alchemtest Documentation

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OVERVIEW

alchemtest is a collection of test datasets for alchemical free energy calculations. The datasets come from a variety of software packages, primarily molecular dynamics engines, and are used as the test set for alchemlyb. The package is standalone, however, and can be used for any purpose.

Datasets are released under an open license that conforms to the Open Definition 2.1 that allows free use, re-use, redistribution, modification, separation, for any purpose and without a charge. All data and code can be found in the public GitHub repository alchemistry/alchemtest.

This library is **under active development**. We use semantic versioning to indicate clearly what kind of changes you may expect between releases. Although it is heavily used for the alchemlyb test suite it may contain bugs. Please raise any issues or questions in the Issue Tracker. Contributions of data sets and code in the form of pull requests are very welcome.

CHAPTER

ONE

INSTALLING ALCHEMTEST

alchemtest is pure-Python, so it can be installed easily via `pip`:

```
pip install alchemtest
```

If you wish to install this in your user `site-packages`, use the `--user` flag:

```
pip install --user alchemtest
```

1.1 Installing from source

from source. Clone the source from GitHub with:

```
git clone https://github.com/alchemistry/alchemtest.git
```

then do:

```
cd alchemtest
pip install .
```

If you wish to install this in your user `site-packages`, use the `--user` flag:

```
pip install --user .
```

CHAPTER

TWO

BASIC USAGE

All datasets in `alchemtest` are accessible via `load_*` functions, organized in submodules by the software package that generated them. The current set of submodules are:

gmx	Gromacs molecular dynamics simulation datasets.
amber	Amber molecular dynamics simulation datasets.
namd	NAMD molecular dynamics simulation datasets.

As an example, we can access the *Gromacs: Benzene in water* dataset with:

```
>>> from alchemtest.gmx import load_benzene
>>> bz = load_benzene()
```

and use the resulting *Bunch* object to introspect what this dataset includes. In particular, it features a `DESCR` attribute with a human-readable description of the dataset:

```
>>> print(bz.DESCR)
Gromacs: Benzene in water
=========================

Benzene in water, alchemically turned into benzene in vacuum separated from water

Notes
-----
Data Set Characteristics:
    :Number of Legs: 2 (Coulomb, VDW)
    :Number of Windows: 5 for Coulomb, 16 for VDW
    :Length of Windows: 40ns

    :Missing Values: None
    :Creator: \I. Kenney
    :Donor: Ian Kenney (ian.kenney@asu.edu)
    :Date: March 2017
    :License: `CC0
              <https://creativecommons.org/publicdomain/zero/1.0/>`_
              Public Domain Dedication

This dataset was generated using `MDPOW <https://github.com/Becksteinlab/MDPOW>`_,␣
↪with
the `Gromacs <http://www.gromacs.org/>`_ molecular dynamics engine.
```

as well as the dataset itself:

```
>>>  bz.data.keys()
['VDW', 'Coulomb']
```

which consists in this case of two alchemical legs, each having several files. For this dataset each file happens to correspond to a simulation sampling a particular λ:

```
>>> bz.data['Coulomb']
['/usr/local/python3.6/site-packages/alchemtest/gmx/benzene/Coulomb/0000/dhdl.xvg.bz2
↪',
 '/usr/local/python3.6/site-packages/alchemtest/gmx/benzene/Coulomb/0250/dhdl.xvg.bz2
↪',
 '/usr/local/python3.6/site-packages/alchemtest/gmx/benzene/Coulomb/0500/dhdl.xvg.bz2
↪',
 '/usr/local/python3.6/site-packages/alchemtest/gmx/benzene/Coulomb/0750/dhdl.xvg.bz2
↪',
 '/usr/local/python3.6/site-packages/alchemtest/gmx/benzene/Coulomb/1000/dhdl.xvg.bz2
↪']
```

These paths can be read by any appropriate parser for further analysis. For this particular dataset, see `alchemlyb.parsing.gmx` for a good set of parsers.

CHAPTER

THREE

HELPER FUNCTIONS AND CLASSES

A small number of functions and classes are included to help organize the data.

class alchemtest.**Bunch**(***kwargs*)

Container object for datasets

Dictionary-like object that exposes its keys as attributes.

```
>>> b = Bunch(a=1, b=2)
>>> b['b']
2
>>> b.b
2
>>> b.a = 3
>>> b['a']
3
>>> b.c = 6
>>> b['c']
6
```

Code taken from sklearn/utils/__init__.py version 0.19.1 under the 'New BSD license' https://github.com/scikit-learn/scikit-learn/blob/master/COPYING

CHAPTER

FOUR

GROMACS DATASETS

Gromacs molecular dynamics simulation datasets.

The `alchemlyb.gmx` module features datasets generated using the Gromacs molecular dynamics engine. They can be accessed using the following accessor functions:

load_benzene()	Load the Gromacs benzene dataset.
load_ABFE()	Load the Gromacs ABFE dataset.
load_expanded_ensemble_case_1()	Load the Gromacs Host CB7 Guest C3 expanded ensemble dataset, case 1 (single simulation visits all states).
load_expanded_ensemble_case_2()	Load the Gromacs Host CB7 Guest C3 expanded ensemble dataset, case 2 (two simulations visit all states independently).
load_expanded_ensemble_case_3()	Load the Gromacs Host CB7 Guest C3 REX dataset, case 3.
load_water_particle_with_total_energy()	Load the Gromacs water particle with total energy dataset.
load_water_particle_with_potential_energy()	Load the Gromacs water particle with potential energy dataset.
load_water_particle_without_energy()	Load the Gromacs water particle without energy dataset.

4.1 Simple TI and FEP

The data sets contain derivatives of the Hamiltonian (TI) and free energy perturbation (FEP) data suitable for processing with FEP estimators as well as BAR/MBAR. Individual λ windows were run independently.

4.1.1 Gromacs: Benzene in water

Benzene in water, alchemically turned into benzene in vacuum separated from water

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 5 for Coulomb, 16 for VDW

Length of Windows 40ns

System Size 1668 atoms

Temperature 300 K

Pressure 1 bar

Alchemical Pathway vdw + coul –> vdw –> vacuum

Experimental Hydration Free Energy -0.90 +- 0.2 kcal/mol

Missing Values None

Energy unit kJ/mol

Time unit ps

Creator I. Kenney

Donor Ian Kenney (ian.kenney@asu.edu)

Date March 2017

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This dataset was generated using MDPOW, with the Gromacs molecular dynamics engine.

Experimental value sourced from [Mobley2013].

`alchemtest.gmx.load_benzene()`

Load the Gromacs benzene dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

4.2 Extended ensemble

Data for *extended ensemble* simulations; case 1 and case 2 are extended ensembles in the alchemical parameters, case 3 includes replica exchange (REX).

4.2.1 Gromacs: Host CB7 and Guest C3 in water

Host CB7 and Guest C3 in water, Guest C3 alchemically turned into Guest C3 in vacuum separated from water and Host CB7. This unpublished data uses Host CB7 and Guest C3 from [Muddana2014a]. Similar published data can be found in [Monroe2014a].

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 32 total, 20 for Coulomb, 12 for VDW

Number of Simulations 1

Length of Simulation 100ns

System Size 8286 atoms

Temperature 300 K

Alchemical Pathway vdw + coul –> vdw –> vacuum

Missing Values None

Energy unit kJ/mol

Time unit ps

Creator T. Jensen

Donor Travis Jensen (travis.jensen@colorado.edu)

Date November 2017

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This dataset was generated using the expanded ensemble algorithm in the Gromacs molecular dynamics engine.

`alchemtest.gmx.load_expanded_ensemble_case_1()`

Load the Gromacs Host CB7 Guest C3 expanded ensemble dataset, case 1 (single simulation visits all states).

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

4.2.2 Gromacs: Host CB7 and Guest C3 in water

Host CB7 and Guest C3 in water, Guest C3 alchemically turned into Guest C3 in vacuum separated from water and Host CB7. This unpublished data uses Host CB7 and Guest C3 from [Muddana2014b]. Similar published data can be found in [Monroe2014b].

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 32 total, 20 for Coulomb, 12 for VDW

Number of Simulations 2

Length of Simulation 50ns

System Size 8286 atoms

Temperature 300 K

Alchemical Pathway vdw + coul –> vdw –> vacuum

Missing Values None

Energy unit kJ/mol

Time unit ps

Creator T. Jensen

Donor Travis Jensen (travis.jensen@colorado.edu)

Date November 2017

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This dataset was generated using the expanded ensemble algorithm in the Gromacs molecular dynamics engine.

`alchemtest.gmx.load_expanded_ensemble_case_2()`

Load the Gromacs Host CB7 Guest C3 expanded ensemble dataset, case 2 (two simulations visit all states independently).

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

4.2.3 Gromacs: Host CB7 and Guest C3 in water

Host CB7 and Guest C3 in water, Guest C3 alchemically turned into Guest C3 in vacuum separated from water and Host CB7. This unpublished data uses Host CB7 and Guest C3 from [Muddana2014c].

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 32 total, 20 for Coulomb, 12 for VDW

Number of Simulations 32

Length of Simulation 5ns

System Size 8286 atoms

Temperature 300 K

Alchemical Pathway vdw + coul –> vdw –> vacuum

Missing Values None

Energy unit kJ/mol

Time unit ps

Creator T. Jensen

Donor Travis Jensen (travis.jensen@colorado.edu)

Date November 2017

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This dataset was generated using the REX algorithm in the Gromacs molecular dynamics engine.

`alchemtest.gmx.load_expanded_ensemble_case_3()`
Load the Gromacs Host CB7 Guest C3 REX dataset, case 3.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

4.3 Water particle TI and FEP

3 simple dH/dl and U_nk datasets of a single water particle from a simulations of water between to hydrophilic surfaces. One dataset contains a total energy column, one contains a potential energy column and one does not contain a energy column.

4.3.1 Gromacs: water particle

Free energy estimation of a water particle between to hydrophilic surfaces

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 17 for Coulomb, 20 for VDW

Length of Windows 10ns

System Size 3312 atoms

Temperature 300 K

Ensemble NVT

Volume 70.204 nm^3

Alchemical Pathway vacuum –> vdw –> vdw + coul

Missing Values None

Creator D. Wille

Donor Dominik Wille (harlor@web.de)

Date November 2018

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Similar free energy estimations can be found in:

`alchemtest.gmx.`**`load_water_particle_with_total_energy`**`()`
Load the Gromacs water particle with total energy dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

`alchemtest.gmx.`**`load_water_particle_with_potential_energy`**`()`
Load the Gromacs water particle with potential energy dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

`alchemtest.gmx.`**`load_water_particle_without_energy`**`()`
Load the Gromacs water particle without energy dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

4.4 Absolute Binding Free Energy of n-phenylglycinonitrile to T4 lysozyme

The dataset for computing the absolute binding free energy of n-phenylglycinonitrile to T4 lysozyme. The calculation has two legs: complex and ligand. In the complex leg, restraint is applied to the ligand and the coulombic as well as the Van der Waals interactions are decoupled sequentially. In the ligand leg, only the coulombic and Van der Waals interactions are decoupled.

4.4.1 Gromacs: n-phenylglycinonitrile in T4 lysozyme

Obtain the absolute binding free energy of the n-phenylglycinonitrile for T4 lysozyme by alchemically turning n-phenylglycinonitrile in T4 lysozyme and water into vacuum.

Notes

Data Set Characteristics:

Number of Legs 2 (Restraint, Coulomb, VDW for protein; Coulomb, VDW for water)

Number of Windows 11 for Restraint, 5 for Coulomb, 16 for VDW

Length of Windows 1ns for protein and 5ns for water

System Size 33005 atoms for protein and 2103 atoms for water

Temperature 300 K

Pressure 1 bar

Alchemical Pathway vdw + coul –> restraint + vdw + coul –> restraint + vdw –> restraint + vacuum

Reference Hydration Free Energy in protein -21.721 +- 0.089 kcal/mol

Reference Hydration Free Energy in water -7.679 +- 0.080 kcal/mol

Missing Values None

Energy unit kJ/mol

Time unit ps

Creator Z. Wu

Donor Zhiyi Wu (zhiyi.wu@bioch.ox.ac.uk)

Date March 2021

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This dataset was generated using tutorial , with the Gromacs molecular dynamics engine.

Data sourced from [Boyce2009].

`alchemtest.gmx.load_ABFE()`
Load the Gromacs ABFE dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

CHAPTER

FIVE

AMBER DATASETS

Amber molecular dynamics simulation datasets.

The `alchemlyb.amber` module features datasets generated using the Amber molecular dynamics engine. They can be accessed using the following accessor functions:

load_bace_improper()	Load Amber Bace improper solvated vdw example :returns: **data** – Dictionary-like object, the interesting attributes are:
load_bace_example()	Load Amber Bace example perturbation.
load_simplesolvated()	Load the Amber solvated dataset.
load_invalidfiles()	Load the invalid files.

5.1 Amber: Small molecule thermodynamic integration free energy difference in water

Improper Bace solvated small molecule perturbation, alchemical vdw perturbation of ligand 1 into ligand 2. This example uses ligands CAT-13a to CAT-13m from [Wang2015].

5.1.1 Notes

Data Set Characteristics:

Number of Legs 1 (vdw)

Number of Windows 12

Length of Windows 1ns

System Size 3920 atoms

Temperature 300 K

Pressure 1 bar

Alchemical Pathway vdw in ligand 1 –> vdw in ligand 2, softcore is used in vdw

Experimental Free Energy difference N/A

Missing Values None

Energy unit kcal/mol

Time unit ps

Date Jan 2018

Donor Silicon Therapeutics

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This dataset was generated using the Amber molecular dynamics engine.

`alchemtest.amber.load_bace_improper()`
Load Amber Bace improper solvated vdw example :returns: **data** – Dictionary-like object, the interesting attributes are:

- 'data' : the data files for improper solvated vdw alchemical leg

Return type *Bunch*

5.2 Amber: Small molecule thermodynamic integration free energy difference in water

Bace complex and solvated small molecule perturbation, alchemical perturbation of ligand 1 into ligand 2. This example uses ligands CAT-13d to CAT-17a from [Wang2015].

5.2.1 Notes

Data Set Characteristics:

Number of Legs 3 (decharge, vdw, recharge)

Number of Windows 5 for decharge, 12 for vdw, 5 for recharge

Length of Windows 1ns

System Size 46594 atoms (complex), 4115 atoms (solvated)

Temperature 300 K

Pressure 1 bar

Alchemical Pathway (decharge + vdw + recharge) in ligand 1 –> (decharge + vdw + recharge) in ligand 2, decharge, vdw, and recharge are running in parellel, soft core is used in vdw

Experimental Free Energy difference -0.26 kcal/mol

Missing Values None

Energy unit kcal/mol

Time unit ps

Date Jan 2018

Donor Silicon Therapeutics

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This dataset was generated using the Amber molecular dynamics engine.

`alchemtest.amber.load_bace_example()`
Load Amber Bace example perturbation. :returns: **data** – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by system and alchemical leg

Return type *Bunch*

5.3 Amber: Small molecule thermodynamic integration free energy difference in water

Small molecule perturbation in water, alchemically turned ligand 1 into ligand 2 in water. This example uses ligands 17124-1 to 18637-1 from [Wang2015].

5.3.1 Notes

Data Set Characteristics:

Number of Legs 2 (charge, vdw)

Number of Windows 5 for charge, 12 for vdw

Length of Windows 1ns

System Size 5979 atoms

Temperature 300 K

Pressure 1 bar

Alchemical Pathway (charge + vdw) in ligand 1 –> (charge + vdw) in ligand 2, charge and vdw are running in parellel, soft core is used in vdw

Experimental Free Energy difference N/A

Missing Values None

Energy unit kcal/mol

Time unit ps

Date Oct 2017

Donor Silicon Therapeutics

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This dataset was generated using the Amber molecular dynamics engine.

`alchemtest.amber.load_simplesolvated()`
Load the Amber solvated dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

5.4 Amber TI invalid output files

Examples for file validation testing.

5.4.1 Notes

- invalid-case-1.out.bz2: file contains no useful data
- invalid-case-2.out.bz2: file contains no control data
- invalid-case-3.out.bz2: file with Non-constant temperature
- invalid-case-4.out.bz2: file with no free energy section
- invalid-case-5.out.bz2: file with no ATOMIC section
- invalid-case-6.out.bz2: file with no RESULTS section

`alchemtest.amber.load_invalidfiles()`
Load the invalid files.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the example of invalid data files
- 'DESCR': the full description of the dataset

Return type *Bunch*

CHAPTER

SIX

NAMD DATASETS

NAMD molecular dynamics simulation datasets.

The `alchemlyb.namd` module features datasets generated using the NAMD molecular dynamics engine. They can be accessed using the following accessor functions:

load_tyr2ala()	Load the NAMD tyrosine to alanine mutation dataset.

6.1 NAMD: free energy of tyrosine to alanine mutation in aqueous solution

Free energy change from mutating a tyrosine (Y) residue into alanine (A) in the Ala-Tyr-Ala tripeptide in aqueous environment.

6.1.1 Notes

Data Set Characteristics:

Number of Legs 2 (forward Y–>A, backward A–>Y)

Number of Windows 20 for each leg

Length of Windows 1000 ps (each window interspersed with 200 ps equilibration)

System Size 1521 atoms

Temperature 300 K

Pressure 1 bar

Alchemical Pathway Point mutation of Tyr to Ala using dual topology hybrid molecule. Non-bonded interactions of perturbed atoms are scaled with their environment.

Experimental Free Energy difference N/A

Missing Values None

Energy unit kcal/mol

Time unit step

Date Oct 2017

Donor JC Gumbart

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This dataset was generated using the NAMD molecular dynamics engine.

alchemtest.namd.**load_tyr2ala**()

Load the NAMD tyrosine to alanine mutation dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

CHAPTER

SEVEN

GOMC DATASETS

GOMC Monte Carlo simulation datasets.

The `alchemlyb.gomc` module features datasets generated using the GPU Optimized Monte Carlo (GOMC) simulation engine. They can be accessed using the following accessor functions:

load_benzene()	Load the GOMC benzene dataset.

7.1 Simple TI and FEP

The data sets contain derivatives of the Hamiltonian (TI) and free energy perturbation (FEP) data suitable for processing with FEP estimators as well as BAR/MBAR. Individual λ windows were run independently.

7.1.1 GOMC: Benzene in water

Hydration free energy of benzene using TraPPE-EH model and SPC water model.

Notes

Data Set Characteristics:

Number of Legs 2 (Coulomb, VDW)

Number of Windows 7 for Coulomb, 15 for VDW

Length of Windows 50 million Monte Carlo steps

System Size 1001 molecules

Temperature 298 K

Pressure 1 bar

Alchemical Pathway vacuum –> vdw –> vdw + coul

Experimental Hydration Free Energy -0.90 +- 0.2 kcal/mol

Missing Values None

Energy unit kJ/mol

Time unit Monte Carlo steps

Creator M. Soroush Barhaghi

Donor Mohammad Soroush Barhaghi (m.soroush@wayne.edu)

Date July 2019

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This dataset was generated using GOMC Monte Carlo simulation engine.

Experimental value sourced from [Mobley2013].

alchemtest.gomc.**load_benzene**()

Load the GOMC benzene dataset.

Returns

data – Dictionary-like object, the interesting attributes are:

- 'data' : the data files by alchemical leg
- 'DESCR': the full description of the dataset

Return type *Bunch*

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PYTHON MODULE INDEX

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