

A different way to write the flexTPC equation

The flexTPC model equation is

$$r(T) = \begin{cases} r_{\max} \left[\left(\frac{T - T_{\min}}{\alpha} \right)^\alpha \left(\frac{T_{\max} - T_{\min}}{1 - \alpha} \right)^{1 - \alpha} \left(\frac{1}{T_{\max} - T_{\min}} \right) \right]^{\frac{\alpha(1 - \alpha)}{\beta}} & T \in [T_{\min}, T_{\max}] \\ 0 & \text{otherwise} \end{cases}$$

This is the most straightforward form of the model, but using this formula directly in the code can lead to numerical issues when some parameters are really small or really large (which can happen during exploration of the MCMC chains).

Because of this, it can be more numerically stable to rewrite it in a different way. For $T \in [T_{\min}, T_{\max}]$ we can also write this model as follows:

$$\begin{aligned} r(T) &= r_{\max} \exp \left(\ln \left[\left(\frac{T - T_{\min}}{\alpha} \right)^\alpha \left(\frac{T_{\max} - T_{\min}}{1 - \alpha} \right)^{1 - \alpha} \left(\frac{1}{T_{\max} - T_{\min}} \right) \right]^{\frac{\alpha(1 - \alpha)}{\beta}} \right) \\ &= r_{\max} \exp \left(\frac{\alpha(1 - \alpha)}{\beta} \left[\alpha \ln \left(\frac{T - T_{\min}}{\alpha} \right) + (1 - \alpha) \ln \left(\frac{T_{\max} - T_{\min}}{1 - \alpha} \right) - \ln(T_{\max} - T_{\min}) \right] \right) \end{aligned}$$

This is the form of the flexTPC equation that is input into `bayesTPC` with two changes:

1. In order to ensure that the function is zero outside the $[T_{\min}, T_{\max}]$ interval, most models in bayes TPC include a factor that looks like

$$(T_{\max} > \text{Temp}) * (T_{\min} < \text{Temp})$$

which will be zero whenever `Temp` is outside this interval. We also add this to the equation.

2. To avoid numerical issues with logarithms of very small numbers (which approach $-\infty$), in the code logarithms of the form

$$f(x) = \ln x$$

are replaced with

$$g(x) = \ln (\max(x, 10^{-20}))$$

which prevents these very small values from causing numerical issues.