Toric Geometry in Brownian motion tree models and their generalizations

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based on the papers:

1. **Tobias Boege, Jane Ivy Coons, Chris Eur**, AM, **Frank Röttger**, *Reciprocal Maximum Likelihood Degrees of Brownian Motion Tree Models*, Le Matematiche 76 (2), 383-398 (2021)

2. **Jane Ivy Coons, Shelby Cox,** AM, **Ikenna Nometa**, *Maximum Likelihood Degrees of Brownian Motion Tree Models: Star Tree and Root Invariance*, arxiv: 2402.10322 (2024)

3. **Emma Cardwell**, AM, **Alvaro Ribot**, *Toric Multivariate Gaussian Models from Symmetries in a Tree*, arxiv: 2412.00895 (2024)

4. AM, **Arpan Pal**, *Symmetry Lie Algebras of Varieties with Applications to Algebraic Statistics*, arxiv: 2309.10741 (2023)

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toric ideals and varieties

ALGEBRA. Take $I \subseteq R = \mathbb{C}[x_1, \ldots, x_n]$ an ideal. I is a binomial ideal if its has a gen. set of binomials $f = x_1^{u_1} \cdots x_n^{u_n} - x_1^{v_1} \cdots x_1^{v_n}$. I is prime if for $fg \in I$ one has $f \in I$ or $g \in I$.

Ideal $I \subseteq R$ is toric if one of the equivalent properties holds:

- I is a prime binomial ideal, or
- I is the kernel of a monomial map $\mathbb{R}[x_1, \ldots, x_n] \to \mathbb{R}[\theta_1^{\pm 1}, \ldots, \theta_m^{\pm 1}]$.

$$\psi : \mathbb{C}[x_1, x_2, x_3] \to \mathbb{C}[\theta_1, \theta_2],\ x_1 \mapsto \theta_1^2,\ x_2 \mapsto \theta_1\theta_2,\ x_3 \mapsto \theta_2^2$$

$$\ker \psi = \langle x_1 x_3 - x_2^2 \rangle$$

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GEOMETRY. $V(I) = \{x \in \mathbb{C}^n \mid f_1(x) = \ldots = f_n(x) = 0\}$ the variety of I. Toric varieties are isomorphic to solutions set to toric ideals.

An ideal I may not be toric and its $V(I)$ may be toric. In this case, a linear change of variables is useful for reveling the toric structure of $V(I)$.

Take $I = \langle x_1 x_3 - x_2^2 - x_1 x_2 \rangle$ and $x_1 = p_1,\ x_2 = p_2 - p_1,\ x_3 = p_3 - p_2$. Then,

$$I = \langle p_1(p_3 - p_2) - (p_2 - p_1)^2 - p_1(p_2 - p_1) \rangle = \langle p_1 p_3 - p_2^2 \rangle \text{ is toric}$$

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Question 1: Why do we prefer toric structures? **optimization over a toric model**

Question 2: Given I not a toric ideal, when can we tell that there is a linear change of variables under which I is toric? **symmetry Lie groups**

Brownian motion tree models

T = a phylogenetic tree with root 0 and other leaves labeled $1, 2, \ldots, n$.

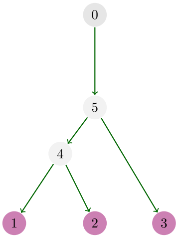
$\mathrm{lca}(i, j)$ = the least common ancestor of leaves i and j.

t_v parameter for non-root node v.

The Brownian motion tree model for T is the set $\mathcal{M}_T = \{\mathcal{N}_n(\mathbf{0}, \Sigma) \mid \Sigma \in \mathcal{L}_T \cap \mathrm{PD}_n\}$, where

$$\mathcal{L}_T = \{\Sigma \in \mathrm{Sym}_n \mid \sigma_{ij} = \sigma_{kl} \text{ if } \mathrm{lca}(i,j) = \mathrm{lca}(k,l)\}.$$

$\mathcal{L}_T^{-1} \cap \mathrm{PD}_n$ is the set of concentration matrices for $\mathcal{M}_T$.



$$\mathcal{L}_T = \{\Sigma = \begin{bmatrix} t_1 & t_4 & t_5 \\ t_4 & t_2 & t_5 \\ t_5 & t_5 & t_3 \end{bmatrix} \mid t_1 \cdots, t_5 \in \mathbb{R}\}$$

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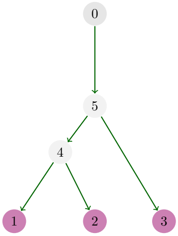

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$$k_{12}k_{23} - k_{13}k_{22} = -(k_{11}k_{23} - k_{12}k_{13})\}$$

$I_T = \langle k_{11}k_{23} - k_{12}k_{13} + k_{12}k_{23} - k_{13}k_{22} \rangle$ is the vanishing ideal of $\mathcal{M}_T$.

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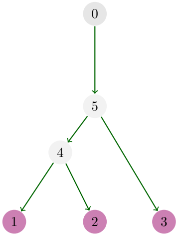

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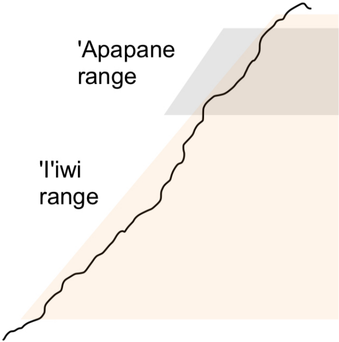
I_T toric under the reduced graph Laplacian.

Genetic Drift

Brownian motion models the evolution of continuous traits under **genetic drift**, which means totally random, non-selective pressure.
→ provide evidence for your model by showing it performs better than a genetic drift model.

'Apapane (short beak)

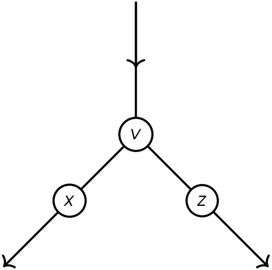
'I'iwi (long beak)



Photos by Daniel Murphy, Macaulay Library at the Cornell Lab of Ornithology ('Apapane) and Jim Denny, ABC's Bird Library ('I'iwi).

Brownian Motion along a tree

* A Brownian motion is a random process that models the movement of a particle subject to a large number of small forces. At each time step, the particle moves according to $\mathcal{N}(0, \sigma^2)$.
Each branch has an independent Brownian motion.



$$Y_x \sim Y_v + B_{\mathrm{dist}(x,v)}$$
$$Y_z \sim Y_v + B_{\mathrm{dist}(z,v)}$$

The Brownian motion at time t is $B_t \sim \mathcal{N}(0, t\sigma^2)$.

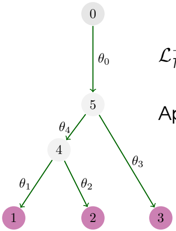
The random variables at the leaves represent averaged continuous trait values (average beak length, gene expression data) for present day species.

Covariance is constrained by common ancestry in the tree:

$$\mathrm{lca}_T(i,j) = \mathrm{lca}_T(k,l) \text{ implies } \mathrm{cov}(Y_i, Y_j) = \mathrm{cov}(Y_k, Y_l)$$

*Felsenstein "Maximum-likelihood estimation of evolutionary trees from continuous characters" (1973).

BMT models are toric and a monomial parametrization



$$\mathcal{L}_T^{-1} = \left\{ \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{12} & k_{22} & k_{23} \\ k_{13} & k_{23} & k_{33} \end{bmatrix} \in \mathbb{R}^{3\times 3} \text{ s.t. } k_{11}k_{23} - k_{12}k_{13} + k_{12}k_{23} - k_{13}k_{22} = 0 \right\}$$

Applying the reduced graph Laplacian over K_{n+1} transform:

$$K = \begin{bmatrix} p_{01} + p_{12} + p_{13} & -p_{12} & -p_{13} \\ -p_{12} & p_{02} + p_{12} + p_{23} & -p_{23} \\ -p_{13} & -p_{23} & p_{03} + p_{13} + p_{23} \end{bmatrix}$$

gives $k_{11}k_{23} - k_{12}k_{13} + k_{12}k_{23} - k_{13}k_{22} = (p_{01} + p_{12} + p_{13})(-p_{23}) - \ldots = p_{01}p_{23} - p_{02}p_{13}$

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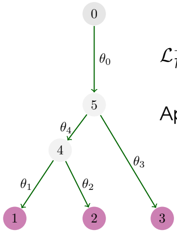

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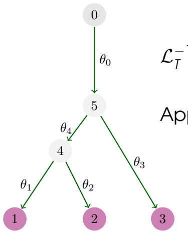
Theorem [Sturmfels-Uhler-Zwiernik, 2020] I is toric under the reduced Laplacian

$$\begin{array}{rcll} p_{ij} & = & -k_{ij} & \text{for } i,j > 0, \text{ and} \\ p_{0i} & = & \sum_{j=1}^{n} k_{ij} & \text{for } 1 \leq i \leq n. \end{array}$$

It is generated by $p_{ik}p_{j\ell} - p_{i\ell}p_{jk}$, where $\{i,j\}$ and $\{k,\ell\}$ are cherries in the induced 4-leaf subtree on any quadruple $i,j,k,\ell \in \{0,\ldots,n\}$.

BMT models are toric and a monomial parametrization



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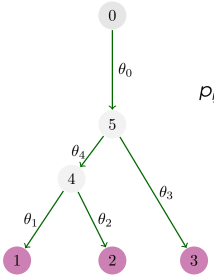
- θ_e parameter to (undirected) edge e in T
- $i \leftrightsquigarrow j$ set of edges in T in the path from vertex i to vertex j

monomial (path) map $\quad \varphi_T : \mathbb{C}[p_{ij} \mid 0 \le i < j \le n] \to \mathbb{C}[\theta_e \mid e \in Edge(T)], \quad p_{ij} \mapsto \prod_{e \in i \leftrightsquigarrow j} \theta_e.$

Theorem [Boege-Coons-Eur-M-Rottger, 2021] $\ker \varphi_T = I_T$ in the variables p_{ij}.

in the θ-s



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$$= \begin{bmatrix} \theta_0\theta_4\theta_1 + \theta_1\theta_2 + \theta_1\theta_4\theta_3 & -\theta_1\theta_2 & -\theta_1\theta_4\theta_3 \\ -\theta_1\theta_2 & \theta_4(\theta_0\theta_2 + \theta_2\theta_3) + \theta_1\theta_2 & -\theta_4\theta_2\theta_3 \\ -\theta_4\theta_1\theta_3 & -\theta_4\theta_2\theta_3 & \theta_4(\theta_1\theta_3 + \theta_2\theta_3) + \theta_0\theta_3 \end{bmatrix}$$

So the model $\mathcal{M}_T$ and any optimization problem on $\mathcal{M}_T$ can be written in terms of the θ-s.

maximum likelihood estimate

Fix T. Given i.i.d. samples $\mathbf{U}_1, \dots, \mathbf{U}_m$ in $\mathbb{R}^n$, find $K \in \mathcal{L}_T^{-1}$ (or $\Sigma \in \mathcal{L}_T$) that *best* fit data $\mathbf{U}$.

The maximum likelihood estimate (MLE) for data $\mathbf{U}_1, \dots, \mathbf{U}_m$ in $\mathcal{M}_T$ is the maximizer of the log-likelihood function

$$\ell(K|S) = \log\det(K) - \mathrm{trace}(SK), \text{ where } S = \frac{1}{m}\sum_{i=1}^{m} \mathbf{U}_i \mathbf{U}_i^T \text{ (in variables } k_{ij} \text{ or } p_{ij}\text{, or } \theta_e\text{)}$$

the MLE is found among solutions to $\frac{\partial \ell}{\partial \theta_e} = 0$ for $e \in E(T)$ in $\mathcal{L}_T^{-1}$ with $\det(K(\theta)) \neq 0$

the nr. of solutions measures the complexity of finding MLE

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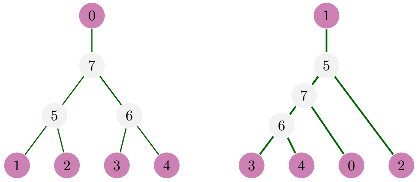
The ML degree of $\mathcal{M}_T$ is the number of complex critical points $K \in \mathcal{L}_T^{-1}$ of $\ell(K|S)$ with $\det(K) \neq 0$, counted with multiplicity, for generic S.

equivalence up to undirected tree topology and star trees

Theorem 1 [Coons, Cox, M, Nometa, 2024]: The ML degree of a BMT model depends only on the undirected tree topology.



$$\max_{K(\theta)} \ \log\det K(\theta) - \mathrm{tr}(SK(\theta))$$
$$\text{s.t. } \det K(\theta) \neq 0.$$

Proof ingredients: path parametrization, ML degree is invariant under generic S,

$$\ell_T(\theta|S) = \ell_{T'}(\theta|S') \qquad \text{for } S' = A \cdot S \text{ where } A \text{ is some invertible matrix}$$

MLE can be recovered: $\mathrm{mle}(\mathcal{M}_T, S) = \mathrm{mle}(\mathcal{M}_{T'}, S')$ for S and $S' = A \cdot S$

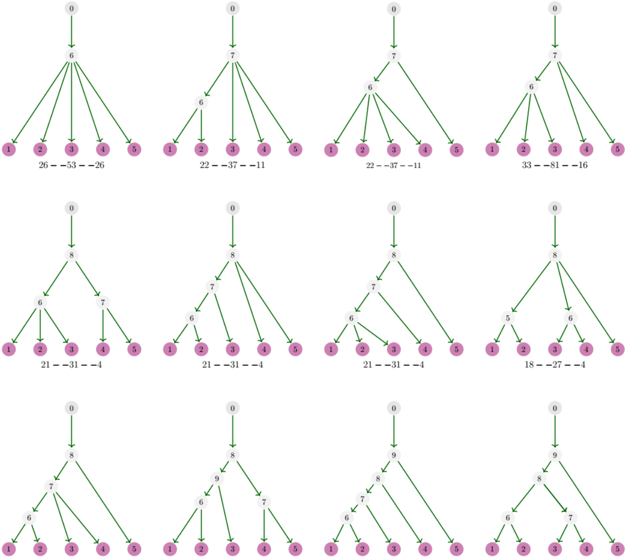
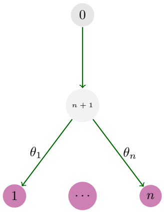


Table 1: $\deg(\mathcal{L}_{\mathcal{T}}^{-1}) - -\mathrm{mld}(\mathcal{M}_{\mathcal{T}}) - -\mathrm{rmld}(\mathcal{M}_{\mathcal{T}})$ *for each phylogenetic tree in* 5 *leaves.*

ML degree of the star tree



> **Theorem 2 [Coons, Cox, M, Nometa, 2024]:** The ML degree of the BMTM with star tree structure on $n+1$ leaves is $2^{n+1} - 2n - 3$.

Previously conjectured by Améndola and Zwiernik (2020)

Sketch of the proof.

1. $\ell(\theta \mid S) = \log(\theta_0 \cdots \theta_n \, (\theta_0 + \cdots + \theta_n)^{n-1}) - \sum_{i<j} c_{ij}\theta_i\theta_j$ and $\theta_0, \dots, \theta_n, \sum_{i=0}^{n} \theta_i \neq 0$
2. Take partial derivatives

$$\frac{\partial \ell(\theta \mid S)}{\partial \theta_i} = \frac{1}{\theta_i} + \frac{n-1}{\theta_0 + \theta_1 + \cdots + \theta_n} - \sum_{\substack{j=0 \\ j \neq i}}^{n} c_{ij}\theta_j, \text{ for } i = 0, \dots, n,$$

3. Set $\psi = (\theta_0 + \cdots + \theta_n)^{-1}$, clear denominators, and homogenize:

$$\frac{\partial \tilde{\ell}_S}{\partial \theta_i} = z^2 + \theta_i \left((n-1)\psi - \sum_{j \neq i} c_{ij}\theta_j \right) \text{ for } i = 0, \dots, n, \text{ and } \tilde{f}_\psi = z^2 - \psi \left(\sum_{i=0}^{n} \theta_i \right)$$

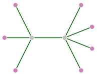
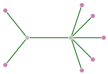
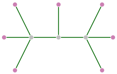
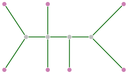
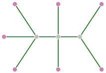
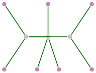
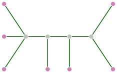
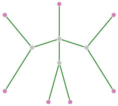
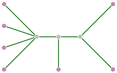
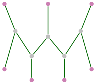
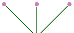
Bezout: 2^{n+2} solutions - points at infinity $= 2^{n+2} - (4n+6)$ solutions in θ.

4. Solutions in p_{ij} (or k_{ij}) are $\dfrac{2^{n+2} - (4n+6)}{2^1} = 2^{n+1} - 2n - 3.$

Questions: ML degree of non-star trees? How many of the critical points are real? Compute MLE, potentially asymptotically? Other optimization tasks on a BMT model...

Theorem 3 [Boege-Coons-Eur-**M**-Rottger, 2021]: The reciprocal (dual) ML-degree is

$$\mathrm{rmldeg}(\mathcal{M}_T) = \prod_{v \in \mathrm{Int}(T)} \left(2^{\deg(v)-1} - \deg(v) - 2\right).$$

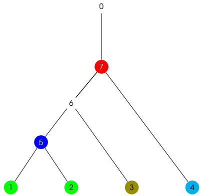
tree topology	deg	rmldeg	mldeg	tree topology	deg	rmldeg	mldeg
	93	44	259		95	26	53
	90	16	221		51	4	83
	77	16	181		47	11	81
	61	4	115		42	4	63
	60	11	101		42	1	61
							

Polyhedral geometry and generalizations of BMT models

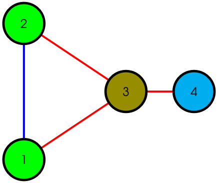
$P_T = \mathrm{conv}\{c^{i\leftrightarrow j} \mid i,j \in \mathrm{Lv}(T)\} \subseteq \mathbb{R}^{E(T)}$, where $c^{i\leftrightarrow j}$ is the edge indicator vector of $i \leftrightarrow j$.

Theorem 4 [Goel, **M**, Ribot, 2025]: Given a tree $T = (V,E)$ with $|V| > 3$ and no internal nodes of degree 2, P_T has dimension $|E| - 1$ and a minimal $\mathcal{H}$-representation

$$\begin{cases} x_{\{u,v\}} & \geq 0 \quad \text{for all } \{u,v\} \in E, \text{with } \mathbf{deg}(u), \mathbf{deg}(v) \neq 3, \\ -x_{\{u,v\}} + \sum\limits_{w \in N(u)\setminus\{v\}} x_{\{u,w\}} & \geq 0 \quad \text{for all } u \in (T) \text{ and all } v \in \mathrm{Neighb}(u), \\ \sum\limits_{\{u,v\}\in E(T)} x_{\{u,v\}} & = 2. \end{cases}$$



$$\begin{bmatrix} t_1 & t_5 & 0 & t_7 \\ t_5 & t_1 & 0 & t_7 \\ 0 & 0 & t_3 & t_7 \\ t_7 & t_7 & t_7 & t_4 \end{bmatrix}$$



Theorem 4 [Cardwell, **M**, Ribot, 2024]: Let $\mathcal{T}$ be a tree with BMT derived graph $\mathcal{G}$. If $\mathcal{G}$ is a vertex-regular block graph, then $\mathcal{L}_{\mathcal{T}}^{-1}$ is toric under the derived Laplacian transformation with vanishing of $I_T + I_G + I_\Lambda$. Monomial parametrization provided.

detecting non-toricness and an algorithm

Let $\mathbb{C}[x] = \mathbb{C}[x_1, \ldots, x_n]$. Determine the group action of $\mathrm{GL}_n(\mathbb{C}) \curvearrowright \mathbb{C}[x]$ by

$$\text{for } g = \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \in \mathrm{GL}_n(\mathbb{C}), p \in \mathbb{C}[x], \quad g \cdot f(x_1, \ldots, x_n) = f(g_1 \cdot x, \ldots, g_n \cdot x).$$

$G_I = \{g \in \mathrm{GL}_n(\mathbb{C}) \mid g \cdot f \in I, \forall f \in I\}$ is the symmetry Lie group of I.

Let $\mathfrak{g}_I$ be its Lie algebra.

Theorem [**M**-Pal, 2023]: Let $I \subseteq \mathbb{C}[x]$ be a prime homogeneous ideal with symmetry Lie group G_I. If $\dim(V(I)) > \dim(G_I) = \dim(\mathfrak{g}_I)$, then I is not toric under any linear change of variables.

Algorithm computing the symmetry Lie algebra of a prime homogeneous ideal provided.

We use it to provide first cases of non-toric one-staged tree models and colored Gaussian graphical models.

Follow up work with a better algorithm: Thomas Kahle and Julian Vill. Efficiently deciding if an ideal is toric after a linear coordinate change. 2024.

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Thank you!