Exercise 10

Markov State Model - Alanine Dipeptide

Deadline: Please, hand in your protocol in pdf format to **saleksic@zedat.fu-berlin.de** by **Thursday, 21st July, 10.15 a.m.**

10.1 Markov State Model - Alanine Dipeptide (100 P)

(a) Generate a single Ramachandran Plot from the ϕ-ψ trajectories of the alanine dipeptide available in Files section, and placed 36x36 grid over the ϕ-ψ space . (10 P)

(b) Discretize ϕ-ψ trajectories by projecting them onto 36x36 grid resulting into 1296 microstates (each microstate has dimensions 10°*10°). Append both microstate trajectories into a list, which will be used for MSM estimation. (20 P)

(c) Calculate the implied time scales (ITS) of the MSM. Present ITS as a plot, and discuss at which times the first two slowest processes occur. (hint: msm.its) (10 P)

(d) Interactively select lag time τ for which MSM should be estimated. (10 P)

(e) Estimate a transition matrix of the MSM (hint: msm.estimate_markov_model). MSM should be computed on the largest connected set with the detailed balance criterion being satisfied. (15 P)

(f) Extract the largest connected set, and the first three right eigenvectors. Are all 1296 microstates contained in the largest connected sets? If no, how many of them are in the largest connected set? (15 P)

(g) In order to visualize the slowest processes reshape extracted right eigenvectors into 36*36 matrices, present them as heat maps, and discuss them by comparing them with the Ramachandran plot previously produced. (20 P)

10.2 Files

Trajectory

```
https://www.dropbox.com/sh/hogphsvfigfo9em/AACmsmED8qcg3Q5NkVsNYIuHa?dl=0
```

PyEMMA

```
http://emma-project.org/latest/
```