
fit_ensemble Documentation

Release 1.0.0

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FitEnsemble is a software package for modeling conformation ensembles of macromolecules. Using the linear virtual biasing potential (LVBP) formalism [R1], FitEnsemble infers conformational ensembles that best capture a set of experimental measurements.

To construct a conformational ensemble, you will need a “prior” ensemble. This guess should ideally be sampled from the approximate equilibrium of your system. To perform an LVBP calculation, you will need three inputs:

- A set of conformations (from MD simulations, for example)
- A set of experimental measurements and their uncertainties
- Predicted experimental observables for each conformation

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1.1 Installation

1.1.1 Installation

FitEnsemble requires Python 2.7 and the following Python packages:

- Numpy
- Scipy
- PyTables
- PyMC
- Pandas
- NumExpr
- MDTraj

The easiest way to install all prerequisites is using the [Enthought](#) or [Anaconda](#) python distributions. These environments come with all prerequisites except PyMC and MDTraj. In Anaconda, PyMC is available as an additional package and can be installed by typing `conda install pymc`.

FitEnsemble is hosted on GitHub (<https://github.com/kyleabeauchamp/FitEnsemble>). The latest version can be downloaded here: (XXX). After unpacking the source code, you can install FitEnsemble with the following command:

```
python setup.py install
```

1.2 Tutorial

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1.2.1 Accessing the FitEnsemble Tutorials

The FitEnsemble tutorials take the form of a set of IPython notebooks. To view these notebooks, you have two options.

First, you can view them on the web. Viewing on the web allows you to see the results of a completed tutorial, but does *not* allow you to perform the calculations yourself. The tutorials are available here:

- [Tutorial1](#)
- [Tutorial2](#)
- [Tutorial3](#)
- [Tutorial4](#)
- [Tutorial5](#)

Alternatively, you can use IPython to interactively complete the tutorials. This requires you to have successfully installed *FitEnsemble*. After installation, go to the *tutorial* directory in the *FitEnsemble* directory. Then type:

```
ipython notebook --pylab=inline
```

A web browser should open to the IPython Notebook manager. Five tutorials should be listed. You should complete the tutorials in order, as each tutorial extends the previous ones.

Bibliography

- [R1] Beauchamp, K. A., Das, R. , Pande, V. S. Inferring Conformational Ensembles from Noisy Experiments. In preparation.