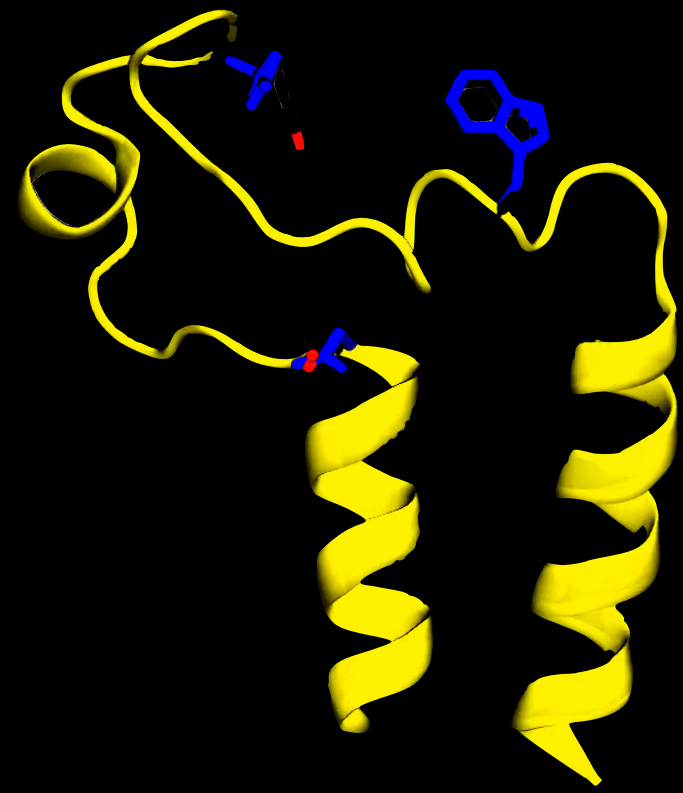


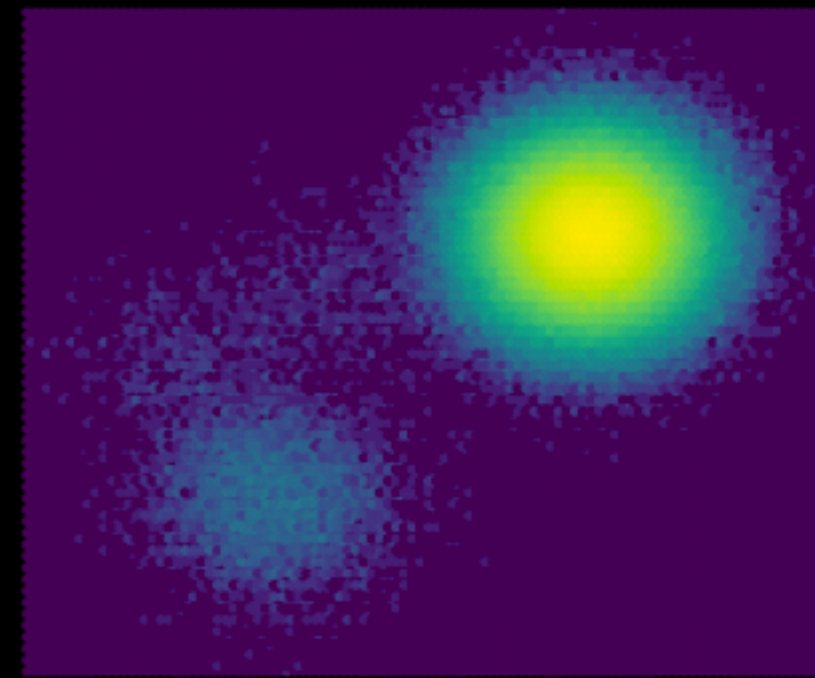
PyEMMA / deeptime typical workflow

Molecular Dynamics data

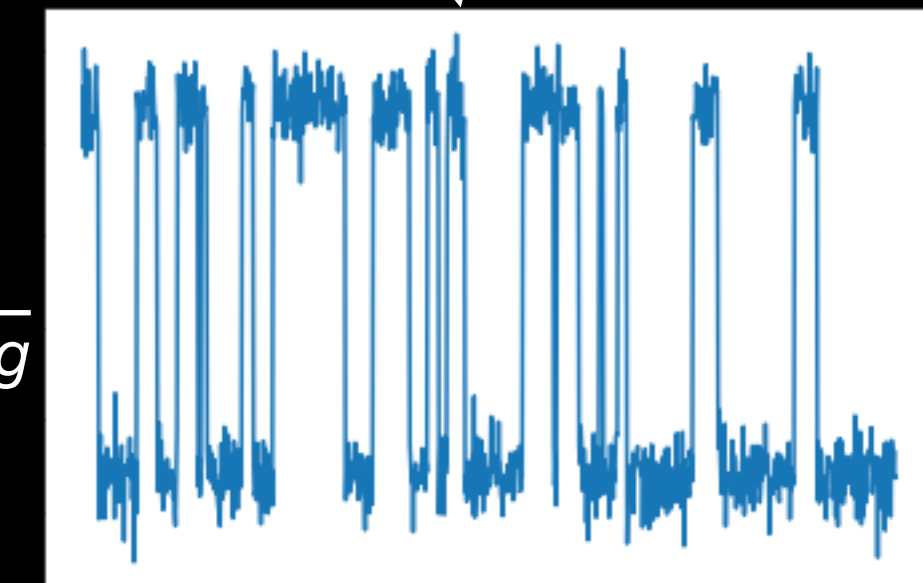


Featurize
(Torsions, distances, angles, ...)
pyemma.coordinates

High-dimensional data



Project onto slow dynamics
deeptime.decomposition



discretize
deeptime.clustering



Markov state model
deeptime.markov

$$P = \begin{pmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{pmatrix}$$