Programming in Python: Final Project

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I. PROJECT

Write a Python program for reducing data dimensionality. Given the high-dimensional representation of data $\mathbf{X}$, implement a Python class (or function) that preprocesses the data, projects the data onto two- or three-dimensional space, and plots the data in the low-dimensional embedding $\mathbf{Y}$.

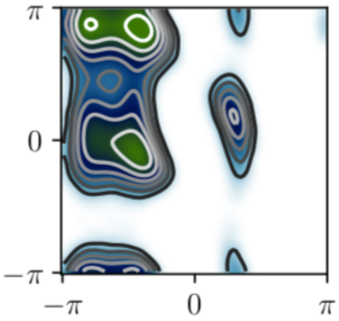
II. WORKFLOW

1. Install `mdshare` and download the high-dimensional data from a public FTP server at Freie Universität Berlin (https://markovmodel.github.io/mdshare/) using:

```
import numpy as np
import mdshare

dataset = mdshare.fetch(’alanine-dipeptide-3x250ns-heavy-atom-distances.npz’)
with np.load(dataset) as f:
  X = np.vstack([f[key] for key in sorted(f.keys())])
```

2. Write a Python program which implements a method called $\mathbf{Y} = \texttt{fit}(\mathbf{X})$ that takes a high-dimensional tensor and returns its projection onto a low-dimensional space.
3. Visualize the low-dimensional embedding using `matplotlib`.
4. Compare your embedding with the following figure:



5. Write a short report summarizing your results.

III. REQUIREMENTS

1. **Tools.** Python 2.7 or 3.*, Jupyter notebook, and Python packages: `numpy, matplotlib, sklearn`.
2. **Command-line Interface.** The package should be able to work in the command-line mode. Use `argparse` to process important flags. For instance:
`./dimred.py -data /path/to/data -parameter_a 1e-5- max_iter=1000 ...`
3. **Documentation.** The code should be documented.
4. **Repository.** Make a git repository `XXX_PPSeminar/` on GitHub; it can be a private or public repository. Each project member must be able to access the repository. It should have the following high-level directory structure:

```
-- doc/
  -- 2020-pp-report/
    -- report.ipynb
    -- report.pdf
-- etc/
  -- 2017-03-25-whitewwq.jpg
  -- 2017-04-03-whiteboard.jpg
  -- 2017-04-06-cow-comments.md
  -- 2017-04-08-jake-comments.pdf
-- src/
  -- checkpoints/
  -- codebase/
  -- log/
  -- out/
  -- script1.py
  -- script2.py
-- README.md
```

5. **Report.** Write a report that explains what is done, how to use the program, and what is the difference between the figure and your projection.

6. **Deadline.** 31 July 2020.