Analyzing Collective Variables Using Machine Learning

BSANNPy folder contains python codes for performing Machine Learning to encode the information from the real dynamical variables.

# The following files are included

# driver\_bsann\_reducedim.py -- it contains the functions to test benchmark data:

# myTest1("data/benchmark1/lorenzmapode45.dat",3) -- accepts as input (X,Y,Z) dynamical variables and encodes this information into the output Z

# Z represents reduced dimension space of the Lorenz map system.

# myTest2("data/benchmark2/coords.pdb",3) -- represents the case of the fragment C2 of the protein G generated using Molecular Dynamics Simulations;

# Inputs -- atomic coordinates in PDB format

# Outputs -- encoded variable (one-dimension array) for each amino acid.

# nnclass.py -- python code for performing BSANN optimization

# trainingData\_mdsim.py --- python code for manipulating input molecular dynamics simulations data.

#

# Auxiliary Libraries

# Numpy is needed to run the python codes.