

1. The acceptance probability is

$$\begin{aligned}
 \text{acceptance prob.} &= \min \left\{ 1, \frac{p(\boldsymbol{\pi} \mid \boldsymbol{\alpha} = A\boldsymbol{\pi}^*)}{p(\boldsymbol{\pi}^* \mid \boldsymbol{\alpha} = A\boldsymbol{\pi})} \right\} \\
 &= \min \left\{ 1, \frac{\left(\frac{\Gamma(A)}{\prod_i \Gamma(A\pi_i^*)} \right) \left(\prod_i \pi_i^{A\pi_i^* - 1} \right)}{\left(\frac{\Gamma(A)}{\prod_i \Gamma(A\pi_i)} \right) \left(\prod_i (\pi_i^*)^{A\pi_i - 1} \right)} \right\} \\
 &= \min \left\{ 1, \frac{\left(\prod_i \Gamma(A\pi_i) \right) \left(\prod_i \pi_i^{A\pi_i^* - 1} \right)}{\left(\prod_i \Gamma(A\pi_i^*) \right) \left(\prod_i (\pi_i^*)^{A\pi_i - 1} \right)} \right\}
 \end{aligned}$$

2. See web page for an R implementation. Nothing actually goes wrong with this implementation. I expected (from previous programming a couple years ago) that the MCMC would be pulled into a corner of the distribution, but this need not be the case.

3. The acceptance probability is

$$\begin{aligned}
 \text{acceptance prob.} &= \min \left\{ 1, \frac{p(\boldsymbol{\pi} \mid \boldsymbol{\alpha} = A\boldsymbol{\pi}^* + \mathbf{1})}{p(\boldsymbol{\pi}^* \mid \boldsymbol{\alpha} = A\boldsymbol{\pi} + \mathbf{1})} \right\} \\
 &= \min \left\{ 1, \frac{\left(\frac{\Gamma(A+4)}{\prod_i \Gamma(A\pi_i^* + 1)} \right) \left(\prod_i \pi_i^{A\pi_i^*} \right)}{\left(\frac{\Gamma(A+4)}{\prod_i \Gamma(A\pi_i + 1)} \right) \left(\prod_i (\pi_i^*)^{A\pi_i} \right)} \right\} \\
 &= \min \left\{ 1, \frac{\left(\prod_i \Gamma(A\pi_i + 1) \right) \left(\prod_i \pi_i^{A\pi_i^*} \right)}{\left(\prod_i \Gamma(A\pi_i^* + 1) \right) \left(\prod_i (\pi_i^*)^{A\pi_i} \right)} \right\}
 \end{aligned}$$

4. We can estimate $\boldsymbol{\pi}$ by using the observed base frequencies for both species. This estimate is: $(\pi_A, \pi_C, \pi_G, \pi_T) = (0.3136, 0.2947, 0.1329, 0.2588)$. A rough point estimate of R is the ratio of the observed number of transitions to the observed number of transversions from a parsimony reconstruction, or $R = (18 + 14 + 42 + 51)/(38 + 6 + 32 + 2 + 3 + 2 + 13 + 2) = 1.2755$. A rough point estimate of ρ is the number of AG or GA sites divided by the number of CT or TC sites, namely $(18 + 14)/(42 + 51) = 0.3441$. Other estimates are possible as well. A fully Bayesian approach would posit prior distributions for these parameters and include them in the MCMC.

The web page has an R program for carrying out MCMC on this problem. This program updates the current edge with a uniform window. The autocorrelation function of the sampled edge lengths is an effective tool for measuring the efficiency of the MCMC sampler. A good rule of thumb is that acceptance probabilities near 0.25 often are associated with autocorrelation functions that decrease relatively rapidly.

Three separate MCMC runs of 10,000 updates using the point estimates above and a window size $w = 0.1$ burn in rapidly and result in these 95% credible regions for the edge length.

Run	Lower	Upper
1	0.200	0.265
2	0.199	0.265
3	0.200	0.264

Computing multiple runs provides a means to assess the error due to simulation. There is a 95% probability that the edge length is between 0.200 and 0.265. given the prior and model.

I also carried out a run where I updated the parameters. I assumed an exponential prior for the parameter ρ with mean 1 and a shifted exponential prior for R (Felsenstein's notation). Notice in equation 13.8 that R has a positive lower bound necessary to ensure the nonnegativity of the rate α_Y .

This run is much slower to mix, partly because there is a strong negative correlation between R and ρ . A better MCMC method would update these two parameters as a pair in an intelligent manner. The posterior mean of R is 1.47 and the similar value for ρ is 0.34. Notice that the crude point estimates were not too bad for R and very good for ρ . The 95% credible region for t is quite similar, (0.201, 0.267).

I also used R to find the MLEs of the three parameters. These were $t = 0.232$, $R = 1.454$ and $\rho = 0.318$, very similar to the posterior means.