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# **pymcmcstat Documentation**

***Release 1.8.0***

**Paul Miles**

**Jul 09, 2019**



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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

This package is an adaptation of the MATLAB toolbox [mcmcstat](#). 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.

Note, advanced plotting routines are available in the [mcmcplot](#) package. Many plotting features are directly available within [pymcmcstat](#), but some user's may find [mcmcplot](#) useful.



# CHAPTER 1

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## Installation

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This code can be found on the [Github project page](#). This package is available on the PyPI distribution site and the latest version can be installed via

```
pip install pymcmcstat
```

The master branch on Github typically matches the latest version on the PyPI distribution site. To install the master branch directly from Github,

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

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





## CHAPTER 2

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### Getting Started

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- [Tutorial notebooks](#)
- [Documentation](#)
- [Release history](#)
- [Contributing guidelines](#)



## CHAPTER 3

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License

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MIT



## CHAPTER 4

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### Contributors

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See the [GitHub contributor page](#)



## CHAPTER 5

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### Citing pymcstat

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Miles, (2019). pymcstat: A Python Package for Bayesian Inference Using Delayed Rejection Adaptive Metropolis. Journal of Open Source Software, 4(38), 1417, <https://doi.org/10.21105/joss.01417>

Also, please cite the appropriate [Zenodo archive](#) for the version of *pymcstat* that you are using.





## CHAPTER 6

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### Feedback

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- Feature Request
- Bug Report



## CHAPTER 7

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Sponsor

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This work was sponsored in part by the NNSA Office of Defense Nuclear Nonproliferation R&D through the Consortium for Nonproliferation Enabling Capabilities.





## 8.1 pymcmcstat package

### 8.1.1 pymcmcstat.MCMC module

Created on Wed Jan 17, 2018

@author: prmls

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, seterr={'over': 'ignore', 'under': 'ignore'})  
    Bases: object
```

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, iiadapt, 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.

## 8.1.2 pymcmcstat.ParallelMCMC module

Created on Tue May 1 15:58:22 2018

@author: prmiles

**class** pymcmcstat.ParallelMCMC.ParallelMCMC

Bases: `object`

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_for_restart_file` (*json\_restart\_file*, *chain\_dir*)

Check if restart directory was specified.

**Args:**

- **json\_restart\_file** (*str*): String specifying path to results directory.
- **chain\_dir** (*str*): String specifying which chain is being restarted.

`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.load_parallel_simulation_results(savedir, extension='h5', chainfile='chainfile', sschainfile='sschainfile', s2chainfile='s2chainfile', covchainfile='covchainfile')`

Load results from parallel simulation directory json files.

Lists in json files are converted to numpy arrays.

**Args:**

- **savedir** (`str`): String indicated path to parallel directory.

**Returns:**

- **pres** (`list`): Each element of list is an MCMC result dictionary.

`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.

### 8.1.3 Subpackages

#### pymcmcstat.chain package

#### pymcmcstat.chain.ChainProcessing module

Created on Tue May 1 09:12:06 2018

@author: prmiles

pymcmcstat.chain.ChainProcessing.**check\_parallel\_directory\_contents** (*parallel\_dir*,  
*cf\_orig*)

Check that items in directory are subdirectories with name “chain\_#”

**Args:**

- **parallel\_dir** (*str*): Directory where parallel log files are saved.
- **cf\_orig** (*list*): List of items contained in parallel directory.

**Returns:**

- **chainfolders** (*list*): List of items that match criteria in parallel directory.

pymcmcstat.chain.ChainProcessing.**generate\_chain\_list** (*pres*, *burnin\_percentage=50*)  
Generate list of chains.

**Args:**

- **pres** (*list*): Parallel results list.
- **burnin\_percentage** (*int*): Percentage of chain to remove for burnin.

**Returns:**

- (*list*): Each element of list corresponds to different chain set.

pymcmcstat.chain.ChainProcessing.**generate\_combined\_chain\_with\_index** (*pres*,  
*burnin\_percentage=50*)  
Generate combined chain with index.

**Args:**

- **pres** (*list*): Parallel results list.
- **burnin\_percentage** (*int*): Percentage of chain to remove for burnin.

**Returns:**

- (*ndarray*, *list*): Combined chain array, index label

pymcmcstat.chain.ChainProcessing.**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.

```
pymcmcstat.chain.ChainProcessing.load_parallel_simulation_results(savedir,  
                                                                extension='h5',  
                                                                chain-  
                                                                file='chainfile',  
                                                                sschain-  
                                                                file='sschainfile',  
                                                                s2chainfile='s2chainfile',  
                                                                covchain-  
                                                                file='covchainfile')
```

Load results from parallel simulation directory json files.

Lists in json files are converted to numpy arrays.

**Args:**

- **savedir** (`str`): String indicated path to parallel directory.

**Returns:**

- **pres** (`list`): Each element of list is an MCMC result dictionary.

```
pymcmcstat.chain.ChainProcessing.load_serial_simulation_results(savedir,  
                                                              json_file=None,  
                                                              extension='h5',  
                                                              chain-  
                                                              file='chainfile',  
                                                              sschain-  
                                                              file='sschainfile',  
                                                              s2chainfile='s2chainfile',  
                                                              covchain-  
                                                              file='covchainfile')
```

Load results from serial simulation directory json files.

Lists in json files are converted to numpy arrays.

**Args:**

- **savedir** (`str`): String indicated path to results directory.

**Returns:**

- **results** (`dict`): Each element of list is an MCMC result dictionary.

```
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
```

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```
2018-05-03 14:15:55      3000      3999
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 an empty list.

**Args:**

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

**Returns:**

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

`pymcmcstat.chain.ChainProcessing.read_in_parallel_json_results_files(parallel_dir)`

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

**Args:**

- **parallel\_dir** (`str`): Directory where parallel log files are saved.

`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', sschainfile='sschainfile', s2chainfile='s2chainfile', covchainfile='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.calculate_psr_f(x, nsimu, nchains)`

Calculate Potential Scale Reduction Factor (PSRF)

Performs analysis of variances for set of chains corresponding to a single parameter. This code follows the MATLAB implementation found here:

<https://users.aalto.fi/~ave/code/mcmcdiag/>

**Args:**

- **x** (*ndarray*): Expect an [nsimu x nchains] array.
- **nsimu** (*int*): Number of simulations in each chain.
- **nchains** (*int*): Number of chains.

**Returns:**

- **dict**
  - R - PSRF
  - B - Between Sequence Variances
  - W - Within Sequence Variances
  - V - Mixture-of-Sequences Variances

– neff - Effective number of samples

```
pymcmcstat.chain.ChainStatistics.chainstats(chain=None, results=None, return-
stats=False, display_details=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.display_gelman_rubin(psrf)
Display results of Gelman-Rubin diagnostic
```

**Args:**

- **psrf** (`dict`): Results from GR diagnostic

```
pymcmcstat.chain.ChainStatistics.gelman_rubin(chains, names=None, results=None, display=True)
Gelman-Rubin diagnostic for multiple chains [GR+92], [BG98].
```

This diagnostic technique compares the variance within a single chain to the variance between multiple chains. This process serves as a method for testing whether or not the chain has converged. If the chain has converged, we would expect the variance within and the variance between to be equal. This diagnostic tool pairs well with the ParallelMCMC module, which generates a set of distinct chains that have all been initialized at different points within the parameter space.

**Args:**

- **chains** (`list`): List of arrays - each array corresponds to different chain set.
- **names** (`list`): List of strings - corresponds to parameter names.
- **results** (`dict`): Results from MCMC simulation.

**Returns:**

- (`dict`): Keywords of the dictionary correspond to the parameter names. Each keyword corresponds to a dictionary outputted from `calculate_psrfs()`.

```
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 [BR98].

**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_acceptance_info(chain,`  
`re-`  
`sults=None)`

Print chain acceptance rate(s)

If results structure is provided, it will try to print acceptance rates with respect to delayed rejection as well.

Example display (if results dictionary provided):

```
-----
Acceptance rate information
-----
Results dictionary:
Stage 1: 3.32%
Stage 2: 22.60%
Net      : 25.92% -> 1296/5000
-----
Chain provided:
```

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```
Net      : 32.10% -> 963/3000
-----
Note, the net acceptance rate from the results dictionary
may be different if you only provided a subset of the chain,
e.g., removed the first part for burnin-in.
-----
```

#### Args:

- **chain** (`ndarray`): Sampling chain.
- **results** (`dict`): Results from MCMC simulation. Default is *None*.

`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: prmiles

**class** pymcmcstat.plotting.MCMCPlotting.Plot

Bases: `object`

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*, *skip=1*, *max-points=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]
- **skip** (`int`): Indicates step size to be used when plotting elements from the chain
- **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*, *return\_kde=False*)

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, figsizeinches=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, figsizeinches=None, skip=1, maxpoints=500)`

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
- **maxpoints** (`py:class:int`): Maximum allowable number of points in plot.

## pymcmcstat.plotting.PredictionIntervals module

Created on Wed Nov 8 12:00:11 2017

@author: prmlies

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

Bases: `object`

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 (' '), 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_settings` (*default\_settings*, *user\_settings=None*)

Check user settings with default.

Recursively checks elements of user settings against the defaults and updates settings as it goes. If a user setting does not exist in the default, then the user setting is added to the settings. If the setting is defined in both the user and default settings, then the user setting overrides the default. Otherwise, the default settings persist.

**Args:**

- **default\_settings** (*dict*): Default settings for particular method.
- **user\_settings** (*dict*): User defined settings.

**Returns:**

- (*dict*): Updated settings.

`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, *sigma2*=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.plotting.utilities.setup_subsample(skip, maxpoints, nsimu)`

Setup subsampling from posterior.

When plotting the sampling chain, it is often beneficial to subsample in order to avoid to dense of plots. This routine determines the appropriate step size based on the size of the chain (`nsimu`) and maximum points allowed to plot (`maxpoints`). The function checks if the size of the chain exceeds the maximum number of points allowed in the plot. If yes, `skip` is defined such that every the max number of points are used and sampled evenly from the start to end of the chain. Otherwise the value of `skip` is return as defined by the user. A subsample index is then generated based on the value of `skip` and the number of simulations.

**Args:**

- `skip` (`int`): User defined skip value.
- `maxpoints` (`int`): Maximum points allowed in each plot.

**Returns:**

- (`int`): Skip value.



## 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

Bases: `object`

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

Bases: `object`

Estimate observation errors.

#### Attributes:

- `update_error_variance()`
- `gammar()`
- `gammar_mt()`

**gammar** (*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

**gammar\_mt** (*m, n, a, b=1*)

Wrapper routine for calculating random deviates from gamma distribution using method of Marsaglia and Tsang (2000) [[MT00](#)].

**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  $\sigma^2$  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  $\sigma_s^2$  are shape and scaling parameters,  $N$  is the number of observations, and  $SS_q$  is the sum-of-squares error. For more details regarding the interpretation of  $N_s$  and  $\sigma_s^2$ , please refer to [[Smi14](#)] page 163.

---

**Note:** The variables  $N_s$  and  $\sigma_s^2$  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=array([0]),  
                                                    sigma=array([inf]))
```

Bases: `object`

Prior distribution functions.

**Attributes:**

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

```
classmethod default_priorfun (theta, mu, sigma)
```

Default prior function - Gaussian.

$$\pi_0(q) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{q - \mu}{\sigma} \right)^2 \right]$$

**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)
```

Bases: `object`

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, custom=None)
```

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: prmls

**class** `pymcmcstat.samplers.Adaptation.Adaptation`

Bases: `object`

Adaptive Metropolis (AM) algorithm based on [HST+01].

**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 threshold

**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-
                                                             rejected, 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, alphatarget, 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: prmiles

**class** `pymcmcstat.samplers.DelayedRejection.DelayedRejection`

Bases: `object`

Delayed Rejection (DR) algorithm based on [HLMS06].

**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, custom=None*)

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`

Bases: `object`

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** `calculate_posterior_ratio(ss1, ss2, sigma2, newprior, oldprior)`

Calculate acceptance ratio

$$\alpha = \min \left[ 1, \frac{\mathcal{L}(\nu_{obs}|q^*, \sigma_{k-1}^2) \pi_0(q^*)}{\mathcal{L}(\nu_{obs}|q^{k-1}, \sigma_{k-1}^2) \pi_0(q^{k-1})} \right]$$

where the Gaussian likelihood function is

$$\mathcal{L}(\nu_{obs}|q, \sigma) = \exp \left( - \frac{SS_q}{2\sigma} \right)$$

and Gaussian prior function is

$$\pi_0(q) = \exp \left[ - \frac{1}{2} \left( \frac{q - \mu_0}{\sigma_0} \right)^2 \right].$$

For the Gaussian likelihood and prior, this yields the acceptance ratio

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

For more details regarding the prior function, please refer to the [PriorFunction](#) class.

---

**Note:** The default behavior of the package is to use Gaussian likelihood and prior functions (as of v1.8.0). Future releases will expand the functionality to allow for alternative likelihood and prior definitions.

---

#### 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,  $\sigma_{k-1}^2$
- **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`, `custom=None`)

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: prmls

**class** pymcmcstat.samplers.SamplingMethods.**SamplingMethods**

Bases: *object*

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: prmls

`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.calculate_log_posterior_ratio(loglikestar, loglike, logpriorstar, logprior)`

Calculate log posterior ratio:

$$\log(\alpha) = \min \left[ 0, \log(\mathcal{L}(\nu_{obs}|q^*)) + \log(\pi_0(q^*)) - \log(\mathcal{L}(\nu_{obs}|q^{k-1})) - \log(\pi_0(q^{k-1})) \right]$$

For more details regarding the prior and likelihood functions, please refer to the [PriorFunction](#) and [LikelihoodFunction](#) class, respectively.

---

**Note:** The default behavior of the package is to use Gaussian likelihood and prior functions (as of v1.8.0). Future releases will expand the functionality to allow for alternative likelihood and prior definitions.

---

**Args:**

- **likestar** (`float`): Likelihood from proposed candidate,  $q^*$
- **like** (`float`): Likelihood from previous sample point,  $q^{k-1}$
- **priorstar** (`float`): Prior for proposal candidate
- **prior** (`float`): Prior for previous sample

**Returns:**

- **alpha** (`float`): Acceptance ratio

`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.log_posterior_ratio_acceptance_test(alpha)`

Run log posterior ratio acceptance test

**Args:**

- **alpha** (`float`): Log posterior ratio

**Returns:**

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

`pymcmcstat.samplers.utilities.posterior_ratio_acceptance_test(alpha)`  
Run posterior ratio acceptance test

**Args:**

- **alpha** (`float`): Posterior ratio

**Returns:**

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

`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: prmls

**class** `pymcmcstat.settings.DataStructure.DataStructure`  
Bases: `object`

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,

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

should return `nds = 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**

Bases: `object`

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, adapt=True*)

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, no\_adapt=None*)

Display parameter settings

**Args:**

- **verbosity** (`int`): Verbosity of display output. 0
- **no\_adapt** (`ndarray`): Boolean array of indices not to be adapted.

**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\_adaptation\_indices** (*parind, adapt*)

Setup adaptation parameter indices.

**Args:**

- **parind** (`ndarray`): Array of boolean flags from parameter structure.
- **adapt** (`ndarray`): Array of boolean flags from parameter structure.

**Returns:**

- **parind** (`ndarray`): Array of indices corresponding to sampling parameters.
- **adapt** (`ndarray`): Array of indices corresponding to adapting parameters.
- **no\_adapt** (`ndarray`): Boolean array of indices not being adapted.

..note:

The size of the returned arrays will equal the number of parameters being sampled.

**classmethod** `setup_adapting` (*adapt*, *sample*)

Setup parameters being adapted.

All parameters that are not being sampled will automatically be thrown out of adaptation. This method checks that the default adaptation status is consistent.

**Args:**

- **adapt** (`bool`): Flag from parameter structure.
- **sample** (`bool`): Flag from parameter structure.

**Returns:**

- `bool`

**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` (*no\_adapt*, *npar*)

Check if noadaptind is None -> Empty List

**Args:**

- **no\_adapt** (`ndarray`): Boolean array of indices not to be adapted.
- **npar** (`int`): Number of parameters.

**Returns:**

- **no\_adapt** (`ndarray`): Boolean array of indices not to be adapted.

`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(no_adapt)`  
Define display settings if index not being adapted.

**Args:**

- **no\_adapt** (`bool`): Flag to determine whether or not it is to be adapted..

**Returns:**

- **st** (`str`): String to be displayed.

`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: prmls

**class** pymcmcstat.settings.ModelSettings.**ModelSettings**

Bases: `object`

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

Bases: `object`

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=True, debug=0, qcov=None, updatesigma=False,  
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, eta-  
param=0.7, initqcovn=None, doram=None, rndseq=None,  
results_filename=None, save_to_json=False, save_to_txt=False,  
json_restart_file=None, save_lightly=False)
```

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).
- **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].
- **adascall** (`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.
- **save\_lightly** (`bool`): Flag to indicate whether results json file should include chains.

---

**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.settings.SimulationOptions.check_lightly_save(save_lightly,
                                                         save_to_json,
                                                         save_to_bin,
                                                         save_to_txt)
```

Check settings for lightly save

If saving to json, chains will be removed if already being stored via one of the logging methods, binary or text. If logging methods not being used, then chains will be included in json file.

#### Args:

- **save\_lightly** (`bool`): Flag to save results w/out arrays
- **save\_to\_json** (`bool`): Flag to save to json
- **save\_to\_bin** (`bool`): Flag to save to binary
- **save\_to\_txt** (`bool`): Flag to save to text

## 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)
```

Bases: `object`

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

Bases: `object`

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, sigma, priortype*)

Add results specific to prior function.

**Args:**

- **mu** (*ndarray*): Prior mean.
- **sigma** (*ndarray*): Prior standard deviation.
- **priortype** (*int*): Flag identifying type of prior.

---

**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\_lightly** (*results*)

Export minimal simulation results to a json file.

This will save the key terms in the results dict, excluding arrays. Ideally, this is used in conjunction with one of the chain saving methods. The goal is to provide a results dict to simplify post- processing and reduces storage overhead.

**Args:**

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

**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.structures.ResultsStructure.lighten_results(results)`  
Saves subset of features of the simulation options in a nested dictionary.

**Args:**

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

## 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,
                                                    ensure_ascii=True,
                                                    check_circular=True,
                                                    allow_nan=True,
                                                    sort_keys=False, indent=None,
                                                    separators=None, 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 9

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### References

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## CHAPTER 10

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### Indices and tables

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- `genindex`
- `modindex`
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