Determinant of the distance matrix of a tree

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Abstract. We present a combinatorial proof of the Graham–Pollak formula for the determinant of the distance matrix of a tree, via sign-reversing involutions and the Lindström–Gessel–Viennot lemma.

Résumé. Nous présentons une preuve combinatoire de la formule de Graham et Pollak pour le déterminant de la matrice des distances d'un arbre, en utilisant des involutions et le lemme de Lindström–Gessel–Viennot.

Keywords: Distance matrix of a tree. Lindström–Gessel–Viennot's Lemma. Sign-reversing involutions. Bijective Combinatorics.

1 Introduction

Consider a tree T with vertices labeled from one to n, and edge set E. Define the *distance* between vertices i and j, denoted by d(i,j), as number of edges in the unique path of T connecting i and j. Define the *distance matrix* of T as $M(T) = (d(i,j))_{1 < i,j < n}$.

In their influential 1971 paper [7], Graham and Pollak established that the determinant of the distance matrix of T obeys the *Graham–Pollak formula*:

$$\det M(T) = (-1)^{n-1}(n-1)2^{n-2} \tag{1.1}$$

Observe that this implies that the determinant of the distance matrix of *T* is solely dependent on its number of vertices, and not on its tree structure.

Multiple techniques drawn from linear algebra, ranging from Gauss elimination to Charles Dodgson's condensation formula, have been used to prove the Graham–Pollak formula [4, 7, 6, 9, 10, 11]. However, the expression $(-1)^{n-1}(n-1)2^{n-2}$ suggests the existence of a signed enumeration problem solved by $\det M(T)$.

Pursuing this trail has led us to a novel combinatorial proof of the Graham–Pollak formula that relies on the existence of sign-reversing involutions, and on the celebrated Lindström–Gessel–Viennot lemma. Our journey concludes by establishing that our combinatorial proof provides a solid framework for many of the existing generalizations and *q*-analogues of the Graham–Pollak formula, and facilitates the derivation of new ones.

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2 Catalysts

Where we introduce the idea of a catalyst for a tree, and demonstrate how det(T) does a signed enumeration of all catalysts of a fixed tree T = ([n], E).

Fix a tree T=([n], E). Let $E^{\pm}=\{(i,j): \{i,j\}\in E\}$ denote the set of arcs supported on T. Given a permutation σ in S_n and a map $f:[n]\to E^{\pm}$, the ordered pair (σ,f) is a catalyst for T if for each vertex i, $f(i)=(v_i,v_{i+1})$ is a pair of successive vertices in the path $P(i,\sigma(i))$ (i.e., an arrow). The sign of a catalyst is the sign of its underlying permutation.

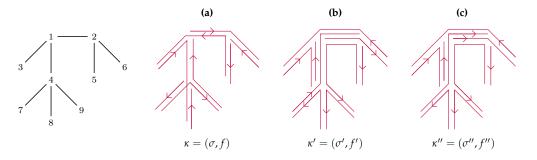


Figure 1: A tree T and the diagrams of three of its catalysts. We can recover a catalyst from its diagram. E.g., from the first diagram we see that $\sigma(1) = 6$ and f(1) = (1,2), that $\sigma(2) = 5$ and f(2) = (2,5), that $\sigma(3) = 8$ and f(3) = (3,1), and so on.

The determinant $\det M(T)$ does a signed enumeration of all catalysts for T. This is so because $d(i, \sigma(i))$ counts the number of edges in the unique path $P(i, \sigma(i))$ in T. Indeed,

$$\det M(T) = \sum_{\sigma \in \mathbb{S}_n} \operatorname{sgn}(\sigma) d(1, \sigma(1)) d(2, \sigma(2)) \dots d(n, \sigma(n)) = \sum_{\kappa \in K} \operatorname{sgn} \kappa, \tag{2.1}$$

where we are summing over K, the set of all catalysts for T. It is worth noting that the definition of catalyst implies that its underlying permutation must be a *derangement*, that is, a permutation without fixed points.

Partitioning catalysts by their underlying permutations proves ineffective in our search of a combinatorial proof of the Graham–Pollak formula, as in general, there are no cancellations between resulting summands.

3 Arrowflows and the Graham-Pollak formula

Where we present the definition of the arrowflow induced on T by a catalyst, and show how the Graham–Pollak formula becomes transparent when catalysts are partitioned according to them.

An *arrowflow on T* is a directed multigraph with vertex set [n], with exactly n arcs when counted with multiplicity, and whose underlying simple graph is a subgraph of T. By definition, given any catalyst $\kappa = (\sigma, f)$, the image of f, considered as a multiset, is always an arrowflow on T. We refer to it as *arrowflow induced* by κ .

We say that an arrowflow A is connected when its underlying simple graph is. If A is a connected arrowflow, there exist precisely two vertices that belong to more than one arrow of A. It turns out that these two vertices always belong to precisely two arrows, that we call the *repeated arrows*. We say that the repeated arrows of a connected arrowflow are *parallel* when they point in the same direction, and *anti-parallel* when they point in opposite directions.

An arrowflow is said to be *unital* when it is connected and its repeated arrows are anti-parallel, as illustrated in Figure 2 (a). Otherwise, it is said to be *zero-sum*. There are two possible causes for an arrowflow to be zero-sum. Either the arrowflow is disconnected, as illustrated in Figure 2 (b), or the arrowflow is connected, but the repeated arrows are parallel, as in Figure 2 (c).

Example 3.1. Figure 2 shows the three arrowflows induced by the three catalysts of Figure 1. The first arrowflow (a) is unital. The second arrowflow (b) is zero-sum because it is disconnected. The last one (c) is zero-sum because arc (1,2) appears twice.

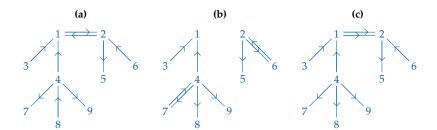


Figure 2: (a) Unital, (b) disconnected zero-sum, (c) connected zero-sum arrowflows.

It is crucial to observe that different catalysts on T can result on the same arrowflow. On the other hand, it is worth pointing out that there exist arrowflows on T that are not induced by any catalyst for T. We leave it to the reader to come up with such examples.

We define the *arrowflow class of A*, denoted by C(A), as the set of catalysts inducing A on T. An arrowflow class C(A) is unital or zero-sum according to whether A is unital or zero-sum. Nonempty arrowflow classes define a partition $K = \bigsqcup_A C(A)$ of the set K of all catalysts for T, that we call the *arrowflow partition of K*. It allows us to rewrite Equation (2.1) as

$$\det M(T) = \sum_{\substack{A \text{arrowflow}}} \sum_{\kappa \in C(A)} \operatorname{sgn}(\kappa), \tag{3.1}$$

where the first sum is taken over all arrowflows on T, and the second one over all catalysts κ in the arrowflow class C(A).

Theorem 3.2. The arrowflow partition defines an optimal way of partitioning the set of catalysts for T. More precisely, if C(A) is an arrowflow class, then

$$\sum_{\kappa \in C(A)} \operatorname{sgn}(\kappa) = \begin{cases} (-1)^{n-1} & \text{if A is a unital arrowflow,} \\ 0 & \text{if A is a zero-sum arrowflow.} \end{cases}$$
(3.2)

The proof of this result will unfold in the following two sections.

We close this section by showing how a combinatorial proof of the Graham–Pollak formula can be obtained by gathering all the elements of our reasoning. First observe that Theorem 3.2 implies that there can be no cancellations between the different summands in Equation (3.1). Therefore, it suffices to show that

$$\sum_{\substack{A \text{ unital} \\ \text{arrowflow}}} (-1)^{n-1} = (-1)^{n-1} (n-1) \, 2^{n-2}.$$

Or equivalently, that there exists $(n-1) 2^{n-2}$ unital arrowflows on T. This is immediate as the factor (n-1) counts the number of ways of selecting the edge of T that gives rise to the anti-parallel repeated arrows, whereas factor 2^{n-2} counts the number of ways in which the remaining n-2 edges can be oriented. Finally, to show that the sign of a unital arrowflow class is $(-1)^{n-1}$, we show that the underlying permutation of the unique catalyst that survives the involution process is always an n-cycle.

4 Zero-sum arrowflows

Where we present a sign-reversing involution without fixed points on each zero-sum arrowflow class, and conclude that the signed sum of catalyst in such a class is always zero.

This is achieved in Lemma 4.1, which implies that the signed sum of catalysts in a zero-sum arrowflow class C(A) is zero. This constitutes one half of Lemma 3.2.

Lemma 4.1. Let A be a zero-sum arrowflow on T. If A is connected, let i and j be the two preimages of the repeated arrow (a,b) of A. On the other hand, if A is disconnected, we let $\{i,j\}$ be an edge of T such that neither (i,j) nor (j,i) is in A. Then, the map $\varphi: C(A) \to C(A)$ that sends the catalyst (σ,f) to the catalyst $(\sigma \circ (i\ j),f \circ (i\ j))$ is a sign-reversing involution without fixed points.

Sketch of proof. It is enough to show that f(i) is an arc in both $P(j,\sigma(i))$ and $P(i,\sigma(i))$. Observe that if A is connected, then i,j and a lie in one connected component of the graph obtained by deleting from T edge $\{a,b\}$, while $\sigma(i),\sigma(j)$ and b lie in the other one. See Figure 3.



Figure 3: Involution φ acting on a zero-sum connected arrowflow A.

On the other hand, when A is disconnected, then $P(j, \sigma(i))$ and $P(i, \sigma(i))$ differ in exactly one arc, either (i, j) or (j, i). Therefore, since f(i) is neither of them, we conclude that f(i) belongs to both paths. See Figure 4.

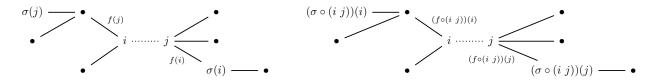


Figure 4: Involution φ acting on zero-sum disconnected arrowflow A.

5 Unital arrowflows

Where we rely on the Lindström–Gessel–Viennot Lemma to compute the signed sum of all catalysts in a unital arrowflow class.

We rely on the following version of the Lindström-Gessel-Viennot lemma here.

Lemma 5.1 (Lindström [8], Gessel–Viennot [5]). Let \mathcal{R} be an acyclic directed graph. Distinguish two sequences of nodes (v(1), ..., v(n)) and (v'(1), ..., v'(n)) with no repeated nodes in either of them. Let \mathcal{P} be the set of all sequences of paths $(P_1, ..., P_n)$ for which there exists a permutation $\sigma_P \in \mathbb{S}_n$ such that, for each i in [n], the path P_i stars at v(i) and finishes at $v'(\sigma(i))$. Then,

$$\sum_{(P_1,...,P_n)\in\mathcal{P}} \operatorname{sgn}(\sigma_P) = \sum_{\substack{(P_1,...,P_n)\in\mathcal{P}\\ \textit{non-intersecting}}} \operatorname{sgn}(\sigma_P).$$

We break down our argument into three parts. First, we prepare for the application of the Lindström–Gessel–Viennot Lemma and create an acyclic directed graph, the *route map* \mathcal{R}_A , from any unital arrowflow A on T. Subsequently, we establish a sign-preserving bijection that sends each catalyst in C(A) to a family of n paths on \mathcal{R}_A , which we refer to as n-paths. The application of the Lindström–Gessel–Viennot Lemma reduces our original quest to the problem of finding a description of the non-intersecting n-paths. Finally,

we establish that in each unital arrowflow class, there exists exactly one catalyst κ that generates a non-intersecting n-path, and that its underlying permutation of κ is always an n-cycle. Therefore, the sole surviving catalyst, has sign $(-1)^{n-1}$.

5.1 The route map \mathcal{R}_A . To construct \mathcal{R}_A , the route map of T, we proceed in several steps. First, we use arrowflow A to define a plane rooted directed tree T_0 . Then, we define the *Southern hemisphere*, an acyclic directed graph; and its anti-isomorphic counterpart, the *Northern hemisphere*. Finally, we add bridges connecting both hemispheres and pointing from South to North.

Step 1. Construct a rooted directed tree A_0 from A.

Let $e = \{a, b\}$ be the edge of T connecting the two vertices appearing in the repeated edge of A. We construct a *rooted directed tree* A_0 from A by adding a new vertex r as a root and substituting the arcs (a, b) and (b, a) by (r, b) and (r, a) respectively. This construction induces a bijection between arcs of A and A_0 . An arc of A_0 will be said to be *ascending* if it points to the root, and *descending* if it points away from the root. A child node u of a parent node v is termed *ascending* when it is descending. See Figures 5 (a) and (b).

We denote the underlying undirected rooted tree of A_0 by T_0 .

Step 2. Give a compatible plane structure to the rooted directed tree A_0 .

A plane structure for A_0 is said to be *compatible* if for each node v with children u_1, \ldots, u_k , every ascending child of v lies to the left of every descending child. In general there exist multiple compatible plane structures on A_0 . We just choose one of them. See Figure 5 (c).

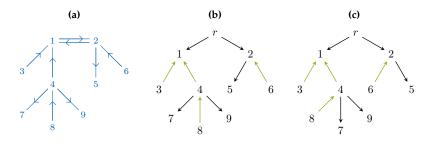


Figure 5: (a) A unital arrowflow A with repeated edge $\{1,2\}$. (b) The rooted directed tree A_0 with root r. (c) A compatible plane structure for A_0 .

The underlying rooted tree T_0 inherits a plane rooted tree structure. The neighbors of a vertex i of T_0 are ordered starting with the children of i in increasing order (as in the plane structure of T_0), and ending with the parent.

Step 3. Construct the Southern hemisphere of T_0 .

The *Southern hemisphere* $S(T_0)$ of an undirected plane rooted tree T_0 is a directed multigraph whose vertex set is composed of three types of nodes (v-node, e-node, and s-node). Each node i of T_0 , including the root, contributes with a node v(i). Each edge $\{i,j\}$ of T_0 , contributes two nodes e(i,j) and e(j,i). Finally, we add two nodes $s_i(j_{k-1},j_k)$ and $s_i(j_k,j_{k-1})$ for each vertex i of T_0 and each pair of consecutive neighbors j_{k-1},j_k of i. See Figure 6.

The arcs of the route map connect these nodes in a natural way, as to allow one to understand the paths of T_0 as paths in the route map. The explicit construction of the set of arcs can be daunting, but these arcs do not need to be included in the graphical representations of $S(T_0)$ as they can be inferred from the set of nodes.

To construct the set of arcs of $S(T_0)$ we add, for each i, two arcs between s-nodes for each three consecutive neighbors j_{k-1} , j_k , j_{k+1} , an arc $(v(i), s_i(j_1, j_2))$ for each node i that is not a leaf, and an arc $(v(i), e(i, j_1))$ for each node i. Additionally, from each e-node e(j, i) there is an arc to (at most) two s-nodes around i, and conversely from each s-node $s_i(j_k, j_{k+1})$ to its corresponding $e(i, j_{k+1})$ node.

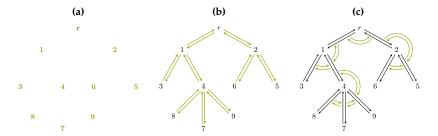


Figure 6: Highlighted, the sets of (a) v-nodes, (b) e-nodes, and (c) s-nodes of $\mathcal{S}(T_0)$.

Step 4. Construct the Northern hemisphere, an anti-isomorphic copy of the Southern hemisphere.

Let T_0 be an undirected plane rooted tree, let T_0' be its *mirror image*; a copy of T_0 in which local orders are inverted. The *Northern hemisphere* $\mathcal{N}(T_0)$ of T_0 is constructed from $\mathcal{S}(T_0')$ by replacing each arc $(v(i), e(i, j_1))$ by the arc $(e(j_1, i), v(i))$, and, whenever i is not a leaf, replacing arc $(v(i), s_i(j_1, j_2))$ by the arc $(s_i(j_2, j_1), v(i))$. We denote nodes of $\mathcal{N}(T_0)$ using primed letters.

Step 5. Construct the route map \mathcal{R}_A .

The *route map* \mathcal{R}_A of the unital arrowflow A is the directed multigraph obtained by adding to $\mathcal{S}(T_0) \cup \mathcal{N}(T_0)$ an arc (e(u,v),e'(u,v)) for each arc (u,v) of A_0 . These arcs are referred to as the *bridges* between hemispheres of \mathcal{R}_A .

The key property of the route map \mathcal{R}_A is that it is always acyclic. The Southern hemisphere $\mathcal{S}(T_0)$ is acyclic because any cycle in $\mathcal{S}(T_0)$ would induce a cycle in the rooted

plane tree T_0 . The Northern hemisphere $\mathcal{N}(T_0)$ is acyclic because it is an anti-isomorphic copy of $\mathcal{S}(T_0)$. Finally, the route map is acyclic because all the bridges point from South to North.

5.2 Catalyst and n-paths. Let A be a unital arrowflow, and (σ, f) be a catalyst in C(A). Let Λ_i be the unique path of \mathcal{R}_A going from v(i) to $v'(\sigma(i))$ and passing through the bridge $(e(u_i, v_i), e'(u_i, v_i))$, where (u_i, v_i) is the arc of A_0 defined by f(i). See Figure 7.

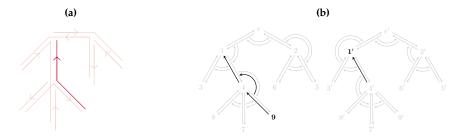


Figure 7: (a) A path $P(9, \sigma(9) = 1)$ marked at f(9) = (4, 1). (b) The path Λ_9 of \mathcal{R}_A .

We define the *n*-path induced by catalyst $\kappa = (\sigma, f)$ on the route map \mathcal{R}_A as $\Lambda(\kappa) = \{\Lambda_1, \ldots, \Lambda_n\}$, and say that κ has been lifted to the *n*-path $\Lambda(\kappa)$. One can recover the permutation σ from $\Lambda(\kappa)$. Thus we define $\operatorname{sgn}(\Lambda(\kappa))$ as $\operatorname{sgn}(\sigma)$.

Example 5.2. Let κ be the catalyst of Figure 1 (a). Figure 8 (b) illustrates the n-path induced by κ , where we mark path Λ_i with subscript i. Moreover, since each node in the route map belongs to at most one path, it is an example of a non-intersecting n-path.

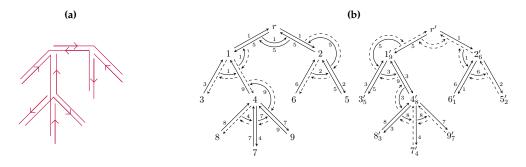


Figure 8: (a) A catalyst and (b) its induced *n*-path $\Lambda(\kappa) = {\Lambda_1, ..., \Lambda_n}$.

We say that an n-path is full when every bridge (e(u,v),e'(u,v)) belongs to exactly one of its paths. Since any n-path that is not full must contain an intersection at some bridge, non-intersecting n-paths are always full. Moreover, the lifting of any catalyst belonging to a unital arrowclass is always full.

Lemma 5.3. The operation of lifting defines a permutation-preserving bijection between the set of catalysts with unital arrowflow A and the set of full n-paths of \mathcal{R}_A .

Sketch of proof. To prove that the lifting map is a bijection, we define its inverse. Any n-path P defines a permutation σ , where P_i is a path from v(i) to $v'(\sigma(i))$. On the other hand, we use the bridges of P to define a map $f:[n]\to E^\pm$. If the arc e defining the bridge of P_i does not include the root, we define f(i)=e. Otherwise, we let f(i) be the repeated edge with the appropriate orientation. It can be shown that $(\sigma,f)\in C(A)$ and, that the map we just defined is the inverse of the lifting map. Since the underlying permutation of a catalyst is the permutation induced by its lifting, we conclude that the lifting map is a permutation-preserving bijection.

Lemma 5.3 allows us to rewrite Equation (3.2) as $\sum_{\kappa \in C(A)} \operatorname{sgn}(\kappa) = \sum \operatorname{sgn}(\Lambda)$, where the second sum is taken over the set of full n-paths on \mathcal{R}_A .

5.3 There is an unique catalyst inducing a non-intersecting n-path. Moreover, its underlying permutation is always an n-cycle.

Proposition 5.4. Let A be a unital arrowflow on T. Consider all n-paths in the route map \mathcal{R}_A induced by catalysts in C(A). There exists precisely one catalyst inducing a non-intersecting n-path in \mathcal{R}_A . Its underlying permutation is an n-cycle. Therefore, its sign is $(-1)^{n-1}$.

Sketch of proof. Fix a plane rooted tree A_0 and let Λ be an n-path. Assume Λ is the lift of catalyst (σ, f) . Consider the set \mathcal{E} consisting of the e-nodes appearing in the paths of Λ . We can show that \mathcal{E} uniquely determines the catalyst (σ, f) . On the other hand, for each arc (i, j) of A_0 , the set \mathcal{E} contains both e(i, j) and e'(i, j). Furthermore, if Λ is non-intersecting, a counting argument allows us to show that (i, j) is ascending if and only if \mathcal{E} contains e'(j, i), and descending if and only if it contains e(j, i). This gives uniqueness.

The argument concludes by noting that the underlying permutation of the sole catalyst inducing a non-intersecting n-path is always an n-cycle, and that the depth-first search algorithm allows us to explicitly describe this cycle, as illustrated in Figure 9. \square

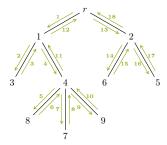


Figure 9: Applying the depth-first search algorithm to this rooted tree results in the word r13148474941r26252r, which we identify with the cycle (384791625).

Example 5.5. Figure 9 illustrates how the depth-first search algorithm describes the non-intersecting path in the route map \mathcal{R}_A of our running example.

The Lindström–Gessel–Viennot Lemma [5, 8] allows us to conclude that when we perform the signed sum of all catalysts in a unital arrowflow class, catalysts that induce intersecting n-paths on \mathcal{R}_A cancel each other out. Finally, since the unique non-intersecting n-path has as its underlying permutation an n-cycle, the signed sum of catalysts in a unital arrowflow class is equal to $(-1)^{n-1}$, which concludes the proof of Lemma 3.2.

6 Beyond the Graham-Pollak formula

Where we show that our combinatorial proof of the Graham–Pollak formula not only establishes a solid framework for the understanding of the existing generalizations but also paves the way for the creation of new ones.

Various generalizations of the Graham–Pollak formula exist in the literature. In [1], a version of this formula is presented for simple trees with weighted edges, while the situation of arc-weighted trees is treated in [2]. In both cases, the weight of a path is defined as the sum of the weights of its edges. In contrast, using q-integers to define the vertex distance results in q-analogues of the results. Simple trees obey the q-Graham–Pollak formula $(-1)^{n-1}(n-1)(1+q)^{n-2}$ [10, Cor. 2.3], and a q-analogue for trees weighted with integers is given in [10, Thm. 2.4]. There also exist q-analogues for the Graham–Pollak formula when q is arc-weighted with integers [2, Thm. 3.1], or over a commutative ring [11, Thm. 4], or with matrices over a commutative ring [11, Thm. 7].

We present a new generalization of the Graham–Pollak formula. Towards this end, we define a *q-sum*, denoted by @, as $a \odot b = a + b + (q-1)ab$. This operation allows us to simplify [10, Thm. 2.4], by noting that $[1]_q = 1$ and $[a+b]_q = [a]_q \odot [b]_q$. More crucially, the *q*-sum operation is well-defined over any commutative ring, and not just integers. This makes our setting more general.

Let e^+ and e^- be the arcs originating from edge e, and let E^\pm be the set of arcs of T. Let R be a commutative ring, and $\alpha: E^\pm \to R[q]$ be a weight function. Let the (i_k, i_{k+1}) 's be the arcs in the unique path from $i=i_0$ to $j=i_{d(i,j)}$. Define the q-distance between vertices i and j as $d_q(i,j)=\alpha(i,i_1)$ @ $\alpha(i_1,i_2)$ @ \cdots @ $\alpha(i_{d(i,j)-1},j)$. For any arc a of E^\pm , we write α_a for $\alpha(a)$. Then, the following theorem holds.

Theorem 6.1. The determinant of the d_q -distance matrix of a tree T is

$$(-1)^{n-1} \sum_{e \in E} \Big(\alpha_{e^+} \alpha_{e^-} \prod_{\substack{f \in E \\ f \neq e}} (\alpha_{f^+} \ \widehat{\mathcal{Q}}) \ \alpha_{f^-} \Big) \Big).$$

Before discussing this result's proof, it's worth noting that the same argument provides a combinatorial proof for the very general Choudhury–Khare formula [3, Thm. A]. It is interesting to note that while the Choudhury–Khare's generalization is, in some precise sense, the most general possible [3, Example 1.13], Theorem 6.1 stands independently from this framework. It represents the most natural simultaneous generalization of [11, Thm. 4] and [10, Thm. 2.4], as depicted in the diagram appearing in Figure 10.

Figure 10: Relationship between the formulas found in the literature.

Both Theorem 6.1 and the Choudhury–Khare formula [3, Thm. A] readily follow from our combinatorial construction. In both situations, we want to compute the determinant of an appropriate matrix M'(T). Towards this end, we define a weight function on the catalyst set of T, in such a way that the determinant of M'(T) does the weighted (q-) sum of all catalysts, as in Equation 3.1.

To show that the weighted (q-) sum of all catalysts in a zero-sum arrowflow class is zero, we show that the involution φ defined in Section 4 is weight-preserving. On the other hand, we use the constructions presented in Section 5 to compute the weighted (q-) sum of all catalysts in a unital arrowflow class. For this, we assign weights to the edges of the route map \mathcal{R}_A , and show that the lifting map is weight-preserving. A weighted version of the Lindström–Gessel–Viennot Lemma allows us to conclude that $\det M'(T)$ does a weighted (q-) sum of non-intersecting n-paths within \mathcal{R}_A . Finally, we use the characterization of the sole catalyst inducing a non-intersecting n-path on \mathcal{R}_A obtained in Proposition 5.4 to deduce the desired formula for the determinant of M'(T).

Acknowledgements

We dedicate this work to Ira Gessel as a token of our gratitude for his lecture on the Lindström–Gessel–Viennot lemma, which he virtually delivered at the University of Seville in March of 2022. The senior authors would also like to express their gratitude to Xavier Viennot for the entrancing memories of his lectures.

This work has been partially supported by the Grant PID2020-117843GB-I00 funded by MICIU/AEI/10.13039/501100011033 and by P2001056 (Junta de Andalucía, FEDER, PAIDI2020).

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