

bhakat_method

October 19, 2018

Table of Contents

```
In [43]: #msmbuilder imports
from msmbuilder.dataset import dataset
from msmbuilder.featurizer import ContactFeaturizer
from msmbuilder.featurizer import DihedralFeaturizer
from msmbuilder.decomposition import tICA
from msmbuilder.cluster import MiniBatchKMeans
from msmbuilder.msm import ContinuousTimeMSM
from msmbuilder.utils import verbose_dump, verbose_load
from msmbuilder.cluster import KCenters

#other imports
import os, glob, shutil
import numpy as np
import mdtraj as md
import pandas as pd
import pickle

#prettier plots
import seaborn as sns
%pylab inline
matplotlib.rcParams['xtick.labelsize'] = 14
matplotlib.rcParams['ytick.labelsize'] = 14
matplotlib.rcParams['font.family'] = "sans-serif"
```

Populating the interactive namespace from numpy and matplotlib

```
In [2]: # some imports
import msmexplorer as msme
import numpy as np
%pylab inline
import seaborn as sns
sns.set_style("whitegrid")
sns.set_context("poster", 1.3)
from msmbuilder.utils import load
```

```
/home/sbhakat/miniconda2/envs/py36/lib/python3.6/site-packages/seaborn/apionly.py:6: UserWarning
warnings.warn(msg, UserWarning)
```

Populating the interactive namespace from numpy and matplotlib

```
In [37]: plot_feat = load("raw_features.pkl")
        train_feat = load("features.pkl")
```

```
In [38]: df = load("feature_descriptor.pkl")
```

```
In [6]: df
```

```
Out[6]:
```

	atominds	featuregroup	featurizer	otherinfo	resids	resnames	\
0	[4, 6, 8, 14]	phi	Dihedral	sin	[0, 1]	[ACE, ALA]	
1	[4, 6, 8, 14]	phi	Dihedral	cos	[0, 1]	[ACE, ALA]	
2	[6, 8, 14, 16]	psi	Dihedral	sin	[1, 2]	[ALA, NME]	
3	[6, 8, 14, 16]	psi	Dihedral	cos	[1, 2]	[ALA, NME]	

	resseqs
0	[1, 2]
1	[1, 2]
2	[2, 3]
3	[2, 3]

```
In [21]: ds = load("traj_list.pkl")
        print("Found %d trajns"%len(ds))
```

Found 2 trajns

```
In [52]: from msmbuilder.io import load_trajns, save_trajns, save_generic
        from msmbuilder.io.sampling import sample_dimension
        from msmbuilder.io import load_trajns, save_generic, preload_top, backup
        from msmbuilder.utils import dump
        %matplotlib inline

        tica_mdl = tICA(lag_time=100,n_components=4, kinetic_mapping=False)
        tica_features = train_feat.fit_transform(tica_mdl, list(train_feat.values()))

        #verbosedump(tica_mdl,"tica_mdl.pkl")
        verbosedump(tica_features,"tica_features.pkl")

        File "<ipython-input-52-d82acb29a618>", line 11
        verbosedump(tica_features,"tica_features.pkl")
        ^
```

SyntaxError: invalid syntax