

The first move type is a *reversible element shift*. A pair of states  $(i, j)$ ,  $i \neq j$ , are selected with uniform probability, and a random number  $\Delta$  is selected uniformly over the interval

$$\Delta \in [\max(-T_{ii}, -\frac{\pi_j}{\pi_i} T_{jj}), T_{ij}]$$

The changed elements in the proposed transition matrix  $\mathbf{T}'$  are then given by:

$$\begin{aligned} T'_{ij} &= T_{ij} - \Delta ; T'_{ji} = T_{ji} - \frac{\pi_i}{\pi_j} \Delta \\ T'_{ii} &= T_{ii} + \Delta ; T'_{jj} = T_{jj} + \frac{\pi_i}{\pi_j} \Delta \end{aligned}$$

This move is accepted with probability

$$P_{\text{accept}}(\mathbf{T} \rightarrow \mathbf{T}') = \min \left\{ 1, \sqrt{\frac{(T'_{ij})^2 + (T'_{ji})^2}{(T_{ij})^2 + (T_{ji})^2}} \right. \\ \left. \times \left( \frac{T'_{ii}}{T_{ii}} \right)^{C_{ii}} \left( \frac{T'_{ij}}{T_{ij}} \right)^{C_{ij}} \left( \frac{T'_{jj}}{T_{jj}} \right)^{C_{jj}} \left( \frac{T'_{ji}}{T_{ji}} \right)^{C_{ji}} \right\} \quad (39)$$

This move will leave the vector of stationary probabilities  $\pi$  unchanged.

The second move type is a *row shift*. A row  $i$  of  $\mathbf{T}$  is selected with uniform probability, and a random number  $\alpha$  chosen uniformly over the interval

$$\alpha \in \left[ 0, \frac{1}{1 - T_{ii}} \right]$$

and used to update row  $i$  of  $\mathbf{T}$  according to

$$T'_{ij} = \begin{cases} \alpha T_{ij} & j = 1, \dots, M, j \neq i \\ \alpha(T_{ii} - 1) + 1 & j = i \end{cases} \quad (40)$$

This move is accepted with probability

$$P_{\text{accept}}(\mathbf{T} \rightarrow \mathbf{T}') = \min \left\{ 1, \alpha^{(M-2)} \alpha^{(C_i - C_{ii})} \left( \frac{1 - \alpha(1 - T_{ii})}{T_{ii}} \right)^{C_{ii}} \right\} \quad (41)$$

The row shift operation will change the stationary distribution of  $\pi'$ , but it may be efficiently updated:

$$\pi'_i = \frac{\pi_i}{\pi_i + \alpha(1 - \pi_i)} ; \pi'_j = \frac{\alpha \pi_j}{\pi_i + \alpha(1 - \pi_i)} \quad j \neq i$$

Since this update scheme is incremental, it will accumulate numerical errors over time that cause the updated  $\pi$  to drift away from the stationary distribution of the current transition matrix. To avoid this,  $\pi$  is recomputed from the current sample of the transition matrix in regular intervals (here, every 100 sampling steps).

### 3. Updating the observable distribution parameters

Following the update of the transition matrix  $\mathbf{T}$ , the observable distribution parameters  $\mathbf{E}$  are updated by sampling  $\mathbf{E}$  from the conditional probability  $P(\mathbf{E}|\mathbf{O}, \mathbf{S})$ . The conditional probability for the observable distribution parameters for state

$$P(\mathbf{E}'|\mathbf{S}', \mathbf{O})$$

$\mathbf{e}_m$ , denoted  $\mathbf{e}_i$ , is given in terms of the output model  $\varphi(o|e)$  by Bayes' theorem:

$$P(\mathbf{E}|\mathbf{O}, \mathbf{S}) = \left[ \prod_{n=1}^N \prod_{t=0}^{T^{(n)}} \varphi(o_{nt} | \mathbf{e}_{s_t^{(n)}}) \right] P(\mathbf{E}) \quad (42)$$

An important choice must be made with regards to the prior,  $P(\mathbf{E})$ . If the prior is chosen to be composed of independent priors for each state, as in

$$P(\mathbf{E}) = \prod_{m=1}^M P(\mathbf{e}_m) \quad (43)$$

then the full BHMM posterior (Eq. 9) will be invariant under any permutation of the states. This behavior might be undesirable, as the states may switch labels during the posterior sampling procedure; this will require any analysis of the models sampled from the posterior to account for the possible permutation symmetry in the states. On the other hand, breaking this symmetry (e.g., by enforcing an ordering on the state mean observables) can artificially restrict the confidence intervals of the states, which might additionally complicate data analysis.

[JDC: Is there anything we can cite on this topic?]

Here, we make the choice that the prior be separable (Eq. 43), which has the benefit of allowing the conditional probability for  $\mathbf{E}$  (Eq. 42) to be decomposed into a separate posterior for each state. For each state  $i$ , collect all the observations  $o_t^{(n)}$  whose updated hidden state labels  $s_t^{(n)} = i$  into a single dataset  $\mathbf{o} \equiv \{o_n\}$ , where  $n = 1, \dots, N$ , for the purposes of this update procedure. Then, the observable parameters  $\mathbf{e}$  for this state are given by

$$P(\mathbf{e}|\mathbf{o}) = P(\mathbf{o}|\mathbf{e})P(\mathbf{e}) = \left[ \prod_{n=1}^N \varphi(o_n|\mathbf{e}) \right] P(\mathbf{e}) \quad (44)$$

In the application presented here, we use a Gaussian output model (Eq. 3) for the state observable distributions  $P(o|e)$ , where  $\mathbf{e} \equiv \{\mu, \sigma^2\}$ , where  $\mu$  is the state mean observable and  $\sigma^2$  the variance (which will include both the distribution of the observable characterizing the state and any broadening from measurement noise). Other models (including multidimensional observation models) are possible, and require only replacing only the observation model  $\varphi(o|e)$  and corresponding prior  $P(\mathbf{e})$ .

We use the (improper) Jeffreys prior [27] which has the information-theoretic interpretation as the prior that maximizes the information content of the data [28],

$$P(\mathbf{e}) \propto \sigma^{-1} \quad (45)$$

which produces the posterior

$$P(\mathbf{e}|\mathbf{o}) \propto \sigma^{-(N+1)} \exp \left[ -\frac{1}{2\sigma^2} \sum_{n=1}^N (o_n - \mu)^2 \right] \quad (46)$$

The conditional distribution of the mean  $\mu$  is then given by

$$P(\mu|\sigma^2, \mathbf{o}) \equiv \frac{P(\mu, \sigma^2|\mathbf{o})}{\int d\mu P(\mu, \sigma^2|\mathbf{o})} \\ \propto \exp \left[ -\frac{1}{2(\sigma^2/N)} (\mu - \hat{\mu})^2 \right] \quad (47)$$

I didn't check any math here beyond basic typos.

don't understand why this is necessary, I think we need a new index since  $N = \# \text{ of traces}$ .

check indices,  $N$ .