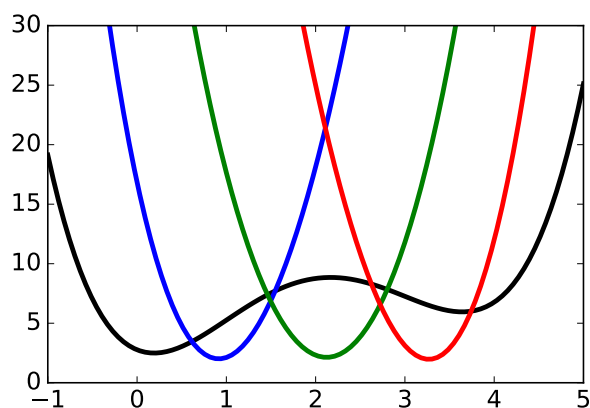


Optimal combination of unbiased and biased data for kinetic estimates

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dTRAM allows to combine unbiased and biased data in one kinetic model. In this project you will investigate how much or how little data of each kind (biased/unbiased) is necessary to get a good kinetic estimates for the asymmetric double-well potential.

- Using the helper function given in the notebook, generate kinetic trajectories that sample from the asymmetric double-well potential. Using an MSM, estimate the mean-first-passage time from the lowest free energy minimum to the higher free energy minimum. Only using purely unbiased trajectories that start from the higher minimum, investigate how the error of the MFPT depends on the amount of data used? Is it better to start many short trajectories or a few long ones? Errors can be determined by repeating the trajectory generation and analysis a couple of times.
- Repeat the experiment by adding Umbrella sampling trajectories that you can generate with the helper function and analyze them with dTRAM this time. Try different compositions of the data, like half of the data being biased and the other half unbiased or 9/10 unbiased and 1/10 biased.