operatorname{cof}(D_{G_j}) - \kappa(D_{G_j}, v_0)) \prod_{i \neq j} \kappa(D_{G_i}, v_0).
\end{aligned} \tag{4.3}$$

In other words, if $\kappa(D_{G_j}, v_0) \in R^\times$ $\forall j$, then

$$\frac{\det(D_G)}{\kappa(D_G, v_0)} = \sum_{j=1}^{k} \frac{\det(D_{G_j})}{\kappa(D_{G_j}, v_0)}, \qquad \frac{\operatorname{cof}(D_G)}{\kappa(D_G, v_0)} - 1 = \sum_{j=1}^{k} \left(\frac{\operatorname{cof}(D_{G_j})}{\kappa(D_{G_j}, v_0)} - 1 \right).$$

Notice these formulas are similar in form to (1.11).

Next, we show that $\kappa(\cdot)$ is indeed an invariant for trees, as stated above:

Theorem 4.3. *Suppose $\mathcal{T} = \{(a_e, m_e, m'_e) : e \in E\}$ comprise the edge-data of T, as in Theorem A. In this case we define $\kappa(D_{\mathcal{T}}, v_0)$ for any vertex $v_0 \in V$, by the same formula as in (4.2). Then $\kappa(D_{\mathcal{T}}, v_0)$ depends on neither the choice of (cut or pendant) node $v_0 \in V$, nor the tree-structure of $D_{\mathcal{T}}$. It only depends on the edge-data, as follows:*

$$\kappa(D_{\mathcal{T}}, v_0) = \prod_{e \in E} a_e(1 - m_e m'_e). \tag{4.4}$$

In particular, $\kappa(D_{\mathcal{T}}, v_0)$ is multiplicative over subgraphs cut by v_0. When $\kappa(D_e)$ is invertible for all edges e, then one has, parallel to Theorem D:

$$\frac{\det(D_{\mathcal{T}})}{\kappa(D_{\mathcal{T}})} = \sum_{e \in E} \frac{\det(D_e)}{\kappa(D_e)}, \qquad \frac{\operatorname{cof}(D_{\mathcal{T}})}{\kappa(D_{\mathcal{T}})} - 1 = \sum_{e \in E} \left(\frac{\operatorname{cof}(D_e)}{\kappa(D_e)} - 1 \right). \tag{4.5}$$

Remark 4.4. Akin to Remark 1.9, while one can use Theorem 4.3 to deduce the formulas for $\det(D_{\mathcal{T}}), \operatorname{cof}(D_{\mathcal{T}})$ in Theorem A, once again the formulas for $\det(\cdot), \operatorname{cof}(\cdot)$ of the more general submatrices $(D_{\mathcal{T}} + xJ)_{I|J'}$ do *not* follow from these results.

Remark 4.5. Given Theorem 4.3, we write $\kappa(D_{\mathcal{T}}, v_0)$ as (the invariant) $\kappa(D_{\mathcal{T}})$ henceforth.

From Theorem 4.3 it is possible to deduce the formulas for $\det(D_{\mathcal{T}})$ and $\operatorname{cof}(D_{\mathcal{T}})$ as in (1.7) (or Theorem A with $I = J' = \emptyset$). Our third result here shows that the converse is also true:

Proposition 4.6. *Notation as in Theorem 4.3. The following can be deduced from each other:*

(1) *For all such trees and all nodes* $v_0 \in V$, $\det(D_{\mathcal{T}}) = \prod_{e\in E}(a_e(1 - m_e m'_e)) \sum_{e\in E} \dfrac{\det(D_e)}{\kappa(D_e)}$, *where the denominators are understood to be placeholders to cancel with a factor outside the sum.*

(2) *For all such trees and all nodes* $v_0 \in V$,

$$\operatorname{cof}(D_{\mathcal{T}}) = \prod_{e\in E} a_e(1 - m_e m'_e) \cdot \left(1 + \sum_{e\in E}\left(\frac{\operatorname{cof}(D_e)}{\kappa(D_e)} - 1\right)\right),$$

where the denominators are again placeholders.

(3) *For all such trees and all nodes* $v_0 \in V$, $\kappa(D_{\mathcal{T}}) = \prod_{e\in E} a_e(1 - m_e m'_e)$. *In particular,* $\kappa(\cdot)$ *is multiplicative across edges of trees.*

Next, from the above three results we deduce a few consequences. First, the Graham–Hoffman–Hosoya type formulas proved in this section hold in slightly greater generality:

Corollary 4.7. *Notation as in Definition 4.1. Let* $G_1, \dots, G_k$ *be strongly connected subgraphs of* G *containing* $v_0 \in V$ *such that the sets* $V(G_j) \setminus \{v_0\}$ *are pairwise disjoint. Also attach finitely many pendant trees* $\mathcal{T}_1, \dots, \mathcal{T}_l$ *to* v_0. *Then the formulas in Theorem D extend to this setting:*

$$\begin{aligned}
\kappa(D_G, v_0) &= \prod_{j=1}^{k} \kappa(D_{G_j}, v_0) \prod_{i=1}^{l} \kappa(D_{\mathcal{T}_i}),\\
\frac{\det(D_G)}{\kappa(D_G, v_0)} &= \sum_{j=1}^{k} \frac{\det(D_{G_j})}{\kappa(D_{G_j}, v_0)} + \sum_{i=1}^{l} \frac{\det(D_{\mathcal{T}_i})}{\kappa(D_{\mathcal{T}_i})},\\
\frac{\operatorname{cof}(D_G)}{\kappa(D_G, v_0)} - 1 &= \sum_{j=1}^{k}\left(\frac{\operatorname{cof}(D_{G_j})}{\kappa(D_{G_j}, v_0)} - 1\right) + \sum_{i=1}^{l}\left(\frac{\operatorname{cof}(D_{\mathcal{T}_i})}{\kappa(D_{\mathcal{T}_i})} - 1\right),
\end{aligned} \tag{4.6}$$

where the denominators on the right are placeholders as earlier, and get cancelled upon multiplying by the denominators on the left.

We skip the proof as this result is a straightforward consequence of Theorems D and 4.3.

Second, when given a graph G with a usual, additive distance matrix $(d(i,j))_{i,j\in V}$, recall that one can treat D_G as the $q = 1$ specialization of the matrix $D_q(G) := \frac{1}{q-1}(q^{d(i,j)} - 1)_{i,j\in V}$. We now claim $\kappa(D_G, v_0) \to \operatorname{cof}(D_G)$ when $q \to 1$. Indeed, beginning with Theorem 4.3, we obtain:

Corollary 4.8. *The formulas in Theorems D and 4.3 with* $m(i,j) = q^{d(i,j)}$ *specialize as* $q \to 1$ *to the classical Graham–Hoffman–Hosoya formulas* (1.11).

Proof. This is easy to see in the setting of Theorem 4.3 (and Proposition 4.6) for trees, using above results with $a_e = 1/(q-1)\ \forall e \in E$. For general graphs, begin with the formula

$$\kappa(D_G, v_0)|_{q\to 1} := \lim_{q\to 1} \det\left([D]_q|_{V\setminus\{v_0\}} - [\mathbf{u}_1]_q\, \mathbf{e}^T - [\mathbf{m}(V \setminus \{v_0\}, v_0)]_q [\mathbf{w}_1]_q^T\right),$$

where $[\mathbf{u}_1]_q$ is the vector with jth coordinate $(q^{u_j} - 1)/(q-1)$, etc. Now by the polynomiality of the determinant in its entries, setting $q = 1$ on the right-hand side after taking the determinant is the same as setting it before; and in the latter scenario, we have

$$\kappa(D_G, v_0)|_{q\to 1} = \det(D_{V\setminus\{v_0\}} - \mathbf{u}_1|_{q\to 1}\mathbf{e}^T - \mathbf{e}\,\mathbf{w}_1^T|_{q\to 1}).$$

But this is precisely $\operatorname{cof}(D_G)$, as observed in [13]. We are done by Theorem D. $\square$

Finally, we present an example which shows that the Graham–Hoffman–Hosoya type identities in Theorem D do not uniformly hold in greater generality.

Example 4.9. While $\det(D_{\mathcal{T}}), \operatorname{cof}(D_{\mathcal{T}})$ for trees $\mathcal{T}$ depend only on the strong blocks – i.e. edges – of $\mathcal{T}$, the same does not hold for general graphs. For example, let G consist of one cut-vertex v_0 and two strong blocks: an edge e with data $(a_e, m_e = m'_e)$; and the clique K_3, with distance matrix

$$D_{K_3} = \begin{pmatrix} 0 & a(m-1) & c(q-1) \\ a(m-1) & 0 & b(n-1) \\ c(q-1) & b(n-1) & 0 \end{pmatrix}.$$

We now claim that the quantity

$$\kappa(D_G, v_0) = \kappa(D_{K_3}, v_0) \cdot a_e(1 - m_e^2)$$

(from above results) does depend on the location of the cut-vertex v_0. Indeed, to show this it suffices to verify that $\kappa(D_{K_3}, 1) \neq \kappa(D_{K_3}, 2) \neq \kappa(D_{K_3}, 3)$. But an easy computation shows that

$$\kappa(D_{K_3}, 3) = \det \begin{pmatrix} c(1-q^2) & a(m-1) - c(q-1) - qb(n-1) \\ a(m-1) - b(n-1) - nc(q-1) & b(1-n^2) \end{pmatrix}.$$

Now a^2m^2, b^2n^2 have coefficients $1, q$ in $\kappa(D_{K_3}, 3)$, respectively. As this is not "symmetric", it follows that $\kappa(D_{K_3}, 3) \neq \kappa(D_{K_3}, 1)$; the remaining verifications are similar. $\square$

4.1. **Proofs.**

Proof of Theorem D. It suffices by induction on k to prove the result when $k = 2$. Thus, suppose

$$G = G_1 \sqcup_{v_0} G_2, \quad \text{with} \quad V(G_1) = \{1, \dots, v_0\},\ V(G_2) = \{v_0, \dots, n\}.$$

Let $V'_j := V(G_j) \setminus \{v_0\}$ for $j = 1, 2$. Corresponding to this notation, write the distance matrix as

$$D_G := \begin{pmatrix} D_1 & \mathbf{u}_1 & \mathbf{u}_1\mathbf{e}^T + \mathbf{m}(V'_1, v_0)\mathbf{w}_2^T \\ \mathbf{w}_1^T & 0 & \mathbf{w}_2^T \\ \mathbf{u}_2\mathbf{e}^T + \mathbf{m}(V'_2, v_0)\mathbf{w}_1^T & \mathbf{u}_2 & D_2 \end{pmatrix}$$

in block form. Let

$$D'_j := D_j - \mathbf{u}_j\mathbf{e}^T - \mathbf{m}(V'_j, v_0)\mathbf{w}_j^T, \qquad j = 1, 2. \tag{4.7}$$

The first claim is that computing $\kappa(D_G, v_0)$ yields precisely the determinant of the block-diagonal matrix $\begin{pmatrix} D'_1 & 0 \\ 0 & D'_2 \end{pmatrix}$. This is straightforward, and it follows that

$$\kappa(D_G, v_0) = \det(D'_1)\det(D'_2) = \kappa(D_{G_1}, v_0)\kappa(D_{G_2}, v_0).$$

We next show the identity for $\det(D_G)$. Begin with the block matrix D_G as above, and carry out the sequence of block row operations

$$R_1 \mapsto R_1 - \mathbf{m}(V'_1, v_0)\, R_2, \qquad R_3 \mapsto R_3 - \mathbf{m}(V'_2, v_0)\, R_2,$$

followed by the sequence of block-column operations

$$C_1 \mapsto C_1 - C_2\, \mathbf{e}^T, \qquad C_3 \mapsto C_3 - C_2\, \mathbf{e}^T.$$

This yields precisely the matrix

$$D' := \begin{pmatrix} D'_1 & \mathbf{u}_1 & 0 \\ \mathbf{w}_1^T & 0 & \mathbf{w}_2^T \\ 0 & \mathbf{u}_2 & D'_2 \end{pmatrix},$$

where D_1', D_2' were defined in (4.7). Now we may assume by a Zariski density argument that (in our setting) D_1', D_2' are invertible, since they are nonzero matrices with no constraints. Carrying out block row and column operations on R_2, C_2 yields a block-triangular matrix, and we obtain:

$$\begin{aligned}\det D_G = \det D' = {} & \det(D_1')\det(D_2') \cdot (-\mathbf{w}_1^T (D_1')^{-1}\mathbf{u}_1 - \mathbf{w}_2^T (D_2')^{-1}\mathbf{u}_2) \\ = {} & \det(D_2') \det \begin{pmatrix} D_1' & \mathbf{u}_1 \\ \mathbf{w}_1^T & 0 \end{pmatrix} + \det(D_1') \det \begin{pmatrix} 0 & \mathbf{w}_2^T \\ \mathbf{u}_2 & D_2' \end{pmatrix},\end{aligned}$$

where the final equality uses two Schur complement expansions of determinants. But now in the two block 2×2 matrices in the final expression, we may replace D_j' by D_j by performing block row and column operations. Hence,

$$\det(D_G) = \det(D_2')\det(D_{G_1}) + \det(D_1')\det(D_{G_2}).$$

This shows (by Zariski density) the formula for $\det(D_G)$, since $\det(D_j') = \kappa(D_{G_j}, v_0)$ for $j = 1, 2$.

Finally, we show the claimed identity for $\operatorname{cof}(D_G)$. Begin with the matrix $D_G + xJ$, where D_G is as above. Carrying out the block-column operations

$$C_1 \mapsto C_1 - C_2\, \mathbf{e}^T, \qquad C_3 \mapsto C_3 - C_2\, \mathbf{e}^T.$$

on $D_G + xJ$, and denoting $\mathbf{m}_j := \mathbf{m}(V_j', v_0)$ for convenience, we compute:

$$\det(D_G) + x \operatorname{cof}(D_G) = \det \begin{pmatrix} D_1 - \mathbf{u}_1\mathbf{e}^T & \mathbf{u}_1 + x\mathbf{e} & \mathbf{m}_1\mathbf{w}_2^T \\ \mathbf{w}_1^T & x & \mathbf{w}_2^T \\ \mathbf{m}_2\mathbf{w}_1^T & \mathbf{u}_2 + x\mathbf{e} & D_2 - \mathbf{u}_2\mathbf{e}^T \end{pmatrix}.$$

By linearity of $\det(\cdot)$ in the second row (treated as a polynomial in x with vector coefficients), and taking the linear term in x, we obtain via Lemma 1.8:

$$\operatorname{cof}(D_G) = \det \begin{pmatrix} D_1 - \mathbf{u}_1\mathbf{e}^T & \mathbf{e} & \mathbf{m}_1\mathbf{w}_2^T \\ \mathbf{w}_1^T & 1 & \mathbf{w}_2^T \\ \mathbf{m}_2\mathbf{w}_1^T & \mathbf{e} & D_2 - \mathbf{u}_2\mathbf{e}^T \end{pmatrix} = \det \begin{pmatrix} D_1' & \mathbf{e} - \mathbf{m}_1 & 0 \\ \mathbf{w}_1^T & 1 & \mathbf{w}_2^T \\ 0 & \mathbf{e} - \mathbf{m}_2 & D_2' \end{pmatrix},$$

where D_1', D_2' are as in (4.7), and the final equality uses two block-row operations. Again assuming D_1', D_2' are invertible over R by Zariski density, we obtain via block-row operations:

$$\operatorname{cof}(D_G) = \kappa(D_{G_1}, v_0)\kappa(D_{G_2}, v_0)(1 - \mathbf{w}_1^T (D_1')^{-1}(\mathbf{e} - \mathbf{m}_1) - \mathbf{w}_2^T (D_2')^{-1}(\mathbf{e} - \mathbf{m}_2)), \tag{4.8}$$

where $\kappa(D_{G_j}, v_0) = \det(D_j')$ s above.

A similar analysis for the matrix D_{G_j} for $j = 1, 2$ reveals that

$$\operatorname{cof}(D_{G_j}) = \det(D_j - \mathbf{e}\mathbf{w}_j^T - \mathbf{u}_j\mathbf{e}^T).$$

But this is the determinant of a rank-one update of D_j', so using Schur complements,

$$\operatorname{cof}(D_{G_j}) = \det(D_j' - (\mathbf{e} - \mathbf{m}_j)\mathbf{w}_j^T) = \det \begin{pmatrix} D_j' & \mathbf{e} - \mathbf{m}_j \\ \mathbf{w}_j^T & 1 \end{pmatrix} = \kappa(D_{G_j}, v_0)(1 - \mathbf{w}_j^T (D_j')^{-1}(\mathbf{e} - \mathbf{m}_j)).$$

Combining this with (4.8), the result follows. □

Proof of Theorem 4.3. Consider a tree with edge-data $\mathcal{T}$ and a node v_0. We prove the result by induction on $|V|$, with the $|V| = 2$ case (of a single edge) easily verified. For the induction step, if v_0 is a cut-vertex then we are done by Theorem D. Thus, suppose v_0 is a pendant node, say $v_0 = n \geqslant 3$ and $n \sim p(n) = n - 1$. Denoting

$$a_{e_0} := a_{n-1,n}, \quad m_{e_0} := m_{n-1,n}, \quad m_{e_0}' := m_{n,n-1}, \quad \mathbf{d} := \mathbf{d}([n-2], n-1), \quad \mathbf{d}' := \mathbf{d}(n-1, [n-2])$$

for notational convenience, the matrix $D_{\mathcal{T}}$ is of the form

$$\begin{pmatrix} D|_{[n-2]} & \mathbf{d} & \mathbf{d} + a_{e_0}(m_{e_0}-1)\mathbf{m}([n-2],n-1) \\ (\mathbf{d}')^T & 0 & a_{e_0}(m_{e_0}-1) \\ a_{e_0}(m'_{e_0}-1)\mathbf{e}^T + m'_{e_0}(\mathbf{d}')^T & a_{e_0}(m'_{e_0}-1) & 0 \end{pmatrix}.$$

Writing $D_{\mathcal{T}} = \begin{pmatrix} D|_{[n-1]} & \mathbf{u}_1 \\ \mathbf{w}_1^T & 0 \end{pmatrix}$, we compute:

$$D_\kappa = \begin{pmatrix} D_0 & a_{e_0}(1-m_{e_0}m'_{e_0})\mathbf{m}([n-2],n-1) \\ (1-m_{e_0}m'_{e_0})(\mathbf{d}')^T + a_{e_0}(1-m_{e_0}m'_{e_0})\mathbf{e}^T & a_{e_0}(1-m_{e_0}m'_{e_0}) \end{pmatrix},$$

where

$$D_0 = D|_{[n-2]} - \mathbf{d}\,\mathbf{e}^T + a_{e_0}(1-m_{e_0}m'_{e_0})\mathbf{m}([n-2],n-1)\mathbf{e}^T - m_{e_0}m'_{e_0}\mathbf{m}([n-2],n-1)\,(\mathbf{d}')^T.$$

Carry out the block-row operation $R_1 \mapsto R_1 - \mathbf{m}([n-2],n-1)R_2$, to obtain a block lower triangular determinant:

$$\kappa(D_{\mathcal{T}},n) = \det D_\kappa = \det \begin{pmatrix} D|_{[n-2]} - \mathbf{d}\,\mathbf{e}^T - \mathbf{m}([n-2],n-1)\,(\mathbf{d}')^T & 0 \\ (1-m_{e_0}m'_{e_0})(a_{e_0}\mathbf{e}^T - (\mathbf{d}')^T) & a_{e_0}(1-m_{e_0}m'_{e_0}). \end{pmatrix}$$

But the $(1,1)$ block on the right-hand side has determinant precisely $\kappa(D_{\mathcal{T}}|_{[n-1]}, n-1)$. We are now done by the induction hypothesis. Finally, (4.5) is now straightforward from Theorem A. ☐

Proof of Proposition 4.6. We first assume that (1) holds, and show (3). Consider a tree with edge-data $\mathcal{T}$ and a node v_0. Attach a pendant edge e_0 to v_0 with edge-data $(a_{e_0}, m_{e_0}, m'_{e_0})$, and call the resulting edge-data $\mathcal{T}_0$ – note that v_0 is a cut-vertex in $\mathcal{T}_0$ satisfying the assumptions in Definition 4.1. Since it is easily verified that $\kappa(D_{e_0}, v_0) = a_{e_0}(1-m_{e_0}m'_{e_0})$, Theorem D yields:

$$\det(D_{\mathcal{T}_0}) = \kappa(D_{\mathcal{T}}, v_0)\det(D_{e_0}) + \kappa(D_{e_0}, v_0)\det(D_{\mathcal{T}}).$$

But in this equation, all terms except $\kappa(D_{\mathcal{T}}, v_0)$ are known by (1) and direct computation. From this, and a Zariski density argument that allows one to cancel $\det(D_{e_0})$, the assertion (3) follows.

A similar argument shows (2) $\implies$ (3) – now assuming by Zariski density that $(\mathrm{cof} - \kappa)(D_e)$ and $\kappa(D_e)$ are invertible for each edge e. Conversely, suppose (3) holds. Then (1) and (2) are direct consequences of Theorem D and direct computation for $\det(D_e)$. ☐

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