Python implementation of the multistate Bennett acceptance ratio (MBAR) method for estimating expectations and free energy differences
1.1 Getting started

1.1.1 Dependencies

pymbar requires numpy and scipy. You’ll also need a working C compiler and build environment, to compile various C-level extensions.

**Easy Way (Recommended)**

The easiest way to get all of the dependencies is to install one of the pre-packaged scientific python distributes like Enthought’s Canopy or Continuum’s Anaconda. These distributions already contain all of the dependences, and are distributed via 1-click installers.

**Medium Way**

**Linux**

If you’re on ubuntu and have root, you can install everything through your package manager.

```bash
$ sudo apt-get install python-dev python-numpy python-nose python-setuptools python-scipy
```

**Mac**

If you’re on mac and want a package manager, you should be using homebrew and brew's python (see this page for details). The best way to install numpy and scipy with brew is to use samueljohn’s tap.

```bash
$ brew tap samueljohn/python
$ brew install python
$ brew install numpy
$ brew install scipy
```

**Harder Way : Compiling from source (no root needed)**

If you don’t already have a python installation you want to use, you can compile a new one.
$ wget http://www.python.org/ftp/python/2.7.5/Python-2.7.5.tgz
$ tar -xzvf Python-2.7.5.tgz
$ cd Python-2.7.5
$ ./configure --prefix=$HOME/local/python
$ make
$ make install
$ export PATH=$HOME/local/python/bin:$PATH

If you don’t have easy_install or pip yet, you can get them with

$ wget http://pypi.python.org/packages/source/s/setuptools/setuptools-0.6c11.tar.gz
$ tar -xzvf setuptools-0.6c11.tar.gz
$ cd setuptools-0.6c11.tar.gz
$ python setup.py install
$ easy_install pip

Now you’re home free

$ pip install numpy
$ pip install scipy

1.1.2 Installing pymbar

pymbar currently runs best on Python 2.7.x; earlier versions of Python are not supported. pymbar is developed and tested on mac and linux platforms.

Easy Way (Recommended)

Just run

$ pip install pymbar

Medium Way (Advanced Users Only)

To get the latest unstable version, clone the source code repository from github:

$ git clone git://github.com/choderalab/pymbar.git

Then, in the directory containing the source code, you can install it with.

$ python setup.py install

1.1.3 Running the tests

Running the tests is a great way to verify that everything is working. The test suite uses nose, which you can pick up via pip if you don’t already have it.

$ pip install nose

Then enter the pymbar the source directory and run

$ nosetests
1.2 The mbar module: `pymbar.mbar`

The mbar module contains the MBAR class, the key object in pymbar.

1.3 The timeseries module: `pymbar.timeseries`

The timeseries module contains tools for dealing with timeseries data.

1.4 The testsystems Module: `pymbar.testsystems`

testsystems contains a number of test systems that you can use with pymbar.
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