
plumitas Documentation

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1.1 API

1.1.1 plumitas.core

`plumitas.core.read_colvar` (*filename='COLVAR', multi=0, unbiased=False*)

Function that takes experimental data and gives us the dependent/independent variables for analysis.

Parameters

- **filename** (*string*) – Name of the COLVAR file to read in.
- **multi** (*int*) – Tells the method to read 1 or more COLVAR files. Default falsy value (0) means read only 1 file.
- **unbiased** (*bool*) – If True, adds a ‘weight’ column of all 1s.

Returns **df** – CVs and bias as columns, time as index.

Return type Pandas DataFrame

`plumitas.core.read_hills` (*filename='HILLS'*)

Function that takes experimental data and gives us the dependent/independent variables for analysis.

Parameters **filename** (*string*) – Name of the COLVAR file to read in.

Returns **df** – CVs and bias as columns, time as index.

Return type Pandas DataFrame

1.1.2 plumitas.analysis

`plumitas.analysis.get_frame_weights` (*df, temp, static_bias=None*)

1.1.3 plumitas.visualization

```
plumitas.visualization.make_2d_free_energy_surface(df, x, y, temp, weight=None,
                                                  bins=20, clim=None, xlim=None,
                                                  ylim=None)
```

Create a 2D FES from a COLVAR file with static 'pb.bias'. This function will be modularized and generalized, but I wanted to include something more exciting than reading colvar/hills files for the first PyPI cut.

Parameters

- **df** (*Pandas DataFrame*) – DataFrame generated from Plumed COLVAR file. This DataFrame must have a column with static 'pb.bias' - most likely generated from *mdrun rerun* - and at two CVs.
- **x** (*string*) – Name of one of the CVs (column name from df).
- **y** (*string*) – Name of one of the CVs (column name from df).
- **bins** (*int*) – Number of bins in each dimension to segment histogram.
- **temp** (*float*) – Temperature of simulation which generated Plumed file.
- **weight** (*str*) – Name of static bias column.
- **clim** (*int*) – Maximum free energy (in kJ/mol) for color bar.
- **xlim** (*tuple/list*) – Limits for x axis in plot (i.e. [x_min, x_max]).
- **ylim** (*tuple/list*) – Limits for y axis in plot (i.e. [y_min, y_max]).

Returns axes

Return type matplotlib.AxesSubplot

```
plumitas.visualization.potential_of_mean_force(df, collective_variables, temp,
                                              weight=None, bins=100, xlim=None,
                                              ylim=None)
```

Create PMF plot for one or several collective variables.

Parameters

- **df** (*Pandas DataFrame*) – DataFrame generated from Plumed COLVAR file. This DataFrame must have a column with static 'pb.bias' - most likely generated from *mdrun rerun* - and at two CVs.
- **collective_variables** (*list*) – List of CVs you'd like to plot. These should be supplied in the form of a list of column names, or an instance of *pd.Index* using *df.columns*
- **temp** (*float*) – Temperature of simulation which generated Plumed file.
- **weight** (*str*) – Name of static bias column.
- **bins** (*int*) – Number of bins in each dimension to segment histogram.
- **xlim** (*tuple/list*) – Limits for x axis in plot (i.e. [x_min, x_max]).
- **ylim** (*tuple/list*) – Limits for y axis in plot (i.e. [y_min, y_max]).

Returns axes

Return type matplotlib.AxesSubplot

1.2 Testing

1.2.1 plumitas.tests

plumitas.tests.test_plumitas

`plumitas.tests.test_plumitas.test_make_2d_free_energy_surface()`

Testing functions to reweight based on COLVAR from biased simulations and generate 2D free energy surface.

`plumitas.tests.test_plumitas.test_potential_of_mean_force()`

Testing functions to reweight based on COLVAR from biased simulations and generate 1D potential of mean force.

`plumitas.tests.test_plumitas.test_read_files()`

Testing function to convert of COLVAR file to pandas DataFrame.

CHAPTER 2

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