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On the interlace polynomials of forests

C. Anderson [a], J. Cutler [b,*], A.J. Radcliffe [a], L. Traldi [c]

[a] *University of Nebraska–Lincoln, Lincoln, NE 68588-0130, United States*

[b] *Montclair State University, Montclair, NJ 07043, United States*

[c] *Lafayette College, Easton, PA 18042, United States*

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ABSTRACT

The interlace polynomials were introduced by Arratia, Bollobás and Sorkin (2004) [3–5]. These invariants generalize to arbitrary graphs some special properties of the Euler circuits of 2-in, 2-out digraphs. Among many other results, Arratia, Bollobás and Sorkin (2004) [3–5] give explicit formulas for the interlace polynomials of certain types of graphs, including paths; it is natural to wonder whether or not it is possible to extend these formulas to larger classes of graphs. We give a combinatorial description of the interlace polynomials of trees and forests.

1. Introduction

A problem involving counting 2-in 2-out digraphs with a fixed number of Euler circuits (which grew out of DNA sequencing by hybridization [2]) led Arratia, Bollobás and Sorkin to introduce a family of new graph polynomials, the interlace polynomials [3–5]. In this paper we introduce a particular type of independent set of vertices in a forest, and prove that the interlace polynomial of a forest is essentially a generating function for these independent sets.

We follow [5] for general notation and terminology, though we restrict our attention to simple graphs. If a and b are distinct vertices of a simple graph G then the *pivot* G^{ab} [3–5,7] is obtained from G by partitioning the vertices in $N_G(a) \cup N_G(b)$ into three sets according to whether they are adjacent only to a, only to b or to both, and then toggling all edges between these sets.

Definition 1 (*[3]*). The *(vertex-nullity) interlace polynomial* of a graph G, denoted q_N, is defined recursively by

$$q_N(G) = \begin{cases} q_N(G-a) + q_N(G^{ab} - b), & \text{if } ab \in E(G), \\ y^n, & \text{if } G = E_n. \end{cases}$$

In [5], a two-variable generalization of the vertex-nullity interlace polynomial was introduced. If $S \subseteq V(G)$ then $G[S]$ is the subgraph of G induced by S; $r(G[S])$ and $n(G[S])$ are the rank and nullity of the adjacency matrix of $G[S]$, considered over $GF(2)$.

* Corresponding author.
E-mail addresses: jonathan.cutler@montclair.edu (J. Cutler), aradcliffe1@math.unl.edu (A.J. Radcliffe), traldil@lafayette.edu (L. Traldi).
URL: http://www.lafayette.edu/~traldil/ (L. Traldi).

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Definition 2. The *(two-variable) interlace polynomial* of a graph G is

$$q(G) = \sum_{S \subseteq V(G)} (x-1)^{r(G[S])} (y-1)^{n(G[S])}.$$

Further, the following recursion was shown to be true when $ab \in E(G)$.

$$q(G) = q(G-a) + q(G^{ab} - b) + ((x^2-1)-1)q(G^{ab} - a - b).$$

This reduces to the recursion in Definition 1 when $x = 2$.

We use standard terminology regarding trees and rooted trees. For a vertex v in a rooted tree, let $p(v)$ be the *parent* of v (for $I \subseteq V(G)$, $p(I) = \cup_{v \in I} p(v)$), and $c(v)$ be the *children* of v. The set of children of $p(v)$ other than v itself is denoted by $s(v)$; its elements are the *siblings* of v. A rooted tree T is *ordered* by assigning an order to the set of children of each parent vertex; non-root vertices may then have *earlier siblings* and *later siblings*. If T is an ordered tree then its *underlying tree* is the ordinary unrooted tree obtained by forgetting the choices of root and child-orders in T.

A subset of $V(T)$ that contains no adjacent pairs is *independent*, and a set of vertices *dominates* a vertex v if it contains v or contains some neighbor of v.

Definition 3. An *earlier sibling cover* (or *es-cover*) in an ordered tree T is an independent set I that dominates r and has the property that for every non-root vertex $v \in I$, every earlier sibling of v is dominated by I.

A different description of sets for which q_N is a generating function was found in [1] when the trees considered are caterpillars.

Definition 4. For integers s and t the *es-number* $c_{s,t}(T)$ is the number of es-covers I in T with $|I| = s$ and $|p(I - \{r\})| = t$; that is, $c_{s,t}(T)$ is the number of s-element es-covers in T whose non-root elements have precisely t different parents.

In Section 2 we show that even though the es-numbers are defined for ordered trees, they are actually independent of the choices of a root and of orders of the children of parent vertices.

Theorem 5. *If T and T' are ordered trees whose underlying unrooted trees are isomorphic, then $c_{s,t}(T) = c_{s,t}(T')$ for all $s, t \in \mathbb{Z}$.*

In Section 3 we show that the es-numbers give a combinatorial description of the interlace polynomials of trees.

Theorem 6. *If T is a tree then the two-variable interlace polynomial of T is*

$$q(T) = \sum_{s,t} c_{s,t}(T) \cdot y^{s-t}(y - 1 + (x-1)^2)^t.$$

Theorem 6 implies Theorem 5, so strictly speaking the proof of Theorem 5 in Section 2 is logically unnecessary. We offer the proof anyway because it is self-contained and lends some insight into the combinatorial significance of earlier sibling covers, without reference to the interlace polynomial.

Theorem 6 is analogous to the spanning forest expansion of the Tutte polynomial (see, e.g., [10] or [6]). Just as there, the number of forests with fixed numbers of internally and externally active edges is invariant under different orderings of the edges of a graph, we have here that the es-numbers $c_{s,t}(T)$ are invariant under different orderings of the vertices of a tree.

Further, we note that setting $x = 2$ in Theorem 6 implies that the vertex-nullity polynomial is a generating function for es-covers in trees.

Corollary 7. *Let T be a tree, and for each integer s let $c_s(T)$ be the number of s-element es-covers in T, i.e., $c_s(T) = \sum_t c_{s,t}(T)$. Then*

$$q_N(T) = \sum_s c_s(T) y^s.$$

Although we focus our attention on trees, the definitions and results above extend directly to forests. An es-cover in a forest F is simply a set of vertices I such that for each component tree T of F, $I \cap V(T)$ is an es-cover in T. (The definition requires the components of F to be ordered individually.) As q is multiplicative on disjoint unions, the formula of Theorem 6 extends directly to forests.

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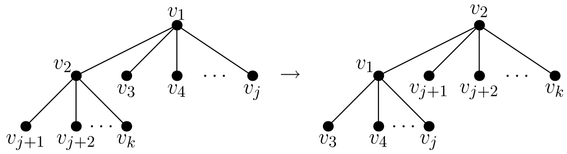

Fig. 1. Moving the root down an edge.

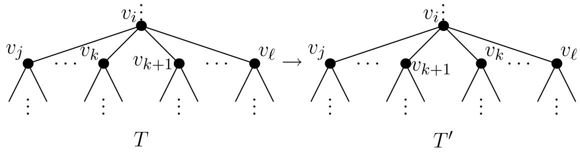

Fig. 2. Swapping the ordering of two vertices.

2. Earlier sibling covers

In this section we prove Theorem 5 by showing that the es-numbers of an ordered tree are invariant under two operations: (a) moving the root along an edge, and (b) switching the positions of two consecutive siblings in the ordering. Using multiple applications of these two operations, we can obtain any ordered tree with a given underlying tree from any other.

(a) We assume that the vertices of T are ordered $v_1, v_2, \dots, v_n$, with root $r = v_1$. Suppose that the children of v_1 are $v_2, v_3, \dots, v_j$ in order, and those of v_2 are $v_{j+1}, v_{j+2}, \dots, v_k$ in order. Let T' be the ordered tree obtained from T by designating v_2 as the root rather than v_1, designating v_1 as the earliest child of v_2, and leaving all other child-orders alone. (See Fig. 1.) This is well-defined because the fact that v_1 and v_2 are neighbors guarantees that all other vertices have the same children in T' as in T.

We claim that the earlier sibling covers in T are exactly the es-covers in T'. To this end, let I be an es-cover in T. Firstly, since T' has the same underlying tree as T, I must be independent in T'. Secondly, if I contains v_1, then I dominates v_2. If I does not contain v_1, then it must contain one of its children and, by the ordering condition, thus must dominate v_2 (the first child). In either case, I dominates the root in T'. Lastly, we must show that I satisfies the ordering condition in T'. For any vertex v other than v_1 and v_2, the ordering of the children of v is the same in T and T'; hence the ordering property for children of v in T' follows immediately from the same property in T. Since $c_{T'}(v_1) \subseteq c_T(v_1)$, the ordering property for children of v_1 in T' is also immediate. For the children of v_2 in T', the ordering property in T guarantees that if some child of v_2, say v_i, is in I, then $v_{i'}$ is dominated by I whenever $j + 1 \leq i' < i$. Also, v_1 is dominated by I since it is the root of T. Thus, the ordering property holds everywhere in T' and so I is an es-cover in T'. Applying this switch again we get T back, so the es-covers in T are exactly those of T'.

The fact that T and T' have the same es-covers is not sufficient for Theorem 5, because a given es-cover may be counted in different es-numbers in the two ordered trees. For instance $\{v_1\}$ is counted in $c_{1,0}(T)$ and $c_{1,1}(T')$, because v_1 has no parent in T but v_1 is a child of v_2 in T'. The only vertices with different parents in T and T' are v_1 and v_2, so the only es-covers that are counted in different es-numbers in T and T' are those that contain one of v_1, v_2 and none of $v_3, \dots, v_k$. If I is such an es-cover then $I \triangle \{v_1, v_2\}$ is also, and if I is counted in $c_{s,t}(T)$ and $c_{s,t'}(T')$ then $I \triangle \{v_1, v_2\}$ is counted in $c_{s,t'}(T)$ and $c_{s,t}(T')$. As $I \leftrightarrow I \triangle \{v_1, v_2\}$ is a one-to-one correspondence between the es-covers I with $I \cap \{v_1, \dots, v_k\} = \{v_1\}$ and those with $I \cap \{v_1, \dots, v_k\} = \{v_2\}$, Theorem 5 is satisfied.

(b) Now we must show that if we interchange the ordering of two children of some vertex in T, say v_i, then the es-numbers remain unchanged. Let the children of v_i be ordered $v_j, v_{j+1}, \dots, v_\ell$. Consider v_k for any $k \in \{j, \dots, \ell - 1\}$. We claim that the number of es-covers remains unchanged if we order the children of x as $v_j, \dots, v_{k+1}, v_k, \dots, v_\ell$, leaving all other child-orders the same, to form an ordered tree T'. (See Fig. 2.) Let I be an es-cover in T and let v_m be the maximal child of v_i that is in I. Note that if v_m does not exist, i.e., $c(v_i) \cap I = \emptyset$, then I is certainly an es-cover in T'. If $m \geq k + 1$, then both v_k and v_{k+1} are dominated by I in both T and T'. Thus, I is an es-cover in T' (although v_k may not be required to be dominated in T'). If $m < k$, then neither v_k nor v_{k+1} is in I, and so I is an es-cover in T'. Finally, we must deal with the case when $m = k$. If v_{k+1} is dominated by I, then I is still an es-cover in T'. However, it may be the case that v_{k+1} is not dominated by I, and thus I is not an es-cover in T'. Since v_{k+1} is not dominated by I, none of its neighbors is in I and thus $I \triangle \{v_k, v_{k+1}\}$ is an independent set in T'. Moreover, in T', v_{k+1} is the latest child of v_i in I and all earlier children are dominated in I since I is an es-cover in T. Further, $I \triangle \{v_k, v_{k+1}\}$ is not an es-cover in T since $v_{k+1} \in I$ but v_k is not dominated by I. Hence, the number of es-covers in T' is at least the number in T. Applying this switch again we get T back, so the number of es-covers in T equals the number of es-covers in T'.

Note further that as T and T' have the same root, they have the same parent-vertex function. Consequently, if I is an es-cover in both T and T' then it is counted in the same es-number in T and T'. Also, if I is an es-cover in T but not T' and I is counted in $c_{s,t}(T)$ then $I \triangle \{v_k, v_{k+1}\}$ is counted in $c_{s,t}(T')$.

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3. Weighted interlace polynomials

It will be convenient to use the weighted version of the interlace polynomial introduced in [9]. Consider a graph G with *vertex weights*, i.e., functions α and β mapping $V(G)$ into some commutative ring R.

Definition 8. If G is a vertex-weighted graph then the *weighted interlace polynomial* of G is

$$q_W(G) = \sum_{S \subseteq V(G)} \left(\prod_{v \in S} \alpha(v) \right) \left(\prod_{v \notin S} \beta(v) \right) (x-1)^{r(G[S])} (y-1)^{n(G[S])}.$$

The weighted interlace polynomial has several useful properties. For instance, q_W is multiplicative on disjoint unions, as is the original unweighted interlace polynomial. A more surprising property of the weighted interlace polynomial is a novel recursive description. As we are interested in trees here, we give only the recursion for simple graphs; a more general result appears in [9].

Proposition 9. *If G is a vertex-weighted simple graph then $q_W(G)$ may be calculated recursively using these two properties.*

1. *If a and b are loopless neighbors in G then*
$$q_W(G) = \beta(a) q_W(G-a) + \alpha(a) q_W((G^{ab} - b)'),$$
where $(G^{ab} - b)'$ is obtained from $G^{ab} - b$ by changing the weights of a to $\alpha'(a) = \beta(b)$ and $\beta'(a) = \alpha(b)(x-1)^2$.
2. *If E_n has no edges then*
$$q_W(E_n) = \prod_{v \in V(E_n)} (\alpha(v)(y-1) + \beta(v)).$$

A tree may be analyzed recursively by pruning its leaves, so for our purposes the most valuable special case of (1) involves a vertex b of degree one. In this special case $G^{ab} = G$ and the assertion of (1) is essentially a weighted version of Proposition 4.12 of [8].

Theorem 6 may be summarized by saying that the definition of $q(T)$ can be organized into sub-totals corresponding to earlier sibling covers. These sub-totals are organized according to the *total weight* of an es-cover.

Definition 10. Let T be an ordered tree with vertex-weights, and let I be an es-cover in T. Let

$$I_r = \{v \in I : \text{either } v = r \text{ or } I \text{ contains a later sibling of } v\},$$
$$I_l = \{v \in I : v \neq r \text{ and } I \text{ contains no later sibling of } v\}, \text{ and}$$
$$I'_c = \{v \notin I : I \text{ contains a child of } v\}.$$

For each vertex v define the *I-weight* $w_I(v)$ as follows:

$$w_I(v) = \begin{cases} \beta(v) + \alpha(v)(y-1) & \text{if } v \in I_r \\ \alpha(v) \cdot \big((y-1)\beta(p(v)) + (x-1)^2 \alpha(p(v))\big) & \text{if } v \in I_l \\ 1 & \text{if } v \in I'_c \\ \beta(v) & \text{if } v \notin I \text{ and } v \notin I'_c. \end{cases}$$

The product

$$\prod_{v \in V(T)} w_I(v)$$

is the *total weight* of I in T, denoted $w_T(I)$.

If T' is a subtree of T that contains the root then we presume that the children of each parent vertex in T' are ordered by restricting the order of the children of that vertex in T. With this convention, it is easy to verify the following.

Lemma 11. *Let T be an ordered tree with a leaf ℓ such that $p(\ell) \neq r \neq \ell$, all the siblings of ℓ are leaves, and ℓ has no later siblings. Further, let $T' = T - \ell$ and $T'' = T - \ell - p(\ell) - s(\ell)$. Then*

$$\{\text{es-covers } I \text{ in } T \text{ with } \ell \notin I\} = \{\text{es-covers in } T'\}$$

and

$$\{\text{es-covers } I \text{ in } T \text{ with } \ell \in I\} = \{\{\ell\} \cup s(\ell) \cup I \text{ with } I \text{ an es-cover in } T''\}.$$

We use T to denote both an ordered tree and its underlying unrooted tree.

Theorem 12. *If T is an ordered tree with vertex-weights then*

$$q_W(T) = \sum_{I \text{ an es-cover}} w_T(I).$$

Proof. If $V(T) = \{r\}$ then $I = \{r\}$ is the only es-cover and $w_T(I) = \beta(r) + \alpha(r)(y-1) = q_W(T)$.

If $V(T) = \{r, v\}$ then $I_1 = \{r\}$ and $I_2 = \{v\}$ are the es-covers in T. As $w_T(I_1) = \beta(v) \cdot (\beta(r) + \alpha(r)(y-1))$ and $w_T(I_2) = \alpha(v) \cdot \left((y-1)\beta(r) + (x-1)^2\alpha(r)\right)$, $w_T(I_1) + w_T(I_2) = \beta(v)\beta(r) + \beta(v)\alpha(r)(y-1) + \alpha(v)\beta(r)(y-1) + \alpha(v)\alpha(r)(x-1)^2$; this agrees with Definition 4.

Suppose $n \geq 3$ and T has only one vertex of degree ≥ 2. Let $V(T) = \{v_1, \ldots, v_n\}$ with v_1 the unique non-leaf, $r \in \{v_1, v_2\}$, and $v_2, \ldots, v_n$ listed in the order used in the ordered tree T. A subset S of $V(T)$ has rank 2 and nullity $|S| - 2$ if $v_1 \in S$ and $|S| \geq 2$; otherwise S has rank 0 and nullity $|S|$. The es-covers of T are $I_1 = \{v_1\}$ and $I_k = \{v_2, \ldots, v_k\}$ for $2 \leq k \leq n$.

If $r = v_1$ then

$$w_T(I_1) = (\beta(v_1) + \alpha(v_1)(y-1)) \prod_{i \geq 2} \beta(v_i)$$

is the sum of the contributions of $S = \emptyset$ and $S = \{v_1\}$ to Definition 8, and

$$w_T(I_2) = \alpha(v_2)\left((y-1)\beta(v_1) + (x-1)^2\alpha(v_1)\right) \prod_{i > 2} \beta(v_i)$$

is the sum of the contributions of $S = \{v_2\}$ and $S = \{v_1, v_2\}$ to Definition 8. If $r = v_2$ then

$$w_T(I_2) = (\beta(v_2) + \alpha(v_2)(y-1)) \prod_{i \neq 2} \beta(v_i)$$

is the sum of the contributions of $S = \emptyset$ and $S = \{v_2\}$ to Definition 8, and

$$w_T(I_1) = \alpha(v_1)\left((y-1)\beta(v_2) + (x-1)^2\alpha(v_2)\right) \prod_{i > 2} \beta(v_i)$$

is the sum of the contributions of $S = \{v_1\}$ and $S = \{v_1, v_2\}$ to Definition 8. For $k > 2$

$$w_T(I_k) = \alpha(v_k)\left((y-1)\beta(v_1) + (x-1)^2\alpha(v_1)\right) \left(\prod_{i=2}^{k-1} (\beta(v_i) + \alpha(v_i)(y-1))\right) \left(\prod_{i=k+1}^{n} \beta(v_i)\right)$$

is the sum of the contributions of those $S \subseteq \{v_1, \ldots, v_k\}$ that contain v_k, regardless of whether r is v_1 or v_2.

Proceeding inductively, suppose $n \geq 3$ and T has more than one vertex of degree ≥ 2. T has a vertex ℓ that satisfies the hypotheses of Lemma 11. Let $p(\ell) = v_p$, let $c(\ell) = \{v_{i_1}, \ldots, v_{i_k}\}$ with $i_1 < \cdots < i_k$ and $v_{i_k} = \ell$, and let $\hat{T} = T - \{v_p, v_{i_1}, \ldots, v_{i_k}\}$. If I is an es-cover in T and $\ell \notin I$ then $\ell \notin I'_c$ so $w_T(I) = \beta(\ell) w_{T - v_n}(I)$. If I is an es-cover in T and $\ell \in I$ then $v_{i_1}, \ldots, v_{i_k} \in I$, with $v_{i_1}, \ldots, v_{i_{k-1}} \in I_r$ and $v_{i_k} = \ell \in I_l$; also $v_p \in I'_c$. $\hat{I} = I - \{v_{i_1}, \ldots, v_{i_k}\}$ is an es-cover in $\hat{T}$ and $w_T(I)$ is

$$\alpha(\ell)\left((y-1)\beta(v_p) + (x-1)^2\alpha(v_p)\right) \left(\prod_{j=1}^{k-1} \left(\beta(v_{i_j}) + \alpha(v_{i_j})(y-1)\right)\right) w_{\hat{T}}(\hat{I}).$$

Lemma 11 and the inductive hypothesis then imply that

$$\begin{aligned} \sum w_T(I) &= \beta(\ell) q_W(T - \ell) + \alpha(\ell)\left((y-1)\beta(v_p) + (x-1)^2\alpha(v_p)\right) \left(\prod_{j=1}^{k-1} \left(\beta(v_{i_j}) + \alpha(v_{i_j})(y-1)\right)\right) q_W(\hat{T}) \\ &= \beta(\ell) q_W(T - v_n) + \alpha(\ell) q_W(\hat{T}) q_W(\{\ell\}') \left(\prod_{j=1}^{k-1} q_W(\{v_{i_j}\})\right) \end{aligned}$$

where $\{\ell\}'$ is the graph with one unlooped vertex ℓ that has weights $\alpha'(\ell) = \beta(v_p)$ and $\beta'(\ell) = \alpha(v_p)(x-1)^2$. As q_W is multiplicative on disjoint unions and $T^{v_p\ell} - v_p$ is the disjoint union of $\hat{T}$ and the isolated vertices $v_{i_1}, \ldots, v_{i_k}$, part (a) of Proposition 9 tells us that $\sum w_T(I) = q_W(T)$. ■

Setting $\alpha \equiv 1$ and $\beta \equiv 1$ we obtain Theorem 6.

Corollary 13. *If T is a tree then the (unweighted) interlace polynomial of T is*

$$q(T) = \sum_{I \text{ an es-cover}} y^{|I_r|} \cdot \left(y - 1 + (x-1)^2\right)^{|I_l|}.$$

Fig. 3. Two graphs with the same q_N polynomial.

4. Discussion

The ideas presented in this paper were developed in three discrete steps over a period of several years. For caterpillars, a different description of $q_N(T)$ as a generating function was given in [1]. Then the first three authors developed the definition of earlier sibling covers in general rooted trees; they proved Corollary 7 and the isomorphism invariance of $c_s(T)$. Later, as the fourth author studied the weighted version of the interlace polynomial discussed in [9] he realized that it provided algorithmic techniques that could be used to improve Corollary 7 to Theorem 6. The invariance proof for $c_s(T)$ needed little modification to provide the invariance proof for $c_{s,t}(T)$ given in Section 2.

One question that remains open is whether there is a combinatorial description of the interlace polynomials of arbitrary graphs. Circuit partitions of 2-in, 2-out digraphs give the fundamental combinatorial description of the interlace polynomials of circle graphs [3,4] but for those circle graphs that happen to be forests the connection between circuit partitions and earlier sibling covers is not immediate. It is possible to give an algorithmic description of the interlace polynomials of arbitrary graphs inspired by the ideas of this paper, but its combinatorial significance is not clear; see [9].

As discussed in [5], it is not generally true that q_N is a generating function for independent sets of any kind. For example, consider the two graphs in Fig. 3. On the left is a tree with $c_4(T) = 1$; it follows that y^4 appears in $q_N(T)$. On the right is the pivot T^{ab}, where a and b are the vertices of degree 3 in T. Remark 18 of [4] tells us that $q_N(T) = q_N(T^{ab})$, even though T^{ab} does not have four independent vertices.

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