# **BayesCMD Documentation** *Release*

Joshua Russell-Buckland

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BayesCMD is a package intended to expand the capabilities of the Brain/Circulation Modelling (BCMD) framework. It introduces the ability to obtain posterior distributions for model parameters by using Approximate Bayesian Computation (ABC).

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**CHAPTER** 

ONE

# **BCMDMODEL**

# 1.1 Running the BCMD Model

```
class bayescmd.bcmdModel.ModelBCMD (model_name, inputs=None, params=None, times=None,
                                              outputs=None, burn_in=999, create_input=True, in-
                                              put_file=None, suppress=False, workdir=None, delete-
                                              Workdir=False, timeout=30, basedir='../bayescmd', de-
                                              bug=False, testing=False)
     BCMD model class. this can be used to create inputs, run simulations etc.
     create_default_input()
          Method to create input file and write to string buffer for access direct from memory.
     create_initialised_input()
          Method to create input file and write to string buffer for access direct from memory.
     output parse()
```

Function to parse the output files into a dictionary.

write\_default\_input()

Function to write a default input to file.

Function to write a default input to file.

write\_initialised\_input()

# 1.2 Input Creation

Input files are required by the BCMD model.

# 1.2.1 input\_creation

Create input files for use with a BCMD model.

Input files are needed in order to set model parameters and provide driving inputs.

```
class bayescmd.bcmdModel.InputCreator(times, inputs, outputs=None, params=None, file-
                                           name=None)
```

Create an input file by passing relevant information to the class.

This input file is then used to create an input file that can either be written to file or kept in buffer and passed directly to the model.

**Parameters** 

- times (list of float or int) List of times at which measurement data has been collected and needs to be simulated.
- inputs (dict) Dictionary of model inputs and their values. Has form {'names': list of str, 'values': list of float} where names should be a list of each model input name, matching up to the model inputs and values would be a list of lists, where each sublist is the input values for that time point. With this in mind, the length of inputs['values']' should equal length of times.
- **filename** (str, optional) Name of the input file to be written to if writing to file is required. Default is None.
- params (dict of str: float, optional) Dictionary of {'parameter': param\_value}
- outputs (list of str, optional) List of model outputs to return.

#### times

list of float or int - List of times at which measurement data has been collected and needs to be simulated

## inputs

dict - Dictionary of model inputs and their values. Has form {'names': list of str, 'values': list of list of float} where names should be a list of each model input name, matching up to the model inputs and values would be a list of lsits, where each sublist is the input values for that time point. With this in mind, the length of inputs['values']' should equal length of times.

## f\_out

StringIO() – String buffer object to which the input file will be written.

## filename

str – Name of the input file to be written to if writing to file is required. Default is None.

# params

```
dict of str: float. - Dictionary of { 'parameter': param_value}
```

## outputs

list of str – List of model outputs to return.

## default\_creation()

Create a default input file from given arguments.

Assumes parameters remain unchanged from default values.

**Returns** Returns the input file as a String.IO() buffer object.

```
Return type String.IO()
```

## initialised creation (burn in)

Create an input file from given arguments.

Creates an input file thatcan have non-default parameter values and outputs, as well as a burn in period. Assumes parameters remain constant for the full duration of the simulation.

Parameters burn\_in (float or int) - Length of burn in period at start of the simulation.

**Returns** Returns the input file as a String.IO() buffer object.

```
Return type String.IO()
```

## input\_file\_write()

Write input file from buffer to file.

**CHAPTER** 

**TWO** 

# **ABC**

The *abc* subpackage is used to handle the Approximate Bayesian Computation (ABC) specific components of BayesCMD. This includes running the model multiple times in a batch process, calculating distances between datasets and generating priors for parameters.

# 2.1 Distances

Use to generate distance measures between simulated and real time series.

bayescmd.abc.distances.DISTANCES

dict – Dictionary contianing the distance aliases, mapping to the functions.

exception bayescmd.abc.distances.Error

Base class for exceptions in this module.

exception bayescmd.abc.distances.ZeroArrayError

Exception raised for errors in the zero array.

bayescmd.abc.distances.check\_for\_key (dictionary, target)

Check that a dictionary contains a key, and if so, return its data.

## **Parameters**

- **dictionary** (*dict*) Dictionary to check for *target* key.
- **target** (str) String containing the target variable that is expected to be found in *dictionary*

**Returns data** – List of data found in *dictionary*. This is likely to be the time series data collected experimentally or generated by the model.

# Return type list

bayescmd.abc.distances.euclidean\_dist(data1, data2)

Get the euclidean distance between two numpy arrays.

# **Parameters**

• data1 (np.ndarray) – First data array.

The shape should match that of data2 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

• data2 (np.ndarray) – Second data array.

The shape should match that of data1 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

Returns d – Euclidean distance measure

Return type float

bayescmd.abc.distances.get\_distance(actual\_data, sim\_data, targets, zero\_flag, distance='euclidean', normalise=False)

Obtain distance between two sets of data.

Get a distance as defined by distance between two sets of data as well as between each signal in the data.

#### **Parameters**

- actual\_data (dict) Dictionary of actual data, as generated by bayescmd.abc. data\_import.import\_actual\_data()
- sim\_data (dict) Dictionary of simulated data, as created by bayescmd. bcmdModel.ModelBCMD.output\_parse()
- targets (list of str) List of model targets, which should all be strings.
- **zero\_flag** (dict) Dictionary of form target(str): bool, where bool indicates whether to zero that target.

Note: zero\_flag keys should match targets list.

- **distance** (str, optional) Name of distance measure to use. One of ['euclidean', 'manhattan', 'MAE', 'MSE'], where default is 'euclidean'.
- **normalise** (bool, optional) Boolean flag to indicate whether the signals need normalising, default is False. Current normalisation is done using z-score but that is likely to change with time.

## Returns

distances -

**Dictionary of form:** {'TOTAL': summed distance of all signals, 'target1: distance of 1st target', ... 'targetN': distance of Nth target }

## Return type dict

bayescmd.abc.distances.manhattan\_dist(data1, data2)

Get the Manhattan distance between two numpy arrays.

# **Parameters**

• data1 (np.ndarray) - First data array.

The shape should match that of data2 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

• data2 (np.ndarray) – Second data array.

The shape should match that of data1 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

**Returns d** – Manhattan distance measure

Return type float

bayescmd.abc.distances.mean\_absolute\_error\_dist(data1, data2)

Get the normalised manhattan distance between two numpy arrays.

## **Parameters**

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• data1 (np.ndarray) – First data array.

The shape should match that of data2 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

• data2 (np.ndarray) – Second data array.

The shape should match that of data1 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

**Returns d** – Normalised Manhattan distance measure

## Return type float

bayescmd.abc.distances.mean\_square\_error\_dist(data1, data2)

Get the Mean Square Error distance between two numpy arrays.

#### **Parameters**

• data1 (np.ndarray) - First data array.

The shape should match that of data2 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

• data2 (np.ndarray) - Second data array.

The shape should match that of data1 and the number of rows should match the number of model outputs i.e. 2 model outputs will be two rows.

**Returns d** – Mean Square Error distance measure

Return type float

bayescmd.abc.distances.zero\_array(array, zero\_flag)

Zero an array of data with its initial values.

## **Parameters**

- array (list) List of data
- zero\_flags (bool) Boolean indicating if data needs zeroing

Returns zerod – Zero'd list

Return type list

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CHAPTER
THREE

# **JSONPARSING**

..automodule:: bayescmd.jsonParsing.modelJSON

CHAPTER
FOLIB

# **MISCELLANEOUS**

Here you will find a number of useful functions that are used throughout the general BayesCMD package.

# CHAPTER

# **FIVE**

# **INDICES AND TABLES**

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