Gene-Tree Statistics: Moments and Limit Laws for Ancestral Configurations

(joint with F. Disanto, C.-Y. Huang, A. R. Paningbatan, and N. A. Rosenberg)

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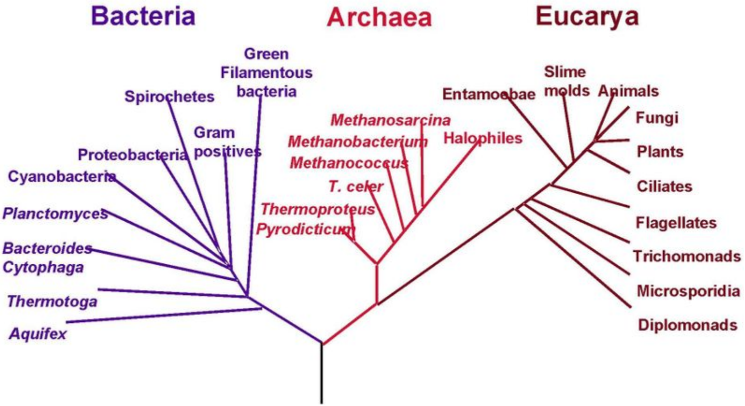

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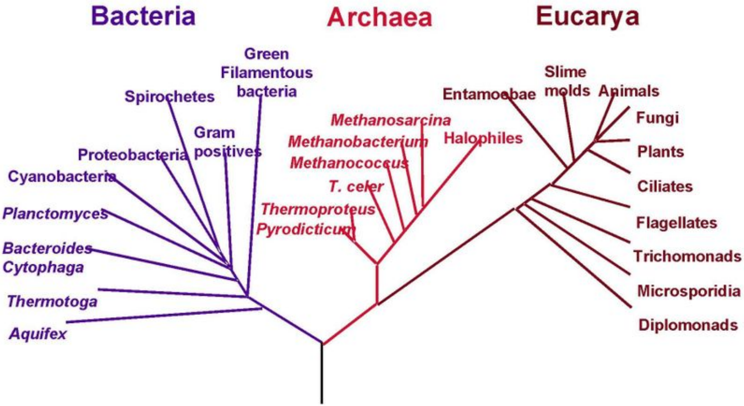

A labeled topology is a rooted, non-plane, binary tree with leaves labeled by X.

Species and Gene Trees

Species tree: tree of evolutionary relationship between species.

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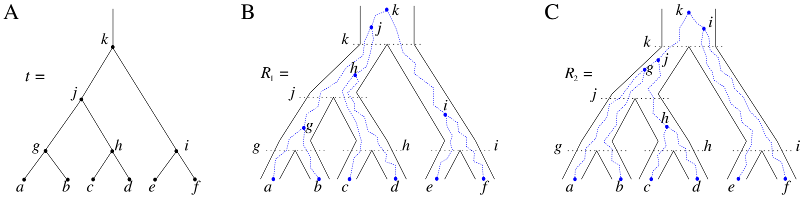

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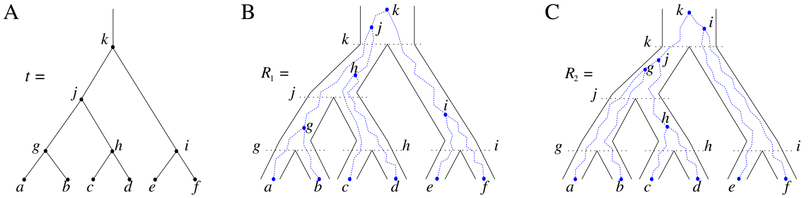

Figure: Two realization of gene trees in the same species tree

We assume throughout the talk that the specific tree and gene tree have the same labeled topology!

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$$c_r(t) = (c_{r_L}(t_L) + 1)(c_{r_R}(t_R) + 1),$$

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$c(t)$ ... total number of ancestral configurations.

Then,

$$c(t) = \sum_v c(t_v).$$

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$$F_n = (n-1)!.$$

Random Labeled Topologies

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Labeled topologies with n leaves are picked uniformly at random, i.e.,

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Thus,

$$P_{\mathsf{YH}}(t) = \frac{2^{n-1}}{n! \prod_{r=3}^{n} (r-1)^{d_r(t)}},$$

where $d_r(t)$ is the number of internal nodes with r leaves below them.

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(ii) For the uniform model:

$$\mathbb{E}_n[c_r(t)] \sim \sqrt{\frac{3}{2}} \left(\frac{4}{3}\right)^n,$$
$$\mathbb{E}_n[c(t)] \bowtie \left(\frac{4}{3}\right)^n$$

and

$$\mathbb{V}_n[c_r(t)] \sim \sqrt{\frac{7(11-\sqrt{2})}{34}} \left(\frac{4}{7(8\sqrt{2}-11)}\right)^n,$$
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For the number R_n of root configurations under the uniform model:

$$R_n \stackrel{d}{=} (R_{I_n} + 1)(R^*_{n-I_n} + 1),$$

where R^*_n is an independent copy of R_n and

$$P(I_n = j) = \frac{C_{j-1}C_{n-j-1}}{C_{n-1}}, \qquad (1 \le j \le n-1).$$

Limit Law under the Uniform Model

Additive tree functional: a function $F(t)$ which satisfies

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Theorem (Disanto, F., Paningbatan, Rosenberg; 2022)

Under the uniform model, $c_r(t)$ is asymptotically lognormal distributed. Moreover,

$$\mathbb{E}_n[\log c_r(t)] \sim \mu n, \qquad \mathbb{V}_n[\log c_r(t)] \sim \sigma^2 n,$$

where $(\mu, \sigma^2) \approx (0.272, 0.034)$.

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Mean under the Yule-Harding Model

Let $e_n := \mathbb{E}[R_n]$.

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Set:

$$E(z) := \sum_{n\geq 1} e_n z^n.$$

Then, $E(z)$ satisfies the Riccati DE

$$zE'(z) = E(z)^2 + \frac{1+z}{1-z}E(z) + \frac{z^2}{(1-z)^2}$$

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with solution

$$E(z) = \frac{2z\sin\left(\frac{\sqrt{3}}{2}\log(1-z)\right)}{(z-1)\left[\sqrt{3}\cos\left(\frac{\sqrt{3}}{2}\log(1-z)\right) + \sin\left(\frac{\sqrt{3}}{2}\log(1-z)\right)\right]}.$$

Mean and Variance under the Yule-Harding Model

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Similarly, but with a more involved analysis, we obtain the variance.

Theorem (Disanto, F., Paningbatan, Rosenberg; 2022)

Under the Yule-Harding model,

$$\mathbb{V}_n[c_r(t)] \sim (2.0449954\cdots)^n.$$

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Set

$$S(z) = \sum_{n\geq 1} s_n z^n.$$

Then,

$$zS'(z) = S(z)^2 + \left[\frac{1+z}{1-z} + 4E(z)\right] S(z) + \frac{(z + 2(1-z)E(z))^2}{(1-z)^2}.$$

This is again a Riccati DE.

Variance under the Yule-Harding Model (ii)

Solving it gives $S(z) = -zU'(z)/U(z)$, where

$$U''(z) - \left(g_1(z) + \frac{g_2'(z)}{g_2(z)}\right)U'(z) + g_2(z)g_0(z)U(z) = 0$$

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$$(g_2(z), g_1(z), g_0(z)) = \left(\frac{1}{z}, \frac{1}{z}\left(\frac{1+z}{1-z} + 4E(z)\right), \frac{(z+2(1-z)E(z))^2}{z(1-z)^2}\right).$$

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Lemma (Disanto, F., Paningbatan, Rosenberg; 2022)

$U(z)$ is analytic in $D(0;1/2)$ and has a unique, simple root β with

$$\beta \approx 0.4889986317.$$

Summary (# of Root Configurations)

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quantity	uniform model	Yule-Harding model
mean	$\mathbb{E}_n[c_r] \sim 1.225 \cdot 1.333^n$	$\mathbb{E}_n[c_r] \sim 1.425^n$
variance	$\mathbb{V}_n[c_r] \sim 1.405 \cdot 1.822^n$	$\mathbb{V}_n[c_r] \sim 2.045^n$
log-mean	$\mathbb{E}_n[\log c_r] \sim 0.272 \cdot n$	$\mathbb{E}_n[\log c_r] \sim 0.351 \cdot n$
log-variance	$\mathbb{V}_n[\log c_r] \sim 0.034 \cdot n$	$\mathbb{V}_n[\log c_r] \sim 0.008 \cdot n$

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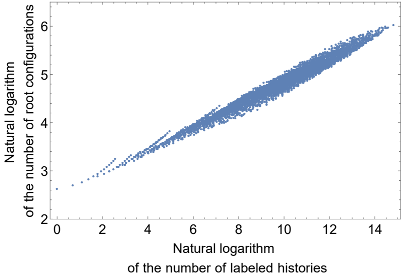
"Balanced" labeled topologies tend to have more root configurations.



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where R^*_n and T^*_n are independent copies of R_n and T_n and

$$P(I_n = j) = \begin{cases} C_{j-1}C_{n-1-j}/C_{n-1}, & \text{uniform model;} \\ 1/(n-1), & \text{Yule-Harding model.} \end{cases}$$

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Also,

$$R_n \leq T_n \leq (2n-1)R_n.$$

Results under Uniform Model

Theorem (Disanto, F., Paningbatan, Rosenberg; 2024)

We have,

$$\mathbb{E}_n[c(t)] \sim \sqrt{6}\left(\frac{4}{3}\right)^n,$$

$$\mathbb{V}_n[c(t)] \sim \frac{2(15+11\sqrt{2})}{17}\sqrt{\frac{7(11-\sqrt{2})}{34}}\left(\frac{4}{7(8\sqrt{2}-11)}\right)^n.$$

In addition,

$$\frac{\log c(t) - \mathbb{E}_n[\log c(t)]}{\sqrt{\mathbb{V}_n[\log c(t)]}} \xrightarrow{d} N(0,1)$$

with

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$\mathbb{E}_n[c_r c]$	$\left(1+\frac{\sqrt{2}}{2}\right)\sqrt{\frac{7(11-\sqrt{2})}{34}}\left(\frac{4}{7(8\sqrt{2}-11)}\right)^n$	$(2.0449954\cdots)^n$
$\mathrm{Cov}_n[c_r, c]$	$\left(1+\frac{\sqrt{2}}{2}\right)\sqrt{\frac{7(11-\sqrt{2})}{34}}\left(\frac{4}{7(8\sqrt{2}-11)}\right)^n$	$(2.0449954\cdots)^n$
$\rho_n[c_r, c]$	$\frac{1+\frac{\sqrt{2}}{2}}{\sqrt{\frac{2(15+11\sqrt{2})}{17}}}$	1

References

1. *F. Disanto, M. Fuchs, A. R. Paningbatan, N. A. Rosenberg (2022). The distribution under two species-tree models of the number of root configurations for matching gene trees and species trees, Ann. Appl. Probab., 32:6, 4426–4458.*

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