Markov State Models

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- MSMs
  - are similar to chemical kinetics models, where there are states and rates of transitions between states
  - there are states and *transition matrices* - which describe the probability of transitions to other states after a certain amount of time
  - are based on Markov chains, which assume that the future of a system only depends on its current state
- They can be used to calculate
  - the rates of transitions between any pair of states
  - the most probable pathways between any pair of states
  - the equilibrium probability of any state
- MSMs are useful because they
  - can combine information from short MD trajectories
  - piece together local equilibria into a global picture