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The package `brian2modelfitting` is a tool for parameter fitting of neuron models in the Brian 2 simulator.

Please contact us at brian-development@googlegroups.com (https://groups.google.com/forum/#!forum/brian-development) if you are interested in contributing.

Please report bugs at the github issue tracker or to briansupport@googlegroups.com (https://groups.google.com/forum/#!forum/briansupport).
The `brian2modelfitting` toolbox offers allows the user to perform data driven optimization for custom neuronal models specified with Brian 2.

The toolbox allows the user to find the best fit of the parameters for recorded traces and spike trains. Just like Brian itself, the Model Fitting Toolbox is designed to be easy to use and save time through automatic parallelization of the simulations using code generation.
2.1 Model Fitting

2.1.1 Introduction

The \texttt{brian2modelfitting} toolbox provides three optimization classes:

- \texttt{TraceFitter}
- \texttt{SpikeFitter}
- \texttt{OnlineTraceFitter}

The classes expect a model and data as an input and returns the best fit of parameters and the corresponding error. The toolbox can optimize over multiple traces (e.g. input currents) at the same time.

In following documentation we assume that \texttt{brian2modelfitting} has been imported like this:

\begin{verbatim}
from brian2modelfitting import *
\end{verbatim}

Installation

To install Model Fitting alongside Brian2 you can use pip, by using a pip utility:

\begin{verbatim}
pip install brian2modelfitting
\end{verbatim}

Testing Model Fitting

Version on master branch gets automatically tested with Travis services. To test the code yourself, you will need to have \texttt{pytest} installed and run the command:

\begin{verbatim}
pytest
\end{verbatim}
2.1.2 How it works

Model fitting script requires three components:

- A **Fitter** of choice: object that will perform the optimization
- A **metric**: to compare results and decide which one is the best
- An **optimization** algorithm: to decide which parameter combinations to try

All of which need to be initialized for fitting application. Each optimization works with a following scheme:

```python
opt = Optimizer()
m= Metric()

fitter = Fitter(...)
result, error = fitter.fit(metric=m, optimizer=opt, ...)
```

The proposed solution is developed using a modular approach, where both the optimization method and metric to be optimized can be easily swapped out by a custom implementation.

**Fitter** objects require ‘model’ defined as an **Equations** object or as a string, that has parameters that will be optimized specified as constants in the following way:

```python
model = '''
...
g_na : siemens (constant)
g_kd : siemens (constant)
gl : siemens (constant)
...'''
```

**Initialization of Fitter requires:**

- `dt` - time step
- `input` - set of input traces (list or array)
- `output` - set of goal output (traces/spike trains) (list or array)
- `input_var` - name of the input trace variable (string)
- `output_var` - name of the output trace variable (string)
- `n_samples` - number of samples to draw in each round (limited by method)
- `reset`, and `threshold` in case of spiking neurons (can take refractory as well)

Additionally, upon call of `fit()`, object requires:

- `n_rounds` - number of rounds to optimize over
- parameters with ranges to be optimized over

...as well as an `optimizer` and a `metric`

Each free parameter of the model that shall be fitted is defined by two values:

```python
param_name = [min, max]
```

**Ready to use elements**

Alongside three optimization classes:
### Brian2modelfitting, Release 0.3

- **TraceFitter**
- **SpikeFitter**
- **OnlineTraceFitter**

We also provide ready optimizers:

- **NevergradOptimizer**
- **SkoptOptimizer**

and metrics:

- **MSEMetric** (for **TraceFitter**)
- **GammaFactor** (for **SpikeFitter**)

Example of **TraceFitter** with all of the necessary arguments:

```python
fitter = TraceFitter(model=model,
                     input=inp_traces,
                     output=out_traces,
                     input_var='I',
                     output_var='v',
                     dt=0.1*ms,
                     n_samples=5)
result, error = fitter.fit(optimizer=optimizer,
                           metric=metric,
                           n_rounds=1,
                           gl=[1e-8*siemens*cm**-2 * area, 1e-3*siemens*cm**-2 * area],)
```

### Remarks

- After performing first fitting, user can continue the optimization with another `fit()` run.
- Number of samples can not be changed between rounds or `fit()` calls, due to parallelization of the simulations.

**Warning:** User is not allowed to change the optimizer or metric between `fit()` calls.

### 2.1.3 Tutorial: TraceFitter

In following documentation we will explain how to get started with using **TraceFitter**. Here we will optimize conductances for a Hodgkin-Huxley cell model.

We start by importing `brian2` and `brian2modelfitting`:

```python
from brian2 import *
from brian2modelfitting import *
```

### Problem description

We have 2 step input currents of different amplitude and two “data samples” recorded from the model with goal parameters. The goal of this exercise is to optimize the conductances of the model `gl`, `g_na`, `g_kd`, for which we know the expected ranges.
Visualization of input currents and corresponding output traces which we will try to fit:

**Procedure**

**Model definition**

We have to specify all of the constants for the model.

- $C_m = 1 \times \text{ufarad} \times \text{cm}^{-2} \times \text{area}$
- $E_l = -65 \times \text{mV}$
- $E_K = -90 \times \text{mV}$
- $E_{Na} = 50 \times \text{mV}$
- $V_T = -63 \times \text{mV}$
Then, we have to define our model:

```python
model = '''
dv/dt = (gL*(E_l-v) - g_na*(m*m*m)*h*(v-ENa) - g_kd*(n*n*n*n)*(v-EK) + I)/Cm : volt

dm/dt = 0.32*(mV**-1)*(13.*mV-v+VT)/
       (exp((13.*mV-v+VT)/(4.*mV))-1.)/ms*(1-m)-0.28*(mV**-1)*(v-VT-40.*mV)/
       (exp((v-VT-40.*mV)/(5.*mV))-1.)/ms*m : 1

dn/dt = 0.032*(mV**-1)*(15.*mV-v+VT)/
        (exp((15.*mV-v+VT)/(5.*mV))-1.)/ms*(1.-n)-.5*exp((10.*mV-v+VT)/(40.*mV))/ms*n : 1

dh/dt = 0.128*exp((17.*mV-v+VT)/(18.*mV))/ms*(1.-h)-4./(1+exp((40.*mV-v+VT)/(5.*mV)))/ms*h : 1

q_na : siemens (constant)
g_kd : siemens (constant)
gl : siemens (constant)
'''
```

**Note:** You have to identify the parameters you want to optimize by adding them as constant variables to the equation.

### Optimizer and metric

Once we know our model and parameters, it’s time to pick an optimizing algorithm and a metric that will be used as a measure.

For simplicity we will use the default method provided by the `NevergradOptimizer`, i.e. “Differential Evolution”, and the `MSEMetric`, calculating the mean squared error between simulated and data traces:

```python
opt = NevergradOptimizer()
metric = MSEMetric()
```

### Fitter Initiation

Since we are going to optimize over traces produced by the model, we need to initiate the fitter `TraceFitter`. The minimum set of input parameters for the fitter, includes the `model` definition, input and output variable names and traces, time step `dt`, number of samples we want to draw in each optimization round.

```python
fitter = TraceFitter(model=model,
                     input_var='I',
                     output_var='v',
                     input=inp_trace * amp,
                     output=out_trace*mV,
                     dt=0.01*ms,
                     n_samples=10,
                     method='exponential_euler',
                     param_init={'v': -65*mV})
```

Additionally, in this example, we pick the integration method to be `exponential_euler`, and we specify the initial value of the state variable `v`, by using the option: `param_init={'v': -65*mV}`.

### Fit

We are now ready to perform the optimization, by calling the `fit` method. We need to pass the `optimizer`, `metric` and pick a number of rounds(`n_rounds`).

2.1. Model Fitting
res, error = fitter.fit(n_rounds=2,
    optimizer=opt,
    metric=metric,
    gl=[2*psiemens, 200*nsiemens],
    g_na=[200*nsiemens, 0.4*msiemens],
    g_kd=[200*nsiemens, 200*usiemens])

Output:

• res: dictionary with best fit values from this optimization
• error: corresponding error

The default output during the optimization run will tell us the best parameters in each round of optimization and the corresponding error:

```
Round 0: fit (4.22867177282197e-05, 7.504100120635022e-08, 4.772988880219001e-05)
    → with error: 0.5165218259614359
Round 1: fit (2.676589777337801e-05, 1.482336088690629e-07, 0.0001772869243329754)
    → with error: 0.1665320942433037
```

Generating traces

To generate the traces that correspond to the new best fit parameters of the model, you can use the `generate_traces` method.

```
traces = fitter.generate_traces()
```

The following plot shows the fit traces in comparison to our target data:
2.2 Optimizer

Optimizer class is responsible for maximizing a fitness function. Our approach uses gradient free global optimization methods (evolutionary algorithms, genetic algorithms, Bayesian optimization). We provided access to two libraries.

- **Nevergrad**
- **Scikit-Optimize (skopt)**
- **Custom Optimizer**

2.2.1 Nevergrad

Offers an extensive collection of algorithms that do not require gradient computation. *NevergradOptimizer* can be specified in the following way:

```python
opt = NevergradOptimizer(method='PSO')
```

where method input is a string with specific optimization algorithm.

Available methods include:

- Differential evolution. ['DE']
- Covariance matrix adaptation.['CMA']
- Particle swarm optimization.['PSO']
- Sequential quadratic programming.['SQP']

Nevergrad is still poorly documented, to check all the available methods use the following code:

```python
from nevergrad.optimization import registry
print(sorted(registry.keys()))
```

2.2.2 Scikit-Optimize (skopt)

Skopt implements several methods for sequential model-based (“blackbox”) optimization and focuses on bayesian methods. Algorithms are based on scikit-learn minimize function.

Available Methods:

- Gaussian process-based minimization algorithms ['GP']
- Sequential optimization using gradient boosted trees ['GBRT']
- Sequential optimisation using decision trees ['ET']
- Random forest regressor ['RF']

User can also provide a custom made sklearn regressor. *SkoptOptimizer* can be specified in the following way:

Parameters:

- method = ['GP', 'RF', 'ET', 'GBRT' or sklearn regressor, default='GP']
- n_initial_points [int, default=10]
- acq_func
2.2.3 Custom Optimizer

To use a different back-end optimization library, user can provide a custom class that inherits from provided abstract class `Optimizer`.

User can plug in different optimization tool, as long as it follows an `ask()` / `tell` interface. The abstract class `Optimizer` is prepared for different back-end libraries. All of the optimizer specific arguments have to be provided upon optimizers initialization.

The `ask()` / `tell` interface is used as follows:

```python
parameters = optimizer.ask()
errors = simulator.run(parameters)
optimizer.tell(parameters, errors)
results = optimizer.recommend()
```

2.3 Metric

A `Metric` specifies the fitness function measuring the performance of the simulation. This function gets applied on each simulated trace. A few metrics are already implemented and included in the toolbox, but the user can also provide their own metric.

- Mean Square Error
- GammaFactor
- FeatureMetric
- Custom Metric

2.3.1 Mean Square Error

`MSEMetric` is provided for use with `TraceFitter`. It calculates the mean squared difference between the data and the simulated trace according to the well known formula:

\[
MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2
\]

It can be initialized in the following way:

```python
metric = MSEMetric()
```
Additionally, \texttt{MSEMetric} accepts an optional input argument start time \texttt{t_start} (as a \texttt{Quantity}). The start time allows the user to ignore an initial period that will not be included in the error calculation.

\begin{verbatim}
metric = MSEMetric(t_start=5*ms)
\end{verbatim}

In \texttt{OnlineTraceFitter}, the mean square error gets calculated in online manner, with no need of specifying a metric object.

### 2.3.2 GammaFactor

\textit{GammaFactor} is provided for use with \texttt{SpikeFitter} and measures the coincidence between spike times in the simulated and the target trace. It is calculated according to:

\[
\Gamma = \left( \frac{2}{1 - 2\Delta r_{\text{exp}}} \right) \left( \frac{N_{\text{coinc}} - 2\delta N_{\text{exp}} r_{\text{exp}}}{N_{\text{exp}} + N_{\text{model}}} \right)
\]

- \( N_{\text{coinc}} \): number of coincidences
- \( N_{\text{exp}} \) and \( N_{\text{model}} \): number of spikes in experimental and model spike trains
- \( r_{\text{exp}} \): average firing rate in experimental train
- \( 2\Delta N_{\text{exp}} r_{\text{exp}} \): expected number of coincidences with a Poisson process

For more details on the gamma factor, see:

- Clopath et al. 2007, “Predicting neuronal activity with simple models of the threshold type: adaptive exponential integrate-and-fire model with two compartments.”, Neurocomp

The coincidence factor \( \Gamma \) is 1 if the two spike trains match exactly and lower otherwise. It is 0 if the number of coincidences matches the number expected from two homogeneous Poisson processes of the same rate. To turn the coincidence factor into an error term (that is lower for better matches), two options are offered. With the \texttt{rate_correction} option (used by default), the error term used is \( 2\left| r_{\text{data}} - r_{\text{model}} \right| - \Gamma \), with \( r_{\text{data}} \) and \( r_{\text{model}} \) being the firing rates in the data/model. This is useful because the coincidence factor \( \Gamma \) on its own can give high values (low errors) if the model generates many more spikes than were observed in the data; this is penalized by the above term. If \texttt{rate_correction} is set to \texttt{False}, \( 1 - \Gamma \) is used as the error.

Upon initialization the user has to specify the \( \Delta \) value, defining the maximal tolerance for spikes to be considered coincident:

\begin{verbatim}
metric = GammaFactor(delta=2*ms)
\end{verbatim}

\textbf{Warning:} The \texttt{delta} parameter has to be smaller than the smallest inter-spike interval in the spike trains.

### 2.3.3 FeatureMetric

\textit{FeatureMetric} is provided for use with \texttt{TraceFitter}. This metric allows the user to optimize the match of certain features between the simulated and the target trace. The features get calculated by Electrophys Feature Extract Library (eFEL) library, for which the documentation is available under following link: \url{https://efel.readthedocs.io}

To get a list of all the available eFEL features, you can run the following code:
import efel
efel.api.getFeatureNames()

Note: Currently, only features that are described by a single value are supported (e.g. the time of the first spike can be used, but not the times of all spikes).

To use the FeatureMetric, you have to provide the following input parameters:

- stim_times - a list of times indicating start and end of the stimulus for each of input traces. This information is used by several features, e.g. the voltage_base feature will consider the average membrane potential during the last 10% of time before the stimulus (see the eFel documentation for details).
- feat_list - list of strings with names of features to be used
- combine - function to be used to compare features between output and simulated traces (uses the absolute difference between the values by default).

Example code usage:

```python
stim_times = [(50*ms, 100*ms), (50*ms, 100*ms), (50*ms, 100*ms), (50, 100*ms)]
feat_list = ['voltage_base', 'time_to_first_spike', 'Spikecount']
metric = FeatureMetric(traces_times, feat_list, combine=None)
```

Note: If times of stimulation are the same for all of the traces, then you can specify a single interval instead:

```python
stim_times = [(50*ms, 100*ms)].
```

### 2.3.4 Custom Metric

Users are not limited to the metrics provided in the toolbox. If needed, they can provide their own metric based on one of the abstract classes TraceMetric and SpikeMetric.

A new metric will need to specify the following functions:

- **get_features()** calculates features / errors for each of the simulations. The representation of the model results and the target data depend on whether traces or spikes are fitted, see below.
- **get_errors()** weights features/multiple errors into one final error per each set of parameters and inputs. The features are received as a 2-dimensional ndarray of shape (n_samples, n_traces) The output has to be an array of length n_samples, i.e. one value for each parameter set.
- **calc()** performs the error calculation across simulation for all parameters of each round. Already implemented in the abstract class and therefore does not need to be reimplemented necessarily.

**TraceMetric**

To create a new metric for TraceFitter, you have to inherit from TraceMetric and overwrite the get_features and/or get_errors method. The model traces for the get_features function are provided as a 3-dimensional ndarray of shape (n_samples, n_traces, time steps), where n_samples are the number of different parameter sets that have been evaluated, and n_traces the number of different stimuli that have been evaluated for each parameter set. The output of the function has to take the shape of (n_samples, n_traces). This array is the input to the get_errors method (see above).
class NewTraceMetric(TraceMetric):
    def get_features(self, model_traces, data_traces, dt):
        ...

    def get_errors(self, features):
        ...

SpikeMetric

To create a new metric for SpikeFitter, you have to inherit from SpikeMetric. Inputs of the metric in `get_features` are a nested list structure for the spikes generated by the model: a list where each element contains the results for a single parameter set. Each of these results is a list for each of the input traces, where the elements of this list are numpy arrays of spike times (without units, i.e. in seconds). For example, if two parameters sets and 3 different input stimuli were tested, this structure could look like this:

```python
[
    [array([0.01, 0.5]), array([]), array([])],
    [array([0.02]), array([]), array([])]
]
```

This means that the both parameter sets only generate spikes for the first input stimulus, but the first parameter sets generates two while the second generates only a single one.

The target spikes are represented in the same way as a list of spike times for each input stimulus. The results of the function have to be returned as in TraceMetric, i.e. as a 2-d array of shape (n_samples, n_traces).

2.4 Advanced Features

This part of documentation list other features provided alongside or inside Fitter objects, to help the user with easier and more flexible applications.

- Parameters initialization
- Restart
- Callback function
- Generate Traces
- Results
- Standalone mode
- OnlineTraceFitter

2.4.1 Parameters initialization

Whilst running Fitter user can specify values with which model evaluation of differential equations start.

The fitting functions accept additional dictionary input to address that. To do so, dictionary argument has to be added to Fitter initialization:
param_init = {'v': -30*mV}

fitter = TraceFitter(..., param_init = {'v': -30*mV})

### 2.4.2 Restart

By default any *Fitter* works in continuous optimization mode between run, where all of the parameters drawn are being evaluated.

Through changing the input flag in *fit()*: *restart* to True, user can reset the optimizer and start the optimization from scratch.

Used by Fitter optimizer and metric can only be changed when the flat is True.

### 2.4.3 Callback function

To visualize the progress of the optimization we provided few possibilities of feedback inside *Fitter*.

The ‘callback’ input provides few default options, updated in each round:

- 'text' (default) that prints out the parameters of the best fit and corresponding error
- 'progressbar' that uses *tqdm.autonotebook* to provide a progress bar
- None for non-verbose option

as well as customized feedback option. User can provide a *callable* (i.e. function), that will provide an output or printout. If callback returns True the fitting execution is interrupted.

User gets four arguments to customize over:

- *params* - set of parameters from current round
- *errors* - set of errors from current round
- *best_params* - best parameters globally, from all rounds
- *best_error* - best parameters globally, from all rounds
- *index* - index of current round

An example function:

```python
def callback(params, errors, best_params, best_error, index):
    print('index {}
 errors minimum: {:.{}'.format(index, min(errors)))
```

```python
fitter = TraceFitter(...)  
result, error = fitter.fit(..., callback=...)  
```

### 2.4.4 Generate Traces

With the same *Fitter* class user can also generate the traces with newly optimized parameters.

To simulate and visualize the traces or spikes for the parameters of choice. For a quick access to best fitted set of parameters Fitter classes provided ready to use functions:

- *generate_traces* inside *TraceFitter*
• `generate_spikes` inside `SpikeFitter`

Functions can be called after fitting in the following manner, without any input arguments:

```python
fitter = TraceFitter(...)  
results, error = fitter.fit(...)  
traces = fitter.generate_traces()
```

```python
fitter = SpikeFitter(...)  
results, error = fitter.fit(...)  
spikes = fitter.generate_traces()
```

**Custom generate**

To create traces for other parameters, or generate traces after spike train fitting, user can call the `-generate` call, that takes in following arguments:

```python
fitter.generate(params=None, output_var=None, param_init=None, level=0)
```

Where `params` is a dictionary of parameters for which the traces we generate. `output_var` provides an option to pick variable for visualization. With `param_init`, user can define the initial values for differential equations. `level` allows for specification of namespace level from which we get the constant parameters of the model.

### 2.4.5 Results

Fitter class stores all of the parameters examined by the optimizer as well as the corresponding error. To retrieve them you can call the `-results`.

```python
fitter = TraceFitter(...)  
...  
traces = fitter.generate_traces()
```

```python
fitter = SpikeFitter(...)  
...  
results = fitter.results(format='dataframe')
```

Results can be returned in one of the following formats:

- `'list'` (default) returns a list of dictionaries with corresponding parameters (including units) and errors
- `'dict'` returns a dictionary of arrays with corresponding parameters (including units) and errors
- `'dataframe'` returns a DataFrame (without units)

**Example output:**

`'list':`

```json
[['gl': 80.61365773 * nsiemens, 'g_kd': 66.00430921 * usiemens, 'g_na': 145.15634566 * usiemens, 'errors': 0.00019059452295872703],
 [{'gl': 83.29319947 * nsiemens, 'g_kd': 168.75187749 * usiemens, 'g_na': 130.64547027 * usiemens, 'errors': 0.00021434415430605653},
 ...]
```

`'dict':`
['g_na': array([[176.4472297 , 212.57019659, ...]) * usiemens,
'g_kd': array([[ 43.82344525,  54.35309635, ...]) * usiemens,
'gl': array([[ 69.23559876, 134.68463669, ...]) * nsiemens,
'errors': array([[1.16788502, 0.5253008 , ...]])}

'dataframe':

<table>
<thead>
<tr>
<th></th>
<th>g_na</th>
<th>gl</th>
<th>g_kd</th>
<th>errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.000280</td>
<td>8.870238e-08</td>
<td>0.000047</td>
<td>0.521425</td>
</tr>
<tr>
<td>1</td>
<td>0.000192</td>
<td>1.121861e-07</td>
<td>0.000118</td>
<td>0.387140</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

### 2.4.6 Standalone mode

Just like with regular Brian script, modelfitting computations can be performed in Runtime mode (default) or Standalone mode. ([https://brian2.readthedocs.io/en/stable/user/computation.html](https://brian2.readthedocs.io/en/stable/user/computation.html))

To enable this mode, add the following line after your Brian import, but before your simulation code:

```python
set_device('cpp_standalone')
```

**Important notes:**

**Warning:** In standalone mode one script can not be used to contain multiple `-Fitter`, use separate scripts!

Before generation of traces, you have to reinitialize the device add additional piece of code before calling `generate`:

```python
device.reinit()
device.activate()
fitter.generate_traces()
```

**Warning:** Device reinitialization causes the device to reset, and disables the possibility for further fitting or retrieving information from fitter monitors.

### 2.4.7 OnlineTraceFitter

`OnlineTraceFitter` was created to work with long traces or big optimization. This `Fitter` uses online Mean Square Error as a metric. When `fit()` is called there is no need of specifying a metric, that is by default set to None. Instead the errors are calculated with use of Brian's `run_regularly`, with each simulation.

```python
fitter = OnlineTraceFitter(model=model,
    input=inp_traces,
    output=out_traces,
    input_var='I',
    output_var='v',
    dt=0.1*ms,
    n_samples=5)
```

(continues on next page)
result, error = fitter.fit(optimizer=optimizer,
    n_rounds=1,
    gl=[[1e-8*siemens*cm**-2 * area, 1e-3*siemens*cm**-2 * area],])

2.5 Examples

2.5.1 Simple Examples

Following pieces of code show an example of Fitter class calls with possible inputs.

TraceFitter

n_opt = NevergradOptimizer(method='PSO')
metric = MSEMetric()
fitter = TraceFitter(model=model,
    input_var='I',
    output_var='v',
    input=inp_trace,
    dt=0.1*ms,
    method='exponential_euler',
    output=out_trace,
    n_samples=5)
results, error = fitter.fit(optimizer=n_opt,
    metric=metric,
    callback='text',
    n_rounds=1,
    param_init={'v': -65*mV},
    gl=[[10*nS*cm**-2 * area, 1*mS*cm**-2 * area],
        g_na=[1*mS*cm**-2 * area, 2000*mS*cm**-2 * area],
        g_kd=[1*mS*cm**-2 * area, 1000*mS*cm**-2 * area]])

SpikeFitter

n_opt = SkoptOptimizer('ET')
metric = GammaFactor(dt, delta=2*ms)
fitter = SpikeFitter(model=eqs,
    input_var='I',
    dt=0.1*ms,
    input=inp_traces,
    output=out_spikes,
    n_samples=30,
    threshold='v > -50*mV',
    reset='v = -70*mV',
    method='exponential_euler')
2.5.2 Multirun of Hodgkin-Huxley

Here you can download the data: input_traces output_traces

```python
import numpy as np
from brian2 import *
from brian2modelfitting import *
```

To load the data, use following code:

```python
import pandas as pd
# Load Input and Output Data
df_inp_traces = pd.read_csv('input_traces_hh.csv')
df_out_traces = pd.read_csv('output_traces_hh.csv')

inp_traces = df_inp_traces.to_numpy()
inp_traces = inp_traces[:, 1:]

out_traces = df_out_traces.to_numpy()
out_traces = out_traces[:, 1:]
```

Then the multiple round optimization can be run with following code:

```python
# Model Fitting
## Parameters
area = 20000*umetre**2
El = -65*mV
EK = -90*mV
ENa = 50*mV
VT = -63*mV
dt = 0.01*ms
defaultclock.dt = dt

## Modle Definition
eqs = Equations(
    'dv/dt = (gl*(El-v) - g_na*(m*m*m)*h*(v-ENa) - g_kd*(n*n*n*n)*(v-EK) + I)/Cm : volt
     dm/dt = 0.32*(mV**-1)*(13.*mV-v+VT)/
           (exp((13.*mV-v+VT)/(4.*mV))-1.)/ms*(1-m)-0.28*(mV**-1)*(v-VT-40.*mV)/
           (exp((v-VT-40.*mV)/(5.*mV))-1.)/ms*m : 1
     dn/dt = 0.032*(mV**-1)*(15.*mV-v+VT)/
           (exp((15.*mV-v+VT)/(5.*mV))-1.)/ms*(1-n)-.5*exp((10.*mV-v+VT)/(40.*mV))/ms*n : 1
     dh/dt = 0.128*exp(((17.*mV-v+VT)/(18.*mV))/ms*(1-h)-4./(1+exp((40.*mV-v+VT)/(5.*mV)))/
           ms*h : 1
    g_na : siemens (constant)
    g_kd : siemens (constant)
    gl : siemens (constant)
    Cm : farad (constant)
)'
```

(results, error = fitter.fit(n_rounds=2,
      optimizer=n_opt,
      metric=metric,
      gL=[20*nS, 40*nS],
      C = [0.5*nF, 1.5*nF])

(continued from previous page)
## Optimization and Metric Choice

```python
n_opt = NevergradOptimizer()
metric = MSEMetric()
```

### Fitting

```python
fitter = TraceFitter(model=eqs, input_var='I', output_var='v',
    input=inp_traces*amp, output=out_traces*mV, dt=dt,
    n_samples=20,
    param_init={'v': -65*mV},
    method='exponential_euler')
```

```python
res, error = fitter.fit(n_rounds=2,
    optimizer=n_opt, metric=metric,
    callback='progressbar',
    gl = [1e-09 *siemens, 1e-07 *siemens],
    g_na = [2e-06*siemens, 2e-04*siemens],
    g_kd = [6e-07*siemens, 6e-05*siemens],
    Cm=0.1*ufarad*cm**-2 * area, 2*ufarad*cm**-2 * area)
```

### Show results

```python
all_output = fitter.results(format='dataframe')
print(all_output)
```

### Second round

```python
res, error = fitter.fit(restart=True,
    n_rounds=20,
    optimizer=n_opt, metric=metric,
    callback='progressbar',
    gl = [1e-09 *siemens, 1e-07 *siemens],
    g_na = [2e-06*siemens, 2e-04*siemens],
    g_kd = [6e-07*siemens, 6e-05*siemens],
    Cm=0.1*ufarad*cm**-2 * area, 2*ufarad*cm**-2 * area)
```

To get the results and traces:

```python
## Visualization of the results
fits = fitter.generate_traces(params=None, param_init={'v': -65*mV})
```

```python
fig, axes = plt.subplots(ncols=5, figsize=(20,5), sharey=True)
for ax, data, fit in zip(axes, out_traces, fits):
    ax.plot(data.transpose())
    ax.plot(fit.transpose()/mV)
plt.show()
```
3.1 brian2modelfitting package

3.1.1 Subpackages and -modules

brian2modelfitting.tests package

brian2modelfitting.tests.run()

brian2modelfitting.metric module

class brian2modelfitting.metric.FeatureMetric(stim_times, feat_list, weights=None, combine=None, t_start=0. * second)
Bases: brian2modelfitting.metric.TraceMetric
calc(model_traces, data_traces, dt)
    Perform the error calculation across all parameters, calculate error between each output trace and corresponding simulation.

Parameters

• model_traces (ndarray) – Traces that should be evaluated and compared to the target data. Provided as an ndarray of shape (n_samples, n_traces, time steps) where n_samples is the number of parameter sets that have been evaluated, and n_traces is the number of stimuli.

• data_traces (ndarray) – The target traces to which the model should be compared. An ndarray of shape (n_traces, time steps).

• dt (Quantity) – The length of a single time step.

Returns Total error for each set of parameters, i.e. an array of shape (n_samples, ).

Return type ndarray
check_values (feat_list)
   Removes all the None values and checks for array features

feat_to_err (d1, d2)

get_errors (features)
   Function weights features/multiple errors into one final error per each set of parameters.
   The output of the function has to take shape of (n_samples,).

   Parameters
   features (ndarray) – 2D array of shape (n_samples, n_traces) with
   the features/errors for each simulated trace

   Returns
   Errors for each parameter set, i.e. of shape (n_samples, )

Return type
   ndarray

get_features (traces, output, dt)
   Calculate the features/errors for each simulated trace, by comparing it to the corresponding data trace.

   Parameters

   model_traces (ndarray) – Traces that should be evaluated and compared to the target data. Provided as an ndarray of shape (n_samples, n_traces, time steps), where n_samples are the number of different parameter sets that have been evaluated, and n_traces are the number of input stimuli.

   data_traces (ndarray) – The target traces to which the model should be compared. An ndarray of shape (n_traces, time steps).

   dt (Quantity) – The length of a single time step.

   Returns
   An ndarray of shape (n_samples, n_traces) returning the error/feature value for each simulated trace.

Return type
   ndarray

class brian2modelfitting.metric.GammaFactor(**kwds)
Bases: brian2modelfitting.metric.SpikeMetric
   Calculate gamma factors between goal and calculated spike trains, with precision delta.

References:


calc (model_spikes, data_spikes, dt)
   Perform the error calculation across all parameters, calculate error between each output trace and corresponding simulation.

   Parameters

   model_spikes (list of list of ndarray) – A nested list structure for the spikes generated by the model: a list where each element contains the results for a single parameter set. Each of these results is a list for each of the input traces, where the elements of this list are numpy arrays of spike times (without units, i.e. in seconds).

   data_spikes (list of ndarray) – The target spikes for the fitting, represented in the same way as model_spikes, i.e. as a list of spike times for each input stimulus.
• \( \text{dt} \) (\text{Quantity}) – The length of a single time step.

**Returns**
Total error for each set of parameters, i.e. an array of shape \((n\_samples, )\)

**Return type** ndarray

**get\_errors** (\text{features})
Function weights features/multiple errors into one final error per each set of parameters.

The output of the function has to take shape of \((n\_samples,)\).

**Parameters**
\text{features} (ndarray) – 2D array of shape \((n\_samples, n\_traces)\) with the features/errors for each simulated trace

**Returns**
Errors for each parameter set, i.e. of shape \((n\_samples, )\)

**Return type** ndarray

**get\_features** (traces, output, dt)
Calculate the features/errors for each simulated spike train by comparing it to the corresponding data spike train.

**Parameters**
• \text{model\_spikes} (list of list of ndarray) – A nested list structure for the spikes generated by the model: a list where each element contains the results for a single parameter set. Each of these results is a list for each of the input traces, where the elements of this list are numpy arrays of spike times (without units, i.e. in seconds).

• \text{data\_spikes} (list of ndarray) – The target spikes for the fitting, represented in the same way as \text{model\_spikes}, i.e. as a list of spike times for each input stimulus.

• \text{dt} (\text{Quantity}) – The length of a single time step.

**Returns**
An ndarray of shape \((n\_samples, n\_traces)\) returning the error/feature value for each simulated trace.

**Return type** ndarray

**class** brian2modelfitting.metric.MSEMetric(**kwds**)
**Bases:** brian2modelfitting.metric.TraceMetric

Mean Square Error between goal and calculated output.

**calc** (model\_traces, data\_traces, dt)
Perform the error calculation across all parameters, calculate error between each output trace and corresponding simulation.

**Parameters**
• \text{model\_traces} (ndarray) – Traces that should be evaluated and compared to the target data. Provided as an ndarray of shape \((n\_samples, n\_traces, time\_steps)\) where \(n\_samples\) is the number of parameter sets that have been evaluated, and \(n\_traces\) is the number of stimuli.

• \text{data\_traces} (ndarray) – The target traces to which the model should be compared. An ndarray of shape \((n\_traces, time\_steps)\).

• \text{dt} (\text{Quantity}) – The length of a single time step.

**Returns**
Total error for each set of parameters, i.e. an array of shape \((n\_samples, )\).

**Return type** ndarray
get_errors (features)
Function weights features/multiple errors into one final error per each set of parameters.

The output of the function has to take shape of (n_samples,).

Parameters features (ndarray) – 2D array of shape (n_samples, n_traces) with the features/errors for each simulated trace

Returns Errors for each parameter set, i.e. of shape (n_samples,)

Return type ndarray

get_features (model_traces, data_traces, dt)
Calculate the features/errors for each simulated trace, by comparing it to the corresponding data trace.

Parameters

• model_traces (ndarray) – Traces that should be evaluated and compared to the target data. Provided as an ndarray of shape (n_samples, n_traces, time steps), where n_samples are the number of different parameter sets that have been evaluated, and n_traces are the number of input stimuli.

• data_traces (ndarray) – The target traces to which the model should be compared. An ndarray of shape (n_traces, time steps).

• dt (Quantity) – The length of a single time step.

Returns An ndarray of shape (n_samples, n_traces) returning the error/feature value for each simulated trace.

Return type ndarray

class brian2modelfitting.metric.Metric(**kwds)
Bases: object

Metric abstract class to define functions required for a custom metric To be used with modelfitting Fitters.

calc (model_results, data_results, dt)
Perform the error calculation across all parameter sets by comparing the simulated to the experimental data.

Parameters

• model_results – Results generated by the model. The type and shape of this data depends on the fitting problem. See TraceMetric.calc and SpikeMetric.calc.

• data_results – The experimental data that the model is fit against. See TraceMetric.calc and SpikeMetric.calc for the type/shape of the data.

• dt (Quantity) – The length of a single time step.

Returns Total error for each set of parameters, i.e. an array of shape (n_samples,).

Return type ndarray

get_errors (features)
Function weights features/multiple errors into one final error per each set of parameters.

The output of the function has to take shape of (n_samples,).

Parameters features (ndarray) – 2D array of shape (n_samples, n_traces) with the features/errors for each simulated trace

Returns Errors for each parameter set, i.e. of shape (n_samples,)

Return type ndarray
**get_features** *(model_results, target_results, dt)*

Function calculates features / errors for each of the input traces.

The output of the function has to take shape of (n_samples, n_traces).

**class** brian2modelfitting.metric.SpikeMetric(**kwds**)

Bases: brian2modelfitting.metric.Metric

A metric for comparing the spike trains.

**calc** *(model_spikes, data_spikes, dt)*

Perform the error calculation across all parameters, calculate error between each output trace and corresponding simulation.

**Parameters**

- **model_spikes** (list of list of ndarray) – A nested list structure for the spikes generated by the model: a list where each element contains the results for a single parameter set. Each of these results is a list for each of the input traces, where the elements of this list are numpy arrays of spike times (without units, i.e. in seconds).

- **data_spikes** (list of ndarray) – The target spikes for the fitting, represented in the same way as model_spikes, i.e. as a list of spike times for each input stimulus.

- **dt** (Quantity) – The length of a single time step.

**Returns** Total error for each set of parameters, i.e. an array of shape (n_samples, )

**Return type** ndarray

**get_errors** *(features)*

Function weights features/multiple errors into one final error per each set of parameters.

The output of the function has to take shape of (n_samples, ).

**Parameters** features (ndarray) – 2D array of shape (n_samples, n_traces) with the features/errors for each simulated trace

**Returns** Errors for each parameter set, i.e. of shape (n_samples, )

**Return type** ndarray

**get_features** *(model_spikes, data_spikes, dt)*

Calculate the features/errors for each simulated spike train by comparing it to the corresponding data spike train.

**Parameters**

- **model_spikes** (list of list of ndarray) – A nested list structure for the spikes generated by the model: a list where each element contains the results for a single parameter set. Each of these results is a list for each of the input traces, where the elements of this list are numpy arrays of spike times (without units, i.e. in seconds).

- **data_spikes** (list of ndarray) – The target spikes for the fitting, represented in the same way as model_spikes, i.e. as a list of spike times for each input stimulus.

- **dt** (Quantity) – The length of a single time step.

**Returns** An ndarray of shape (n_samples, n_traces) returning the error/feature value for each simulated trace.

**Return type** ndarray

**class** brian2modelfitting.metric.TraceMetric(**kwds**)

Bases: brian2modelfitting.metric.Metric
Input traces have to be shaped into 2D array.

**calc** *(model_traces, data_traces, dt)*

Perform the error calculation across all parameters, calculate error between each output trace and corresponding simulation.

**Parameters**

- **model_traces** *(ndarray)* – Traces that should be evaluated and compared to the target data. Provided as an *ndarray* of shape *(n_samples, n_traces, time steps)* where *n_samples* is the number of parameter sets that have been evaluated, and *n_traces* is the number of stimuli.
- **data_traces** *(ndarray)* – The target traces to which the model should be compared. An *ndarray* of shape *(n_traces, time steps)*.
- **dt** *(Quantity)* – The length of a single time step.

**Returns** Total error for each set of parameters, i.e. an array of shape *(n_samples, )*.

**Return type** *ndarray*

**get_errors** *(features)*

Function weights features/multiple errors into one final error per each set of parameters.

The output of the function has to take shape of *(n_samples, ).*

**Parameters** **features** *(ndarray)* – 2D array of shape *(n_samples, n_traces)* with the features/errors for each simulated trace

**Returns** Errors for each parameter set, i.e. of shape *(n_samples, )*

**Return type** *ndarray*

**get_features** *(model_traces, data_traces, dt)*

Calculate the features/errors for each simulated trace, by comparing it to the corresponding data trace.

**Parameters**

- **model_traces** *(ndarray)* – Traces that should be evaluated and compared to the target data. Provided as an *ndarray* of shape *(n_samples, n_traces, time steps)*, where *n_samples* are the number of different parameter sets that have been evaluated, and *n_traces* are the number of input stimuli.
- **data_traces** *(ndarray)* – The target traces to which the model should be compared. An *ndarray* of shape *(n_traces, time steps)*.
- **dt** *(Quantity)* – The length of a single time step.

**Returns** An *ndarray* of shape *(n_samples, n_traces)* returning the error/feature value for each simulated trace.

**Return type** *ndarray*

**brian2modelfitting.metric.calc_eFEL** *(traces, inp_times, feat_list, dt)*

**brian2modelfitting.metric.firing_rate** *(spikes)*

Returns rate of the spike train

**brian2modelfitting.metric.get_gamma_factor** *(model, data, delta, time, dt, rate_correction=True)*

Calculate gamma factor between model and target spike trains, with precision delta.

**Parameters**

- **model** *(list or ndarray)* – model trace
Brian2modelfitting, Release 0.3

- **data** (list or ndarray) – data trace
- **delta** (Quantity) – time window
- **dt** (Quantity) – time step
- **time** (Quantity) – total time of the simulation
- **rate_correction** (bool) – Whether to include an error term that penalizes differences in firing rate, following Clopath et al., Neurocomputing (2007).

**Returns**
An error based on the Gamma factor. If `rate_correction` is used, then the returned error is $2 \left| \frac{r_{\text{data}} - r_{\text{model}}}{r_{\text{data}}} \right| - \Gamma$ (with $r_{\text{data}}$ and $r_{\text{model}}$ being the firing rates in the data/model, and $\Gamma$ the coincidence factor). Without `rate_correction`, the error is $1 - \Gamma$. Note that the coincidence factor $\Gamma$ has a maximum value of 1 (when the two spike trains are exactly identical) and a value of 0 if there are only as many coincidences as expected from two homogeneous Poisson processes of the same rate. It can also take negative values if there are fewer coincidences than expected by chance.

**Return type** float

**brian2modelfitting.fitter module**

```python
class brian2modelfitting.fitter.Fitter(dt, model, input, output, input_var, output_var, 
n_samples, threshold, reset, refractory, method, 
param_init)
```

**Bases:** object

Base Fitter class for model fitting applications.

Creates an interface for model fitting of traces with parameters draw by gradient-free algorithms (through ask/tell interfaces).

Initiates $n_{\text{neurons}} = \text{num input traces} \times \text{num samples}$, to which drawn parameters get assigned and evaluates them in parallel.

**Parameters**
- **dt** (Quantity) – The size of the time step.
- **model** (Equations or str) – The equations describing the model.
- **input** (ndarray or Quantity) – A 2D array of shape ($n_{\text{traces}}$, time steps) given the input that will be fed into the model.
- **output** (ndarray or Quantity or list) – Recorded output of the model that the model should reproduce. Should be a 2D array of the same shape as the input when fitting traces with `TraceFitter`, a list of spike times when fitting spike trains with `SpikeFitter`.
- **input_var** (str) – The name of the input variable in the model. Note that this variable should be used in the model (e.g. a variable $I$ that is added as a current in the membrane potential equation), but not defined.
- **output_var** (str) – The name of the output variable in the model. Only needed when fitting traces with `TraceFitter`.
- **n_samples** (int) – Number of parameter samples to be optimized over in a single iteration.
- **threshold** (str, optional) – The condition which produces spikes. Should be a boolean expression as a string.
- **reset** (str, optional) – The (possibly multi-line) string with the code to execute on reset.
• **refractory** *(str or Quantity, optional)* – Either the length of the refractory period (e.g. 2*ms), a string expression that evaluates to the length of the refractory period after each spike (e.g. `(1 + rand())*ms`), or a string expression evaluating to a boolean value, given the condition under which the neuron stays refractory after a spike (e.g. `v > -20*mV`)

• **method** *(str, optional)* – Integration method

• **param_init** *(dict, optional)* – Dictionary of variables to be initialized with respective values

**calc_errors** *(metric)*

Abstract method required in all Fitter classes, used for calculating errors

**Parameters**

- **metric** *(Metric children)* – Child of Metric class, specifies optimization metric

**fit** *(optimizer, metric=None, n_rounds=1, callback='text', restart=False, **params)*

Run the optimization algorithm for given amount of rounds with given number of samples drawn. Return best set of parameters and corresponding error.

**Parameters**

- **optimizer** *(Optimizer children)* – Child of Optimizer class, specific for each library.
- **metric** *(Metric children)* – Child of Metric class, specifies optimization metric
- **n_rounds** *(int)* – Number of rounds to optimize over (feedback provided over each round).
- **callback** *(str or Callable)* – Either the name of a provided callback function (text or progressbar), or a custom feedback function `func(results, errors, parameters, index)`. If this function returns `True` the fitting execution is interrupted.
- **restart** *(bool)* – Flag that reinitializes the Fitter to reset the optimization. With restart True user is allowed to change optimizer/metric.
- ****params – bounds for each parameter

**Returns**

- **best_results** *(dict)* – dictionary with best parameter set
- **error** *(float)* – error value for best parameter set

**generate** *(params=None, output_var=None, param_init=None, level=0)*

Generates traces for best fit of parameters and all inputs. If provided with other parameters provides those.

**Parameters**

- **params** *(dict)* – Dictionary of parameters to generate fits for.
- **output_var** *(str)* – Name of the output variable to be monitored.
- **param_init** *(dict)* – Dictionary of initial values for the model.
- **level** *(int, optional)* – How much farther to go down in the stack to find the namespace.

**optimization_iter** *(optimizer, metric)*

Function performs all operations required for one iteration of optimization. Drawing parameters, setting them to simulator and calculating the error.

**Returns**

- **results** *(list)* – recommended parameters
- **parameters** *(list of list)* – drawn parameters


- **errors** (*list*) – calculated errors

### results (*format='list'*)

Returns all of the gathered results (parameters and errors). In one of the 3 formats: ‘dataframe’, ‘list’, ‘dict’.

- **Parameters**
  - **format** (*str*) – The desired output format. Currently supported: *dataframe*, *list*, *dict*.

- **Returns**
  - ‘dataframe’: returns pandas *DataFrame* without units
  - ‘list’: list of dictionaries
  - ‘dict’: dictionary of lists

- **Return type**
  - *object*

### setup_neuron_group (*n_neurons, namespace, name='neurons'*)

Setup neuron group, initialize required number of neurons, create namespace and initialize the parameters.

- **Parameters**
  - **n_neurons** (*int*) – number of required neurons
  - **namespace** – arguments to be added to NeuronGroup namespace

- **Returns**
  - *neurons* – group of neurons

- **Return type**
  - *NeuronGroup*

---

**class** brian2modelfitting.fitter.OnlineTraceFitter(*model, input_var, input, output_var, output, dt, n_samples=30, method=None, reset=None, refractory=False, threshold=None, level=0, param_init=None, t_start=0. * second)

Bases: *brian2modelfitting.fitter.Fitter*

Input nad output have to have the same dimensions.

- **calc_errors** (*metric=None*)

  Calculates error in online fashion. To be used inside optim_iter.

- **fit** (*optimizer, metric=None, n_rounds=1, callback='text', restart=False, **params*)

  Run the optimization algorithm for given amount of rounds with given number of samples drawn. Return best set of parameters and corresponding error.

- **Parameters**
  - **optimizer** (*Optimizer* children) – Child of Optimizer class, specific for each library.
  - **metric** (*Metric* children) – Child of Metric class, specifies optimization metric
  - **n_rounds** (*int*) – Number of rounds to optimize over (feedback provided over each round).
  - **callback** (*str* or *Callable*) – Either the name of a provided callback function (*text* or *progressbar*), or a custom feedback function *func(results, errors, parameters, index)*. If this function returns *True* the fitting execution is interrupted.
  - **restart** (*bool*) – Flag that reinitializes the Fitter to reset the optimization. With restart True user is allowed to change optimizer/metric.
  - **params** – bounds for each parameter

- **Returns**
  - **best_results** (*dict*) – dictionary with best parameter set

---

3.1. brian2modelfitting package
• **error** *(float)* – error value for best parameter set

**generate** *(params=None, output_var=None, param_init=None, level=0)*
Generates traces for best fit of parameters and all inputs. If provided with other parameters provides those.

Parameters

• **params** *(dict)* – Dictionary of parameters to generate fits for.

• **output_var** *(str)* – Name of the output variable to be monitored.

• **param_init** *(dict)* – Dictionary of initial values for the model.

• **level** *(int, optional)* – How much farther to go down in the stack to find the namespace.

**generate_traces** *(params=None, param_init=None, level=0)*
Generates traces for best fit of parameters and all inputs

**optimization_iter** *(optimizer, metric)*
Function performs all operations required for one iteration of optimization. Drawing parameters, setting them to simulator and calculating the error.

Returns

• **results** *(list)* – recommended parameters

• **parameters** *(list of list)* – drawn parameters

• **errors** *(list)* – calculated errors

**results** *(format='list')*
Returns all of the gathered results (parameters and errors). In one of the 3 formats: ‘dataframe’, ‘list’, ‘dict’.

Parameters **format** *(str)* – The desired output format. Currently supported: dataframe, list, or dict.

Returns

• ‘dataframe’: returns pandas **DataFrame** without units

• ‘list’: list of dictionaries

• ‘dict’: dictionary of lists

Return type **object**

**setup_neuron_group** *(n_neurons, namespace, name='neurons')*
Setup neuron group, initialize required number of neurons, create namespace and initialize the parameters.

Parameters

• **n_neurons** *(int)* – number of required neurons

• ****namespace – arguments to be added to NeuronGroup namespace

Returns **neurons** – group of neurons

Return type **NeuronGroup**

**class** **brian2modelfitting.fitter.SpikeFitter** *(model, input, output, dt, reset, threshold, input_var='I', refractory=False, n_samples=30, method=None, level=0, param_init=None)*

Bases: **brian2modelfitting.fitter.Fitter**

**calc_errors** *(metric)*
Returns errors after simulation with SpikeMonitor. To be used inside optim_iter.

**fit** *(optimizer, metric=None, n_rounds=1, callback='text', restart=False, **params)*
Run the optimization algorithm for given amount of rounds with given number of samples drawn. Return best set of parameters and corresponding error.
Parameters

- **optimizer** *(Optimizer children)* – Child of Optimizer class, specific for each library.
- **metric** *(Metric children)* – Child of Metric class, specifies optimization metric
- **n_rounds** *(int)* – Number of rounds to optimize over (feedback provided over each round).
- **callback** *(str or Callable)* – Either the name of a provided callback function (text or progressbar), or a custom feedback function func(results, errors, parameters, index). If this function returns True the fitting execution is interrupted.
- **restart** *(bool)* – Flag that reinitializes the Fitter to reset the optimization. With restart True user is allowed to change optimizer/metric.
- ****params – bounds for each parameter

Returns

- **best_results** *(dict)* – dictionary with best parameter set
- **error** *(float)* – error value for best parameter set

**generate** *(params=None, output_var=None, param_init=None, level=0)*

Generates traces for best fit of parameters and all inputs. If provided with other parameters provides those.

Parameters

- **params** *(dict)* – Dictionary of parameters to generate fits for.
- **output_var** *(str)* – Name of the output variable to be monitored.
- **param_init** *(dict)* – Dictionary of initial values for the model.
- **level** *(int, optional)* – How much farther to go down in the stack to find the namespace.

**generate_spikes** *(params=None, param_init=None, level=0)*

Generates traces for best fit of parameters and all inputs

**optimization_iter** *(optimizer, metric)*

Function performs all operations required for one iteration of optimization. Drawing parameters, setting them to simulator and calculating the error.

Returns

- **results** *(list)* – recommended parameters
- **parameters** *(list of list)* – drawn parameters
- **errors** *(list)* – calculated errors

**results** *(format='list')*

Returns all of the gathered results (parameters and errors). In one of the 3 formats: ‘dataframe’, ‘list’, ‘dict’.

Parameters **format** *(str)* – The desired output format. Currently supported: dataframe, list, or dict.

Returns ‘dataframe’: returns pandas DataFrame without units ‘list’: list of dictionaries ‘dict’: dictionary of lists

Return type **object**

**setup_neuron_group** *(n_neurons, namespace, name='neurons')*

Setup neuron group, initialize required number of neurons, create namespace and initialize the parameters.
Parameters

- **n_neurons** (*int*) – number of required neurons
- **namespace** – arguments to be added to NeuronGroup namespace

Returns **neurons** – group of neurons

Return type **NeuronGroup**

class brian2modelfitting.fitter.TraceFitter(model, input_var, input, output_var, output, dt, n_samples=30, method=None, reset=None, refractory=False, threshold=None, level=0, param_init=None)

Bases: brian2modelfitting.fitter.Fitter

Input and output have to have the same dimensions.

calc_errors(metric)
Returns errors after simulation with StateMonitor. To be used inside optim_iter.

fit(optimizer, metric=None, n_rounds=1, callback='text', restart=False, **params)
Run the optimization algorithm for given amount of rounds with given number of samples drawn. Return best set of parameters and corresponding error.

Parameters

- **optimizer** (*Optimizer children*) – Child of Optimizer class, specific for each library.
- **metric** (*Metric children*) – Child of Metric class, specifies optimization metric
- **n_rounds** (*int*) – Number of rounds to optimize over (feedback provided over each round).
- **callback** (*str or Callable*) – Either the name of a provided callback function (text or progressbar), or a custom feedback function `func(results, errors, parameters, index)`. If this function returns `True` the fitting execution is interrupted.
- **restart** (*bool*) – Flag that reinitializes the Fitter to reset the optimization. With restart True user is allowed to change optimizer/metric.
- ****params** – bounds for each parameter

Returns

- **best_results** (*dict*) – dictionary with best parameter set
- **error** (*float*) – error value for best parameter set

generate(params=None, output_var=None, param_init=None, level=0)
Generates traces for best fit of parameters and all inputs. If provided with other parameters provides those.

Parameters

- **params** (*dict*) – Dictionary of parameters to generate fits for.
- **output_var** (*str*) – Name of the output variable to be monitored.
- **param_init** (*dict*) – Dictionary of initial values for the model.
- **level** (*int, optional*) – How much farther to go down in the stack to find the namespace.

generate_traces(params=None, param_init=None, level=0)
Generates traces for best fit of parameters and all inputs.
**optimization_iter** *(optimizer, metric)*
Function performs all operations required for one iteration of optimization. Drawing parameters, setting them to simulator and calculating the error.

**Returns**
- **results** *(list)* – recommended parameters
- **parameters** *(list of list)* – drawn parameters
- **errors** *(list)* – calculated errors

**results** *(format=’list’)*
Returns all of the gathered results (parameters and errors). In one of the 3 formats: ‘dataframe’, ‘list’, ‘dict’.

**Parameters**
- **format** *(str)* – The desired output format. Currently supported: dataframe, list, or dict.

**Returns**
- ‘dataframe’: returns pandas DataFrame without units
- ‘list’: list of dictionaries
- ‘dict’: dictionary of lists

**Return type** *object*

**setup_neuron_group** *(n_neurons, namespace, name=’neurons’)*
Setup neuron group, initialize required number of neurons, create namespace and initialize the parameters.

**Parameters**
- **n_neurons** *(int)* – number of required neurons
- **namespace** – arguments to be added to NeuronGroup namespace

**Returns** *neurons* – group of neurons

**Return type** *NeuronGroup*

brian2modelfitting.fitter.get_param_dic(params, param_names, n_traces, n_samples)
Transform parameters into a dictionary of appropriate size

brian2modelfitting.fitter.get_spikes(monitor, n_samples, n_traces)
Get spikes from spike monitor change format from dict to a list, remove units.

brian2modelfitting.fitter.setup_fit()
Function sets up simulator in one of the two available modes: runtime or standalone.

**Returns** *simulator*

**Return type** *Simulator*

### brian2modelfitting.optimizer module

**class** *brian2modelfitting.optimizer.NevergradOptimizer*(method=’DE’, **kwds)*
Bases: *brian2modelfitting.optimizer.Optimizer*

NevergradOptimizer instance creates all the tools necessary for the user to use it with Nevergrad library.

**Parameters**
- **parameter_names** *(list or dict)* – List/Dict of strings with parameters to be used as instruments.
- **bounds** *(list)* – List with appropriate bounds for each parameter.
- **method** *(str, optional)* – The optimization method. By default differential evolution, can be chosen from any method in Nevergrad registry
- **budget** *(int or None)* – number of allowed evaluations
- **num_workers** *(int)* – number of evaluations which will be run in parallel at once

```python
ask(n_samples)
```
Returns the requested number of samples of parameter sets

```python
Parameters
n_samples (int) – number of samples to be drawn

Returns
parameters – list of drawn parameters [n_samples x n_params]

Return type
list
```

```python
initialize(parameter_names, popsize, **params)
```
Initialize the instrumentation for the optimization, based on parameters, creates bounds for variables and attaches them to the optimizer

```python
Parameters

* parameter_names (list[str]) – list of parameter names in use
* popsize (int) – population size
* **params – bounds for each parameter

recommend()
```
Returns best recommendation provided by the method

```python
Returns
result – list of best fit parameters[n_params]

Return type
list
```

```python
tell(parameters, errors)
```
Provides the evaluated errors from parameter sets to optimizer

```python
Parameters

* parameters (list) – list of parameters [n_samples x n_params]
* errors (list) – list of errors [n_samples]
```

```python
class brian2modelfitting.optimizer.Optimizer
```
Bases: object

Optimizer class created as a base for optimization initialization and performance with different libraries. To be used with modelfitting Fitter.

```python
ask(n_samples)
```
Returns the requested number of samples of parameter sets

```python
Parameters
n_samples (int) – number of samples to be drawn

Returns
parameters – list of drawn parameters [n_samples x n_params]

Return type
list
```

```python
initialize(parameter_names, popsize, **params)
```
Initialize the instrumentation for the optimization, based on parameters, creates bounds for variables and attaches them to the optimizer

```python
Parameters

* parameter_names (list[str]) – list of parameter names in use
* popsize (int) – population size
• **params** – bounds for each parameter

**recommend()**

Returns best recommendation provided by the method

Returns **result** – list of best fit parameters[n_params]

Return type **list**

**tell (parameters, errors)**

Provides the evaluated errors from parameter sets to optimizer

Parameters

• **parameters** (**list**) – list of parameters [n_samples x n_params]

• **errors** (**list**) – list of errors [n_samples]

**class** *brian2modelfitting.optimizer.SkoptOptimizer (method='GP', **kwds)*

Bases: *brian2modelfitting.optimizer.Optimizer*

SkoptOptimizer instance creates all the tools necessary for the user to use it with scikit-optimize library.

Parameters

• **parameter_names** (**list**{str}) – Parameters to be used as instruments.

• **bounds** (**list**) – List with appropriate bounds for each parameter.

• **method** (**str**, optional) – The optimization method. Possibilities: “GP”, “RF”, “ET”, “GBRT” or sklearn regressor, default=”GP”

• **n_calls** (**int**) – Number of calls to **func**. Defaults to 100.

**ask (n_samples)**

Returns the requested number of samples of parameter sets

Parameters **n_samples** (**int**) – number of samples to be drawn

Returns **parameters** – list of drawn parameters [n_samples x n_params]

Return type **list**

**initialize (parameter_names, popsize, **params)**

Initialize the instrumentation for the optimization, based on parameters, creates bounds for variables and attaches them to the optimizer

Parameters

• **parameter_names** (**list**{str}) – list of parameter names in use

• **popsize** (**int**) – population size

• **params** – bounds for each parameter

**recommend()**

Returns best recommendation provided by the method

Returns **result** – list of best fit parameters[n_params]

Return type **list**

**tell (parameters, errors)**

Provides the evaluated errors from parameter sets to optimizer

Parameters

• **parameters** (**list**) – list of parameters [n_samples x n_params]
• `errors (list)` – list of errors [n_samples]

`brian2modelfitting.optimizer.calc_bounds (parameter_names, **params)`

Verify and get the provided for parameters bounds

Parameters

• `parameter_names (list [str])` – list of parameter names in use
• `**params` – bounds for each parameter

`brian2modelfitting.simulator` module

class `brian2modelfitting.simulator.CPPStandaloneSimulator`

Bases: `brian2modelfitting.simulator.Simulator`

Simulation class created for use with CPPStandaloneDevice

`initialize (network, var_init, name='neurons')`

Prepares the simulation for running

Parameters

• `network (Network)` – Network consisting of a NeuronGroup named neurons and a monitor named monitor.
• `var_init (dict)` – dictionary to initialize the variable states
• `name (str, optional)` – name of the network

`run (duration, params, params_names, name='neurons')`

Simulation has to be run in two stages in order to initialize the code generation

class `brian2modelfitting.simulator.RuntimeSimulator`

Bases: `brian2modelfitting.simulator.Simulator`

Simulation class created for use with RuntimeDevice

`initialize (network, var_init, name='neurons')`

Prepares the simulation for running

Parameters

• `network (Network)` – Network consisting of a NeuronGroup named neurons and a monitor named monitor.
• `var_init (dict)` – dictionary to initialize the variable states
• `name (str, optional)` – name of the network

`run (duration, params, params_names, name='neurons')`

Restores the network, sets neurons to required parameters and runs the simulation

Parameters

• `duration (Quantity)` – Simulation duration
• `params (dict)` – parameters to be set
• `params_names (list [str])` – names of parameters to set the dictionary

class `brian2modelfitting.simulator.Simulator`

Bases: `object`

Simulation class created to perform a simulation for fit_traces
**initialize** *(network, var_init, name)*
Prepares the simulation for running

**Parameters**
- **network** *(Network)* – Network consisting of a NeuronGroup named neurons and a monitor named monitor.
- **var_init** *(dict)* – dictionary to initialize the variable states
- **name** *(str, optional)* – name of the network

**run** *(duration, params, params_names)*
Restores the network, sets neurons to required parameters and runs the simulation

**Parameters**
- **duration** *(Quantity)* – Simulation duration
- **params** *(dict)* – parameters to be set
- **params_names** *(list [str])* – names of parameters to set the dictionary

**brian2modelfitting.simulator.initialize_neurons** *(params_names, neurons, params)*
initialize each parameter for NeuronGroup returns dictionary of Dummy devices

**brian2modelfitting.simulator.initialize_parameter** *(variableview, value)*
initialize parameter variable in static file, returns Dummy device

**brian2modelfitting.simulator.run_again** *
re-run the NeuronGroup on cpp file

**brian2modelfitting.simulator.set_parameter_value** *(identifier, value)*
change parameter value in cpp file

**brian2modelfitting.simulator.set_states** *(init_dict, values)*
set parameters values in the file for the NeuronGroup

**brian2modelfitting.utils module**

**class** *brian2modelfitting.utils.ProgressBar*(toolbar_width=10, **kwds)*
Setup for tqdm progress bar in Fitter

**brian2modelfitting.utils.callback_none** *(params, errors, best_params, best_error, index)*
Non-verbose callback

**brian2modelfitting.utils.callback_setup** *(set_type, n_rounds)*
Helper function for callback setup in Fitter, loads option: 'text', 'progressbar' or custion FunctionType

**brian2modelfitting.utils.callback_text** *(params, errors, best_params, best_error, index)*
Default callback print-out for Fitters

**brian2modelfitting.utils.make_dic** *(names, values)*
Create dictionary based on list of strings and 2D array
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