
pymcmcstat Documentation

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The *pymcmcstat* package is a Python program for running Markov Chain Monte Carlo (MCMC) simulations. Included in this package is the ability to use different Metropolis based sampling techniques:

- Metropolis-Hastings (MH): Primary sampling method.
- Adaptive-Metropolis (AM): Adapts covariance matrix at specified intervals.
- Delayed-Rejection (DR): Delays rejection by sampling from a narrower distribution. Capable of n -stage delayed rejection.
- Delayed Rejection Adaptive Metropolis (DRAM): DR + AM

The [pymcmcstat homepage](#) contains tutorials for users as well as installation instructions.

Python implementation of MATLAB toolbox “mcmcstat”. This code is designed to replicate the functionality of the MATLAB routines developed and posted here: <http://helios.fmi.fi/~lainema/mcmc/>

The user interface is designed to be as similar to the MATLAB version as possible, but this implementation has taken advantage of certain data structure concepts more amenable to Python.

CHAPTER 1

Installation

This code can be found on the [Github project page](#). It is open source and provided under the MIT license. To install directly from Github,

```
pip install git+https://github.com/prmiles/pymcmcstat.git
```

You can also clone the repository and run `python setup.py install`.

Package is also available on the PyPI distribution site.

```
pip install pymcmcstat
```


CHAPTER 2

Getting Started

- [Tutorial notebooks](#)
- [Documentation](#)

CHAPTER 3

License

MIT

CHAPTER 4

Contributors

See the [GitHub contributor page](#)

5.1 pymcmcstat package

5.1.1 pymcmcstat.MCMC module

Created on Wed Jan 17, 2018

@author: prmiles

Description: This module is intended to be the main class from which to run these Markov Chain Monte Carlo type simulations. The user will create an MCMC object, initialize data, simulation options, model settings and parameters.

class pymcmcstat.MCMC.MCMC (*rngseed=None*)
Markov Chain Monte Carlo (MCMC) simulation object.

This class type is the primary feature of this Python package. All simulations are run through this class type, and for the most part the user will interact with an object of this type. The class initialization provides the option for setting the random seed, which can be very useful for testing the functionality of the code. It was found that setting the random seed at object initialization was the simplest interface.

Args:

- **rngseed** (*float*): Seed for numpy's random number generator.

Attributes:

- *run_simulation()*
- *display_current_mcmc_settings()*
- **data** (*DataStructure*): MCMC data structure.
- **simulation_options** (*SimulationOptions*): MCMC simulation options.
- **model_settings** (*ModelSettings*): MCMC model settings.
- **parameters** (*ModelParameters*): MCMC model parameters.

display_current_mcmc_settings()

Display model settings, simulation options, and current covariance values.

Example display:

```
model settings:
  sos_function = <function test_ssfun at 0x1c13c5d400>
  model_function = None
  sigma2 = [1.]
  N = [100.]
  N0 = [0.]
  S20 = [1.]
  nsos = 1
  nbatch = 1
simulation options:
  nsimu = 5000
  adaptint = 100
  ntry = 2
  method = dram
  printint = 100
  lastadapt = 5000
  drscale = [5. 4. 3.]
  qcov = None
covariance:
  qcov = [[0.01  0.    ]
 [0.    0.0625]]
  R = [[0.1  0.    ]
 [0.    0.25]]
  RDR = [array([[0.1 , 0.   ],
 [0.   , 0.25]]), array([[0.02, 0.   ],
 [0.   , 0.05]])]
  invR = [array([[10.,  0.],
 [ 0.,  4.]]), array([[50.,  0.],
 [ 0., 20.]])]
  last_index_since_adaptation = 0
  covchain = None
```

run_simulation (*use_previous_results=False*)

Run MCMC Simulation

Note: This is the method called by the user to run the simulation. The user must specify a data structure, setup simulation options, and define the model settings and parameters before calling this method.

Args:

- **use_previous_results** (*bool*): Flag to indicate whether simulation is being restarted.

pymcmcstat.MCMC.print_rejection_statistics (*rejected, isimu, iadapt, verbosity*)

Print Rejection Statistics.

Threshold for printing is verbosity greater than or equal to 2. If the rejection counters are as follows:

- *total*: 144
- *in_adaptation_interval*: 92
- *outside_bounds*: 0

Then we would expect the following display at the 200th simulation with an adaptation interval of 100.


```
i:200 (72.0, 92.0, 0.0)
```

Args:

- **isimu** (`int`): Simulation counter
- **iiadapt** (`int`): Adaptation counter
- **verbosity** (`int`): Verbosity of display output.

5.1.2 pymcmcstat.ParallelMCMC module

Created on Tue May 1 15:58:22 2018

@author: prmiles

class pymcmcstat.ParallelMCMC.**ParallelMCMC**
Run Parallel MCMC Simulations.

Attributes:

- `setup_parallel_simulation()`
- `run_parallel_simulation()`
- `display_individual_chain_statistics()`

display_individual_chain_statistics()

Display chain statistics for different chains in parallel simulation.

Example display:

```
*****
Displaying results for chain 0
Files: <parallel_dir>/chain_0

-----
name      :      mean      std    MC_err      tau      geweke
m         :      1.9869    0.1295    0.0107    320.0997    0.9259
b         :      3.0076    0.2489    0.0132    138.1260    0.9413
-----

*****
Displaying results for chain 1
Files: <parallel_dir>/chain_1

-----
name      :      mean      std    MC_err      tau      geweke
m         :      1.8945    0.4324    0.0982   2002.6361    0.3116
b         :      3.2240    1.0484    0.2166   1734.0201    0.4161
-----
```

run_parallel_simulation()

Run MCMC simulations in parallel.

The code is run in parallel by using `Pool`. While running, you can expect a display similar to

```
Processing: <parallel_dir>/chain_1
Processing: <parallel_dir>/chain_0
Processing: <parallel_dir>/chain_2
```

The simulation is complete when you see the run time displayed.

```
Parallel simulation run time: 16.15234899520874 sec
```

setup_parallel_simulation (*mcset*, *initial_values=None*, *num_cores=1*, *num_chain=1*)

Setup simulation to run in parallel.

Settings defined in *mcset* object will be copied into different instances in order to run parallel chains.

Args:

- **mcset** (*MCMC*): Instance of MCMC object with serial simulation setup.
- **initial_values** (*ndarray*): Array of initial parameter values - [num_chain,npar].
- **num_cores** (*int*): Number of cores designated by user.
- **num_chain** (*int*): Number of sampling chains to be generated.

`pymcmcstat.ParallelMCMC.assign_number_of_cores` (*num_cores=1*)

Assign number of cores to use in parallel process

Args:

- **num_cores** (*int*): Number of cores designated by user.

Returns:

- **num_cores** (*int*): Number of cores designated by user or maximum number of cores available on machine.

`pymcmcstat.ParallelMCMC.check_directory` (*directory*)

Check and make sure directory exists

Args:

- **directory** (*str*): Folder/directory path name.

`pymcmcstat.ParallelMCMC.check_initial_values` (*initial_values*, *num_chain*, *npar*, *low_lim*, *upp_lim*)

Check if initial values satisfy requirements.

Args:

- **initial_values** (*ndarray*): Array of initial parameter values - [num_chain,npar].
- **num_chain** (*int*): Number of sampling chains to be generated.
- **npar** (*int*): Number of model parameters.
- **low_lim** (*ndarray*): Lower limits.
- **upp_lim** (*ndarray*): Upper limits.

Returns:

- **initial_values** (*ndarray*): Array of initial parameter values - [num_chain,npar].
- **num_chain** (*int*): Number of sampling chains to be generated.

`pymcmcstat.ParallelMCMC.check_options_output` (*options*)

Check output settings defined in options

Args:

- **options** (*SimulationOptions*): MCMC simulation options.

Returns:

- **options** (*SimulationOptions*): MCMC simulation options with at least binary save flag set to True.

`pymcmcstat.ParallelMCMC.check_shape_of_users_initial_values` (*initial_values*,
num_chain, *npar*)

Check shape of users initial values

Args:

- **initial_values** (*ndarray*): Array of initial parameter values - expect [num_chain,npar]
- **num_chain** (*int*): Number of sampling chains to be generated.
- **npar** (*int*): Number of model parameters.

Returns:

- **num_chain** (*int*): Number of sampling chains to be generated - equal to number of rows in initial values array.
- **initial_values**

`pymcmcstat.ParallelMCMC.check_users_initial_values_wrt_limits` (*initial_values*,
low_lim,
upp_lim)

Check users initial values wrt parameter limits

Args:

- **initial_values** (*ndarray*): Array of initial parameter values - expect [num_chain,npar]
- **low_lim** (*ndarray*): Lower limits.
- **upp_lim** (*ndarray*): Upper limits.

Returns:

- **initial_values** (*ndarray*): Array of initial parameter values - expect [num_chain,npar]

Raises:

- *SystemExit* if initial values are outside parameter bounds.

`pymcmcstat.ParallelMCMC.generate_initial_values` (*num_chain*, *npar*, *low_lim*, *upp_lim*)
Generate initial values by sampling from uniform distribution between limits

Args:

- **num_chain** (*int*): Number of sampling chains to be generated.
- **npar** (*int*): Number of model parameters.
- **low_lim** (*ndarray*): Lower limits.
- **upp_lim** (*ndarray*): Upper limits.

Returns:

- **initial_values** (*ndarray*): Array of initial parameter values - [num_chain,npar]

`pymcmcstat.ParallelMCMC.get_parameter_features` (*parameters*)
Get features of model parameters.

Args:

- **parameters** (*list*): List of MCMC model parameter dictionaries.

Returns:

- `npar` (`int`): Number of model parameters.
- `low_lim` (`ndarray`): Lower limits.
- `upp_lim` (`ndarray`): Upper limits.

`pymcmcstat.ParallelMCMC.run_serial_simulation` (*mcstat*)
Run serial MCMC simulation

Args:

- `mcstat` (`MCMC.MCMC`): MCMC object.

Returns:

- `results` (`dict`): Results dictionary for serial simulation.

`pymcmcstat.ParallelMCMC.unpack_mcmc_set` (*mcset*)
Unpack attributes of MCMC object.

Args:

- `mcset` (`MCMC`): MCMC object.

Returns:

- `data` (`DataStructure`): MCMC data structure.
- `options` (`SimulationOptions`): MCMC simulation options.
- `model` (`ModelSettings`): MCMC model settings.
- `parameters` (`ModelParameters`): MCMC model parameters.

5.1.3 Subpackages

`pymcmcstat.chain` package

`pymcmcstat.chain.ChainProcessing` module

Created on Tue May 1 09:12:06 2018

@author: prmiles

`pymcmcstat.chain.ChainProcessing.print_log_files` (*savedir*)
Print log files to screen.

Args:

- `savedir` (`str`): Directory where log files are saved.

The output display will include a date/time stamp, as well as indices of the chain that were saved during that export sequence.

Example display:

```
-----
Display log file: <savedir>/binlogfile.txt
2018-05-03 14:15:54      0      999
2018-05-03 14:15:54    1000    1999
2018-05-03 14:15:55    2000    2999
2018-05-03 14:15:55    3000    3999
```

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```
2018-05-03 14:15:55      4000      4999
-----
```

`pymcmcstat.chain.ChainProcessing.read_in_bin_file(filename)`

Read in information from file containing binary data.

If file exists, it will read in the array elements. Otherwise, it will return and empty list.

Args:

- **filename** (`str`): Name of file to read.

Returns:

- **out** (`ndarray`): Array of chain elements.

`pymcmcstat.chain.ChainProcessing.read_in_parallel_savedir_files(parallel_dir,`

*extension='h5',
chainfile='chainfile',
sschainfile='sschainfile',
s2chainfile='s2chainfile',
covchainfile='covchainfile')*

Read in log files from directory containing results from parallel MCMC simulation.

Args:

- **parallel_dir** (`str`): Directory where parallel log files are saved.
- **extension** (`str`): Extension of files being loaded.
- **chainfile** (`str`): Name of chain log file.
- **sschainfile** (`str`): Name of sschain log file.
- **s2chainfile** (`str`): Name of s2chain log file.
- **covchainfile** (`str`): Name of covchain log file.

`pymcmcstat.chain.ChainProcessing.read_in_savedir_files(savedir,`

*extension='h5',
chainfile='chainfile', ss-
chainfile='sschainfile',
s2chainfile='s2chainfile',
covchain-
file='covchainfile')*

Read in log files from directory.

Args:

- **savedir** (`str`): Directory where log files are saved.
- **extension** (`str`): Extension of files being loaded.
- **chainfile** (`str`): Name of chain log file.
- **sschainfile** (`str`): Name of sschain log file.
- **s2chainfile** (`str`): Name of s2chain log file.
- **covchainfile** (`str`): Name of covchain log file.

`pymcmcstat.chain.ChainProcessing.read_in_txt_file(filename)`

Read in information from file containing text data.

If file exists, it will read in the array elements. Otherwise, it will return an empty list.

Args:

- **filename** (`str`): Name of file to read.

Returns:

- **out** (`ndarray`): Array of chain elements.

pymcmcstat.chain.ChainStatistics module

Created on Thu Apr 26 10:23:51 2018

@author: prmls

`pymcmcstat.chain.ChainStatistics.batch_mean_standard_deviation(chain, b=None)`

Standard deviation calculated from batch means

Args:

- **chain** (`ndarray`): Sampling chain.
- **b** (`int`): Step size.

Returns:

- **s** (`ndarray`): Batch mean standard deviation.

`pymcmcstat.chain.ChainStatistics.chainstats(chain=None, results=None, returnstats=False)`

Calculate chain statistics.

Args:

- **chain** (`ndarray`): Sampling chain.
- **results** (`dict`): Results from MCMC simulation.
- **returnstats** (`bool`): Flag to return statistics.

Returns:

- **stats** (`dict`): Statistical measures of chain convergence.

`pymcmcstat.chain.ChainStatistics.get_parameter_names(nparam, results)`

Get parameter names from results dictionary.

If no results found, then default names are generated. If some results are found, then an extended set is generated to complete the list requirement. Uses the functions: `generate_default_names()` and `extend_names_to_match_nparam()`

Args:

- **nparam** (`int`): Number of parameter names needed

Returns:

- **names** (`list`): List of length `nparam` with strings.

`pymcmcstat.chain.ChainStatistics.geweke(chain, a=0.1, b=0.5)`

Geweke's MCMC convergence diagnostic

Test for equality of the means of the first `a%` (default 10%) and last `b%` (50%) of a Markov chain - see [brooks1998assessing].

Args:

- **chain** (`ndarray`): Sampling chain.
- **a** (`float`): First `a%` of chain.
- **b** (`float`): Last `b%` of chain.

Returns:

- **z** (`ndarray`): Convergence diagnostic prior to CDF.
- **p** (`ndarray`): Geweke's MCMC convergence diagnostic.

Note: The percentage of the chain should be given as a decimal between zero and one. So, for the first 10% of the chain, define `a = 0.1`. Likewise, for the last 50% of the chain, define `b = 0.5`.

`pymcmcstat.chain.ChainStatistics.integrated_autocorrelation_time(chain)`

Estimates the integrated autocorrelation time using Sokal's adaptive truncated periodogram estimator.

Args:

- **chain** (`ndarray`): Sampling chain.

Returns:

- **tau** (`ndarray`): Autocorrelation time.
- **m** (`ndarray`): Counter.

`pymcmcstat.chain.ChainStatistics.power_spectral_density_using_hanning_window(x, nfft=None, nw=None)`

Power spectral density using Hanning window.

Args:

- **x** (`ndarray`): Array of points - portion of chain.
- **nfft** (`int`): Length of Fourier transform.
- **nw** (`int`): Size of window.

Returns:

- **y** (`ndarray`): Power spectral density.

`pymcmcstat.chain.ChainStatistics.print_chain_statistics(names, meanii, stdii, mcerr, tau, p)`

Print chain statistics to terminal window.

Args:

- **names** (`list`): List of parameter names.
- **meanii** (`list`): Parameter mean values.
- **stdii** (`list`): Parameter standard deviation.
- **mcerr** (`ndarray`): Normalized batch mean standard deviation.

- **tau** (`ndarray`): Integrated autocorrelation time.
- **p** (`ndarray`): Geweke's convergence diagnostic.

Example display:

name	:	mean	std	MC_err	tau	geweke
\$p_{0}\$:	1.9680	0.0319	0.0013	36.3279	0.9979
\$p_{1}\$:	3.0818	0.0803	0.0035	37.1669	0.9961

`pymcmcstat.chain.ChainStatistics.spectral_estimate_for_variance(x)`
Spectral density at frequency zero.

Args:

- **x** (`ndarray`): Array of points - portion of chain.

Returns:

- **s** (`ndarray`): Spectral estimate for variance.

pymcmcstat.plotting package

pymcmcstat.plotting.MCMCPlotting module

Created on Wed Jan 31 12:54:16 2018

@author: prmls

class `pymcmcstat.plotting.MCMCPlotting.Plot`
Plotting routines for analyzing sampling chains from MCMC process.

Attributes:

- `plot_density_panel()`
- `plot_chain_panel()`
- `plot_pairwise_correlation_panel()`
- `plot_histogram_panel()`
- `plot_chain_metrics()`

`pymcmcstat.plotting.MCMCPlotting.plot_chain_metrics(chain, name=None, fig-sizeinches=None)`

Plot chain metrics for individual chain

- Scatter plot of chain
- Histogram of chain

Args:

- **chains** (`ndarray`): Sampling chain for specific parameter
- **names** (`str`): Name of each parameter
- **figsizeinches** (`list`): Specify figure size in inches [Width, Height]

`pymcmcstat.plotting.MCMCPlotting.plot_chain_panel` (*chains*, *names=None*, *fig-sizeinches=None*, *maxpoints=500*)

Plot sampling chain for each parameter

Args:

- **chains** (`ndarray`): Sampling chain for each parameter
- **names** (`list`): List of strings - name of each parameter
- **figsizeinches** (`list`): Specify figure size in inches [Width, Height]
- **maxpoints** (`int`): Max number of display points - keeps scatter plot from becoming overcrowded

`pymcmcstat.plotting.MCMCPlotting.plot_density_panel` (*chains*, *names=None*, *hist_on=False*, *fig-sizeinches=None*)

Plot marginal posterior densities

Args:

- **chains** (`ndarray`): Sampling chain for each parameter
- **names** (`list`): List of strings - name of each parameter
- **hist_on** (`bool`): Flag to include histogram on density plot
- **figsizeinches** (`list`): Specify figure size in inches [Width, Height]

`pymcmcstat.plotting.MCMCPlotting.plot_histogram_panel` (*chains*, *names=None*, *fig-sizeinches=None*)

Plot histogram from each parameter's sampling history

Args:

- **chains** (`ndarray`): Sampling chain for each parameter
- **names** (`list`): List of strings - name of each parameter
- **hist_on** (`bool`): Flag to include histogram on density plot
- **figsizeinches** (`list`): Specify figure size in inches [Width, Height]

`pymcmcstat.plotting.MCMCPlotting.plot_pairwise_correlation_panel` (*chains*, *names=None*, *fig-sizeinches=None*, *skip=1*)

Plot pairwise correlation for each parameter

Args:

- **chains** (`ndarray`): Sampling chain for each parameter
- **names** (`list`): List of strings - name of each parameter
- **figsizeinches** (`list`): Specify figure size in inches [Width, Height]
- **skip** (`int`): Indicates step size to be used when plotting elements from the chain

pymcmcstat.plotting.PredictionIntervals module

Created on Wed Nov 8 12:00:11 2017

@author: prmiles

class pymcmcstat.plotting.PredictionIntervals.**PredictionIntervals**

Prediction/Credible interval methods.

Attributes:

- `setup_prediction_interval_calculation()`
- `generate_prediction_intervals()`
- `plot_prediction_intervals()`

generate_prediction_intervals (*sstype=None, nsample=500, calc_pred_int=True, waitbar=False*)

Generate prediction/credible interval.

Args:

- **sstype** (*int*): Sum-of-squares type
- **nsample** (*int*): Number of samples to use in generating intervals.
- **calc_pred_int** (*bool*): Flag to turn on prediction interval calculation.
- **waitbar** (*bool*): Flag to turn on progress bar.

plot_prediction_intervals (*plot_pred_int=True, adddata=False, addlegend=True, figsizeinches=None, model_display={}, data_display={}, interval_display={}*)

Plot prediction/credible intervals.

Args:

- **plot_pred_int** (*bool*): Flag to include PI on plot.
- **adddata** (*bool*): Flag to include data on plot.
- **addlegend** (*bool*): Flag to include legend on plot.
- **figsizeinches** (*list*): Specify figure size in inches [Width, Height].
- **model_display** (*dict*): Model display settings.
- **data_display** (*dict*): Data display settings.
- **interval_display** (*dict*): Interval display settings.

Available display options (defaults in parantheses):

- **model_display**: *linestyle ('-'), marker ('r'), color ('r'), linewidth (2), markersize (5), label (model), alpha (1.0)*
- **data_display**: *linestyle (' '), marker ('. '), color ('b'), linewidth (1), markersize (5), label (data), alpha (1.0)*
- **data_display**: *linestyle (': '), linewidth (1), alpha (1.0), edgecolor ('k')*

setup_prediction_interval_calculation (*results, data, modelfunction, burnin=0*)

Setup calculation for prediction interval generation

Args:

- **results** (*ResultsStructure*): MCMC results structure
- **data** (*DataStructure*): MCMC data structure
- **modelfunction**: Model function handle

pymcmcstat.plotting.utilities module

Created on Mon May 14 06:24:12 2018

@author: prmls

`pymcmcstat.plotting.utilities.append_to_nrow_ncol_based_on_shape` (*sh*, *nrow*,
ncol)

Append to list based on shape of array

Args:

- **sh** (`tuple`): Shape of array.
- **nrow** (`list`): List of number of rows
- **ncol** (`list`): List of number of columns

Returns:

- **nrow** (`list`): List of number of rows
- **ncol** (`list`): List of number of columns

`pymcmcstat.plotting.utilities.check_defaults` (*kwargs*, *defaults*)

Check if defaults are defined in kwargs

Args:

- **kwargs** (`dict`): Keyword arguments.
- **defaults** (`dict`): Default settings.

Returns:

- **kwargs** (`dict`): Updated keyword arguments with at least defaults set.

`pymcmcstat.plotting.utilities.check_symmetric` (*a*, *tol=1e-08*)

Check if array is symmetric by comparing with transpose.

Args:

- **a** (`ndarray`): Array to test.
- **tol** (`float`): Tolerance for testing equality.

Returns:

- (`bool`): True -> symmetric, False -> not symmetric.

`pymcmcstat.plotting.utilities.convert_flag_to_boolean` (*flag*)

Convert flag to boolean for backwards compatibility.

Args:

- **flag** (`bool` or `int`): Flag to specify something.

Returns:

- **flag** (`bool`): Flag to converted to boolean.

`pymcmcstat.plotting.utilities.empirical_quantiles` (*x*, *p=array([0.25, 0.5, 0.75])*)

Calculate empirical quantiles.

Args:

- **x** (`ndarray`): Observations from which to generate quantile.
- **p** (`ndarray`): Quantile limits.

Returns:

- (`ndarray`): Interpolated quantiles.

`pymcmcstat.plotting.utilities.extend_names_to_match_nparam` (*names*, *nparam*)

Append names to list using default convention until length of names matches number of parameters.

For example, if *names* = [`'name_1'`, `'name_2'`] and *nparam* = 4, then two additional names will be appended to the *names* list. E.g.,:

```
names = ['name_1', 'name_2', 'p_{2}', 'p_{3}']
```

Args:

- **names** (`list`): Names of parameters provided by user
- **nparam** (`int`): Number of parameter names to generate

Returns:

- **names** (`list`): List of strings - extended list of parameter names

`pymcmcstat.plotting.utilities.gaussian_density_function` (*x*, *mu*=0, *sigma*2=1)

Standard normal/Gaussian density function.

Args:

- **x** (`float`): Value of which to calculate probability.
- **mu** (`float`): Mean of Gaussian distribution.
- **sigma2** (`float`): Variance of Gaussian distribution.

Returns:

- **y** (`float`): Likelihood of *x*.

`pymcmcstat.plotting.utilities.generate_default_names` (*nparam*)

Generate generic parameter name set.

For example, if *nparam* = 4, then the generated names are:

```
names = ['p_{0}', 'p_{1}', 'p_{2}', 'p_{3}']
```

Args:

- **nparam** (`int`): Number of parameter names to generate

Returns:

- **names** (`list`): List of strings - parameter names

`pymcmcstat.plotting.utilities.generate_ellipse` (*mu*, *cmat*, *ndp*=100)

Generates points for a probability contour ellipse

Args:

- **mu** (`ndarray`): Mean values
- **cmat** (`ndarray`): Covariance matrix
- **ndp** (`int`): Number of points to generate

Returns:

- `x` (`ndarray`): x-points
- `y` (`ndarray`): y-points

`pymcmcstat.plotting.utilities.generate_names(nparam, names)`

Generate parameter name set.

For example, if `nparam = 4`, then the generated names are:

```
names = ['p_{0}', 'p_{1}', 'p_{2}', 'p_{3}']
```

Args:

- `nparam` (`int`): Number of parameter names to generate
- `names` (`list`): Names of parameters provided by user

Returns:

- `names` (`list`): List of strings - parameter names

`pymcmcstat.plotting.utilities.generate_subplot_grid(nparam=2)`

Generate subplot grid.

For example, if `nparam = 2`, then the subplot will have 2 rows and 1 column.

Args:

- `nparam` (`int`): Number of parameters

Returns:

- `ns1` (`int`): Number of rows in subplot
- `ns2` (`int`): Number of columns in subplot

`pymcmcstat.plotting.utilities.iqrangle(x)`

Interquantile range of each column of `x`.

Args:

- `x` (`ndarray`): Array of points.

Returns:

- (`ndarray`): Interquantile range - single element array, $q3 - q1$.

`pymcmcstat.plotting.utilities.is_semi_pos_def_chol(x)`

Check if matrix is semi positive definite by calculating Cholesky decomposition.

Args:

- `x` (`ndarray`): Matrix to check

Returns:

- If matrix is *not* semi positive definite return `False`, `None`
- If matrix is semi positive definite return `True` and the Upper triangular form of the Cholesky decomposition matrix.

`pymcmcstat.plotting.utilities.make_x_grid(x, npts=100)`

Generate x grid based on extrema.

1. If `len(x) > 200`, then generates grid based on difference between the max and min values in the array.
2. Otherwise, the grid is defined with respect to the array mean plus or minus four standard deviations.

Args:

- `x` (`ndarray`): Array of points
- `npts` (`int`): Number of points to use in generated grid

Returns:

- Uniformly spaced array of points with shape = `(npts, 1)`. (`ndarray`)

`pymcmcstat.plotting.utilities.scale_bandwidth(x)`
Scale bandwidth of array.

Args:

- `x` (`ndarray`): Array of points - column of chain.

Returns:

- `s` (`ndarray`): Scaled bandwidth - single element array.

`pymcmcstat.plotting.utilities.set_local_parameters(ii, local)`
Set local parameters based on tests.

Test 1

- `local == 0`

Test 2

- `local == ii`

Args:

- `ii` (`int`): Index.
- `local` (`ndarray`): Local flags.

Returns:

- `test` (`ndarray`): Array of Booleans indicated test results.

`pymcmcstat.plotting.utilities.setup_plot_features(nparam, names, figsizeinches)`
Setup plot features.

Args:

- `nparam` (`int`): Number of parameters
- `names` (`list`): Names of parameters provided by user
- `figsizeinches` (`list`): [Width, Height]

Returns:

- `ns1` (`int`): Number of rows in subplot
- `ns2` (`int`): Number of columns in subplot
- `names` (`list`): List of strings - parameter names
- `figsizeiches` (`list`): [Width, Height]

pymcmcstat.procedures package

pymcmcstat.procedures.CovarianceProcedures module

Created on Thu Jan 18 07:55:46 2018

Description: Support methods for initializing and updating the covariance matrix. Additional routines associated with Cholesky Decomposition.

@author: prmiles

class pymcmcstat.procedures.CovarianceProcedures.**CovarianceProcedures**
Covariance matrix variables and methods.

Attributes:

- `display_covariance_settings()`
- `setup_covariance_matrix()`

display_covariance_settings (*print_these=None*)
Display subset of the covariance settings.

Args:

- **print_these** (*list*): List of strings corresponding to keywords. Default below.

```
print_these = ['qcov', 'R', 'RDR', 'invR', 'last_index_since_adaptation',
               ↪ 'covchain']
```

setup_covariance_matrix (*qcov, thetasig, value*)
Initialize covariance matrix.

If no proposal covariance matrix is provided, then the default is generated by squaring 5% of the initial value. This yields a diagonal covariance matrix.

$$V = \text{diag}([(0.05\theta_i)^2])$$

If the initial value was one, this would lead to zero variance. In those instances the variance is set equal to `qcov[qcov==0] = 1.0`.

Args:

- **qcov** (*ndarray*): Parameter covariance matrix.
- **thetasig** (*ndarray*): Prior variance.
- **value** (*ndarray*): Current parameter value.

pymcmcstat.procedures.ErrorVarianceEstimator module

Created on Thu Jan 18 13:12:50 2018

@author: prmiles

class pymcmcstat.procedures.ErrorVarianceEstimator.**ErrorVarianceEstimator**
Estimate observation errors.

Attributes:

- `update_error_variance()`
- `gamma`

- `gamma_mt()`

gamma(*m*, *n*, *a*, *b*=1)

Random deviates from gamma distribution.

Returns a m x n matrix of random deviates from the Gamma distribution with shape parameter A and scale parameter B:

$$p(x|A, B) = \frac{B^{-A}}{\Gamma(A)} * x^{A-1} * \exp(-x/B)$$

Args:

- **m** (`int`): Number of rows in return
- **n** (`int`): Number of columns in return
- **a** (`float`): Shape parameter
- **b** (`float`): Scaling parameter

gamma_mt(*m*, *n*, *a*, *b*=1)

Wrapper routine for calculating random deviates from gamma distribution using method of Marsaglia and Tsang (2000) [marsaglia2000simple].

Args:

- **m** (`int`): Number of rows in return
- **n** (`int`): Number of columns in return
- **a** (`float`): Shape parameter
- **b** (`float`): Scaling parameter

update_error_variance(*sos*, *model*)

Update observation error variance.

Strategy: Treat error variance σ^2 as parameter to be sampled.

Definition: The property that the prior and posterior distributions have the same parametric form is termed conjugacy.

Starting from the likelihood function, it can be shown

$$\sigma^2 | (\nu, q) \sim \text{Inv-Gamma} \left(\frac{N_s + N}{2}, \frac{N_s \sigma_s^2 + SS_q}{2} \right)$$

where N_s and σ_s^2 are shape and scaling parameters, N is the number of observations, and SS_q is the sum-of-squares error.

Note: The variables N_s and σ_s^2 correspond to N0 and S20 in the `ModelSettings` class, respectively.

Args:

- **sos** (`ndarray`): Return argument from evaluation of sum-of-squares function.
- **model** (`ModelSettings`): MCMC model settings.

pymcmcstat.procedures.PriorFunction module

Created on Thu Jan 18 09:10:21 2018

Description: Prior function

@author: prmls

class pymcmcstat.procedures.PriorFunction.**PriorFunction** (*priorfun=None, mu=None, sigma=None*)

Prior distribution functions.

Attributes:

- `default_priorfun()`
- `evaluate_prior()`

classmethod `default_priorfun(theta, mu, sigma)`

Default prior function.

$$\pi_0(q) = \sum_{i=1}^N \left(\frac{\theta_i - \mu_i}{\sigma_i^2} \right)^2$$

Args:

- **theta** (`ndarray`): Current parameter values.
- **mu** (`ndarray`): Prior mean.
- **sigma** (`ndarray`): Prior standard deviation.

evaluate_prior(theta)

Evaluate the prior function.

Args:

- **theta** (`ndarray`): Current parameter values.

pymcmcstat.procedures.SumOfSquares module

Created on Wed Jan 17 16:21:48 2018

@author: prmls

class pymcmcstat.procedures.SumOfSquares.**SumOfSquares** (*model, data, parameters*)

Sum-of-squares function evaluation.

Description: Sum-of-squares (sos) class intended for used in MCMC simulator. Each instance will contain the sos function. If the user did not specify a sos-function, then the user supplied model function will be used in the default mcmc sos-function.

Attributes:

- `evaluate_sos_function()`
- `mcmc_sos_function()`

evaluate_sos_function(theta)

Evaluate sum-of-squares function.

Args:

- **theta** (`ndarray`): Parameter values.

Returns:

- `ss` (`ndarray`): Sum-of-squares error(s)

classmethod `mcmc_sos_function` (*theta*, *data*, *nbatch*, *model_function*)

Default sum-of-squares function.

Note: This method requires specifying a model function instead of a sum of squares function. Not recommended for most applications.

Basic formulation:

$$SS_{q,i} = \sum [w_i (y_i^{data} - y_i^{model})^2]$$

where w_i is the weight of a particular data set, and $SS_{q,i}$ is the sum-of-squares error for the i -th data set.

Args:

- **theta** (`ndarray`): Parameter values.

Returns:

- `ss` (`ndarray`): Sum-of-squares error(s)

pymcmcstat.samplers package

pymcmcstat.samplers.Adaptation module

Created on Thu Jan 18 11:14:11 2018

@author: prmiles

class `pymcmcstat.samplers.Adaptation.Adaptation`

Adaptive Metropolis (AM) algorithm based on [haario2001adaptive].

Attributes:

- `run_adaptation()`

run_adaptation (*covariance*, *options*, *isimu*, *iiadapt*, *rejected*, *chain*, *chainind*, *u*, *npar*, *alpha*)

Run adaptation step

Args:

- **covariance** (`CovarianceProcedures`): Covariance methods and variables
- **options** (`SimulationOptions`): Options for MCMC simulation
- **isimu** (`int`): Simulation counter
- **iiadapt** (`int`): Adaptation counter
- **rejected** (`dict`): Rejection counter
- **chain** (`ndarray`): Sampling chain
- **chainind** (`ind`): Relative point in chain
- **u** (`ndarray`): Latest random sample points
- **npar** (`int`): Number of parameters being sampled
- **alpha** (`float`): Latest Likelihood evaluation

Returns:

- **covariance** (*CovarianceProcedures*): Updated covariance object

`pymcmcstat.samplers.Adaptation.adjust_cov_matrix` (*upcov*, *R*, *npar*, *qcov_adjust*,
qcov_scale, *rejected*, *iiadapt*,
verbosity)

Adjust covariance matrix if found to be singular.

Args:

- **upcov** (*ndarray*): Parameter covariance matrix.
- **R** (*ndarray*): Cholesky decomposition of covariance matrix.
- **npar** (*int*): Number of parameters.
- **qcov_adjust** (*float*): Covariance adjustment factor.
- **qcov_scale** (*float*): Scale parameter
- **rejected** (*dict*): Rejection counters.
- **iiadapt** (*int*): Adaptation counter.
- **verbosity** (*int*): Verbosity of display output.

Returns:

- **R** (*ndarray*): Cholesky decomposition of covariance matrix.

`pymcmcstat.samplers.Adaptation.below_burnin_threshold` (*rejected*, *iiadapt*, *R*,
burnin_scale, *verbosity*)

Update Cholesky Matrix using below burnin thershold

Args:

- **rejected** (*dict*): Rejection counters.
- **iiadapt** (*int*): Adaptation counter
- **R** (*ndarray*): Cholesky decomposition of covariance matrix.
- **burnin_scale** (*float*): Scale for burnin.
- **verbosity** (*int*): Verbosity of display output.

Returns:

- **R** (*ndarray*): Scaled Cholesky matrix.

`pymcmcstat.samplers.Adaptation.check_for_singular_cov_matrix` (*upcov*, *R*, *npar*,
qcov_adjust,
qcov_scale, *re-*
jected, *iiadapt*,
verbosity)

Check if singular covariance matrix

Args:

- **upcov** (*ndarray*): Parameter covariance matrix.
- **R** (*ndarray*): Cholesky decomposition of covariance matrix.
- **npar** (*int*): Number of parameters.
- **qcov_adjust** (*float*): Covariance adjustment factor.
- **qcov_scale** (*float*): Scale parameter

- **rejected** (`dict`): Rejection counters.
- **iiadapt** (`int`): Adaptation counter.
- **verbosity** (`int`): Verbosity of display output.

Returns:

- **R** (`ndarray`): Adjusted Cholesky decomposition of covariance matrix.

`pymcmcstat.samplers.Adaptation.cholupdate` (*R*, *x*)
Update Cholesky decomposition

Args:

- **R** (`ndarray`): Weighted Cholesky decomposition
- **x** (`ndarray`): Weighted sum based on local chain update

Returns:

- **R1** (`ndarray`): Updated Cholesky decomposition

`pymcmcstat.samplers.Adaptation.initialize_covariance_mean_sum` (*x*, *w*)
Initialize covariance chain, local mean, local sum

Args:

- **x** (`ndarray`): Chain segment
- **w** (`ndarray`): Weights

Returns:

- **xcov** (`ndarray`): Initial covariance matrix
- **xmean** (`ndarray`): Initial mean chain values
- **wsum** (`ndarray`): Initial weighted sum

`pymcmcstat.samplers.Adaptation.is_semi_pos_def_chol` (*x*)
Check if matrix is semi-positive definite using Cholesky Decomposition

Args:

- **x** (`ndarray`): Covariance matrix

Returns:

- *Boolean*
- **c** (`ndarray`): Cholesky decomposition (upper triangular form) or *None*

`pymcmcstat.samplers.Adaptation.scale_cholesky_decomposition` (*Ra*, *qcov_scale*)
Scale Cholesky decomposition

Args:

- **R** (`ndarray`): Cholesky decomposition of covariance matrix.
- **qcov_scale** (`float`): Scale factor

Returns:

- **R** (`ndarray`): Scaled Cholesky decomposition of covariance matrix.

`pymcmcstat.samplers.Adaptation.setup_cholupdate` (*R*, *oldwsum*, *wsum*, *oldmean*, *xi*)
Setup input arguments to the Cholesky update function

Args:

- **R** (`ndarray`): Previous Cholesky decomposition matrix
- **oldwsum** (`ndarray`): Previous weighted sum
- **w** (`ndarray`): Current Weights
- **oldmean** (`ndarray`): Previous mean chain values
- **xi** (`ndarray`): Row of chain segment

Returns:

- **Rin** (`ndarray`): Scaled Cholesky decomposition matrix
- **xin** (`ndarray`): Updated mean chain values for Cholesky function

`pymcmcstat.samplers.Adaptation.setup_w_R(w, oldR, n)`
Setup weights and Cholesky matrix

Args:

- **x** (`ndarray`): Chain segment
- **w** (`ndarray`): Weights
- **oldcov** (`ndarray` or `None`): Previous covariance matrix
- **oldmean** (`ndarray`): Previous mean chain values
- **oldwsum** (`ndarray`): Previous weighted sum
- **oldR** (`ndarray`): Previous Cholesky decomposition matrix

Returns:

- **w** (`ndarray`): Weights
- **R** (`ndarray`): Previous Cholesky decomposition matrix

`pymcmcstat.samplers.Adaptation.unpack_covariance_settings(covariance)`
Unpack covariance settings

Args:

- **covariance** (`CovarianceProcedures`): Covariance methods and variables

Returns:

- **last_index_since_adaptation** (`int`): Last index since adaptation occurred.
- **R** (`ndarray`): Cholesky decomposition of covariance matrix.
- **oldcovchain** (`ndarray`): Covariance matrix history.
- **oldmeanchain** (`ndarray`): Current mean chain values.
- **oldwsum** (`ndarray`): Weights
- **no_adapt_index** (`numpy.ndarray`): Indices of parameters not being adapted.
- **qcov_scale** (`float`): Scale parameter
- **qcov** (`ndarray`): Covariance matrix

`pymcmcstat.samplers.Adaptation.unpack_simulation_options(options)`
Unpack simulation options

Args:

- **options** (`SimulationOptions`): Options for MCMC simulation

Returns:

- **burnintime** (`int`):
- **burnin_scale** (`float`): Scale for burnin.
- **ntry** (`int`): Number of tries to take before rejection. Default is method dependent.
- **drscale** (`ndarray`): Reduced scale for sampling in DR algorithm. Default is [5,4,3].
- **alphatarget** (`float`): Acceptance ratio target.
- **etaparam** (`float`):
- **qcov_adjust** (`float`): Adjustment scale for covariance matrix.
- **doram** (`int`): Flag to perform 'ram' algorithm (Obsolete).
- **verbosity** (`int`): Verbosity of display output.

`pymcmcstat.samplers.Adaptation.update_cov_from_covchain` (*covchain*, *qcov*,
no_adapt_index)

Update covariance matrix from covariance matrix chain

Args:

- **covchain** (`ndarray`): Covariance matrix history.
- **qcov** (`ndarray`): Parameter covariance matrix
- **no_adapt_index** (`numpy.ndarray`): Indices of parameters not being adapted.

Returns:

- **upcov** (`ndarray`): Updated covariance matrix

`pymcmcstat.samplers.Adaptation.update_cov_via_ram` (*u*, *isimu*, *etaparam*, *npar*, *alphatar-*
get, *alpha*, *R*)

Update covariance matrix via RAM

Args:

- **u** (`ndarray`): Latest random sample points
- **isimu** (`int`): Simulation counter
- **alphatarget** (`float`): Acceptance ratio target.
- **npar** (`int`): Number of parameters.
- **etaparam** (`float`):
- **alpha** (`float`): Latest Likelihood evaluation
- **R** (`ndarray`): Cholesky decomposition of covariance matrix.

Returns:

- **upcov** (`ndarray`): Updated parameter covariance matrix.

`pymcmcstat.samplers.Adaptation.update_covariance_mean_sum` (*x*, *w*, *oldcov*, *oldmean*,
oldwsum, *oldR=None*)

Update covariance chain, local mean, local sum

Args:

- **x** (`ndarray`): Chain segment
- **w** (`ndarray`): Weights

- **oldcov** (`ndarray` or `None`): Previous covariance matrix
- **oldmean** (`ndarray`): Previous mean chain values
- **oldwsum** (`ndarray`): Previous weighted sum
- **oldR** (`ndarray`): Previous Cholesky decomposition matrix

Returns:

- **xcov** (`ndarray`): Updated covariance matrix
- **xmean** (`ndarray`): Updated mean chain values
- **wsum** (`ndarray`): Updated weighted sum

`pymcmcstat.samplers.Adaptation.update_delayed_rejection(R, npar, ntry, drscale)`

Update Cholesky/Inverse matrix for Delayed Rejection

Args:

- **R** (`ndarray`): Cholesky decomposition of covariance matrix.
- **npar** (`int`): Number of parameters.
- **ntry** (`int`): Number of tries to take before rejection. Default is method dependent.
- **drscale** (`ndarray`): Reduced scale for sampling in DR algorithm. Default is [5,4,3].

Returns:

- **RDR** (`list`): List of Cholesky decomposition of covariance matrices for each stage of DR.
- **InvR** (`list`): List of Inverse Cholesky decomposition of covariance matrices for each stage of DR.

pymcmcstat.samplers.DelayedRejection module

Created on Thu Jan 18 10:42:07 2018

@author: prmls

class `pymcmcstat.samplers.DelayedRejection.DelayedRejection`

Delayed Rejection (DR) algorithm based on [haario2006dram].

Attributes:

- `run_delayed_rejection()`
- `initialize_next_metropolis_step()`
- `alphafun()`

alphafun (`trypath`, `invR`)

Calculate likelihood according to DR

Args:

- **trypath** (`list`): Sequence of DR steps
- **invR** (`ndarray`): Inverse Cholesky decomposition matrix

Returns:

- **alpha** (`float`): Result of likelihood function according to delayed rejection

classmethod `initialize_next_metropolis_step` (`npar`, `old_theta`, `sigma2`, `RDR`)

Take metropolis step according to DR

Args:

- **npar** (`int`): Number of parameters
- **old_theta** (`ndarray`): q^{k-1}
- **sigma2** (`float`): Observation error variance
- **RDR** (`ndarray`): Cholesky decomposition of parameter covariance matrix for DR steps
- **itry** (`int`): DR step counter

Returns:

- **next_set** (`ParameterSet`): New proposal set
- **u** (`numpy.ndarray`): Numbers sampled from standard normal distributions (`u.shape = (1, npar)`)

run_delayed_rejection (`old_set`, `new_set`, `RDR`, `ntry`, `parameters`, `invR`, `sosobj`, `priorobj`)

Perform delayed rejection step - occurs in standard metropolis is not accepted.

Args:

- **old_set** (`ParameterSet`): Features of q^{k-1}
- **new_set** (`ParameterSet`): Features of q^*
- **RDR** (`ndarray`): Cholesky decomposition of parameter covariance matrix for DR steps
- **ntry** (`int`): Number of DR steps to perform until rejection
- **parameters** (`ModelParameters`): Model parameters
- **invR** (`ndarray`): Inverse Cholesky decomposition matrix
- **sosobj** (`SumOfSquares`): Sum-of-Squares function
- **priorobj** (`PriorFunction`): Prior function

Returns:

- **accept** (`int`): 0 - reject, 1 - accept
- **out_set** (`ParameterSet`): If `accept == 1`, then latest DR set; Else, $q^k = q^{k-1}$
- **outbound** (`int`): 1 - rejected due to sampling outside of parameter bounds

`pymcmcstat.samplers.DelayedRejection.extract_state_elements` (`iq`, `stage`, `trypath`)

Extract elements from tried paths.

Args:

- **iq** (`int`): Stage number.
- **stage** (`int`): Number of stages - 2
- **trypath** (`list`): Sequence of DR steps

`pymcmcstat.samplers.DelayedRejection.log_posterior_ratio` (`x1`, `x2`)

Calculate the logarithm of the posterior ratio.

Args:

- **x1** (`ParameterSet`): Old set - q^{k-1}
- **x2** (`ParameterSet`): New set - q^*

Returns:

- **zq** (`float`): Logarithm of posterior ratio.

`pymcmcstat.samplers.DelayedRejection.nth_stage_log_proposal_ratio` (*iq*, *trypath*,
invR)

Gaussian nth stage log proposal ratio.

Logarithm of $q_i(y_n, \dots, y_{n-j})/q_i(x, y_1, \dots, y_j)$

Args:

- **iq** (`int`): Stage number.
- **trypath** (`list`): Sequence of DR steps
- **invR** (`ndarray`): Inverse Cholesky decomposition matrix

Returns:

- **zq** (`float`): Logarithm of Gaussian nth stage proposal ratio.

`pymcmcstat.samplers.DelayedRejection.update_set_based_on_acceptance` (*accept*,
old_set,
next_set)

Define output set based on acceptance

If $u_\alpha < \alpha$,
Set $q^k = q^*$, $SS_{q^k} = SS_{q^*}$
Else
Set $q^k = q^{k-1}$, $SS_{q^k} = SS_{q^{k-1}}$

Args:

- **accept** (`int`): 0 - reject, 1 - accept
- **old_set** (`ParameterSet`): Features of q^{k-1}
- **next_set** (`ParameterSet`): New proposal set

Returns:

- **out_set** (`ParameterSet`): If `accept == 1`, then latest DR set; Else, $q^k = q^{k-1}$

pymcmcstat.samplers.Metropolis module

Created on Thu Jan 18 10:30:29 2018

@author: prmls

class `pymcmcstat.samplers.Metropolis.Metropolis`

Pseudo-Algorithm:

1. Sample $z_k \sim N(0, 1)$
2. Construct candidate $q^* = q^{k-1} + Rz_k$
3. Compute $SS_{q^*} = \sum_{i=1}^N [v_i - f_i(q^*)]^2$
4. Compute $\alpha = \min \left(1, e^{[SS_{q^*} - SS_{q^{k-1}}]/(2\sigma_{k-1}^2)} \right)$
5. If $u_\alpha < \alpha$, Set $q^k = q^*$, $SS_{q^k} = SS_{q^*}$
Else Set $q^k = q^{k-1}$, $SS_{q^k} = SS_{q^{k-1}}$

Attributes:

- `acceptance_test()`
- `run_metropolis_step()`
- `unpack_set()`

classmethod `evaluate_likelihood_function` (*ss1, ss2, sigma2, newprior, oldprior*)

Evaluate likelihood function:

$$\alpha = \exp \left[-0.5 \left(\sum \left(\frac{SS_{q^*} - SS_{q^{k-1}}}{\sigma_{k-1}^2} \right) + p_1 - p_2 \right) \right]$$

Args:

- **ss1** (`ndarray`): SS error from proposed candidate, q^*
- **ss2** (`ndarray`): SS error from previous sample point, q^{k-1}
- **sigma2** (`ndarray`): Error variance estimate from previous sample point, σ_{k-1}^2
- **newprior** (`ndarray`): Prior for proposal candidate
- **oldprior** (`ndarray`): Prior for previous sample

Returns:

- **alpha** (`float`): Result of likelihood function

run_metropolis_step (*old_set, parameters, R, prior_object, sos_object*)

Run Metropolis step.

Args:

- **old_set** (`ParameterSet`): Features of q^{k-1}
- **parameters** (`ModelParameters`): Model parameters
- **R** (`ndarray`): Cholesky decomposition of parameter covariance matrix
- **priorobj** (`PriorFunction`): Prior function
- **sosobj** (`SumOfSquares`): Sum-of-Squares function

Returns:

- **accept** (`int`): 0 - reject, 1 - accept
- **newset** (`ParameterSet`): Features of q^*
- **outbound** (`int`): 1 - rejected due to sampling outside of parameter bounds
- **npar_sample_from_normal** (`ndarray`): Latent random sample points

classmethod `unpack_set` (*parset*)

Unpack parameter set

Args:

- **parset** (`ParameterSet`): Parameter set to unpack

Returns:

- **theta** (`ndarray`): Value of sampled model parameters
- **ss** (`ndarray`): Sum-of-squares error using sampled value
- **prior** (`ndarray`): Value of prior

- **sigma2** (`ndarray`): Error variance

pymcmcstat.samplers.SamplingMethods module

Created on Thu Jan 18 10:11:40 2018

@author: prmiles

class pymcmcstat.samplers.SamplingMethods.**SamplingMethods**
Metropolis sampling methods.

Attributes:

- *Metropolis*
- *DelayedRejection*
- *Adaptation*

pymcmcstat.samplers.utilities module

Created on Wed Jun 27 12:07:11 2018

Utility functions used by different samplers

@author: prmiles

pymcmcstat.samplers.utilities.**acceptance_test** (*alpha*)
Run standard acceptance test

If $u_\alpha < \alpha$,
Set $q^k = q^*$, $SS_{q^k} = SS_{q^*}$
Else
Set $q^k = q^{k-1}$, $SS_{q^k} = SS_{q^{k-1}}$

Args:

- **alpha** (`float`): Result of likelihood function

Returns:

- **accept** (`bool`): False - reject, True - accept

pymcmcstat.samplers.utilities.**is_sample_outside_bounds** (*theta*, *lower_limits*, *upper_limits*)

Check whether proposal value is outside parameter limits

Args:

- **theta** (`ndarray`): Value of sampled model parameters
- **lower_limits** (`ndarray`): Lower limits
- **upper_limits** (`ndarray`): Upper limits

Returns:

- **outsidebounds** (`bool`): True -> Outside of parameter limits

`pymcmcstat.samplers.utilities.sample_candidate_from_gaussian_proposal` (*npar*,
old-par,
R)

Sample candidate from Gaussian proposal distribution

Args:

- **npar** (`int`): Number of parameters being samples
- **oldpar** (`ndarray`): q^{k-1} Old parameter set.
- **R** (`ndarray`): Cholesky decomposition of parameter covariance matrix.

Returns:

- **newpar** (`ndarray`): q^* - candidate
- **npar_sample_from_sample** (`ndarray`): Sampled values from normal distribution: $N(0, 1)$.

`pymcmcstat.samplers.utilities.set_outside_bounds` (*next_set*)

Assign set features based on being outside bounds

Args:

- **next_set** (`ParameterSet`): q^*

Returns:

- **next_set** (`ParameterSet`): q^* with updated features
- **outbound** (`bool`): True

pymcmcstat.settings package

pymcmcstat.settings.DataStructure module

Created on Wed Jan 17 09:03:37 2018

@author: prmiles

class `pymcmcstat.settings.DataStructure.DataStructure`

Structure for storing data in MCMC object. The following random data sets will be referenced in examples for the different class methods:

```
x1 = np.random.random_sample(size = (5, 1))
y1 = np.random.random_sample(size = (5, 2))

x2 = np.random.random_sample(size = (10, 1))
y2 = np.random.random_sample(size = (10, 3))
```

Attributes:

- `add_data_set()`
- `get_number_of_batches()`
- `get_number_of_data_sets()`
- `get_number_of_observations()`

add_data_set (*x*, *y*, *n=None*, *weight=1*, *user_defined_object=0*)

Add data set to MCMC object.

This method must be called first before using any of the other methods within *DataStructure*.

```
mcstat = MCMC ()
mcstat.data.add_data_set (x = x1, y = y1)
mcstat.data.add_data_set (x = x2, y = y2)
```

This yields the following variables in the data structure.

- **xdata** (*list*): List of numpy arrays

- `xdata[0] = x1`, `xdata[0].shape = (5, 1)`
- `xdata[1] = x2`, `xdata[1].shape = (10, 1)`

- **ydata** (*list*): List of numpy arrays

- `ydata[0] = y1`, `ydata[0].shape = (5, 2)`
- `ydata[1] = y2`, `ydata[1].shape = (10, 3)`

- **n** (*list*): List of integers. `n = [5, 10]`

- **shape** (*list*): List of *y.shape*. `shape = [(5, 2), (10, 3)]`

- **weight** (*list*): List of weights. `weight = [1, 1]`

- **user_defined_object** (*list*): List of objects. `user_defined_object = [0, 0]`

Args:

- **x** (*ndarray*): Independent data. Recommend input as column vectors.
- **y** (*ndarray*): Dependent data. Recommend input as column vectors.
- **n** (*list*): List of integers denoting number of data points.
- **weight** (*list*): Weight of each data set.
- **user_defined_object** (*User Defined*): Any object can be stored in this variable.

Note: In general, it is recommended that user's format their data as a column vector. So, if you have *nds* independent data points, *x* and *y* should be `[nds, 1]` or `[nds,]` numpy arrays. Note if a list is sent, the code will convert it to a numpy array.

get_number_of_batches ()

Get number of batches in data structure. Essentially, each time you call the `add_data_set()` method you are adding another batch. It is also equivalent to say the number of batches is equal to the length of the list *ydata*. For example,

```
nb = mcstat.data.get_number_of_batches()
```

should return `nb = 2` because `len(mcstat.data.ydata) = 2`.

Returns:

- **nbatch** (*int*): Number of batches.

get_number_of_data_sets ()

Get number of data sets in data structure. A data set is strictly speaking defined as the total number of columns in each element of the *ydata* list. For example,

```
nbs = mcstat.data.get_number_of_data_sets()
```

should return `nbs = 2 + 3 = 5` because the number of columns in `y1` is 2 and the number of columns in `y2` is 3.

Returns:

- Number of columns in `ydata` (`int`)

get_number_of_observations()

Get number of observations in data structure. An observation is essentially the total number of rows from each element of the `ydata` list. For example,

```
nobs = mcstat.data.get_number_of_observations()
```

should return `nobs = 5 + 10 = 15` because the number of rows in `y1` is 5 and the number of rows in `y2` is 10.

Returns:

- Number of rows in `ydata` (`ndarray`)

pymcmcstat.settings.ModelParameters module

Created on Wed Jan 17 09:13:03 2018

@author: prmiles

class pymcmcstat.settings.ModelParameters.**ModelParameters**
MCMC Model Parameters.

Example:

```
mcstat = MCMC()

mcstat.parameters.add_model_parameter(name = 'm', theta0 = 1., minimum = -10,
↪maximum = 10)
mcstat.parameters.add_model_parameter(name = 'b', theta0 = -5., minimum = -10,
↪maximum = 100)
mcstat.parameters.display_model_parameter_settings()
```

This will display to screen:

```
Sampling these parameters:
name      start [  min,   max] N( mu, sigma^2)
m         :   1.00 [-10.00,  10.00] N(0.00, inf)
b         :  -5.00 [-10.00, 100.00] N(0.00, inf)
```

Attributes:

- `add_model_parameter()`
- `display_parameter_settings()`

add_model_parameter (`name=None`, `theta0=None`, `minimum=-inf`, `maximum=inf`,
`prior_mu=array([0.])`, `prior_sigma=inf`, `sample=True`, `local=0`)
Add model parameter to MCMC simulation.

Args:

- `name (str)`: Parameter name
- `theta0 (float)`: Initial value
- `minimum (float)`: Lower parameter bound
- `maximum (float)`: Upper parameter bound
- `prior_mu (float)`: Mean value of prior distribution
- `prior_sigma (float)`: Standard deviation of prior distribution
- `sample (bool)`: Flag to turn sampling on (True) or off (False)
- `local (int)`: Local flag - still testing.

The default prior is a uniform distribution from minimum to maximum parameter value.

display_parameter_settings (*verbosity=None, noadaptind=None*)

Display parameter settings

Args:

- **verbosity** (`int`): Verbosity of display output. 0
- **noadaptind** (`int`): Indices not to be adapted in covariance matrix. []

classmethod scan_for_local_variables (*nbatch, parameters*)

Scan for local variables

Args:

- **nbatch** (`int`): Number of data batches
- **parameters** (`list`): List of model parameters.

Returns:

- **local** (`ndarray`): Array with local flag indices.

classmethod setup_prior_mu (*mu, value*)

Setup prior mean.

Args:

- **mu** (`float`): defined mean
- **value** (`float`): default value

Returns:

- Prior mean

classmethod setup_prior_sigma (*sigma*)

Setup prior variance.

Args:

- **sigma** (`float`): defined variance

Returns:

- Prior mean

`pymcmcstat.settings.ModelParameters.check_noadaptind` (*noadaptind*)

Check if noadaptind is None -> Empty List

Args:

- **noadaptind** (`list`): Indices not to be adapted in covariance matrix.

Returns:

- **noadaptind** (`list`): Indices not to be adapted in covariance matrix.

`pymcmcstat.settings.ModelParameters.check_verbosity(verbosity)`
Check if verbosity is None -> 0

Args:

- **verbosity** (`int`): Verbosity level

Returns:

- **verbosity** (`int`): Returns 0 if verbosity was initially *None*

`pymcmcstat.settings.ModelParameters.format_number_to_str(number)`
Format number for display

Args:

- **number** (`float`): Number to be formatted

Returns:

- (`str`): Formatted string display

`pymcmcstat.settings.ModelParameters.generate_default_name(nparam)`
Generate generic parameter name. For example, if `nparam = 4`, then the generated name is:

```
names = 'p_{3}'
```

Args:

- **nparam** (`int`): Number of parameter names to generate

Returns:

- **name** (`str`): Name based on size of parameter list

`pymcmcstat.settings.ModelParameters.less_than_or_equal_to_zero(x)`
Return result of test on number based on less than or equal to

Args:

- **x** (`float`): Number to be tested

Returns:

- (`bool`): Result of test: $x \leq 0$

`pymcmcstat.settings.ModelParameters.noadapt_display_setting(ii, noadaptind)`
Define display settings if index not being adapted.

Args:

- **ii** (`int`): Current index number
- **noadaptind** (`list`): List of indices not being adapted.

Returns:

- **st** (`str`): String to be displayed, depending on if in *noadaptind*.

`pymcmcstat.settings.ModelParameters.prior_display_setting(x)`
Define display string for prior.

Args:

- `x (float)`: Prior mean

Returns:

- `h2 (str)`: String to be displayed, depending on if x is infinity.

`pymcmcstat.settings.ModelParameters.replace_list_elements(x, testfunction, value)`

Replace list elements based on results from testfunction.

Args:

- `x (list)`: List of numbers to be tested
- `testfunction (testfunction())`: Test function
- `value (float)`: Value to assign if test function return True

Returns:

- `x (list)`: Updated list

pymcmcstat.settings.ModelSettings module

Created on Wed Jan 17 09:06:51 2018

@author: prmiles

class `pymcmcstat.settings.ModelSettings.ModelSettings`
MCMC Model Settings

Attributes:

- `define_model_settings()`
- `display_model_settings()`

define_model_settings (*sos_function=None, prior_function=None, prior_type=1, prior_update_function=None, prior_pars=None, model_function=None, sigma2=None, N=None, S20=nan, N0=None, nbatch=None*)

Define model settings.

Args:

- **sos_function**: Handle for sum-of-squares function
- **prior_function**: Handle for prior function
- **prior_type**: Pending...
- **prior_update_function**: Pending...
- **prior_pars**: Pending...
- **model_function**: Handle for model function (needed if `sos_function` not specified)
- **sigma2 (float)**: List of initial error observations.
- **N (int)**: Number of observations - see [DataStructure](#).
- **S20 (float)**: List of scaling parameter in observation error estimate.
- **N0 (float)**: List of scaling parameter in observation error estimate.
- **nbatch (int)**: Number of batch data sets - see [get_number_of_batches\(\)](#).

Note: Variables `sigma2`, `N`, `S20`, `N0`, and `nbatch` converted to `ndarray` for subsequent processing.

display_model_settings (*print_these=None*)

Display subset of the simulation options.

Args:

- **print_these** (*list*): List of strings corresponding to keywords. Default below.

```
print_these = ['sos_function', 'model_function', 'sigma2', 'N', 'N0', 'S20',  
↪ 'nsos', 'nbatch']
```

pymcmcstat.settings.SimulationOptions module

Created on Wed Jan 17 09:08:13 2018

@author: prmiles

class pymcmcstat.settings.SimulationOptions.SimulationOptions

MCMC simulation options.

Attributes:

- `define_simulation_options()`
- `display_simulation_options()`

define_simulation_options (*nsimu=10000*, *adaptint=None*, *ntry=None*, *method='dram'*, *printint=None*, *adaptend=0*, *lastadapt=0*, *burnintime=0*, *waitbar=1*, *debug=0*, *qcov=None*, *updatesigma=False*, *noadaptind=None*, *stats=0*, *drscale=array([5., 4., 3.])*, *adascale=None*, *savesize=0*, *maxmem=0*, *chainfile='chainfile'*, *s2chainfile='s2chainfile'*, *sschainfile='sschainfile'*, *covchainfile='covchainfile'*, *savedir=None*, *save_to_bin=False*, *skip=1*, *label=None*, *RDR=None*, *verbosity=1*, *maxiter=None*, *priorupdatestart=0*, *qcov_adjust=1e-08*, *burnin_scale=10*, *alphatarget=0.234*, *etaparam=0.7*, *initqcovn=None*, *doram=None*, *rndseq=None*, *results_filename=None*, *save_to_json=False*, *save_to_txt=False*, *json_restart_file=None*)

Define simulation options.

Args:

- **nsimu** (*int*): Number of parameter samples to simulate. Default is 1e4.
- **adaptint** (*int*): Number of iterates between adaptation. Default is method dependent.
- **ntry** (*int*): Number of tries to take before rejection. Default is method dependent.
- **method** (*str*): Sampling method ('mh', 'am', 'dr', 'dram'). Default is 'dram'.
- **printint** (*int*): Printing interval.
- **adaptend** (*int*): Obsolete.
- **lastadapt** (*int*): Last adaptation iteration (i.e., no more adaptation beyond this point).
- **burnintime** (*int*):

- **waitbar** (`int`): Flag to use progress bar. Default is 1 -> on (otherwise -> off).
- **debug** (`int`): Flag to perform debug. Default is 0 -> off.
- **qcov** (`ndarray`): Proposal parameter covariance matrix.
- **updatesigma** (`bool`): Flag for updating measurement error variance. Default is 0 -> off (1 -> on).
- **noadaptind** (`int`): Indices not to be adapted in covariance matrix. Default is [] (untested).
- **stats** (`int`): Calculate convergence statistics. Default is 0 -> off (1 -> on).
- **drscale** (`ndarray`): Reduced scale for sampling in DR algorithm. Default is [5,4,3].
- **adascale** (`float`): User defined covariance scale. Default is method dependent (untested).
- **savesize** (`int`): Size of chain segments when saving to log files. Default is 0.
- **maxmem** (`int`): Maximum memory available in mega bytes (Obsolete).
- **chainfile** (`str`): File name for chain log file.
- **sschainfile** (`str`): File name for sschain log file.
- **s2chainfile** (`str`): File name for s2chain log file.
- **covchainfile** (`str`): File name for qcov log file.
- **savedir** (`str`): Output directory of log files. Default is current directory.
- **save_to_bin** (`bool`): Save log files to binary. Default is False.
- **save_to_txt** (`bool`): Save log files to text. Default is False.
- **skip** (`int`):
- **label** (`str`):
- **RDR** (`ndarray`): R matrix for each stage of DR.
- **verbosity** (`int`): Verbosity of display output.
- **maxiter** (`int`): Obsolete.
- **priorupdatestart**
- **qcov_adjust** (`float`): Adjustment scale for covariance matrix.
- **burnin_scale** (`float`): Scale for burnin.
- **alphatarget** (`float`): Acceptance ratio target.
- **etaparam** (`float`):
- **initqcovn** (`float`): Proposal covariance weight in update.
- **doram** (`int`): Flag to perform 'ram' algorithm (Obsolete).
- **rndseq** (`ndarray`): Random number sequence (Obsolete).
- **results_filename** (`str`): Output file name when saving results structure with json.
- **save_to_json** (`bool`): Save results structure to json file. Default is False.
- **json_restart_file** (`str`): Extract parameter covariance and last sample value from saved json file.

Note: For the log file names `chainfile`, `sschainfile`, `s2chainfile` and `covchainfile` do not include the extension. By specifying whether to save to text or to binary, the appropriate extension will be added.

display_simulation_options (*print_these=None*)

Display subset of the simulation options.

Args:

- **print_these** (*list*): List of strings corresponding to keywords. Default below.

```
print_these = ['nsimu', 'adaptint', 'ntry', 'method', 'printint', 'lastadapt',
↪ 'drscale', 'qcov']
```

pymcmcstat.structures package

pymcmcstat.structures.ParameterSet module

Created on Thu Jan 18 10:15:37 2018

@author: prmls

```
class pymcmcstat.structures.ParameterSet.ParameterSet (theta=None,      ss=None,
                                                         prior=None,  sigma2=None,
                                                         alpha=None)
```

Basic MCMC parameter set.

Description: Storage device for passing parameter sets back and forth between sampling methods.

Args:

- **theta** (*ndarray*): Sampled values.
- **ss** (*ndarray*): Sum-of-squares error(s).
- **prior** (*ndarray*): Result from prior function.
- **sigma2** (*ndarray*): Observation errors.
- **alpha** (*float*): Result from evaluating likelihood function.

pymcmcstat.structures.ResultsStructure module

Created on Wed Jan 17 09:18:19 2018

@author: prmls

```
class pymcmcstat.structures.ResultsStructure.ResultsStructure
Results from MCMC simulation.
```

Description: Class used to organize results of MCMC simulation.

Attributes:

- `export_simulation_results_to_json_file()`
- `determine_filename()`
- `save_json_object()`

- `load_json_object()`
- `add_basic()`
- `add_updatesigma()`
- `add_dram()`
- `add_prior()`
- `add_options()`
- `add_model()`
- `add_chain()`
- `add_s2chain()`
- `add_sschain()`
- `add_time_stats()`
- `add_random_number_sequence()`

add_basic (*nsimu, covariance, parameters, rejected, simutime, theta*)
Add basic results from MCMC simulation to structure.

Args:

- **nsimu** (`int`): Number of MCMC simulations.
- **model** (`ModelSettings`): MCMC model settings.
- **covariance** (`CovarianceProcedures`): Covariance variables.
- **parameters** (`ModelParameters`): Model parameters.
- **rejected** (`dict`): Dictionary of rejection stats.
- **simutime** (`float`): Simulation run time in seconds.
- **theta** (`ndarray`): Last sampled values.

add_chain (*chain=None*)
Add chain to results structure.

Args:

- **chain** (`ndarray`): Model parameter sampling chain.

add_dram (*drscale, RDR, total_rejected, drsettings*)
Add results specific to performing DR algorithm.

Args:

- **drscale** (`ndarray`): Reduced scale for sampling in DR algorithm. Default is [5,4,3].
- **RDR** (`ndarray`): Cholesky decomposition of covariance matrix based on DR.
- **total_rejected** (`int`): Number of rejected samples.
- **drsettings** (`DelayedRejection`): Need access to counters within DR class.

add_model (*model=None*)
Saves subset of features of the model settings in a nested dictionary.

Args:

- **model** (`ModelSettings`): MCMC model settings.

add_options (*options=None*)

Saves subset of features of the simulation options in a nested dictionary.

Args:

- **options** (*SimulationOptions*): MCMC simulation options.

add_prior (*mu, sig, priorfun, priortype, priorpars*)

Add results specific to prior function.

Args:

- **mu** (*float*): Prior mean.
- **sig** (*float*): Prior standard deviation.
- **priorfun**: Handle for prior function.
- **priortype** (*int*): Flag identifying type of prior.
- **priorpars** (*float*): Prior parameter for prior update function.

Note: This feature is not currently implemented.

add_random_number_sequence (*rndseq*)

Add random number sequence to results structure.

Args:

- **rndseq** (*ndarray*): Sequence of sampled random numbers.

Note: This feature is not currently implemented.

add_s2chain (*s2chain=None*)

Add observation error chain to results structure.

Args:

- **s2chain** (*ndarray*): Sampling chain of observation errors.

add_sschain (*sschain=None*)

Add sum-of-squares chain to results structure.

Args:

- **sschain** (*ndarray*): Calculated sum-of-squares error for each parameter chains set.

add_time_stats (*mtime, drtime, adtime*)

Add time spend using each sampling algorithm.

Args:

- **mtime** (*float*): Time spent performing standard Metropolis.
- **drtime** (*float*): Time spent performing Delayed Rejection.
- **adtime** (*float*): Time spent performing Adaptation.

Note: This feature is not currently implemented.

add_updatesigma (*updatesigma*, *sigma2*, *S20*, *N0*)

Add information to results structure related to observation error.

Args:

- **updatesigma** (`bool`): Flag to update error variance(s).
- **sigma2** (`ndarray`): Latest estimate of error variance(s).
- **S20** (`ndarray`): Scaling parameter(s).
- **N0** (`ndarray`): Shape parameter(s).

If `updatesigma` is `True`, then

```
results['sigma2'] = np.nan
results['S20'] = S20
results['N0'] = N0
```

Otherwise

```
results['sigma2'] = sigma2
results['S20'] = np.nan
results['N0'] = np.nan
```

classmethod determine_filename (*options*)

Determine results filename.

If not specified by *results_filename* in the simulation options, then a default naming format is generated using the date string associated with the initialization of the simulation.

Args:

- **options** (*SimulationOptions*): MCMC simulation options.

Returns:

- **filename** (`str`): Filename string.

export_simulation_results_to_json_file (*results*)

Export simulation results to a json file.

Args:

- **results** (*ResultsStructure*): Dictionary of MCMC simulation results/settings.

classmethod load_json_object (*filename*)

Load object stored in json file.

Note: Filename should include extension.

Args:

- **filename** (`str`): Load object from file with this name.

Returns:

- **results** (`dict`): Object loaded from file.

classmethod save_json_object (*results*, *filename*)

Save object to json file.

Note: Filename should include extension.

Args:

- **results** (`dict`): Object to save.
- **filename** (`str`): Write object into file with this name.

pymcmcstat.utilities package

pymcmcstat.utilities.NumpyEncoder module

Created on Mon Apr 2 08:42:56 2018

@author: prmiles

```
class pymcmcstat.utilities.NumpyEncoder.NumpyEncoder (skipkeys=False,          en-
                                                    sure_ascii=True,
                                                    check_circular=True,
                                                    allow_nan=True,
                                                    sort_keys=False,          in-
                                                    dent=None, separators=None,
                                                    encoding='utf-8',          de-
                                                    fault=None)
```

Bases: `json.encoder.JSONEncoder`

Encoder used for storing numpy arrays in json files.

default (*obj*)

Implement this method in a subclass such that it returns a serializable object for `o`, or calls the base implementation (to raise a `TypeError`).

For example, to support arbitrary iterators, you could implement default like this:

```
def default(self, o):
    try:
        iterable = iter(o)
    except TypeError:
        pass
    else:
        return list(iterable)
    # Let the base class default method raise the TypeError
    return JSONEncoder.default(self, o)
```

pymcmcstat.utilities.general module

Created on Tue Jun 26 06:16:02 2018

General functions used throughout package

@author: prmiles

`pymcmcstat.utilities.general.message` (*verbosity, level, printthis*)

Display message

Args:

- **verbosity** (`int`): Verbosity of display output.
- **level** (`int`): Print level relative to verbosity.
- **printthis** (`str`): String to be printed.

`pymcmcstat.utilities.general.removekey(d, key)`
 Removed elements from dictionary and return the remainder.

Args:

- **d** (`dict`): Original dictionary.
- **key** (`str`): Keyword to be removed.

Returns:

- **r** (`dict`): Updated dictionary without the keyword, value pair.

pymcmcstat.utilities.progressbar module

`pymcmcstat.utilities.progressbar.progress_bar(iters)`
 Simulation progress bar.

A simple progress bar to monitor MCMC sampling progress. Modified from original code by Corey Goldberg (2010).

Args:

- **iters** (`int`): Number of iterations in simulation.

Example display:

[-----	21%] 2109 of 10000 complete in 0.5 sec
--------	-----	-------------------------------------

Note: Will display a progress bar as simulation runs, providing feedback as to the status of the simulation. Depending on the available resources, the appearance of the progress bar may differ.

CHAPTER 6

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