

An Exact Singular-Locus Formula for Rooted-Tree Compartmental Models

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Abstract

We compute the coefficient-map Jacobian determinant of every bidirected-tree linear compartmental model whose sole input, output and leak are at one root. The determinant is a product of explicit edge powers and squared resultants of characteristic polynomials of sibling branches. If a descendant subtree has size s , the rates away from and toward the root have exact multiplicities $s - 1$ and s , respectively. The formula proves the catenary singular-locus conjecture of Gross, Meshkat and Shiu and the tree multiplicity conjecture credited by them to Hoch, Sweeney and Tung. It also specifies all additional factors caused by branching. The proof factors the coefficient map into a polynomial gluing map and a leafwise change of rate coordinates. All identities hold polynomially, including at zero rates and coincident branch spectra.

1 Model and main result

Let T be a finite tree with n vertices, rooted at o . Each undirected edge is replaced by both directed edges. If $v \neq o$ has parent u , let p_v be the rate $u \rightarrow v$ and q_v the rate $v \rightarrow u$. There is one leak, of rate ℓ , at o , and both input and output are at o . In the destination-row/source-column convention the compartmental matrix is

$$A_{v,u} = p_v, \quad A_{u,v} = q_v, \quad (1)$$

$$A_{o,o} = -\ell - \sum_{v \in \text{ch}(o)} p_v, \quad A_{u,u} = -q_u - \sum_{v \in \text{ch}(u)} p_v \quad (u \neq o). \quad (2)$$

All other off-diagonal entries vanish. Positive rates give the usual compartmental model; for the polynomial identity we allow arbitrary real or complex parameters.

For each vertex v , let T_v be its descendant subtree, let $s_v = |T_v|$, and define monic polynomials

$$P_v(z) = \det(zI - A[T_v, T_v]), \quad Q_v(z) = \prod_{w \in \text{ch}(v)} P_w(z). \quad (3)$$

The empty product is 1. Principal submatrices retain the full physical diagonal. Thus q_v , the rate back to the parent, is still present in the diagonal of $A[T_v, T_v]$.

The input-output equation has denominator P_o and numerator $Q_o = \det(zI - A[V(T) \setminus \{o\}, V(T) \setminus \{o\}])$. Following [1, Definitions 2.8–2.9], let $\mathbf{c}$ be the list of all nonleading coefficients of P_o and Q_o . It has $2n - 1$ coordinates, as does $(\ell, (p_v, q_v)_{v \neq o})$. We use the full polynomial coefficient map, without canceling common factors at exceptional parameter values.

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Theorem 1.1. *For every rooted tree T , the coefficient-map Jacobian satisfies*

$$\det Dc = \pm \left(\prod_{v \neq o} p_v^{s_v-1} q_v^{s_v} \right) \prod_{u \in V(T)} \prod_{\{v,w\} \subseteq \text{ch}(u)} \text{Res}_z(P_v, P_w)^2. \quad (4)$$

The sign depends only on the chosen coordinate orders. This is an identity of polynomials with integer coefficients. The exact multiplicities of the individual variables p_v, q_v, ℓ are, respectively, $s_v - 1, s_v, 0$.

In particular, the determinant is not identically zero. Its zero set is exactly the rank-drop locus of this square coefficient map. Over the positive parameter region, the edge monomial is nonzero, so rank drops exactly when two sibling principal-subtree matrices, at some vertex of the tree, have a common characteristic root. This statement concerns the differential; it does not identify every critical point with a failure of set-theoretic local injectivity.

Relation to prior work and scope

Gross, Meshkat and Shiu [1] compute singular-locus equations for mammillary and directed-cycle models. Their Conjecture 5.5 specifies the catenary equation; their Conjecture 5.9 gives the exact variable multiplicities for a bidirected tree and is attributed there to Molly Hoch, Mark Sweeney and Hwai-Ray Tung. Theorem 1.1 proves both conjectures and gives the remaining factors for every tree. We retain the version-3 numbering of [1]. Generic identifiability of these tree models and global identifiability of the endpoint-rooted catenary model are not new assertions here.

The catenary conjecture also appears in Gross's Oberwolfach abstract [2, p. 3136, Conjecture 1]. The next question, continued on page 3137, asks about the covariance Jacobian of general structural equation models. These are different maps. The frozen `ulamai/UnsolvedMath` v1.6.0 record `OWR-11695865-007` extracts that broader covariance question together with the caption of the catenary figure. Our theorem resolves the adjacent catenary conjecture and its tree extension, not that general covariance question. Ahmed et al. [3, Sections 5–6] give catenary coefficient formulas and still discuss [1, Conjecture 5.5] as a target.

2 A polynomial gluing determinant

We first isolate a coefficient-space identity. For a monic polynomial we use its nonleading coefficients as coordinates; for a polynomial of bounded degree we use all coefficients up to that bound.

Lemma 2.1. *Let P_i be monic of degree $m_i \geq 1$, and let $\deg S_i < m_i$, for $1 \leq i \leq k$. Put $m = \sum_i m_i$ and*

$$Q = \prod_i P_i, \quad R = \sum_i S_i \prod_{j \neq i} P_j.$$

The map $(P_i, S_i)_i \mapsto (Q, R)$ has Jacobian determinant

$$\pm \prod_{i < j} \text{Res}(P_i, P_j)^2. \quad (5)$$

For $k = 0$, both coordinate spaces have dimension zero and the determinant is 1.

Proof. Order the source coordinates first by all P_i coefficients and then by all S_i coefficients, and order the target as (Q, R) . The derivative is block triangular. Its two diagonal blocks represent the same linear map

$$L : (U_1, \dots, U_k) \mapsto \sum_i U_i \prod_{j \neq i} P_j, \quad \deg U_i < m_i.$$

For two factors, this is the Sylvester coefficient map, so its determinant is the resultant up to sign. For more factors, factor the product map through $\tilde{P} = \prod_{i < k} P_i$ and P_k . The chain rule and the two-factor case multiply the determinant for the first $k - 1$ factors by

$$\text{Res}(\tilde{P}, P_k) = \prod_{i < k} \text{Res}(P_i, P_k).$$

Induction gives $\det L = \pm \prod_{i < j} \text{Res}(P_i, P_j)$, and the two diagonal blocks give (5). This calculation uses coefficient matrices, not division by resultants; it remains valid when factors have common roots. $\square$

3 Independent diagonal and edge-product coordinates

Temporarily take $b_v = -A_{v,v}$ and $r_v = p_v q_v$ as independent coordinates, with one b_v per vertex and one r_v per nonroot vertex. The tree determinant recurrence is

$$P_u = (z + b_u)Q_u - \sum_{v \in \text{ch}(u)} r_v Q_v \prod_{\substack{w \in \text{ch}(u) \\ w \neq v}} P_w, \quad Q_u = \prod_{v \in \text{ch}(u)} P_v. \quad (6)$$

For example, when the child blocks are invertible, the Schur complement gives the correction $r_v Q_v / P_v$. Multiplication by their determinants gives (6). Both sides are polynomials, so the identity holds without the invertibility restriction. It also follows from the matching expansion of a tree determinant.

Let J_u denote the determinant of the coefficient map (P_u, Q_u) in the $2s_u - 1$ independent b and r coordinates of T_u . The rate product r_u on the edge back to the parent is not among these coordinates.

Proposition 3.1. *For these independent coordinates,*

$$J_o = \pm \prod_{v \neq o} r_v^{s_v - 1} \prod_u \prod_{\{v, w\} \subseteq \text{ch}(u)} \text{Res}(P_v, P_w)^2. \quad (7)$$

Proof. At a leaf, $P_u = z + b_u$ and $Q_u = 1$, so $J_u = 1$. For an internal vertex, first replace each child's internal parameters by the coefficients of (P_v, Q_v) . These maps contribute $\prod_{v \in \text{ch}(u)} J_v$; b_u and the connecting r_v remain separate coordinates.

Next replace (r_v, Q_v) by the polynomial $S_v = r_v Q_v$. Since Q_v is monic of degree $s_v - 1$, the leading coefficient of S_v is r_v , and each of its other $s_v - 1$ coefficients is multiplied by r_v . The determinant of this change is $\pm r_v^{s_v - 1}$. This is valid also for a leaf, where $S_v = r_v$. Apply Lemma 2.1 to these (P_v, S_v) :

$$Q_u = \prod_v P_v, \quad R_u = \sum_v S_v \prod_{w \neq v} P_w.$$

It contributes the squared sibling resultants.

Finally pass from (b_u, Q_u, R_u) to (P_u, Q_u) , where $P_u = (z + b_u)Q_u - R_u$ and $\deg R_u < s_u - 1$. Keeping Q_u fixed, the coefficient of z^{s_u-1} in P_u has derivative 1 in b_u . The remaining coefficients have derivative -1 in the respective coefficients of R_u . This final map has determinant ± 1 . Consequently

$$J_u = \pm \left(\prod_{v \in \text{ch}(u)} J_v r_v^{s_v-1} \right) \prod_{\{v,w\} \subseteq \text{ch}(u)} \text{Res}(P_v, P_w)^2.$$

Induction proves (7). Every map used here is polynomial and square; no local inverse is assumed at a singular point. $\square$

4 Physical rate coordinates and exact multiplicities

Lemma 4.1. *The map $(\ell, (p_v, q_v)_{v \neq o}) \mapsto ((b_u)_u, (r_v)_{v \neq o})$, where*

$$b_o = \ell + \sum_{v \in \text{ch}(o)} p_v, \quad b_u = q_u + \sum_{v \in \text{ch}(u)} p_v \ (u \neq o), \quad r_v = p_v q_v,$$

has Jacobian determinant $\pm \prod_{v \neq o} q_v$.

Proof. Choose a nonroot leaf v and put source coordinates (q_v, p_v) and target coordinates (b_v, r_v) first. The first two target functions are $(q_v, p_v q_v)$, with derivative block

$$\begin{pmatrix} 1 & 0 \\ p_v & q_v \end{pmatrix}.$$

The upper-right block is zero. The lower-left block need not vanish, because p_v occurs in the parent diagonal, but does not affect the block-triangular determinant. The complementary block is the derivative for the smaller tree, with a fixed additive shift in that parent diagonal. Its determinant is therefore computed by the same induction. After all nonroot leaves have been removed, the final derivative of the root diagonal with respect to ℓ is 1. $\square$

Proof of Theorem 1.1. Substituting $r_v = p_v q_v$ into Proposition 3.1 and multiplying by Lemma 4.1 proves (4). It remains to show that the displayed rate exponents are exact.

Write H for the product of all squared resultants in (4). Set every p_v to zero and choose all q_v distinct and positive. For a proper descendant subtree, the principal matrix is triangular and its characteristic polynomial is the product of $z + q_x$ over its vertices x . Sibling subtrees have disjoint vertex sets, hence disjoint root sets. Thus $H \neq 0$ at this specialization. In particular, no individual p_v divides H .

For any fixed nonroot vertex x , additionally set $q_x = 0$, retaining distinct positive values for all other q_v . At each branching, at most one child subtree contains x . Hence zero is a root of at most one sibling polynomial, while the remaining roots are all distinct. Again $H \neq 0$. No individual q_x divides H . Finally, H is independent of ℓ , since the root diagonal occurs in none of the proper child-subtree polynomials.

It follows that the displayed monomial gives precisely the individual variable multiplicities. The same specializations show that H is a nonzero polynomial; multiplication by the nonzero monomial cannot give the zero polynomial. Thus the generic rank is $2n - 1$, and the determinant zero set is exactly its rank-drop locus. $\square$

5 Catenary and tree conjectures

Corollary 5.1 (Catenary formula). *For the path $1, \dots, n$ rooted at endpoint 1, put $p_i = a_{i+1,i}$ and $q_i = a_{i,i+1}$ for the edge $i-(i+1)$. Then, up to coordinate sign,*

$$\det Dc = \prod_{i=1}^{n-1} p_i^{n-i-1} q_i^{n-i}. \quad (8)$$

This proves [1, Conjecture 5.5].

Proof. There are no sibling pairs, and the subtree beyond edge i has $n - i$ vertices. Formula (8) is exactly

$$a_{12}^{n-1} (a_{21}a_{23})^{n-2} (a_{32}a_{34})^{n-3} \cdots (a_{n-1,n-2}a_{n-1,n}).$$

For $n = 2$ it is a_{12} . □

Corollary 5.2 (Tree multiplicities). *The recursive multiplicity rule of Hoch, Sweeney and Tung in [1, Conjecture 5.9] holds for every bidirected tree with the sole input, output and leak at one vertex.*

Proof. For an outward edge to v , a leaf gives exponent $0 = s_v - 1$. The source rule adds one to the label on each outward child edge and sums, yielding $\sum_{w \in \text{ch}(v)} s_w = s_v - 1$. For an inward edge from v , a leaf gives $1 = s_v$; the rule adds one to the sum of the inward child labels, giving $1 + \sum_{w \in \text{ch}(v)} s_w = s_v$. Theorem 1.1 shows that these are the exact multiplicities, not merely lower bounds. □

For a rooted star, $P_v = z + q_v$ for each child and

$$\det Dc = \pm \prod_v q_v \prod_{\{v,w\}} (q_v - q_w)^2,$$

recovering the known mammillary formula [1, Theorem 5.1]. For a root with two children v, w , each with one leaf, let the rates from child v to its leaf and back be p_x, q_x . Its branch polynomial is

$$P_v(z) = (z + q_v + p_x)(z + q_x) - p_x q_x = z^2 + (q_v + p_x + q_x)z + q_v q_x.$$

There is an analogous P_w . In this five-vertex example the determinant is, up to sign,

$$p_v q_v^2 p_w q_w^2 q_x q_y \text{Res}(P_v, P_w)^2.$$

Thus the extra factors can involve entire branch spectra, not just equalities of individual rates. Collisions below the root contribute as well.

6 Reproducibility and limitations

The accompanying standard-library Python program differentiates the coefficient map by exact rational first-order arithmetic. It obtains characteristic coefficients by matrix multiplication via Faddeev–LeVerrier and compares their Jacobian determinant with a separate subtree recurrence and Sylvester-resultant calculation. Tests include every increasing-parent representation through six vertices, longer paths and stars, signed and zero rates, and sibling collisions at and below the root. Negative controls reject a monomial-only formula, unsquared resultants, and replacing the

answer by the discriminant of the full characteristic polynomial. These finite tests supplement the general proof; they do not establish it.

The theorem assumes a single collocated input, output and leak. It does not classify multiple leaks, separated input and output, arbitrary directed graphs or general mixed-graph covariance models. Classical determinant recurrences, resultants and the chain rule are used explicitly. A bounded primary-source search found no earlier proof of the stated full factorization; no absolute-priority claim is made. This preprint is unrefereed. Its preparation used AI-assisted mathematical exploration, literature retrieval, exact computation and typesetting; the author is responsible for the submitted text and claims. No independent review or proof-assistant certification is asserted.

References

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