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). Then,

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

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:

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

As the piecewise approximation is linear, computing the derivatives of these two functions (later 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 the main body of this article, Constant Distance was extended to be compatible with the *quant* parameterisation.

In this appendix, two of the remaining operators are extended, and the Hastings-Green ratio of Constant Distance is further explicated.

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 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:

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

where $\alpha \sim$ Uniform$(-w, w)$, for some window size w. 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 $C \in \{L, R\}$:

$$
\begin{aligned}
{q_C}' \leftarrow & \hat{F}\Big({r_C}'\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times r_C\Big) \\
\leftarrow & \hat{F}\Big(\frac{t_X - t_C}{{t_X}' - t_C} \times \hat{F}^{-1}(q_C)\Big).
\end{aligned} \tag{9}
$$

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

$$
r_C(t_X - t_C) = {r_C}'({t_X}' - t_C). \tag{10}
$$

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.

$$
\begin{aligned}
J = & \begin{bmatrix} \frac{\partial {t_X}'}{\partial t_X} & \frac{\partial {t_X}'}{\partial q_L} & \frac{\partial {t_X}'}{\partial q_R} \\ \frac{\partial {q_L}'}{\partial t_X} & \frac{\partial {q_L}'}{\partial q_L} & \frac{\partial {q_L}'}{\partial q_R} \\ \frac{\partial {q_R}'}{\partial t_X} & \frac{\partial {q_R}'}{\partial q_L} & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix} \\
= & \begin{bmatrix} \frac{\partial {t_X}'}{\partial t_X} & 0 & 0 \\ \frac{\partial {q_L}'}{\partial t_X} & \frac{\partial {q_L}'}{\partial q_L} & 0 \\ \frac{\partial {q_R}'}{\partial t_X} & 0 & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix}.
\end{aligned} \tag{11}
$$

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

$$
\begin{aligned}
\ln|J| &= \ln\{\frac{\partial {t_X}'}{\partial t_X} \times \frac{\partial {q_L}'}{\partial q_L} \times \frac{\partial {q_R}'}{\partial q_R}\} \\
&= \ln\frac{\partial {t_X}'}{\partial t_X} + \ln\frac{\partial {q_L}'}{\partial q_L} + \ln\frac{\partial {q_R}'}{\partial q_R} \\
&= \ln 1 \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_L}{{t_X}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln\frac{\partial}{\partial q_L}\frac{t_X - t_L}{{t_X}' - t_L}\hat{F}^{-1}\Big(q_L\Big) \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{{t_X}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln\frac{\partial}{\partial q_R}\frac{t_X - t_R}{{t_X}' - t_R}\hat{F}^{-1}\Big(q_R\Big) \\
&= \ln\ D\hat{F}\Big(\frac{t_X - t_L}{{t_X}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln\ D\hat{F}^{-1}\Big(q_L\Big) + \ln\frac{t_X - t_L}{{t_X}' - t_L} \\
&\quad + \ln\ D\hat{F}\Big(\frac{t_X - t_R}{{t_X}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln\ D\hat{F}^{-1}\Big(q_R\Big) + \ln\frac{t_X - t_R}{{t_X}' - t_R}.
\end{aligned}
\tag{12}
$$

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

2.2 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:

$$
{d_L}' \leftarrow d_L + \alpha \tag{13}
$$

$$
{d_R}' \leftarrow d_R - \alpha \tag{14}
$$

where $\alpha \sim$ Uniform$(-w, w)$, for some window size w. 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:

$$
\begin{aligned}
{q_L}' &\leftarrow \hat{F}(\frac{{d_L}'}{t_X - t_L}) \\
&\leftarrow \hat{F}(\frac{\hat{F}^{-1}(q_L)(t_X - t_L) + \alpha}{t_X - t_L}) \qquad (15) \\
{q_R}' &\leftarrow \hat{F}(\frac{{d_R}'}{t_X - t_R}) \\
&\leftarrow \hat{F}(\frac{\hat{F}^{-1}(q_R)(t_X - t_R) - \alpha}{t_X - t_R}). \qquad (16)
\end{aligned}
$$

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

$$
\begin{aligned}
J &= \begin{bmatrix} \frac{\partial {q_L}'}{\partial q_L} & \frac{\partial {q_L}'}{\partial q_R} \\ \frac{\partial {q_R}'}{\partial q_L} & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial {q_L}'}{\partial q_L} & 0 \\ 0 & \frac{\partial {q_R}'}{\partial q_R} \end{bmatrix} \qquad (17)
\end{aligned}
$$

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

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

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

2.3 Constant Distance

The Jacobian matrix J of this operator is defined as

$$
\begin{aligned}
J &= \begin{bmatrix}
\frac{\partial t_X{}'}{\partial t_X} & \frac{\partial t_X{}'}{\partial q_X} & \frac{\partial t_X{}'}{\partial q_L} & \frac{\partial t_X{}'}{\partial q_R} \\
\frac{\partial q_X{}'}{\partial t_X} & \frac{\partial q_X{}'}{\partial q_X} & \frac{\partial q_X{}'}{\partial q_L} & \frac{\partial q_X{}'}{\partial q_R} \\
\frac{\partial q_L{}'}{\partial t_X} & \frac{\partial q_L{}'}{\partial q_X} & \frac{\partial q_L{}'}{\partial q_L} & \frac{\partial q_L{}'}{\partial q_R} \\
\frac{\partial q_R{}'}{\partial t_X} & \frac{\partial q_R{}'}{\partial q_X} & \frac{\partial q_R{}'}{\partial q_L} & \frac{\partial q_R{}'}{\partial q_R}
\end{bmatrix} \\
&= \begin{bmatrix}
\frac{\partial t_X{}'}{\partial t_X} & 0 & 0 & 0 \\
\frac{\partial q_X{}'}{\partial t_X} & \frac{\partial q_X{}'}{\partial q_X} & 0 & 0 \\
\frac{\partial q_L{}'}{\partial t_X} & 0 & \frac{\partial q_L{}'}{\partial q_L} & 0 \\
\frac{\partial q_R{}'}{\partial t_X} & 0 & 0 & \frac{\partial q_R{}'}{\partial q_R}
\end{bmatrix}.
\end{aligned} \tag{19}
$$

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

$$
\begin{aligned}
\ln|J| =& \ln\{\frac{\partial t_X{}'}{\partial t_X} \times \frac{\partial q_X{}'}{\partial q_X} \times \frac{\partial q_L{}'}{\partial q_L} \times \frac{\partial q_R{}'}{\partial q_R}\} \\
=& \ln 1 + \ln\ D\hat{F}\Big(\frac{t_P - t_X}{t_P - t_X{}'} \times \hat{F}^{-1}(q_X)\Big) + \ln \frac{\partial}{\partial q_X}\frac{t_P - t_X}{t_P - t_X{}'}\hat{F}^{-1}\Big(q_X\Big) \\
&+ \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln \frac{\partial}{\partial q_L}\frac{t_X - t_L}{t_X{}' - t_L}\hat{F}^{-1}\Big(q_L\Big) \\
&+ \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln \frac{\partial}{\partial q_R}\frac{t_X - t_R}{t_X{}' - t_R}\hat{F}^{-1}\Big(q_R\Big) \\
=& \ln\ D\hat{F}\Big(\frac{t_P - t_X}{t_P - t_X{}'} \times \hat{F}^{-1}(q_X)\Big) + \ln\ D\hat{F}^{-1}\Big(q_X\Big) + \ln \frac{t_P - t_X}{t_P - t_X{}'} \\
&+ \ln\ D\hat{F}\Big(\frac{t_X - t_L}{t_X{}' - t_L} \times \hat{F}^{-1}(q_L)\Big) + \ln\ D\hat{F}^{-1}\Big(q_L\Big) + \ln \frac{t_X - t_L}{t_X{}' - t_L} \\
&+ \ln\ D\hat{F}\Big(\frac{t_X - t_R}{t_X{}' - t_R} \times \hat{F}^{-1}(q_R)\Big) + \ln\ D\hat{F}^{-1}\Big(q_R\Big) + \ln \frac{t_X - t_R}{t_X{}' - t_R}.
\end{aligned} \tag{20}
$$

References