S1 Appendix: Rate quantiles

1 Linear piecewise approximation

In this article we introduced a linear piecewise approximation of the i-cdf to improve the *quant* method. Let $\hat{F}^{-1}(\mathcal{R}_i)$ be the piecewise approximation of $F^{-1}(\mathcal{R}_i)$. The approximation is comprised of n pieces (where n is fixed).

$$\hat{F}^{-1}(\mathcal{R}_i) = F^{-1}(\lfloor b_i \rfloor) + \begin{cases} \Big(F^{-1}(\lfloor b_i \rfloor + 1) - F^{-1}(\lfloor b_i \rfloor)\Big)\Big(b_i - \lfloor b_i \rfloor\Big) & \text{if } \lfloor b_i \rfloor < n-1 \\ 0 & \text{if } \lfloor b_i \rfloor = n-1 \end{cases} \tag{1}$$

where $b_i = \min\{\max\{\frac{n \times \mathcal{R}_i}{n-1}, \frac{n_0}{n-1}\}, \frac{n-1-n_0}{n-1}\}$ indexes $\mathcal{R}_i$ into one of the n pieces $\lfloor b_i \rfloor$. $n_0 = 0.1$ provides a lower and upper limits of the piecewise approximation, corresponding to $r_{\min}$ and $r_{\max}$ respectively. The lower and upper rate limits are equal to:

$$r_{\min} = F^{-1}\Big(\frac{n_0}{n-1}\Big) = F^{-1}\Big(0.001\Big) \tag{2}$$

$$r_{\max} = F^{-1}\Big(\frac{n-1-n_0}{n-1}\Big) = F^{-1}\Big(0.999\Big), \tag{3}$$

when $n = 101$ and $n_0 = 0.1$. It is important to ensure that any operators which act in rate space (as opposed to quantile space) respect these boundaries. The inverse of the approximation function (ie. the cdf $\hat{F}$) is

$$\hat{F}(r_i) = \begin{cases} \max\Big(0, \frac{1}{n-1} \times \Big(v_i + \frac{r_i - F^{-1}(\lfloor v_i \rfloor)}{F^{-1}(\lfloor v_i \rfloor + 1) - F^{-1}(\lfloor v_i \rfloor)}\Big)\Big) & \text{if } \lfloor v_i \rfloor < n-1 \\ 1 & \text{if } \lfloor v_i \rfloor = n-1 \end{cases} \tag{4}$$

where $v_i \in (0, 1, \ldots, n-1)$ is the piece which r_i corresponds to:

$$v_i = \max_{j=0}^{n-1}\{j : \hat{F}^{-1}(\frac{j}{n-1}) < r_i\}. \tag{5}$$

As the piecewise approximation is linear, computing the derivatives of these two functions (required for computing Hastings ratios) are trivial:

$$\frac{\partial}{\partial \mathcal{R}_i}\hat{F}^{-1}(\mathcal{R}_i) = D\hat{F}^{-1}(\mathcal{R}_i) = \begin{cases} \Big(\hat{F}^{-1}(\lfloor b_i \rfloor + 1) - \hat{F}^{-1}(\lfloor b_i \rfloor)\Big) \times (n-1) & \text{if } \lfloor b_i \rfloor < n-1 \\ 0 & \text{if } \lfloor b_i \rfloor = n-1 \end{cases} \tag{6}$$

$$\frac{\partial}{\partial r_i}\hat{F}(r_i) = D\hat{F}(r_i) = \frac{1}{\hat{F}^{-1}\Big(\hat{F}(r_i)\Big)} \tag{7}$$

2 Tree operators for rate quantiles

Zhang and Drummond 2020 introduced several tree operators for the *real* parameterisation – including Constant Distance, Simple Distance, and Small Pulley. In this appendix, these three operators are extended to the the *quant* parameterisation.

Following the notation presented in the main article, let t_i be the time of node i, let $0 < q_i < 1$ be the rate quantile of node i, and let $r_i = \hat{F}^{-1}(q_i)$ be the natural rate of node i.

2.1 Constant Distance

Let X be a uniformly-at-random sampled internal node on tree $\mathcal{T}$. Let L and R be the left and right child of X, respectively, and let P be the parent of X. Under the *quant* parameterisation, the Constant Distance operator works as follows:

Step 1. Propose a new height for t_X:

$$t_X{}' \leftarrow t_X + \Sigma \tag{8}$$

where $\Sigma \sim$ Uniform$(-s, s)$, for some random walk step size s. Ensure that $\max\{t_L, t_R\} < t_X{}' < t_P$, and if the constrant is broken then reject the proposal.

Step 2. Recalculate q_X as:

$$
\begin{aligned}
{q_X}' \leftarrow & \hat{F}\Big({r_X}'\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_P - t_X}{t_P - {t_X}'} r_X\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_P - t_X}{t_P - {t_X}'} \hat{F}^{-1}(q_X)\Big).
\end{aligned} \tag{9}
$$

This ensures that the genetic distance between X and P remains constant after the operation by enforcing the constraint:

$$
r_X(t_P - t_X) = {r_X}'(t_P - {t_X}'). \tag{10}
$$

Step 3. Similarly, propose new rate quantiles for the two children $C \in \{L, R\}$:

$$
\begin{aligned}
{q_C}' \leftarrow & \hat{F}\Big({r_C}'\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times r_C\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times \hat{F}^{-1}(q_C)\Big).
\end{aligned} \tag{11}
$$

Ensure that $r_{\min} < {r_i}' < r_{\max}$ for all proposed nodes $i \in \{X, L, R\}$, and if the constraint is broken then reject the proposal.

Step 4. Finally, compute the natural logarithm of the Hastings ratio as that of the determinant of the Jacobian matrix:

$$
\begin{aligned}
J = & \begin{bmatrix}
\frac{\partial {t_X}'}{\partial t_X} & \frac{\partial {t_X}'}{\partial q_X} & \frac{\partial {t_X}'}{\partial q_L} & \frac{\partial {t_X}'}{\partial q_R} \\
\frac{\partial {q_X}'}{\partial t_X} & \frac{\partial {q_X}'}{\partial q_X} & \frac{\partial {q_X}'}{\partial q_L} & \frac{\partial {q_X}'}{\partial q_R} \\
\frac{\partial {q_L}'}{\partial t_X} & \frac{\partial {q_L}'}{\partial q_X} & \frac{\partial {q_L}'}{\partial q_L} & \frac{\partial {q_L}'}{\partial q_R} \\
\frac{\partial {q_R}'}{\partial t_X} & \frac{\partial {q_R}'}{\partial q_X} & \frac{\partial {q_R}'}{\partial q_L} & \frac{\partial {q_R}'}{\partial q_R}
\end{bmatrix} \\
= & \begin{bmatrix}
\frac{\partial {t_X}'}{\partial t_X} & 0 & 0 & 0 \\
\frac{\partial {q_X}'}{\partial t_X} & \frac{\partial {q_X}'}{\partial q_X} & 0 & 0 \\
\frac{\partial {q_L}'}{\partial t_X} & 0 & \frac{\partial {q_L}'}{\partial q_L} & 0 \\
\frac{\partial {q_R}'}{\partial t_X} & 0 & 0 & \frac{\partial {q_R}'}{\partial q_R}
\end{bmatrix}.
\end{aligned} \tag{12}
$$

As J is triangular, its determinant $|J|$ is equal to the product of diagonal elements:

$$\begin{aligned}
\ln|J| &= \ln\{\frac{\partial t_X{}'}{\partial t_X} \times \frac{\partial q_X{}'}{\partial q_X} \times \frac{\partial q_L{}'}{\partial q_L} \times \frac{\partial q_R{}'}{\partial q_R}\} \\
&= \ln 1 + \ln\ D\hat{F}\Big(\frac{t_P - t_X}{t_P - t_X{}'} \times \hat{F}^{-1}(q_X)\Big) + \ln \frac{\partial}{\partial q_X}\frac{t_P - t_X}{t_P - t_X{}'}\hat{F}^{-1}\Big(q_X\Big) \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln \frac{\partial}{\partial q_L}\frac{t_X - t_L}{t_X{}' - t_L}\hat{F}^{-1}\Big(q_L\Big) \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln \frac{\partial}{\partial q_R}\frac{t_X - t_R}{t_X{}' - t_R}\hat{F}^{-1}\Big(q_R\Big) \\
&= \ln\ D\hat{F}\Big(\frac{t_P - t_X}{t_P - t_X{}'} \times \hat{F}^{-1}(q_X)\Big) + \ln\ D\hat{F}^{-1}\Big(q_X\Big) + \ln \frac{t_P - t_X}{t_P - t_X{}'} \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln\ D\hat{F}^{-1}\Big(q_L\Big) + \ln \frac{t_X - t_L}{t_X{}' - t_L} \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln\ D\hat{F}^{-1}\Big(q_R\Big) + \ln \frac{t_X - t_R}{t_X{}' - t_R}.
\end{aligned} \tag{13}$$

The derivatives $D\hat{F}$ and $D\hat{F}^{-1}$ are readily computed under the linear piecewise approximation. As its final step, the operator returns $\ln|J|$.

2.2 Simple Distance

While Constant Distance proposes internal node heights, Simple Distance operates on the root. Let X be the root node and let L and R be its two children.

Step 1. Propose a new height for t_X:

$$t_X{}' \leftarrow t_X + \Sigma \tag{14}$$

where $\Sigma \sim$ Uniform$(-s, s)$, for some window size s. Ensure that $\max\{t_L, t_R\} < t_X{}'$, and if the constraint is broken then reject the proposal.

Step 2. Propose new rate quantiles for the two children $C \in \{L, R\}$:

$$
\begin{aligned}
{q_C}' \leftarrow & \hat{F}\Big({r_C}'\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times r_C\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times \hat{F}^{-1}(q_C)\Big).
\end{aligned} \tag{15}
$$

These proposals ensure that the genetic distance between X and its children C remain constant after the operation by enforcing the constraint:

$$
r_C(t_X - t_C) = {r_C}'({t_X}' - t_C). \tag{16}
$$

Ensure that $r_{\min} < {r_C}' < r_{\max}$, and if the constraint is broken then reject the proposal.

Step 3. Return the natural logarithm of the Green ratio by calculating the determinant of the Jacobian matrix J.

$$
\begin{aligned}
J = & \begin{bmatrix} \frac{\partial {t_X}'}{\partial t_X} & \frac{\partial {t_X}'}{\partial q_L} & \frac{\partial {t_X}'}{\partial q_R} \\ \frac{\partial {q_L}'}{\partial t_X} & \frac{\partial {q_L}'}{\partial q_L} & \frac{\partial {q_L}'}{\partial q_R} \\ \frac{\partial {q_R}'}{\partial t_X} & \frac{\partial {q_R}'}{\partial q_L} & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix} \\
= & \begin{bmatrix} \frac{\partial {t_X}'}{\partial t_X} & 0 & 0 \\ \frac{\partial {q_L}'}{\partial t_X} & \frac{\partial {q_L}'}{\partial q_L} & 0 \\ \frac{\partial {q_R}'}{\partial t_X} & 0 & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix}.
\end{aligned} \tag{17}
$$

As J is triangular, its determinant $|J|$ is equal to the product of diagonal elements:

$$
\begin{aligned}
\ln|J| &= \ln\{\frac{\partial t_X{}'}{\partial t_X} \times \frac{\partial q_L{}'}{\partial q_L} \times \frac{\partial q_R{}'}{\partial q_R}\} \\
&= \ln \frac{\partial t_X{}'}{\partial t_X} + \ln \frac{\partial q_L{}'}{\partial q_L} + \ln \frac{\partial q_R{}'}{\partial q_R} \\
&= \ln 1 \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln \frac{\partial}{\partial q_L} \frac{t_X - t_L}{t_X{}' - t_L} \hat{F}^{-1}\Big(q_L\Big) \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln \frac{\partial}{\partial q_R} \frac{t_X - t_R}{t_X{}' - t_R} \hat{F}^{-1}\Big(q_R\Big) \\
&= \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln\ D\hat{F}^{-1}\Big(q_L\Big) + \ln \frac{t_X - t_L}{t_X{}' - t_L} \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln\ D\hat{F}^{-1}\Big(q_R\Big) + \ln \frac{t_X - t_R}{t_X{}' - t_R}.
\end{aligned}
\tag{18}
$$

$D\hat{F}(x)$ and $D\hat{F}^{-1}(x)$ are readily computed from the linear piecewise approximation. As its final step, the operator returns $\ln|J|$.

2.3 Small Pulley

Just like the previous operator, Small Pulley operates on the root. Let X be the root node and let L and R be its two children. However, unlike Simple Distance, this operator alters the two genetic distances $d_L = r_L(t_X - t_L) = \hat{F}^{-1}(q_L)(t_X - t_L)$ and $d_R = r_R(t_X - t_R) = \hat{F}^{-1}(q_R)(t_X - t_R)$, while conserving their sum $d_L + d_R$.

Step 1. Propose new genetic distances for d_L and d_R:

$$d_L{}' \leftarrow d_L + \Sigma \tag{19}$$

$$d_R{}' \leftarrow d_R - \Sigma \tag{20}$$

where $\Sigma \sim$ Uniform$(-s, s)$, for some window size s. Ensure that $0 < d_L{}' < d_L + d_R$ and that $r_{\min} < r_C{}' < r_{\max}$ for $C \in \{L, R\}$, and if either constrant is broken then reject the proposal.

Step 2. Propose new rate quantiles for the two children L and R:

$$
\begin{aligned}
{q_L}' &\leftarrow \hat{F}(\frac{{d_L}'}{t_X - t_L}) \\
&\leftarrow \hat{F}(\frac{\hat{F}^{-1}(q_L)(t_X - t_L) + \Sigma}{t_X - t_L})
\end{aligned}
\tag{21}
$$

$$
\begin{aligned}
{q_R}' &\leftarrow \hat{F}(\frac{{d_R}'}{t_X - t_R}) \\
&\leftarrow \hat{F}(\frac{\hat{F}^{-1}(q_R)(t_X - t_R) - \Sigma}{t_X - t_R}).
\end{aligned}
\tag{22}
$$

Step 3. Return the natural logarithm of the Green ratio by calculating the determinant of the Jacobian matrix J.

$$
\begin{aligned}
J &= \begin{bmatrix} \frac{\partial {q_L}'}{\partial q_L} & \frac{\partial {q_L}'}{\partial q_R} \\ \frac{\partial {q_R}'}{\partial q_L} & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial {q_L}'}{\partial q_L} & 0 \\ 0 & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix}
\end{aligned}
\tag{23}
$$

As J is triangular/diagonal, its determinant $|J|$ is equal to the product of diagonal elements:

$$
\begin{aligned}
\ln|J| &= \ln\{\frac{\partial {q_L}'}{\partial q_L} \times \frac{\partial {q_R}'}{\partial q_R}\} \\
&= \ln\frac{\partial {q_L}'}{\partial q_L} + \ln\frac{\partial {q_R}'}{\partial q_R} \\
&= \ln\ D\hat{F}(\frac{\hat{F}^{-1}(q_L)(t_X - t_L) + \Sigma}{t_X - t_L}) + \ln\frac{\partial {q_L}'}{\partial q_L}\frac{\hat{F}^{-1}(q_L)(t_X - t_L) + \Sigma}{t_X - t_L} \\
&\quad + \ln\ D\hat{F}(\frac{\hat{F}^{-1}(q_R)(t_X - t_R) - \Sigma}{t_X - t_R}) + \ln\frac{\partial {q_R}'}{\partial q_R}\frac{\hat{F}^{-1}(q_R)(t_X - t_R) - \Sigma}{t_X - t_R} \\
&= \ln\ D\hat{F}(\frac{\hat{F}^{-1}(q_L)(t_X - t_L) + \Sigma}{t_X - t_L}) + \ln\ D\hat{F}^{-1}(q_L) \\
&\quad + \ln\ D\hat{F}(\frac{\hat{F}^{-1}(q_R)(t_X - t_R) - \Sigma}{t_X - t_R}) + \ln\ D\hat{F}^{-1}(q_R).
\end{aligned}
\tag{24}
$$

Thus, as its final step, the operator returns $\ln|J|$.

References