

PCA analysis of molecular simulation

- In a molecular simulation, it could be helpful to visualize
 - the principal components themselves
 - the variance and cumulated variance
 - the projections onto the principal components in one or more dimensions
 - time series
 - histograms
- See [PCA.ipynb](#), which shows PCA analysis for a simulation of ubiquitin

Time-lagged independent component analysis (TICA)

- Like PCA, based on eigenvector and eigenvalues of a matrix
 - autocorrelation instead of covariance matrix
 - isolates slow motions into coordinates
- Often used in Markov state models (MSMs)
- Slow is often but not always functionally relevant