

Appendix to “Generating heterogeneous data on gene trees”

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Lemma 1. *Given a time-reversible Markov matrix M with stationary distribution π , let $\tilde{M} = (1 - a)M + aI$. If $a \in (0, 1)$, then \tilde{M} is a Markov matrix with stationary distribution π .*

Proof. As the set of Markov matrices is a convex space, \tilde{M} is also a Markov matrix if $a \in (0, 1)$.

The matrix M is time-reversible with stationary distribution π if and only if

$$\pi = \pi M \quad \text{and} \quad D_\pi M = M^t D_\pi, \quad (1)$$

where D_π is the diagonal matrix with π on its diagonal elements (t denotes transpose here).

To show that these conditions hold for \tilde{M} is immediate: $\pi \tilde{M} = (1 - a)\pi M + a\pi = \pi$ and $D_\pi \tilde{M} = (1 - a)D_\pi M + aD_\pi = (1 - a)M^t D_\pi + aD_\pi = ((1 - a)M^t + aI) D_\pi = \tilde{M}^t D_\pi$. \square

Remark 2. Note that if $M = ADA^{-1}$ is an eigendecomposition of M with eigenvalues 1, λ_2 , λ_3 , and λ_4 , we have $\tilde{M}_2 = A((1 - a)D + aI)A^{-1}$ and its determinant can be computed as

$$p(a) = ((1 - a)\lambda_2 + a)((1 - a)\lambda_3 + a)((1 - a)\lambda_4 + a).$$

We compute the roots of the polynomial $p(a) - d_2$ and choose the root a in $(0, 1)$ if exists (it may happen that the real root of this polynomial is not in this interval, and then we repeat the process in Algorithm 2 starting with another M).