

**SUPPLEMENTARY MATERIALS: A NOVEL ALGEBRAIC  
APPROACH TO TIME-REVERSIBLE EVOLUTIONARY MODELS\***

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**SM1. Gluing parameters.**

*Proof of Lemma 4.5.* By rooting the tree  $T'$  at  $s$  we have

$$\begin{aligned} \bar{p}_{\mathbf{i}_\alpha, k, \mathbf{i}_\beta}^T &= \sum_{j \in \text{ext}(\mathbf{i}_\alpha, k, \mathbf{i}_\beta)} \pi_k \prod_{e \in E(T')} M_{j_{p(e)}, j_{c(e)}}^e = \\ &= \frac{1}{\pi_k} \sum_{\substack{v \in \text{Int}(T_1) \cup \text{Int}(T_2) \\ j_v \in \Sigma}} \left( \pi_k \prod_{e \in E(T_1)} M_{j_{p(e)}, j_{c(e)}}^e \right) \left( \pi_k \prod_{e \in E(T_2)} M_{j_{p(e)}, j_{c(e)}}^e \right) = \\ &= \frac{1}{\pi_k} \left( \sum_{\substack{v \in \text{Int}(T_1) \\ j_v \in \Sigma}} \pi_k \prod_{e \in E(T_1)} M_{j_{p(e)}, j_{c(e)}}^e \right) \left( \sum_{\substack{v \in \text{Int}(T_2) \\ j_v \in \Sigma}} \pi_k \prod_{e \in E(T_2)} M_{j_{p(e)}, j_{c(e)}}^e \right) \end{aligned}$$

and the claim follows. □

**SM2. Computations.**

**SM2.1. Computations for the tripod.** The list of 9 quadric binomials, 29 cubic binomials, and 3 quintic binomials generating  $I_T$  for a tripod  $T$  mentioned in Proposition 5.3 is:

**Generators of degree 2**

- |   |  |
|---|--|
| <p>(1) <math>\bar{p}_{222}\bar{p}_{441} - \frac{\pi_{34}-\pi_{12}}{\pi_{34}}\bar{p}_{221}\bar{p}_{442}</math></p> <p>(2) <math>\bar{p}_{332}\bar{p}_{441} + \frac{\pi_{12}}{\pi_{34}}\bar{p}_{331}\bar{p}_{442}</math></p> <p>(3) <math>\bar{p}_{222}\bar{p}_{414} - \frac{\pi_{34}-\pi_{12}}{\pi_{34}}\bar{p}_{212}\bar{p}_{424}</math></p> <p>(4) <math>\bar{p}_{323}\bar{p}_{414} + \frac{\pi_{12}}{\pi_{34}}\bar{p}_{313}\bar{p}_{424}</math></p> | <p>(5) <math>\bar{p}_{144}\bar{p}_{222} - \frac{\pi_{34}-\pi_{12}}{\pi_{34}}\bar{p}_{122}\bar{p}_{244}</math></p> <p>(6) <math>\bar{p}_{332}\bar{p}_{221} - \frac{\pi_{12}}{\pi_{12}-\pi_{34}}\bar{p}_{331}\bar{p}_{222}</math></p> <p>(7) <math>\bar{p}_{144}\bar{p}_{233} + \frac{\pi_{12}}{\pi_{34}}\bar{p}_{133}\bar{p}_{244}</math></p> <p>(8) <math>\bar{p}_{122}\bar{p}_{233} - \frac{\pi_{12}}{\pi_{12}-\pi_{34}}\bar{p}_{133}\bar{p}_{222}</math></p> <p>(9) <math>\bar{p}_{323}\bar{p}_{212} - \frac{\pi_{12}}{\pi_{12}-\pi_{34}}\bar{p}_{313}\bar{p}_{222}</math></p> |
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## Generators of degree 3

- (10)  $\bar{p}_{144}\bar{p}_{424}\bar{p}_{442} - \frac{\pi_1\pi_2\pi_{34}}{(\pi_1-\pi_2)^2}\bar{p}_{122}\bar{p}_{444}^2$
- (11)  $\bar{p}_{244}\bar{p}_{414}\bar{p}_{442} - \frac{\pi_1\pi_2\pi_{34}}{(\pi_1-\pi_2)^2}\bar{p}_{212}\bar{p}_{444}^2$
- (12)  $\bar{p}_{244}\bar{p}_{424}\bar{p}_{441} - \frac{\pi_1\pi_2\pi_{34}}{(\pi_1-\pi_2)^2}\bar{p}_{221}\bar{p}_{444}^2$
- (13)  $\bar{p}_{144}\bar{p}_{414}\bar{p}_{441} - \frac{\pi_1\pi_2\pi_{12}}{(\pi_1-\pi_2)^2}\bar{p}_{111}\bar{p}_{444}^2$
- (14)  $\bar{p}_{122}\bar{p}_{414}\bar{p}_{441} - \frac{\pi_{12}}{\pi_{34}}\bar{p}_{111}\bar{p}_{424}\bar{p}_{442}$
- (15)  $\bar{p}_{144}\bar{p}_{212}\bar{p}_{441} - \frac{\pi_{12}}{\pi_{34}}\bar{p}_{111}\bar{p}_{244}\bar{p}_{442}$
- (16)  $\bar{p}_{122}\bar{p}_{212}\bar{p}_{441} - \frac{\pi_{12}}{\pi_{34}-\pi_{12}}\bar{p}_{111}\bar{p}_{222}\bar{p}_{442}$
- (17)  $\bar{p}_{133}\bar{p}_{212}\bar{p}_{441} + \bar{p}_{111}\bar{p}_{233}\bar{p}_{442}$
- (18)  $\bar{p}_{122}\bar{p}_{313}\bar{p}_{441} + \bar{p}_{111}\bar{p}_{323}\bar{p}_{442}$
- (19)  $\bar{p}_{122}\bar{p}_{313}\bar{p}_{441} + \bar{p}_{111}\bar{p}_{323}\bar{p}_{442}$
- (20)  $\bar{p}_{144}\bar{p}_{221}\bar{p}_{414} - \frac{\pi_{12}}{\pi_{34}}\bar{p}_{111}\bar{p}_{244}\bar{p}_{424}$
- (21)  $\bar{p}_{122}\bar{p}_{221}\bar{p}_{414} - \frac{\pi_{12}}{\pi_{34}-\pi_{12}}\bar{p}_{111}\bar{p}_{222}\bar{p}_{424}$
- (22)  $\bar{p}_{133}\bar{p}_{221}\bar{p}_{414} + \bar{p}_{111}\bar{p}_{233}\bar{p}_{424}$
- (23)  $\bar{p}_{122}\bar{p}_{331}\bar{p}_{414} + \bar{p}_{111}\bar{p}_{332}\bar{p}_{424}$
- (24)  $\bar{p}_{144}\bar{p}_{212}\bar{p}_{221} - \frac{\pi_{12}}{\pi_{34}-\pi_{12}}\bar{p}_{111}\bar{p}_{222}\bar{p}_{244}$
- (25)  $\bar{p}_{122}\bar{p}_{212}\bar{p}_{221} - \frac{\pi_{12}\pi_{34}}{(\pi_{12}-\pi_{34})^2}\bar{p}_{111}\bar{p}_{222}^2$
- (26)  $\bar{p}_{133}\bar{p}_{212}\bar{p}_{221} - \frac{\pi_{34}}{\pi_{12}-\pi_{34}}\bar{p}_{111}\bar{p}_{233}\bar{p}_{222}$
- (27)  $\bar{p}_{144}\bar{p}_{313}\bar{p}_{221} + \bar{p}_{111}\bar{p}_{323}\bar{p}_{244}$
- (28)  $\bar{p}_{122}\bar{p}_{313}\bar{p}_{221} - \frac{\pi_{34}}{\pi_{12}-\pi_{34}}\bar{p}_{111}\bar{p}_{323}\bar{p}_{222}$
- (29)  $\bar{p}_{331}\bar{p}_{323}\bar{p}_{233} - \frac{\pi_3\pi_4\pi_{12}}{(\pi_3-\pi_4)^2}\bar{p}_{333}^2\bar{p}_{221}$
- (30)  $\bar{p}_{111}\bar{p}_{323}\bar{p}_{233} - \frac{\pi_{12}}{\pi_{34}}\bar{p}_{133}\bar{p}_{313}\bar{p}_{221}$
- (31)  $\bar{p}_{144}\bar{p}_{331}\bar{p}_{212} + \bar{p}_{111}\bar{p}_{332}\bar{p}_{244}$
- (32)  $\bar{p}_{122}\bar{p}_{331}\bar{p}_{212} - \frac{\pi_{34}}{\pi_{12}-\pi_{34}}\bar{p}_{111}\bar{p}_{332}\bar{p}_{222}$
- (33)  $\bar{p}_{133}\bar{p}_{331}\bar{p}_{212} - \frac{\pi_{34}}{\pi_{12}}\bar{p}_{111}\bar{p}_{332}\bar{p}_{233}$
- (34)  $\bar{p}_{122}\bar{p}_{333}^2 - \frac{(\pi_3-\pi_4)^2}{\pi_3\pi_4\pi_{12}}\bar{p}_{133}\bar{p}_{332}\bar{p}_{323}$
- (35)  $\bar{p}_{122}\bar{p}_{313}\bar{p}_{331} - \frac{\pi_{34}}{\pi_{12}}\bar{p}_{111}\bar{p}_{332}\bar{p}_{323}$
- (36)  $\bar{p}_{133}\bar{p}_{313}\bar{p}_{331} - \frac{\pi_3\pi_4\pi_{34}}{(\pi_3-\pi_4)^2}\bar{p}_{111}\bar{p}_{333}^2$
- (37)  $\bar{p}_{244}\bar{p}_{424}\bar{p}_{442} - \frac{\pi_1\pi_2(\pi_3+\pi_4)^2}{(\pi_1-\pi_2)^2(\pi_{34}-\pi_{12})}\bar{p}_{222}\bar{p}_{444}^2$
- (38)  $\bar{p}_{332}\bar{p}_{323}\bar{p}_{233} - \frac{\pi_3\pi_4\pi_{12}^2}{(\pi_3-\pi_4)^2(\pi_{12}^2-\pi_{34}^2)}\bar{p}_{333}^2\bar{p}_{222}$
- (39)  $\bar{p}_{333}^2\bar{p}_{212} - \frac{(\pi_{12}-\pi_{34})(\pi_3-\pi_4)^2}{\pi_3\pi_4\pi_{12}}\bar{p}_{313}\bar{p}_{332}\bar{p}_{233}$

## Generators of degree 5

- (40)  $\bar{p}_{144}\bar{p}_{333}^2\bar{p}_{414}\bar{p}_{442} + \frac{\pi_1\pi_2(\pi_3-\pi_4)^2}{\pi_3\pi_4(\pi_1-\pi_2)^2}\bar{p}_{133}\bar{p}_{313}\bar{p}_{332}\bar{p}_{444}^2$
- (41)  $\bar{p}_{144}\bar{p}_{333}^2\bar{p}_{424}\bar{p}_{441} + \frac{\pi_1\pi_2(\pi_3-\pi_4)^2}{\pi_3\pi_4(\pi_1-\pi_2)^2}\bar{p}_{133}\bar{p}_{331}\bar{p}_{323}\bar{p}_{444}^2$
- (42)  $\bar{p}_{333}^2\bar{p}_{244}\bar{p}_{414}\bar{p}_{441} + \frac{\pi_1\pi_2(\pi_3-\pi_4)^2}{\pi_3\pi_4(\pi_1-\pi_2)^2}\bar{p}_{313}\bar{p}_{331}\bar{p}_{233}\bar{p}_{444}^2$

**SM2.2. Computations for quartets.** In the following lemma we compute the coordinates in  $B_n$  for any point in evolving on  $T = 12|34$  under the TN93 model. The coordinates for points on the variety of  $T = 13|24$  or  $14|23$  can be obtained by correspondingly permuting the subindices of the coordinates. This result is used in Proposition 5.11.

LEMMA SM2.1. *Consider the tree  $T = 12|34$  evolving under the evolutionary model  $\mathcal{M} = TN93$ . In the basis  $B_4$ , any tensor  $p = \varphi_T(\Lambda^1, \dots, \Lambda^5)$  has monomial coordinates except for  $\bar{p}_{iiii}$  and  $\bar{p}_{ijij}$  for  $i, j \in \{2, 3, 4\}$ . These coordinates can be obtained by (4.4) from the following expressions of the coordinates of  $q = \varphi_T(\text{Id}, \text{Id}, \text{Id}, \text{Id}, \Lambda)$ , where  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$  (non listed coordinates are zero):*

- (1)  $\bar{q}_{1111} = \lambda_1$
- (2)  $\bar{q}_{1122} = \bar{q}_{2211} = \frac{1}{\pi_{12}\pi_{34}}\lambda_1$
- (3)  $\bar{q}_{1133} = \bar{q}_{3311} = \frac{\pi_{34}}{\pi_3\pi_4}\lambda_1$

- (4)  $\bar{q}_{1144} = \bar{q}_{4411} = \frac{\pi_{12}}{\pi_1 \pi_2} \lambda_1$
- (5)  $\bar{q}_{1212} = \bar{q}_{1221} = \bar{q}_{2112} = \bar{q}_{2121} = \frac{1}{\pi_{12} \pi_{34}} \lambda_2$
- (6)  $\bar{q}_{1222} = \bar{q}_{2122} = \bar{q}_{2212} = \bar{q}_{2221} = \frac{\pi_{34} - \pi_{12}}{\pi_{34} \pi_{12}} \lambda_2$
- (7)  $\bar{q}_{1233} = \bar{q}_{2133} = \bar{q}_{3312} = \bar{q}_{3321} = -\frac{1}{\pi_3 \pi_4} \lambda_2$
- (8)  $\bar{q}_{1244} = \bar{q}_{2144} = \bar{q}_{4412} = \bar{q}_{4421} = \frac{1}{\pi_1 \pi_2} \lambda_2$
- (9)  $\bar{q}_{1313} = \bar{q}_{1331} = \bar{q}_{3113} = \bar{q}_{3131} = \frac{\pi_{34}}{\pi_3 \pi_4} \lambda_3$
- (10)  $\bar{q}_{1323} = \bar{q}_{1332} = \bar{q}_{2313} = \bar{q}_{2331} = \bar{q}_{3123} = \bar{q}_{3132} = \bar{q}_{3213} = \bar{q}_{3231} = -\frac{1}{\pi_3 \pi_4} \lambda_3$
- (11)  $\bar{q}_{1333} = \bar{q}_{3133} = \bar{q}_{3313} = \bar{q}_{3331} = \frac{\pi_{34}(\pi_4 - \pi_3)}{\pi_3^2 \pi_4} \lambda_3$
- (12)  $\bar{q}_{1414} = \bar{q}_{1441} = \bar{q}_{4114} = \bar{q}_{4141} = \frac{\pi_{12}}{\pi_1 \pi_2} \lambda_4$
- (13)  $\bar{q}_{1424} = \bar{q}_{1442} = \bar{q}_{2414} = \bar{q}_{2441} = \bar{q}_{4124} = \bar{q}_{4142} = \bar{q}_{4214} = \bar{q}_{4241} = \frac{1}{\pi_1 \pi_2} \lambda_4$
- (14)  $\bar{q}_{1444} = \bar{q}_{4144} = \bar{q}_{4414} = \bar{q}_{4441} = \frac{\pi_{12}(\pi_2 - \pi_1)}{\pi_1^2 \pi_2} \lambda_4$
- (15)  $\bar{q}_{2222} = \frac{1}{\pi_{12}^2 \pi_{34}^2} \lambda_1 + \frac{(\pi_{12} - \pi_{34})^2}{\pi_{12}^3 \pi_{34}^3} \lambda_2$
- (16)  $\bar{q}_{2233} = \bar{q}_{3322} = \frac{1}{\pi_{12} \pi_3 \pi_4} \lambda_1 + \frac{\pi_{12} - \pi_{34}}{\pi_3 \pi_4 \pi_{12} \pi_{34}} \lambda_2$
- (17)  $\bar{q}_{2244} = \bar{q}_{4422} = \frac{1}{\pi_1 \pi_2 \pi_{34}} \lambda_1 + \frac{\pi_{34} - \pi_{12}}{\pi_1 \pi_2 \pi_{12} \pi_{34}} \lambda_2$
- (18)  $\bar{q}_{2323} = \bar{q}_{2332} = \bar{q}_{3223} = \bar{q}_{3232} = \frac{1}{\pi_3 \pi_4 \pi_{34}} \lambda_3$
- (19)  $\bar{q}_{2333} = \bar{q}_{3233} = \bar{q}_{3323} = \bar{q}_{3332} = \frac{\pi_3 - \pi_4}{\pi_3^2 \pi_4} \lambda_3$
- (20)  $\bar{q}_{2424} = \bar{q}_{2442} = \bar{q}_{4224} = \bar{q}_{4242} = \frac{1}{\pi_1 \pi_2 \pi_{12}} \lambda_4$
- (21)  $\bar{q}_{2444} = \bar{q}_{4244} = \bar{q}_{4424} = \bar{q}_{4442} = \frac{\pi_2 - \pi_1}{\pi_1^2 \pi_2} \lambda_4$
- (22)  $\bar{q}_{3333} = \frac{\pi_{34}^2}{\pi_3^2 \pi_4} \lambda_1 + \frac{\pi_{12} \pi_{34}}{\pi_3^2 \pi_4} \lambda_2 + \frac{\pi_{34}(\pi_3 - \pi_4)^2}{\pi_3^3 \pi_4^3} \lambda_3$
- (23)  $\bar{q}_{3344} = \bar{q}_{4433} = \frac{\pi_{12} \pi_{34}}{\pi_1 \pi_2 \pi_3 \pi_4} \lambda_1 - \frac{\pi_{12} \pi_{34}}{\pi_1 \pi_2 \pi_3 \pi_4} \lambda_2$
- (24)  $\bar{q}_{4444} = \frac{\pi_{12}^2}{\pi_1^2 \pi_2} \lambda_1 + \frac{\pi_{12} \pi_{34}}{\pi_1^2 \pi_2} \lambda_2 + \frac{\pi_{12}(\pi_1 - \pi_2)^2}{\pi_1^3 \pi_2^3} \lambda_4$

*Proof.* Let  $T_1$  be the tripod with leaves  $l_1, l_2, l_s$  and  $T_2$  be the tripod with leaves  $l_s, l_3, l_4$  so that  $T$  is the gluing  $T_1 * T_2$ . Define tensors  $q^{T_1} = \varphi_{T_1}(Id, Id, \Lambda)$  and  $\bar{p}^{T_2} = \varphi_{T_2}(Id, Id, Id)$  evolving on  $T_1$  and  $T_2$  respectively; hence  $q = q_1 * q_2$ .

By Theorem 4.6 the coordinates of  $q$  in the basis  $B_n$  can be obtained by the matrix product

$$\begin{pmatrix} & 1 & 2 & 3 & 4 \\ 11 & * & 0 & 0 & 0 \\ 22 & * & * & 0 & 0 \\ 33 & * & * & * & 0 \\ 44 & * & * & 0 & * \\ 12 & 0 & * & 0 & 0 \\ 21 & 0 & * & 0 & 0 \\ 13 & 0 & 0 & * & 0 \\ 31 & 0 & 0 & * & 0 \\ 23 & 0 & 0 & * & 0 \\ 32 & 0 & 0 & * & 0 \\ 14 & 0 & 0 & 0 & * \\ 41 & 0 & 0 & 0 & * \\ 24 & 0 & 0 & 0 & * \\ 42 & 0 & 0 & 0 & * \\ 34 & 0 & 0 & 0 & 0 \\ 43 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} & 11 & 22 & 33 & 44 & 12 & 21 & 13 & 31 & 23 & 32 & 14 & 41 & 24 & 42 & 34 & 43 \\ 1 & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & * & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & * & 0 & 0 & 0 & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & 0 & 0 \end{pmatrix}$$

in the sense that  $q_{i_1 i_2 i_3 i_4}$  is the product of row  $(i_1, i_2)$  of the first matrix and column  $(i_3, i_4)$  of the second matrix up to multiplication by a scalar product. As  $*$  entries are monomials in (actually they are linear entries in some  $\lambda_k$  in the first matrix and scalar entries in the second), non-monomial entries only appear when multiplying rows and columns with indices  $(2, 2), (3, 3), (4, 4)$ . From this matrix product we get the entries that appear in the list.  $\square$

**SM3. Flattening matrices.**











