

# Project: Transition matrix sampling

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Consider the following transition matrix for a birth-death chain,

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & & & & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & & & & & \\ 0 & 1 - 10^{-b} & 0 & 10^{-b} & 0 & & & & \\ & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & & & \\ & & 0 & 10^{-b} & 0 & 1 - 10^{-b} & 0 & & \\ & & & 0 & \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & & & 0 & \frac{1}{2} & 0 & \frac{1}{2} & \\ & & & & & 0 & \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$

We want to use sampling of *non-reversible* transition matrices to characterize the convergence of largest implied time-scale and the mean first-passage time for the transition between the two meta-stable sets in the system.

1. Which states belong to the two meta-stable sets  $A$ ,  $B$ ? What determines the meta-stability of the system.
2. For  $b = 3$  generate system trajectories of different length  $N = 10^4, \dots, 10^6$  starting in state  $X_0 = 1$  using the `evolve_chain` function in `chaintools.py`.
3. Estimate mean,  $\mu$ , and standard-deviation,  $\sigma$ , for the two observables for different trajectory lengths using the `sample` function in `sampletools.py`. What do you observe?
4. Compare to values computed from a non-reversible maximum likelihood transition matrix. Do the estimates match?

Repeat your experiment for the alanine-dipeptide data from the tutorial. The input count-matrix for sampling needs to be estimated using the `sliding=False` option. What can you say about the uncertainty of the largest implied time-scale and the mean-first passage time for the  $C_5$  to  $\alpha_L$  transition. What about the opposite transition from  $\alpha_L$  to  $C_5$ .