

PESTO

1.0

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1 PESTO Documentation

1.1 Introduction

Computational models are commonly used in diverse disciplines such as computational biology, engineering, or meteorology. The parameterization of these models is usually based on measurements or observations. The process of inferring model parameters from such data is called model calibration or parameter estimation. This parameter estimation is often not straightforward due to non-linearities in the model equations or due to the mere size and the resulting computational challenges. Therefore, efficient algorithms are required to provide robust results within acceptable time.

PESTO is a freely available Parameter EStimation TOolbox for MATLAB (MathWorks) implementing a number of state-of-the-art algorithms for parameter estimation. It provides the following features, which are explained in more detail [below](#):

- Parameter estimation from measurement data by global optimization based on multi-start local optimization (requires [MATLAB Optimization Toolbox](#))
- Parameter sampling using Markov Chain Monte Carlo (MCMC) algorithms
- Uncertainty analysis based on local approximations, parameter samples and profile-likelihood analysis (requires [MATLAB Optimization Toolbox](#))
- Visualization routines for all analyses
- Parallel processing (requires [MATLAB Parallel Computing Toolbox](#))
- ...

PESTO functions can be applied to any user-provided formulation of an optimization problem with an objective function that can be evaluated in MATLAB. Besides the objective function, upper and lower bounds for the function parameters need to be specified.

1.2 Availability

PESTO can be freely obtained from <https://github.com/ICB-DCM/PESTO/> by downloading the zip archive at <https://github.com/ICB-DCM/PESTO/archive/master.zip> or cloning the git repository via

```
1 git clone git@github.com:ICB-DCM/PESTO.git
```

1.3 Installation

If the zip archive was downloaded, it needs to be unzipped and the main folder has to be added to the MATLAB search path (non-recursively).

If the repository was cloned, the main folder needs to be added to the MATLAB search path (non-recursively).

Note: Detailed instructions on how to modify your MATLAB search path are provided here: https://de.mathworks.com/help/matlab/matlab_env/add-remove-or-reorder-folders-on-the-search-path.html

Third-party packages

PESTO provides an interfaces to several other toolboxes which are not included in the PESTO archive:

- PSwarm: <http://www.norg.uminho.pt/aivaz/pswarm/>
- MEIGO: <http://gingproc.iim.csic.es/meigo.html>
- DRAM: <http://helios.fmi.fi/~lainema/dram/>

To use their functionality, these toolboxes have to be installed separately. Please consult the respective user manuals for details.

1.4 Licensing

See `LICENSE` file in the PESTO source directory.

1.5 How to cite

This section will be updated upon publication of PESTO.

1.6 Code organization

The end-user interface is provided by the MATLAB functions and classes in the top-level directory. PESTO examples applications are provided in `/examples/`. All other folders only contain files used internally in PESTO.

1.7 Features

PESTO implements a number of state-of-the-art algorithms related to parameter estimations. The main features are described below. Various Examples demonstrate their application.

Notations and Terminology

Since most of the examples use analytical approaches for computing the gradient of the respective objective function, which quantifies the deviation of the fit for the current model parameters from the actual measurement data, the usage of the term ‚sensitivity analysis‘ may be misleading. In our context, ‚sensitivity analysis‘ is used in the context of ODE or PDE models and describes the sensitivity of the ODE/PDE state with respect to the model parameters. Those state sensitivities can be implemented in the ODE/PDE system and then used for an analytical calculation of the sensitivity of the objective function. This objective functions sensitivity will always be called the objective function gradient in our context. Finally, the behavior of the objective function by the variation of single parameters in order to find possible (non-)identifiabilities will always be referred to as ‚uncertainty analysis‘.

1.7.1 Global optimization

Non-linear optimization problems like those in parameter estimation problems tend to have multiple optima. Usually, nothing is known beforehand about their number or their location, but the user is interested in finding the global optimum. There are different techniques for this kind of problem. PESTO provides a multi-start local optimization framework and provides an interface to two global optimizers.

Multi-start local optimization

Multi-start local optimization has turned out to be a very efficient method for "global optimization": Here, random points from across the parameter space are chosen as starting points for local optimization. If an adequate number of starting points spanning the domain of interest of the parameter space is selected, the lowest/highest minimum/maximum is accepted to be the global minimum/maximum. By default, `fmincon` is used as a local solver.

This functionality is provided in [getMultiStarts.m](#), [getPropertyMultiStarts.m](#) and the respective plotting routines [plotMultiStarts.m](#) and [plotPropertyMultiStarts.m](#). See `mainConversionReaction.m` for an example.

Global optimizers

PESTO provides an interface to `PSwarm` and `MEIGO`. Once these toolboxes have been installed - they are not included in the PESTO archive - they can be used for parameter estimation. These optimizers are also accessed via [getMultiStarts.m](#) by setting `PestoOptions::localOptimizer` and `PestoOptions::localOptimizerOptions` accordingly. In principle, a single optimizer run (`PestoOptions::n_starts = 1`) should be enough for these global optimizers.

An example is included in `mainConversionReaction.m`.

1.7.2 Uncertainty analysis

When parameters are inferred from measurement data, the deviation of the data from the fit for the best parameter guess is usually supposed to be of stochastic nature. This means that the estimated parameters themselves underly are stochastic and underly an uncertainty. This can be quantified by performing uncertainty analysis and computing confidence intervals.

The easiest way to do this is using local approximations (based on the Hessian matrix of the objective function) at the best parameter guess. From those approximations, either threshold-based or mass-based methods can be used to compute confidence intervals for the inferred parameters. Another approach uses sampling based methods in combination with local approximations.

The most reliable way to compute confidence intervals is a third approach, based on profile likelihoods. Here, each model parameter is varied separately while the others are constantly reoptimized. In this way one finds profiles for every parameter. By fixing a confidence level using the inverse chi-squared-distribution, one gets a threshold which, together with the profile likelihood, gives reliable confidence intervals for each parameter. In this way, non-identifiable parameter can be found.

Those functionalities are provided in [getParameterProfiles.m](#), [getPropertyProfiles.m](#) (for the profile likelihoods), [getParameterConfidenceIntervals.m](#) and [getPropertyConfidenceIntervals.m](#) (for the confidence intervals). In order to get confidence intervals based on local approximations or sampling methods, one needs to run the routines `getMultiStart.m/getPropertyMultiStarts.m` or [getParameterSamples.m/getPropertySamples.m](#) first. The respective visualization routines are [plotParameterProfiles.m](#) and [plotPropertyProfiles.m](#). See `mainConversionReaction.m` for an example.

1.7.3 Parameter sampling

PESTO provides Markov Chain Monte Carlo (MCMC) algorithms for sampling the posterior distribution. Sampling methods such as the `Metropolis-Hastings (MH)`, adaptive Metropolis (AM) and `Metropolis-adjusted Langevin algorithm (MALA)` are currently implemented. Additionally, PESTO provides an interface to the `Delayed Rejection Adaptive Metropolis (DRAM)` toolbox.

See [getParameterSamples\(\)](#) for details and `mainConversionReaction.m` for examples.

1.7.4 Plotting

An integral part of PESTO are its highly customizable plotting functions for each type of analysis.

Details are provided in the documentation of the specific plotting functions:

- [plotMultiStarts.m](#)
- [plotParameterProfiles.m](#)
- [plotParameterSamples.m](#)
- [plotParameterUncertainty.m](#)
- [plotPropertyMultiStarts.m](#)
- [plotPropertyProfiles.m](#)
- [plotPropertySamples.m](#)
- [plotPropertyUncertainty.m](#)

Here some examples:

Plot of model fit using [plotMultiStarts.m](#):

Plot of different variants of parameter confidence intervals using [plotParameterUncertainty.m](#):

2D plot of parameter samples using [plotParameterSamples.m](#):

Plot of parameter samples using [plotParameterSamples.m](#):

Plot of property samples using [plotPropertySamples.m](#):

See `mainConversionReaction.m` for live examples.

1.7.5 Properties

The above-mentioned methods for parameter estimation, confidence intervals, parameter profiles and parameter samples ([getMultiStarts.m](#), [getParameterConfidenceIntervals.m](#), [getParameterProfiles.m](#), [getParameterSamples.m](#)) all operate on the objective function parameters directly. However, sometimes not the parameters themselves, but some function thereof is of interest. To this end, PESTO provides a simple interface to achieve this without having to change the objective function. Arbitrary user-provided functions which take the objective function parameter vector as an argument are referred to as 'properties'. After having used any of the `getParameter*.m` functions, the respective `getProperty*.m` function can be called, to evaluate a user-provided property function with the parameters values/samples/confidences obtained from the `getParameter*.m` functions.

The following functions are available to analyze and plot properties:

- [getPropertyConfidenceIntervals.m](#)
- [getPropertyMultiStarts.m](#)
- [getPropertyProfiles.m](#)
- [getPropertySamples.m](#)
- [plotPropertyMultiStarts.m](#)
- [plotPropertyProfiles.m](#)
- [plotPropertySamples.m](#)
- [plotPropertyUncertainty.m](#)

See `mainConversionReaction.m` for examples.

2 Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

SetGet

PestoPlottingOptions 8

3 Class Index

3.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

PestoPlottingOptions
PestoPlottingOptions is class for checking and holding information on optimization parameters 8

4 File Index

4.1 File List

Here is a list of all documented files with brief descriptions:

collectResults.m
CollectResults() collects and plots the results stored in a common folder 20

getBins.m ??

getMultiStarts.m
GetMultiStarts() computes the maximum a posterior estimate of the parameters of a user-supplied posterior function. Therefore, a multi-start local optimization is used. The parameters from the best value of the posterior function are then used as the global optimum. To ensure that the found maximum is a global one, a sufficiently high number of multistarts must be done. Those starts can be initialized with either randomly sampled parameter values, following either a uniform distribution or a latin hypercube, or they can be sampled by a user provided initial function (provided as option.init_fun) 21

getParameterConfidenceIntervals.m
GetParameterConfidenceIntervals() calculates the confidence intervals for the model parameters. This is done by four approaches: The values of CI.local_PL and CI.PL are determined by the point on which a threshold according to the confidence level alpha (calculated by a chi2-distribution) is reached. local_PL computes this point by a local approximation around the MAP estimate using the Hessian matrix, PL uses the profile likelihoods instead. The value of CI.local_B is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate. The value of CI.S is calculated using samples for the model parameters and the according percentiles based on the confidence levels alpha 24

getParameterProfiles.m

GetParameterProfiles.m calculates the profiles likelihoods for the model parameters, starting from the maximum a posteriori estimate. This calculation is done by fixing the *i*-th parameter and repeatedly reoptimizing the likelihood/posterior estimate (for all *i*). The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization

25

getParameterSamples.m

GetParameterSamples.m performs adaptive MCMC sampling of the posterior distribution. The DRAM library routine `tooparameters.minox` is used internally

28

getPropertyConfidenceIntervals.m

GetPropertyConfidenceIntervals.m calculates the confidence intervals for the model properties. This is done by three approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level α (calculated by a χ^2 -distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate

29

getPropertyMultiStarts.m

GetPropertyMultiStarts.m evaluates the properties for the different multi-start results

31

getPropertyProfiles.m

GetPropertyProfiles.m calculates the profiles of user-supplied property functions, starting from the maximum a posteriori estimate. This calculation is done by varying the value of each property function respectively, starting from the value of this function at the global optimum and by reoptimizing the likelihood/posterior estimate in each variational step of the property. The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization

33

getPropertySamples.m

GetPropertySamples.m evaluates the properties for the sampled parameters

36

meigoDummy.m

Objective function wrapper for MEIGO / PSwarm / ... which need objective function *file*name* and cannot use function handles directly

38

plotConfidenceIntervals.m

PlotConfidenceIntervals.m visualizes confidence intervals stored in either the parameters or properties struct `.CI`

39

plotMCMCdiagnosis.m

PlotMCMCdiagnosis.m visualizes the Markov chains generated by `getSamples.m`

41

plotMultiStartDiagnosis.m

??

plotMultiStarts.m

PlotMultiStarts plots the result of the multi-start optimization stored in parameters

42

plotParameterProfiles.m

PlotParameterProfiles.m visualizes profile likelihood. Note: This routine provides an interface for `plotUncertainty.m`

43

plotParameterSamples.m

PlotParameterSamples.m visualizes MCMC samples. Note: This routine provides an interface for `plotUncertainty.m`

45

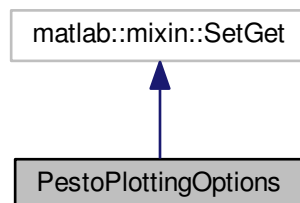
plotParameterUncertainty.m	
PlotParameterUncertainty.m visualizes profile likelihood and MCMC samples stored in parameters	47
plotPropertyMultiStarts.m	
PlotPropertyMultiStarts plots the result of the multi-start optimization stored in properties	49
plotPropertyProfiles.m	
PlotPropertyProfiles.m visualizes profile likelihood of model properties. Note: This routine provides an interface for plotPropertyUncertainty.m	50
plotPropertySamples.m	
PlotPropertySamples.m visualizes samples of model properties. Note: This routine provides an interface for plotPropertyUncertainty.m	52
plotPropertyUncertainty.m	
PlotPropertyUncertainty.m visualizes profile likelihood and MCMC samples stored in properties	54
runPestoTests.m	
RunPestoTests Run a set of PESTO unit tests	55
testGradient.m	
TestGradient.m calculates finite difference approximations to the gradient to check an analytical version	56
@PestoOptions/PestoOptions.m	??
@PestoPlottingOptions/PestoPlottingOptions.m	??

5 Class Documentation

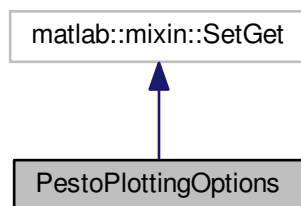
5.1 PestoPlottingOptions Class Reference

[PestoPlottingOptions](#) is class for checking and holding information on optimization parameters.

Inheritance diagram for PestoPlottingOptions:



Collaboration diagram for PestoPlottingOptions:



Public Member Functions

- [PestoPlottingOptions](#) (matlabtypesubstitute varargin)
PestoPlottingOptions Construct a new *PestoPlottingOptions* object.
- `mlhsInnerSubst` < matlabtypesubstitute, new > **copy** ()

Public Attributes

- matlabtypesubstitute `title` = true
Title of PESTO-generated plots.
- matlabtypesubstitute `add_points`
Additional points to include in the plots, e.g. true parameter in the case of test examples.
- matlabtypesubstitute `mark_constraint` = false
TODO: from plotmultistarts.
- matlabtypesubstitute `subplot_size_1D` = "[]"
TODO from plotparameteruncertainty.
- matlabtypesubstitute `subplot_indexing_1D` = "[]"
TODO.
- matlabtypesubstitute `labels`
TODO.
- matlabtypesubstitute `hold_on` = false
Indicates whether plots are redrawn or whether something is added to the plot.
- matlabtypesubstitute `interval` = "dynamic"
Way of choosing x limits for plotting.
- matlabtypesubstitute `draw_bounds` = true
Draw bounds.
- matlabtypesubstitute `bounds` = {""}
Bounds used for visualization if options.interval = static
- matlabtypesubstitute `P`
Options for profile plots.
- matlabtypesubstitute `S`
Options for sample plots.
- matlabtypesubstitute `MS`
Options for multi-start optimization plots.
- matlabtypesubstitute `A`

- Options for distribution approximation plots.*
 - matlabtypesubstitute **MCMC** = "multistart"
 - Option if a user provided sampling initialization should be used for plotting an approximation of the distribution.*
 - matlabtypesubstitute **boundary**
 - Options for boundary visualization.*
 - matlabtypesubstitute **CL**
 - Options for confidence level plots.*
 - matlabtypesubstitute **group_CI_by** = "parprop"
 - Options for the way to plot confidence intervals.*
 - matlabtypesubstitute **op2D** = struct("b1", 0.15, 'b2', 0.02, 'r', 0.95")
 - Settings for 2D plot to position subplot axes.*
 - matlabtypesubstitute **legend**
 - Legend options.*
 - matlabtypesubstitute **fontsize** = struct ("tick", 12")
 - Fontsize for labels.*
 - matlabtypesubstitute **fh_logPost_trace** = ""
 - figure handle for log-posterior trace plot*
 - matlabtypesubstitute **fh_par_trace** = ""
 - figure handle for parameter trace plots.*
 - matlabtypesubstitute **fh_par_dis_1D** = ""
 - figure handle for the parameter distribution plot. fh_par_dis = [];*
 - matlabtypesubstitute **fh_par_dis_2D** = ""
 - matlabtypesubstitute **plot_type** = {"parameter", 'posterior'}
 - matlabtypesubstitute **n_max** = 1e4

5.1.1 Detailed Description

PestoPlottingOptions is class for checking and holding information on optimization parameters.

This file is based on AMICI amioptions.m (<http://icb-dcm.github.io/AMICI/>)

Definition at line 17 of file PestoPlottingOptions.m.

5.1.2 Constructor & Destructor Documentation

5.1.2.1 PestoPlottingOptions::PestoPlottingOptions (matlabtypesubstitute *varargin*)

PestoPlottingOptions Construct a new **PestoPlottingOptions** object.

OPTS = **PestoPlottingOptions**() creates a set of options with each option set to its default value.

OPTS = **PestoPlottingOptions**(PARAM, VAL, ...) creates a set of options with the named parameters altered with the specified values.

OPTS = **PestoPlottingOptions**(OLDOPTS, PARAM, VAL, ...) creates a copy of OLDOPTS with the named parameters altered with the specified value

Note to see the parameters, check the documentation page for **PestoPlottingOptions**

Definition at line 472 of file PestoPlottingOptions.m.

References draw_bounds, group_CI_by, hold_on, interval, mark_constraint, MCMC, n_max, and title.

5.1.3 Member Data Documentation

5.1.3.1 PestoPlottingOptions::A

Initial value:

```
= struct("plot_type", 1, \
        'col', [0,0,1], \
        'lw', 2, \
        'sigma_level', 2, \
        'name', 'P_{app}')
```

Options for distribution approximation plots.

Struct with

- .plot_type: plot type
 - = 0 (default if no MS are provided) ... no plot
 - = 1 (default if MS are provided) ... likelihood ratio
 - = 2 ... negative log-likelihood
- .col: color of approximation lines (default: [0,0,1])
- .lw: line width of approximation lines (default: 1.5)
- .sigma_level: sigma-level which is visualized (default = 2)
- .name: name of legend entry (default = $P_{\{app\}}$)

Default: struct("plot_type", 1, \ 'col', [0,0,1], \ 'lw', 2, \ 'sigma_level', 2, \ 'name', 'P_{app}')

Definition at line 277 of file PestoPlottingOptions.m.

5.1.3.2 PestoPlottingOptions::add_points

Initial value:

```
= struct("par", [], \
        'logPost', [], \
        'col', [0,0.8,0], \
        'ls', '-', \
        'lw', 1, \
        'm', 'd', \
        'ms', 8, \
        'name', 'add. point')
```

Additional points to include in the plots, e.g. true parameter in the case of test examples.

Struct with the following fields

- .par: n x m matrix of m additional points
- .col: color used for additional points (default = [0,0,0]). This can also be a m x 3 matrix of colors.
- .ls: line style (default = -)
- .lw: line width (default = 2)
- .m: marker style (default = s)
- .ms: line width (default = 8)
- .name: name of legend entry (default = add. point)
- .property_MS: line width (default = 8).
- .logPost

Default: struct("par", [], \ 'logPost', [], \ 'col', [0,0.8,0], \ 'ls', '-', \ 'lw', 1, \ 'm', 'd', \ 'ms', 8, \ 'name', 'add. point')

Definition at line 42 of file PestoPlottingOptions.m.

5.1.3.3 PestoPlottingOptions::boundary

Initial value:

```
= struct('mark', true, \
        'eps', 1e-4)
```

Options for boundary visualization.

Struct with

- .mark: marking of profile points which are on the boundary
 - = 0 ... no visualization
 - = 1 (default) ... indicates points which are close to the boundaries in one or more dimensions.
- .eps: minimal distance from boundary for which points are considered to be close to the boundary (default = 1e-4). Note that a one-norm is used.

Default: struct('mark', true, \ 'eps', 1e-4)

Definition at line 318 of file PestoPlottingOptions.m.

5.1.3.4 PestoPlottingOptions::bounds = {}

Bounds used for visualization if options.interval = static

struct with

- .min: lower bound
- .max: upper bound

Default: {}

Definition at line 152 of file PestoPlottingOptions.m.

5.1.3.5 PestoPlottingOptions::CL

Initial value:

```
= struct("plot_type", 0, \
        'alpha', 0.95, \
        'type', 'point-wise', \
        'col', [0,0,0], \
        'lw', 2, \
        'name', 'cut-off')
```

Options for confidence level plots.

Struct with

- `.plot_type`: plot type
 - = 0 (default) ... no plot
 - = 1 ... likelihood ratio
 - = 2 ... negative log-likelihood
- `.alpha`: visualized confidence level (default = 0.95)
- `.type`: type of confidence interval
 - = `point-wise` (default) ... point-wise confidence interval
 - = `simultaneous` ... point-wise confidence interval
 - = `{point-wise,simultaneous}` ... both
- `.col`: color of profile lines (default: [0,0,0])
- `.lw`: line width of profile lines (default: 1.5)
- `.name`: name of legend entry (default = `cut-off`)

Default: `struct("plot_type", 0, \ 'alpha', 0.95, \ 'type', 'point-wise', \ 'col', [0,0,0], \ 'lw', 2, \ 'name', 'cut-off')`

Definition at line 339 of file `PestoPlottingOptions.m`.

5.1.3.6 PestoPlottingOptions::draw_bounds = true

Draw bounds.

- `true`: yes
- `false`: no

Default: `true`

Note

This property has custom functionality when its value is changed.

Definition at line 141 of file `PestoPlottingOptions.m`.

Referenced by `PestoPlottingOptions()`.

5.1.3.7 PestoPlottingOptions::fh_logPost_trace = "[]"

figure handle for log-posterior trace plot

Default: "[]"

Definition at line 430 of file PestoPlottingOptions.m.

5.1.3.8 PestoPlottingOptions::fh_par_dis_1D = "[]"

figure handle for the parameter distribution plot. fh_par_dis = [];

Default: "[]"

Definition at line 448 of file PestoPlottingOptions.m.

5.1.3.9 PestoPlottingOptions::fh_par_trace = "[]"

figure handle for parameter trace plots.

Default: "[]"

Definition at line 439 of file PestoPlottingOptions.m.

5.1.3.10 PestoPlottingOptions::fontsize = struct ("tick", 12)

Fontsize for labels.

- .tick: fontsize for ticklabels (default = 12)

Default: struct ("tick", 12)

Definition at line 420 of file PestoPlottingOptions.m.

5.1.3.11 PestoPlottingOptions::group_CI_by = "parprop"

Options for the way to plot confidence intervals.

Either all confidence intervals of one method are plotted to one window `params`, or the confidence intervals for one parameter from all methods are plotted to one window `methods`, or everthing is grouped together `all`.

Default: "parprop"

Note

This property has custom functionality when its value is changed.

Definition at line 373 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.12 PestoPlottingOptions::hold_on = false

Indicates whether plots are redrawn or whether something is added to the plot.

- true: extension of plot
- false: new plot

Default: false

Note

This property has custom functionality when its value is changed.

Definition at line 116 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.13 PestoPlottingOptions::interval = "dynamic"

Way of choosing x limits for plotting.

- `dynamic`: x limits depending on analysis results
- `static`: x limits depending on parameters.min and .max or on user-defined bound options.bounds.min and .max. The later are used if provided.

Default: "dynamic"

Note

This property has custom functionality when its value is changed.

Definition at line 128 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.14 PestoPlottingOptions::labels

Initial value:

```
= struct('y_always', true, \
        'y_name', [])
```

TODO.

Default: struct("y_always", true, \ 'y_name', [])

Definition at line 105 of file PestoPlottingOptions.m.

5.1.3.15 PestoPlottingOptions::legend

Initial value:

```
= struct("'color', 'none', \
        'box', 'on', \
        'orientation', 'vertical', \
        'position', [])")
```

Legend options.

- .color: background color (default = none).
- .box: legend outline (default = on).
- .orientation: orientation of list (default = vertical)

Default: struct("'color', 'none', \ 'box', 'on', \ 'orientation', 'vertical', \ 'position', [])")

Definition at line 402 of file PestoPlottingOptions.m.

5.1.3.16 PestoPlottingOptions::mark_constraint = false

TODO: from plotmultistarts.

Default: false

Note

This property has custom functionality when its value is changed.

Definition at line 78 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.17 PestoPlottingOptions::MCMC = "multistart"

Option if a user provided sampling initialization should be used for plotting an approximation of the distribution.

- user-provided
- multistart (default)

Default: "multistart"

Note

This property has custom functionality when its value is changed.

Definition at line 305 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.18 PestoPlottingOptions::MS

Initial value:

```
= struct("plot_type", 1, \
        'col', [1,0,0], \
        'lw', 2, \
        'name_conv', 'MS - conv.', \
        'name_nconv', 'MS - not conv.', \
        'only_optimum', false")
```

Options for multi-start optimization plots.

Struct with

- .plot_type: plot type
 - = 0 (default if no MS are provided) ... no plot
 - = 1 (default if MS are provided) ... likelihood ratio and position of optima above threshold
 - = 2 ... negative log-likelihood and position of optima above threshold
- .col: color of local optima (default: [1,0,0])
- .lw: line width of local optima (default: 1.5)
- .name_conv: name of legend entry (default = MS - conv.)
- .name_nconv: name of legend entry (default = MS - not conv.)
- .only_optimum: only optimum is plotted

Default: struct("plot_type", 1, \ 'col', [1,0,0], \ 'lw', 2, \ 'name_conv', 'MS - conv.', \ 'name_nconv', 'MS - not conv.', \ 'only_optimum', false")

Definition at line 244 of file PestoPlottingOptions.m.

5.1.3.19 PestoPlottingOptions::n_max = 1e4

Note

This property has custom functionality when its value is changed.

Definition at line 462 of file PestoPlottingOptions.m.

Referenced by PestoPlottingOptions().

5.1.3.20 PestoPlottingOptions::op2D = struct("b1", 0.15, 'b2', 0.02, 'r', 0.95")

Settings for 2D plot to position subplot axes.

Struct with

- .b1 ... offset from left and bottom border (default = 0.15)
- .b2 ... offset from left and bottom border (default = 0.02)
- .r ... relative width of subplots (default = 0.95)

Default: struct("b1", 0.15, 'b2', 0.02, 'r', 0.95")

Definition at line 387 of file PestoPlottingOptions.m.

5.1.3.21 PestoPlottingOptions::P

Initial value:

```
= struct("plot_type", 1, \
        'col', [1,0,0], \
        'lw', 2, \
        'name', 'P')
```

Options for profile plots.

Struct with

- .plot_type: plot type
 - = 0 (default if no profiles are provided) ... no plot
 - = 1 (default if profiles are provided) ... likelihood ratio
 - = 2 ... negative log-likelihood
- .col: color of profile lines (default: [1,0,0])
- .lw: line width of profile lines (default: 1.5)

Default: struct("plot_type", 1, \ 'col', [1,0,0], \ 'lw', 2, \ 'name', 'P')

Definition at line 165 of file PestoPlottingOptions.m.

5.1.3.22 PestoPlottingOptions::S

Initial value:

```
= struct("plot_type", 0, \
        'bins', 'conservative', \
        'scaling', [], \
        'hist_col', [0.7,0.7,0.7], \
        'sp_col', [0.7,0.7,0.7], \
        'lin_col', [1,0,0], \
        'lin_lw', 2, \
        'sp_m', '.', \
        'sp_ms', 5, \
        'col', [1,0,0], 'lw', 2, \
        'PT', struct('sp_m', '.', \
        'sp_ms', 5, \
        'lw', 1.5, \
        'ind', [], \
        'col', [], \
        'plot_type', 0), \
        'name', 'S')
```

Options for sample plots.

- .plot_type: plot type
 - = 0 (default if no samples are provided) ... no plot
 - = 1 (default if samples are provided) ... histogram
 - = 2 ... kernel-density estimates
- .col ... color of profile lines (default: [0.7,0.7,0.7])
- .hist_col ... color of histogram (default = [0.7,0.7,0.7])

- `.bins` ... number of histogram bins (default: 30)
 - `= optimal` ... selection using Scott's rule
 - `= conservative` ... selection using Scott's rule / 2
 - `= N` (with N being an integer) ... N bins
- `.sp_col`: color of scatter plot (default = [0.7,0.7,0.7])
- `.sp_m`: marker for scatter plot (default = `.`)
- `.sp_ms`: marker size for scatter plot (default = 5)
- `.name`: name of legend entry (default = `S`)

Default: `struct('plot_type', 0, \ 'bins', 'conservative', \ 'scaling', [], \ 'hist_col', [0.7,0.7,0.7], \ 'sp_col', [0.7,0.7,0.7], \ 'lin_col', [1,0,0], \ 'lin_lw', 2, \ 'sp_m', '.', \ 'sp_ms', 5, \ 'col', [1,0,0], 'lw', 2, \ 'PT', struct('sp_m', '.', \ 'sp_ms', 5, \ 'lw', 1.5, \ 'ind', [], \ 'col', [], \ 'plot_type', 0), \ 'name', 'S')`

Definition at line 188 of file `PestoPlottingOptions.m`.

5.1.3.23 PestoPlottingOptions::subplot_indexing_1D = "[]"

TODO.

Default: "[]"

Definition at line 96 of file `PestoPlottingOptions.m`.

5.1.3.24 PestoPlottingOptions::subplot_size_1D = "[]"

TODO from `plotparameteruncertainty`.

Default: "[]"

Definition at line 87 of file `PestoPlottingOptions.m`.

5.1.3.25 PestoPlottingOptions::title = true

Title of PESTO-generated plots.

- `true`: show
- `false`: don't show

Default: `true`

Note

This property has custom functionality when its value is changed.

Definition at line 30 of file `PestoPlottingOptions.m`.

Referenced by `PestoPlottingOptions()`.

The documentation for this class was generated from the following file:

- `@PestoPlottingOptions/PestoPlottingOptions.m`

6 File Documentation

6.1 collectResults.m File Reference

`collectResults()` collects and plots the results stored in a common folder

Functions

- `mlhsInnerSubst< matlabtypesubstitute, obj > collectResults (matlabtypesubstitute foldername)`
`collectResults()` collects and plots the results stored in a common folder

6.1.1 Detailed Description

`collectResults()` collects and plots the results stored in a common folder

6.1.2 Function Documentation

6.1.2.1 `mlhsInnerSubst< matlabtypesubstitute, obj > collectResults (matlabtypesubstitute foldername)`

`collectResults()` collects and plots the results stored in a common folder

USAGE

`[parameters] = collectResults(foldername)`

History

2014/06/12 Jan Hasenauer % Initialization

Parameters

<i>foldername</i>	Name of folder from which results are collected.
-------------------	--

Return values

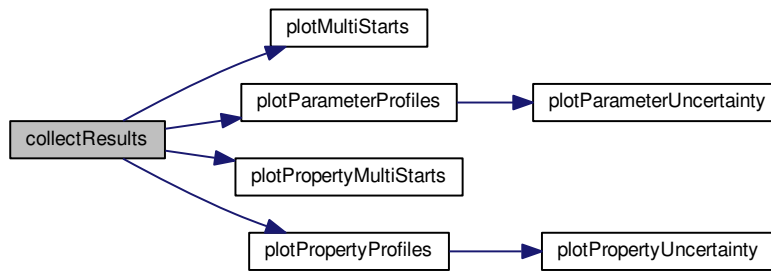
<i>parameters</i>	parameter struct.
-------------------	-------------------

Generated fields of obj:

Definition at line 17 of file `collectResults.m`.

References `plotMultiStarts()`, `plotParameterProfiles()`, `plotPropertyMultiStarts()`, and `plotPropertyProfiles()`.

Here is the call graph for this function:



6.2 getMultiStarts.m File Reference

[getMultiStarts\(\)](#) computes the maximum a posterior estimate of the parameters of a user-supplied posterior function. Therefore, a multi-start local optimization is used. The parameters from the best value of the posterior function are then used as the global optimum. To ensure that the found maximum is a global one, a sufficiently high number of multistarts must be done. Those starts can be initialized with either randomly sampled parameter values, following either a uniform distribution or a latin hypercube, or they can be sampled by a user provided initial function (provided as `option.init_fun`).

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh > > getMultiStarts` (`matlabtypesubstitute parameters`, `matlabtypesubstitute objective_function`, `matlabtypesubstitute varargin`)
[getMultiStarts\(\)](#) computes the maximum a posterior estimate of the parameters of a user-supplied posterior function. Therefore, a multi-start local optimization is used. The parameters from the best value of the posterior function are then used as the global optimum. To ensure that the found maximum is a global one, a sufficiently high number of multistarts must be done. Those starts can be initialized with either randomly sampled parameter values, following either a uniform distribution or a latin hypercube, or they can be sampled by a user provided initial function (provided as `option.init_fun`).
- `mlhsInnerSubst< matlabtypesubstitute, vararginout > mtoc_subst_getMultiStarts_m_tsbust_cotm_obj` (`matlabtypesubstitute varargin`)
- `mlhsInnerSubst< matlabtypesubstitute, vararginout > mtoc_subst_getMultiStarts_m_tsbust_cotm_obj ↔ w_error_count` (`matlabtypesubstitute varargin`)
- `mlhsInnerSubst< matlabtypesubstitute, stringTimePrediction > mtoc_subst_getMultiStarts_m_tsbust_cotm_updateWaitBar` (`matlabtypesubstitute timePredicted`)
- `noret::substitute mtoc_subst_getMultiStarts_m_tsbust_cotm_saveResults` (`matlabtypesubstitute parameters`, `matlabtypesubstitute options`, `matlabtypesubstitute i`)

6.2.1 Detailed Description

[getMultiStarts\(\)](#) computes the maximum a posterior estimate of the parameters of a user-supplied posterior function. Therefore, a multi-start local optimization is used. The parameters from the best value of the posterior function are then used as the global optimum. To ensure that the found maximum is a global one, a sufficiently high number of multistarts must be done. Those starts can be initialized with either randomly sampled parameter values, following either a uniform distribution or a latin hypercube, or they can be sampled by a user provided initial function (provided as `option.init_fun`).

6.2.2 Function Documentation

6.2.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh > >`
`getMultiStarts (matlabtypesubstitute parameters, matlabtypesubstitute objective_function, matlabtypesubstitute`
`varargin)`

`getMultiStarts()` computes the maximum a posterior estimate of the parameters of a user-supplied posterior function. Therefore, a multi-start local optimization is used. The parameters from the best value of the posterior function are then used as the global optimum. To ensure that the found maximum is a global one, a sufficiently high number of multistarts must be done. Those starts can be initialized with either randomly sampled parameter values, following either a uniform distribution or a latin hypercube, or they can be sampled by a user provided initial function (provided as `option.init_fun`).

Note: This function can exploit up to $(n_start + 1)$ workers when running in `parallel` mode.

USAGE

- `[...] = getMultiStarts(parameters,objective_function)`
- `[...] = getMultiStarts(parameters,objective_function,options)`
- `[parameters,fh] = getMultiStarts(...)`

`getMultiStarts()` uses the following `PestoOptions` members

- `PestoOptions::start_index`
- `PestoOptions::n_starts`
- `PestoOptions::mode`
- `PestoOptions::fh`
- `PestoOptions::fmincon`
- `PestoOptions::rng`
- `PestoOptions::proposal`
- `PestoOptions::save`
- `PestoOptions::foldername`
- `PestoOptions::trace`
- `PestoOptions::comp_type`
- `PestoOptions::tempsave`
- `PestoOptions::resetobjective`
- `PestoOptions::obj_type`
- `PestoOptions::init_threshold`
- `PestoOptions::plot_options`

History

- 2012/05/31 Jan Hasenauer
- 2012/07/11 Jan Hasenauer
- 2014/06/11 Jan Hasenauer
- 2015/07/28 Fabian Froehlich
- 2015/11/10 Fabian Froehlich
- 2016/06/07 Paul Stapor
- 2016/10/04 Daniel Weindl
- 2016/12/04 Paul Stapor

Parameters

<i>parameters</i>	parameter struct
<i>objective_function</i>	objective function to be optimized. This function should accept one input, the parameter vector.
<i>varargin</i>	<pre>1 getMultiStarts (..., options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> options A PestoOptions object holding various options for the algorithm.

Return values

<i>parameters</i>	updated parameter object
<i>fh</i>	figure handle

Required fields of parameters:

- *number* -- Number of parameters
- *min* -- Lower bound for each parameter
- *max* -- upper bound for each parameter name = {name1, ...}: names of the parameters
- *guess* -- initial guess for the parameters (Optional, will be initialized empty if not provided)
- *init_fun* -- function to draw starting points for local optimization, must have the structure `init_fun(theta_0, theta_min, theta_max)`. (Only required if `proposal == user-supplied`)

Generated fields of parameters:

- *MS* -- information about multi-start optimization
 - *par0(:,i)*: starting point yielding ith MAP
 - *par(:,i)*: ith MAP
 - *logPost(i)*: log-posterior for ith MAP
 - *logPost0(i)*: log-posterior for starting point yielding ith MAP
 - *gradient(_,i)*: gradient of log-posterior at ith MAP
 - *hessian(:,i)*: hessian of log-posterior at ith MAP
 - *n_objfun(i)*: # objective evaluations used to calculate ith MAP
 - *n_iter(i)*: # iterations used to calculate ith MAP
 - *t_cpu(i)*: CPU time for calculation of ith MAP
 - *exitflag(i)*: exitflag the optimizer returned for ith MAP
 - *par_trace(:,i)*: parameter trace for ith MAP (if `options.trace == true`)
 - *fval_trace(:,i)*: objective function value trace for ith MAP (if `options.trace == true`)
 - *time_trace(:,i)*: computation time trace for ith MAP (if `options.trace == true`)

Definition at line 17 of file getMultiStarts.m.

References plotMultiStarts().

Here is the call graph for this function:



6.3 `getParameterConfidenceIntervals.m` File Reference

`getParameterConfidenceIntervals()` calculates the confidence intervals for the model parameters. This is done by four approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a `chi2`-distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate. The value of `CI.S` is calculated using samples for the model parameters and the according percentiles based on the confidence levels `alpha`.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, parameters > getParameterConfidenceIntervals` (`matlabtypesubstitute parameters, matlabtypesubstitute alpha, matlabtypesubstitute varargin`)

`getParameterConfidenceIntervals()` calculates the confidence intervals for the model parameters. This is done by four approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a `chi2`-distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate. The value of `CI.S` is calculated using samples for the model parameters and the according percentiles based on the confidence levels `alpha`.

6.3.1 Detailed Description

`getParameterConfidenceIntervals()` calculates the confidence intervals for the model parameters. This is done by four approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a `chi2`-distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate. The value of `CI.S` is calculated using samples for the model parameters and the according percentiles based on the confidence levels `alpha`.

6.3.2 Function Documentation

- ##### 6.3.2.1 `mlhsInnerSubst< matlabtypesubstitute, parameters > getParameterConfidenceIntervals` (`matlabtypesubstitute parameters, matlabtypesubstitute alpha, matlabtypesubstitute varargin`)

`getParameterConfidenceIntervals()` calculates the confidence intervals for the model parameters. This is done by four approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a `chi2`-distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate. The value of `CI.S` is calculated using samples for the model parameters and the according percentiles based on the confidence levels `alpha`.

USAGE

- `parameters = getParameterConfidenceIntervals(parameters, alpha)`

History

- 2013/11/29 Jan Hasenauer
- 2016/12/01 Paul Stapor

Parameters

<i>parameters</i>	parameter struct
<i>alpha</i>	vector with desired confidence levels for the intervals

Return values

<i>parameters</i>	updated parameter struct
-------------------	--------------------------

Required fields of parameters:

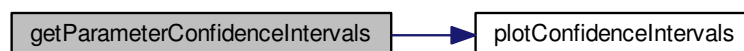
Generated fields of parameters:

- `CI` -- Information about confidence levels
 - `local_PL`: Threshold based approach, uses a local approximation by the Hessian matrix at the MAP estimate (requires `parameters.MS`, e.g. from `getMultiStarts`)
 - `PL`: Threshold based approach, uses profile likelihoods (requires `parameters.P`, e.g. from `getParameterProfiles`)
 - `local_B`: Mass based approach, uses a local approximation by the Hessian matrix at the MAP estimate (requires `parameters.MS`, e.g. from `getMultiStarts`)
 - `S`: Bayesian approach, uses percentiles based on samples (requires `parameters.S`, e.g. from `getParameterSamples`)

Definition at line 17 of file `getParameterConfidenceIntervals.m`.

References `plotConfidenceIntervals()`.

Here is the call graph for this function:

6.4 `getParameterProfiles.m` File Reference

[getParameterProfiles.m](#) calculates the profiles likelihoods for the model parameters, starting from the maximum a posteriori estimate. This calculation is done by fixing the *i*-th parameter and repeatedly reoptimizing the likelihood/posterior estimate (for all *i*). The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh > > getParameterProfiles (matlabtypesubstitute parameters, matlabtypesubstitute objective_function, matlabtypesubstitute varargin)`

[getParameterProfiles.m](#) calculates the profiles likelihoods for the model parameters, starting from the maximum a posteriori estimate. This calculation is done by fixing the i -th parameter and repeatedly reoptimizing the likelihood/posterior estimate (for all i). The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

6.4.1 Detailed Description

[getParameterProfiles.m](#) calculates the profiles likelihoods for the model parameters, starting from the maximum a posteriori estimate. This calculation is done by fixing the i -th parameter and repeatedly reoptimizing the likelihood/posterior estimate (for all i). The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

6.4.2 Function Documentation

- 6.4.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh > > getParameterProfiles (matlabtypesubstitute parameters, matlabtypesubstitute objective_function, matlabtypesubstitute varargin)`

[getParameterProfiles.m](#) calculates the profiles likelihoods for the model parameters, starting from the maximum a posteriori estimate. This calculation is done by fixing the i -th parameter and repeatedly reoptimizing the likelihood/posterior estimate (for all i). The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

Note: This function can exploit up to $(n_theta + 1)$ workers when running in `parallel` mode.

USAGE

```
[...] = getParameterProfiles(parameters, objective_function) [...] = getParameterProfiles(parameters,
objective_function, options) [parameters, fh] = getParameterProfiles(...)
```

`getParameterProfiles()` uses the following `PestoOptions` members

- `PestoOptions::calc_profiles`
- `PestoOptions::comp_type`
- `PestoOptions::dJ`
- `PestoOptions::dR_max`
- `PestoOptions::fh`
- `PestoOptions::MAP_index`
- `PestoOptions::mode`
- `PestoOptions::obj_type`
- `PestoOptions::options_getNextPoint .guess .min .max .update .mode`
- `PestoOptions::parameter_index`
- `PestoOptions::parameter_method_index`
- `PestoOptions::profile_method`
- `PestoOptions::profileReoptimizationOptions`

- `PestoOptions::plot_options`
- `PestoOptions::R_min`
- `PestoOptions::save`

History

- 2012/05/16 Jan Hasenauer
- 2014/06/12 Jan Hasenauer
- 2016/10/04 Daniel Weindl
- 2016/10/12 Paul Stapor

Parameters

<i>parameters</i>	parameter struct
<i>objective_function</i>	objective function to be optimized. This function should accept one input, the parameter vector.
<i>varargin</i>	<pre>1 getParameterProfiles (..., options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • options A <code>PestoOptions</code> object holding various options for the algorithm.

Return values

<i>parameters</i>	updated parameter struct
<i>fh</i>	figure handle

Required fields of parameters:

- `number` -- Number of parameters
- `min` -- Lower bound for each parameter
- `max` -- upper bound for each parameter name = {`name1`, ...}: names of the parameters
- `MS` -- results of global optimization, obtained using for instance the routine `getMultiStarts.m`. `MS` has to contain at least
 - `par`: sorted list `n_theta` x `n_starts` of parameter estimates. The first entry is assumed to be the best one.
 - `logPost`: sorted list `n_starts` x 1 of log-posterior values corresponding to the parameters listed in `.par`.
 - `hessian`: Hessian matrix (or approximation) at the optimal point

Generated fields of parameters:

- `P(i)` -- profile for i-th parameter
 - `par`: MAPs along profile
 - `logPost`: maximum log-posterior along profile
 - `R`: ratio

Definition at line 17 of file `getParameterProfiles.m`.

References `plotParameterProfiles()`.

Here is the call graph for this function:



6.5 `getParameterSamples.m` File Reference

`getParameterSamples.m` performs adaptive MCMC sampling of the posterior distribution. The DRAM library routine `tooparameters.minox` is used internally.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh_logPost_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_1D >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_2D > > getParameterSamples` (`matlabtypesubstitute parameters`, `matlabtypesubstitute objective_function`, `matlabtypesubstitute varargin`)
`getParameterSamples.m` performs adaptive MCMC sampling of the posterior distribution. The DRAM library routine `tooparameters.minox` is used internally.
- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, fh_logPost_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_1D >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_2D > > mtoc_subst_getParameterSamples_m_tsbust_cotm_visualize` (`Results` (`matlabtypesubstitute parameters`, `matlabtypesubstitute options`))

6.5.1 Detailed Description

`getParameterSamples.m` performs adaptive MCMC sampling of the posterior distribution. The DRAM library routine `tooparameters.minox` is used internally.

6.5.2 Function Documentation

6.5.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, parameters >,mlhsInnerSubst< matlabtypesubstitute, fh_logPost_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_trace >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_1D >,mlhsInnerSubst< matlabtypesubstitute, fh_par_dis_2D > > getParameterSamples (matlabtypesubstitute parameters, matlabtypesubstitute objective_function, matlabtypesubstitute varargin)`

`getParameterSamples.m` performs adaptive MCMC sampling of the posterior distribution. The DRAM library routine `tooparameters.minox` is used internally.

USAGE

```
[...] = getParameterSamples(parameters,objective_function) [...] = getParameterSamples(parameters,objective_↵
_function,options) [parameters] = getParameterSamples(...) [parameters,fh_logPost_trace] = getParameter_↵
Samples(...) [parameters,fh_logPost_trace,fh_par_trace] = getParameterSamples(...) [parameters,fh_logPost_↵
trace,fh_par_trace,fh_par_dis] = getParameterSamples(...)
```

2012/07/11 Jan Hasenauer 2015/04/29 Jan Hasenauer 2016/10/17 Benjamin Ballnus 2016/10/19 Daniel Weindl
2016/11/04 Paul Stapor

Parameters

<i>parameters</i>	parameter struct
<i>varargin</i>	<pre>1 getParameterSamples (..., logPosterior, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • <code>logPosterior</code> log-posterior of model as function of the parameters. • <code>options</code> A <code>PestoOptions</code> object holding various options for the sampling

Return values

<i>parameters</i>	updated parameter object
<i>fh_logPost_trace</i>	figure handle for log-posterior trace
<i>fh_par_trace</i>	figure handle for parameter traces
<i>fh_par_dis</i>	figure handle for parameter distribution

Required fields of parameters:

- `number` -- Number of parameters
- `min` -- Lower bound for each parameter
- `max` -- upper bound for each parameter
- `ml` -- maximum likelihood estimate

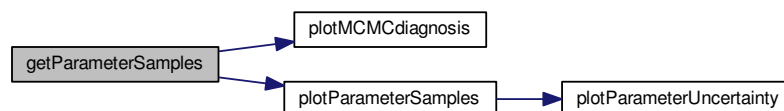
Generated fields of parameters:

- `S` -- parameter and posterior sample.
 - `logPost`: log-posterior function along chain
 - `par`: parameters along chain

Definition at line 17 of file `getParameterSamples.m`.

References `plotMCMCdiagnosis()`, and `plotParameterSamples()`.

Here is the call graph for this function:

6.6 `getPropertyConfidenceIntervals.m` File Reference

[getPropertyConfidenceIntervals.m](#) calculates the confidence intervals for the model properties. This is done by three approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level α (calculated by a χ^2 -distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, properties > getPropertyConfidenceIntervals` (`matlabtypesubstitute properties, matlabtypesubstitute alpha, matlabtypesubstitute varargin`)

[getPropertyConfidenceIntervals.m](#) calculates the confidence intervals for the model properties. This is done by three approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a χ^2 -distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate.

6.6.1 Detailed Description

[getPropertyConfidenceIntervals.m](#) calculates the confidence intervals for the model properties. This is done by three approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a χ^2 -distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate.

6.6.2 Function Documentation

- 6.6.2.1 `mlhsInnerSubst< matlabtypesubstitute, properties > getPropertyConfidenceIntervals (matlabtypesubstitute properties, matlabtypesubstitute alpha, matlabtypesubstitute varargin)`

[getPropertyConfidenceIntervals.m](#) calculates the confidence intervals for the model properties. This is done by three approaches: The values of `CI.local_PL` and `CI.PL` are determined by the point on which a threshold according to the confidence level `alpha` (calculated by a χ^2 -distribution) is reached. `local_PL` computes this point by a local approximation around the MAP estimate using the Hessian matrix, `PL` uses the profile likelihoods instead. The value of `CI.local_B` is computed by using the cumulative distribution function of a local approximation of the profile based on the Hessian matrix at the MAP estimate.

USAGE

- `properties = getPropertyConfidenceIntervals(properties, alpha)`

History

- 2013/11/29 Jan Hasenauer
- 2016/12/01 Paul Stapor

Parameters

<i>properties</i>	property struct
<i>alpha</i>	vector with desired confidence levels for the intervals

Return values

<i>properties</i>	updated properties struct
-------------------	---------------------------

Required fields of properties:

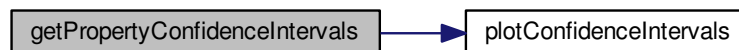
Generated fields of properties:

- `CI` -- Information about confidence levels
 - `local_PL`: Threshold based approach, uses a local approximation by the Hessian matrix at the MAP estimate (requires `parameters.MS`, e.g. from `getMultiStarts`)
 - `PL`: Threshold based approach, uses profile likelihoods (requires `parameters.P`, e.g. from `getParameterProfiles`)
 - `local_B`: Mass based approach, uses a local approximation by the Hessian matrix at the MAP estimate (requires `parameters.MS`, e.g. from `getMultiStarts`)

Definition at line 17 of file `getPropertyConfidenceIntervals.m`.

References `plotConfidenceIntervals()`.

Here is the call graph for this function:



6.7 `getPropertyMultiStarts.m` File Reference

[getPropertyMultiStarts.m](#) evaluates the properties for the different multi-start results.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh > > getPropertyMultiStarts` (matlabtypesubstitute properties, matlabtypesubstitute parameters, matlabtypesubstitute varargin)

[getPropertyMultiStarts.m](#) evaluates the properties for the different multi-start results.

6.7.1 Detailed Description

[getPropertyMultiStarts.m](#) evaluates the properties for the different multi-start results.

6.7.2 Function Documentation

6.7.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh > >`
`getPropertyMultiStarts (matlabtypesubstitute properties, matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

[getPropertyMultiStarts.m](#) evaluates the properties for the different mutli-start results.

USAGE

`[...] = getPropertyMultiStarts(properties,parameters) [...] = getPropertyMultiStarts(properties,parameters,options)`
`[parameters,fh] = getPropertyMultiStarts(...)`

`getPropertyMultiStarts()` uses the following `PestoOptions` members

- `PestoOptions::mode`
- `PestoOptions::fh`
- `PestoOptions::save`
- `PestoOptions::foldername`
- `PestoOptions::comp_type`

History

- 2015/03/03 Jan Hasenauer
- 2016/04/10 Daniel Weindl

Parameters

<i>properties</i>	property struct containing at least:
<i>parameters</i>	parameter struct containing at least:
<i>varargin</i>	<pre>1 getPropertyMultiStarts (..., MS, number, min, max, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • MS information about multi-start optimization • number Number of properties • min lower bound for property values • max upper bound for property values <code>name = {name1,...}</code>: names of the properties <code>function = {function1,...}</code>: functions to evaluate property values. These functions provide the values of the respective properties and the corresponding 1st and 2nd order derivatives. • options A <code>PestoOptions</code> object holding the options for the algorithm.

Return values

<i>properties</i>	updated parameter object containing:
<i>fh</i>	figure handle

Return values

<i>MS</i>	properties for multi-start optimization results <ul style="list-style-type: none"> • <code>par(:,i)</code>: ith MAP • <code>logPost(i)</code>: log-posterior for ith MAP • <code>exitflag(i)</code>: exit flag of ith MAP • <code>prop(j,i)</code>: values of jth property for ith MAP • <code>prop_Sigma(:, :, i)</code>: covariance of properties for ith MAP
-----------	--

Required fields of parameters:

Required fields of properties:

Generated fields of properties:

Definition at line 17 of file `getPropertyMultiStarts.m`.

References `plotPropertyMultiStarts()`.

Here is the call graph for this function:

6.8 `getPropertyProfiles.m` File Reference

[getPropertyProfiles.m](#) calculates the profiles of user-supplied property functions, starting from the maximum a posteriori estimate. This calculation is done by varying the value of each property function respectively, starting from the value of this function at the global optimum and by reoptimizing the likelihood/posterior estimate in each variational step of the property. The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh > > getPropertyProfiles` (matlabtypesubstitute properties, matlabtypesubstitute parameters, matlabtypesubstitute objective_function, matlabtypesubstitute varargin)

[getPropertyProfiles.m](#) calculates the profiles of user-supplied property functions, starting from the maximum a posteriori estimate. This calculation is done by varying the value of each property function respectively, starting from the value of this function at the global optimum and by reoptimizing the likelihood/posterior estimate in each variational step of the property. The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

- `mlhsInnerSubst< matlabtypesubstitute, varargout > mtoc_subst_getPropertyProfiles_m_tsbust_cotm_↔
_obj` (matlabtypesubstitute theta, matlabtypesubstitute fun, matlabtypesubstitute type)
- `mlhsInnerSubst< matlabtypesubstitute, varargout > mtoc_subst_getPropertyProfiles_m_tsbust_cotm_↔
_obj_con` (matlabtypesubstitute theta, matlabtypesubstitute fun, matlabtypesubstitute fun_min, matlabtypesubstitute type)
- `mlhsInnerSubst< matlabtypesubstitute, varargout > mtoc_subst_getPropertyProfiles_m_tsbust_cotm_↔
prop_fun` (matlabtypesubstitute theta, matlabtypesubstitute fun, matlabtypesubstitute prop_min, matlabtypesubstitute prop_max, matlabtypesubstitute s)
- `mlhsInnerSubst< matlabtypesubstitute, varargout > mtoc_subst_getPropertyProfiles_m_tsbust_cotm_↔
_prop_con_fun` (matlabtypesubstitute theta, matlabtypesubstitute fun, matlabtypesubstitute prop_min, matlabtypesubstitute prop_max, matlabtypesubstitute s)

6.8.1 Detailed Description

[getPropertyProfiles.m](#) calculates the profiles of user-supplied property functions, starting from the maximum a posteriori estimate. This calculation is done by varying the value of each property function respectively, starting from the value of this function at the global optimum and by reoptimizing the likelihood/posterior estimate in each variational step of the property. The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

6.8.2 Function Documentation

- 6.8.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh > > getPropertyProfiles` (matlabtypesubstitute *properties*, matlabtypesubstitute *parameters*, matlabtypesubstitute *objective_function*, matlabtypesubstitute *varargin*)

[getPropertyProfiles.m](#) calculates the profiles of user-supplied property functions, starting from the maximum a posteriori estimate. This calculation is done by varying the value of each property function respectively, starting from the value of this function at the global optimum and by reoptimizing the likelihood/posterior estimate in each variational step of the property. The initial guess for the next reoptimization point is computed by extrapolation from the previous points to ensure a quick optimization.

Note: This function can exploit up to (n_theta + 1) workers when running in `parallel` mode.

USAGE

[...] = [getPropertyProfiles](#)(properties, parameters, objective_function) [...] = [getPropertyProfiles](#)(properties, parameters, objective_function, options) [parameters, fh] = [getPropertyProfiles](#)(...)

%

[getPropertyProfiles\(\)](#) uses the following `PestoOptions` members

- `PestoOptions::boundary`

- PestoOptions::calc_profiles
- PestoOptions::comp_type
- PestoOptions::dJ
- PestoOptions::dR_max
- PestoOptions::fh
- PestoOptions::fmincon
- PestoOptions::foldername
- PestoOptions::MAP_index
- PestoOptions::mode
- PestoOptions::obj_type
- PestoOptions::options_getNextPoint .guess .min .max .update .mode
- PestoOptions::plot_options
- PestoOptions::property_index
- PestoOptions::R_min
- PestoOptions::save

History

- 2012/03/02 Jan Hasenauer
- 2016/04/10 Daniel Weindl
- 2016/10/12 Paul Stapor

Parameters

<i>properties</i>	property struct
<i>parameters</i>	parameter struct
<i>objective_function</i>	objective function to be optimized. This function should accept one input, the parameter vector.
<i>varargin</i>	<pre>1 getPropertyProfiles (..., options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • options A PestoOptions object holding various options for the algorithm.

Return values

<i>properties</i>	updated property struct
<i>fh</i>	figure handle

Required fields of properties:

- `number` -- Number of properties
- `min` -- Lower bound for each properties
- `max` -- upper bound for each properties
`name = {name1, ...}`: names of the properties
`function = {function1, ...}`: functions to evaluate property values. These functions provide the values of the respective properties and the corresponding 1st and 2nd order derivatives.

Required fields of parameters:

- `number` -- Number of parameters
- `min` -- Lower bound for each parameter
- `max` -- upper bound for each parameter name = {name1, ...}: names of the parameters
- `MS` -- results of global optimization, obtained using for instance the routine [getMultiStarts.m](#). MS has to contain at least
 - `par`: sorted list `n_theta` x `n_starts` of parameter estimates. The first entry is assumed to be the best one.
 - `logPost`: sorted list `n_starts` x 1 of log-posterior values corresponding to the parameters listed in `.par`.
 - `hessian`: Hessian matrix (or approximation) at the optimal point

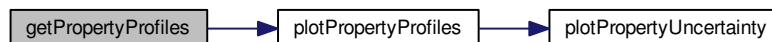
Generated fields of properties:

- `P(i)` -- profile for i-th parameter
 - `prop`: MAPs along profile
 - `par`: MAPs along profile
 - `logPost`: maximum log-posterior along profile
 - `R`: ratio

Definition at line 17 of file `getPropertyProfiles.m`.

References `plotPropertyProfiles()`.

Here is the call graph for this function:



6.9 `getPropertySamples.m` File Reference

[getPropertySamples.m](#) evaluates the properties for the sampled parameters.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh > >` [getPropertySamples](#) (matlabtypesubstitute properties, matlabtypesubstitute parameters, matlabtypesubstitute varargin)

[getPropertySamples.m](#) evaluates the properties for the sampled parameters.

6.9.1 Detailed Description

[getPropertySamples.m](#) evaluates the properties for the sampled parameters.

6.9.2 Function Documentation

6.9.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, properties >,mlhsInnerSubst< matlabtypesubstitute, fh >`
`> getPropertySamples (matlabtypesubstitute properties, matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

`getPropertySamples.m` evaluates the properties for the sampled parameters.

USAGE

```
[...] = getPropertySamples(properties,parameters) [...] = getPropertySamples(properties,parameters,options)
[parameters,fh] = getPropertySamples(...)
```

`getPropertySamples()` uses the following `PestoOptions` members

- `PestoOptions::property_index`
- `PestoOptions::mode`
- `PestoOptions::fh`
- `PestoOptions::save`
- `PestoOptions::foldername`
- `PestoOptions::comp_type`
- `PestoOptions::plot_options`
- `PestoOptions::MCMC.thinning`

History

- 2015/04/01 Jan Hasenauer
- 2016/10/04 Daniel Weindl

Parameters

<i>properties</i>	property struct
<i>parameters</i>	parameter struct
<i>varargin</i>	<pre>1 getPropertySamples (..., options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • <code>options</code> A <code>PestoOptions</code> object holding various options for the algorithm.

Return values

<i>properties</i>	updated parameter object
<i>fh</i>	figure handle

Required fields of `properties`:

- `number` -- number of parameter
- `min` -- lower bound for property values

- `max` -- upper bound for property values
- `name` -- = {`name1`,...} ... names of the parameters
- `function` -- = {`function1`,...} ... functions to evaluate property values. These functions provide the values of the respective properties and the corresponding 1st and 2nd order derivatives.

Required fields of parameters:

- `S` -- parameter and posterior sample. `logPost` ... log-posterior function along chain `par` ... parameters along chain *Note* This struct is obtained using `getSamples.m`.

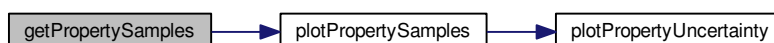
Generated fields of properties:

- `S` -- properties for sampling results
 - `par(*,i)`: *i*th samples parameter vector
 - `logPost(i)`: log-posterior for *i*th samples parameter vector
 - `prop(j,i)`: values of *j*th property for *i*th samples parameter vector
 - `prop_Sigma(*,*,i)`: covariance of properties for *i*th samples parameter vector

Definition at line 17 of file `getPropertySamples.m`.

References `plotPropertySamples()`.

Here is the call graph for this function:



6.10 meigoDummy.m File Reference

Objective function wrapper for MEIGO / PSwarm / ... which need objective function *file*name* and cannot use function handles directly.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, f > meigoDummy` (`matlabtypesubstitute theta`, `matlabtypesubstitute fun`, `matlabtypesubstitute varargin`)

*Objective function wrapper for MEIGO / PSwarm / ... which need objective function file*name and cannot use function handles directly.*

6.10.1 Detailed Description

Objective function wrapper for MEIGO / PSwarm / ... which need objective function *file*name* and cannot use function handles directly.

6.10.2 Function Documentation

- ##### 6.10.2.1 `mlhsInnerSubst< matlabtypesubstitute, f > meigoDummy` (`matlabtypesubstitute theta`, `matlabtypesubstitute fun`, `matlabtypesubstitute varargin`)

Objective function wrapper for MEIGO / PSwarm / ... which need objective function *file*name* and cannot use function handles directly.

Parameters

<i>theta</i>	parameter vector
<i>fun</i>	objective function handle
<i>varargin</i>	

Definition at line 17 of file `meigoDummy.m`.

6.11 `plotConfidenceIntervals.m` File Reference

[plotConfidenceIntervals.m](#) visualizes confidence intervals stored in either the parameters or properties struct `.CI`

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotConfidenceIntervals` (`matlabtypesubstitute pStruct`, `matlabtypesubstitute alpha`, `matlabtypesubstitute varargin`)
[plotConfidenceIntervals.m](#) visualizes confidence intervals stored in either the parameters or properties struct `.CI`
- `mlhsInnerSubst< matlabtypesubstitute, methodsOut > mtoc_subst_plotConfidenceIntervals_m_tsbus↔_cotm_checkMeth` (`matlabtypesubstitute methodsIn`, `matlabtypesubstitute pStruct`, `matlabtypesubstitute boolWarning`)

6.11.1 Detailed Description

[plotConfidenceIntervals.m](#) visualizes confidence intervals stored in either the parameters or properties struct `.CI`

6.11.2 Function Documentation

- 6.11.2.1 `mlhsInnerSubst< matlabtypesubstitute, fh > plotConfidenceIntervals` (`matlabtypesubstitute pStruct`, `matlabtypesubstitute alpha`, `matlabtypesubstitute varargin`)

[plotConfidenceIntervals.m](#) visualizes confidence intervals stored in either the parameters or properties struct `.CI`

USAGE

`fh = plotParameterUncertainty(pStruct)` `fh = plotParameterUncertainty(pStruct, methods)` `fh = plotParameter↔Uncertainty(pStruct, methods, options)`

`plotMultiStarts()` uses the following `PestoPlottingOptions` members

- `PestoPlottingOptions::P`
- `PestoPlottingOptions::S`
- `PestoPlottingOptions::MS`
- `PestoPlottingOptions::boundary`
- `PestoPlottingOptions::subplot_size_1D`
- `PestoPlottingOptions::subplot_indexing_1D`
- `PestoPlottingOptions::CL`
- `PestoPlottingOptions::hold_on`

- [PestoPlottingOptions::interval](#)
- [PestoPlottingOptions::bounds](#)
- [PestoPlottingOptions::A](#)
- [PestoPlottingOptions::add_points](#)
- [PestoPlottingOptions::labels](#)
- [PestoPlottingOptions::legend](#)
- [PestoPlottingOptions::op2D](#)
- [PestoPlottingOptions::fontsize](#)

History

- 2016/11/14 Paul Stapor

Parameters

<i>pStruct</i>	either the parameter or the property struct containing information about parameters and results of optimization (.MS) and uncertainty analysis (.P and .S). This structures is the output of plotMultiStarts.m , getProfiles.m or plotSamples.m .
<i>varargin</i>	<pre>1 plotConfidenceIntervals (..., method, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • method integer array, from which method confidence intervals should be plotted: • options options of plotting as instance of PestoPlottingOptions

Return values

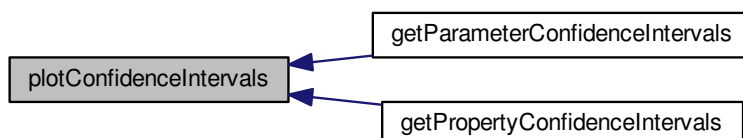
<i>fh</i>	figure handle
-----------	---------------

Required fields of pStruct:

Definition at line 17 of file `plotConfidenceIntervals.m`.

Referenced by `getParameterConfidenceIntervals()`, and `getPropertyConfidenceIntervals()`.

Here is the caller graph for this function:



6.12 plotMCMCdiagnosis.m File Reference

[plotMCMCdiagnosis.m](#) visualizes the Markov chains generated by [getSamples.m](#).

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotMCMCdiagnosis (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`
[plotMCMCdiagnosis.m](#) visualizes the Markov chains generated by [getSamples.m](#).

6.12.1 Detailed Description

[plotMCMCdiagnosis.m](#) visualizes the Markov chains generated by [getSamples.m](#).

6.12.2 Function Documentation

- 6.12.2.1 `mlhsInnerSubst< matlabtypesubstitute, fh > plotMCMCdiagnosis (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

[plotMCMCdiagnosis.m](#) visualizes the Markov chains generated by [getSamples.m](#).

USAGE

```
fh = plotMCMCdiagnosis(parameters) fh = plotMCMCdiagnosis(parameters,type) fh = plotMCMCdiagnosis(parameters,type,fh) fh = plotMCMCdiagnosis(parameters,type,fh,l) fh = plotMCMCdiagnosis(parameters,type,fh,l,options)
```

History

- 2014/06/20 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>parameters</i>	parameter struct containing information about parameters and results of optimization (.MS) and uncertainty analysis (.S). This structures is the output of plotMultiStarts.m , getProfiles.m or plotSamples.m .
<i>varargin</i>	

Definition at line 17 of file [plotMCMCdiagnosis.m](#).

Referenced by [getParameterSamples\(\)](#).

Here is the caller graph for this function:



6.13 plotMultiStarts.m File Reference

plotMultiStarts plots the result of the multi-start optimization stored in parameters.

Functions

- mlhsInnerSubst< matlabtypesubstitute, fh > [plotMultiStarts](#) (matlabtypesubstitute parameters, matlabtypesubstitute varargin)
plotMultiStarts plots the result of the multi-start optimization stored in parameters.

6.13.1 Detailed Description

plotMultiStarts plots the result of the multi-start optimization stored in parameters.

6.13.2 Function Documentation

6.13.2.1 mlhsInnerSubst< matlabtypesubstitute, fh > plotMultiStarts (matlabtypesubstitute *parameters*, matlabtypesubstitute *varargin*)

plotMultiStarts plots the result of the multi-start optimization stored in parameters.

USAGE

fh = plotMultiStarts(parameters) fh = plotMultiStarts(parameters,fh) fh = plotMultiStarts(parameters,fh,options)

plotMultiStarts() uses the following PestoPlottingOptions members

- [PestoPlottingOptions::add_points](#)
- [PestoPlottingOptions::title](#)
- [PestoPlottingOptions::draw_bounds](#)

History:

- 2012/05/31 Jan Hasenauer
- 2016/10/07 Daniel Weindl

Parameters

<i>parameters</i>	parameter struct containing information about parameters and log-posterior.
<i>varargin</i>	<pre>1 plotMultiStarts (..., fh, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> fh handle of figure in which profile likelihood is plotted. If no figure handle is provided, a new figure is opened. options options of plotting as instance of PestoPlottingOptions

Return values

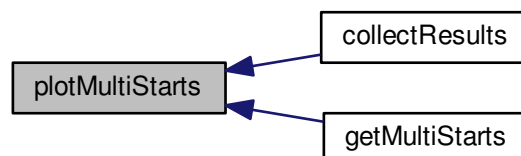
<i>fh</i>	figure handle
-----------	---------------

Required fields of parameters:

Definition at line 17 of file `plotMultiStarts.m`.

Referenced by `collectResults()`, and `getMultiStarts()`.

Here is the caller graph for this function:

6.14 `plotParameterProfiles.m` File Reference

[plotParameterProfiles.m](#) visualizes profile likelihood. Note: This routine provides an interface for `plotUncertainty.m`.

Functions

- `mlhsInnerSubst < matlabtypesubstitute, fh > plotParameterProfiles` (`matlabtypesubstitute` parameters, `matlabtypesubstitute` varargin)
[plotParameterProfiles.m](#) visualizes profile likelihood. Note: This routine provides an interface for `plotUncertainty.m`.

6.14.1 Detailed Description

[plotParameterProfiles.m](#) visualizes profile likelihood. Note: This routine provides an interface for [plotUncertainty.m](#).

6.14.2 Function Documentation

6.14.2.1 `mlhslInnerSubst< matlabtypesubstitute, fh > plotParameterProfiles (matlabtypesubstitute parameters,
matlabtypesubstitute varargin)`

[plotParameterProfiles.m](#) visualizes profile likelihood. Note: This routine provides an interface for [plotUncertainty.m](#).

USAGE

```
fh = plotParameterProfiles(parameters) fh = plotParameterProfiles(parameters,type) fh = plotParameterProfiles(parameters,type,fh) fh = plotParameterProfiles(parameters,type,fh,I) fh = plotParameterProfiles(parameters,type,fh,I,options)
```

History

- 2012/05/31 Jan Hasenauer
- 2014/06/20 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>parameters</i>	parameter struct containing information about parameters and results of optimization (.MS) and uncertainty analysis (.P and .S). This structure is the output of plotMultiStarts.m , getProfiles.m or plotSamples.m .
<i>varargin</i>	<pre>1 plotParameterProfiles (..., type, fh, I, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D or 2D • fh handle of figure. If no figure handle is provided, a new figure is opened. • I index of parameters which are updated. If no index is provided all parameters are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

<i>fh</i>	figure handle
-----------	---------------

Definition at line 17 of file [plotParameterProfiles.m](#).

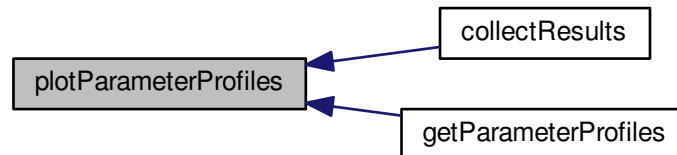
References [plotParameterUncertainty\(\)](#).

Referenced by [collectResults\(\)](#), and [getParameterProfiles\(\)](#).

Here is the call graph for this function:



Here is the caller graph for this function:



6.15 `plotParameterSamples.m` File Reference

[plotParameterSamples.m](#) visualizes MCMC samples. Note: This routine provides an interface for `plotUncertainty.m`.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotParameterSamples (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

[plotParameterSamples.m](#) visualizes MCMC samples. Note: This routine provides an interface for `plotUncertainty.m`.

6.15.1 Detailed Description

[plotParameterSamples.m](#) visualizes MCMC samples. Note: This routine provides an interface for `plotUncertainty.m`.

6.15.2 Function Documentation

- #### 6.15.2.1 `mlhsInnerSubst< matlabtypesubstitute, fh > plotParameterSamples (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

[plotParameterSamples.m](#) visualizes MCMC samples. Note: This routine provides an interface for `plotUncertainty.m`.

USAGE

```
fh = plotParameterSamples(parameters) fh = plotParameterSamples(parameters,type) fh = plotParameterSamples(parameters,type,fh) fh = plotParameterSamples(parameters,type,fh,l) fh = plotParameterSamples(parameters,type,fh,l,options)
```

History

- 2012/05/31 Jan Hasenauer
- 2014/06/20 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>parameters</i>	parameter struct containing information about parameters and results of optimization (.MS) and uncertainty analysis (.P and .S). This structures is the output of plotMultiStarts.m , getProfiles.m or plotSamples.m .
<i>varargin</i>	<pre>1 plotParameterSamples (..., type, fh, l, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D or 2D • fh handle of figure. If no figure handle is provided, a new figure is opened. • l index of parameters which are updated. If no index is provided all parameters are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

<i>fh</i>	figure handle
-----------	---------------

Definition at line 17 of file `plotParameterSamples.m`.

References `plotParameterUncertainty()`.

Referenced by `getParameterSamples()`.

Here is the call graph for this function:



Here is the caller graph for this function:



6.16 plotParameterUncertainty.m File Reference

[plotParameterUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in parameters.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotParameterUncertainty (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`
[plotParameterUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in parameters.

6.16.1 Detailed Description

[plotParameterUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in parameters.

6.16.2 Function Documentation

- 6.16.2.1 `mlhsInnerSubst< matlabtypesubstitute, fh > plotParameterUncertainty (matlabtypesubstitute parameters, matlabtypesubstitute varargin)`

[plotParameterUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in parameters.

USAGE

```
fh = plotParameterUncertainty(parameters) fh = plotParameterUncertainty(parameters,type) fh = plot↵
ParameterUncertainty(parameters,type,fh) fh = plotParameterUncertainty(parameters,type,fh,l) fh = plot↵
ParameterUncertainty(parameters,type,fh,l,options)
```

`plotMultiStarts()` uses the following `PestoPlottingOptions` members

- [PestoPlottingOptions::P](#)
- [PestoPlottingOptions::S](#)
- [PestoPlottingOptions::MS](#)
- [PestoPlottingOptions::boundary](#)
- [PestoPlottingOptions::subplot_size_1D](#)
- [PestoPlottingOptions::subplot_indexing_1D](#)
- [PestoPlottingOptions::CL](#)

- [PestoPlottingOptions::hold_on](#)
- [PestoPlottingOptions::interval](#)
- [PestoPlottingOptions::bounds](#)
- [PestoPlottingOptions::A](#)
- [PestoPlottingOptions::add_points](#)
- [PestoPlottingOptions::labels](#)
- [PestoPlottingOptions::legend](#)
- [PestoPlottingOptions::op2D](#)
- [PestoPlottingOptions::fontsize](#)

History

- 2012/05/31 Jan Hasenauer
- 2014/06/20 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>parameters</i>	parameter struct containing information about parameters and results of optimization (.MS) and uncertainty analysis (.P and .S). This structures is the output of plotMultiStarts.m , getProfiles.m or plotSamples.m .
<i>varargin</i>	<pre>1 plotParameterUncertainty (..., type, fh, I, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D or 2D • fh handle of figure. If no figure handle is provided, a new figure is opened. • I index of parameters which are updated. If no index is provided all parameters are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

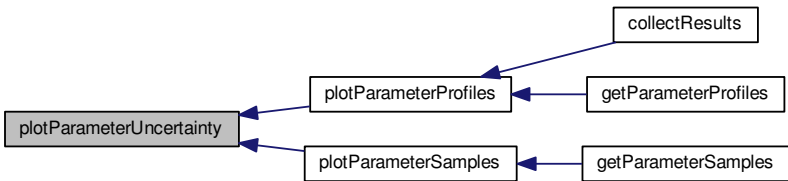
<i>fh</i>	figure handle
-----------	---------------

Required fields of parameters:

Definition at line 17 of file `plotParameterUncertainty.m`.

Referenced by `plotParameterProfiles()`, and `plotParameterSamples()`.

Here is the caller graph for this function:



6.17 plotPropertyMultiStarts.m File Reference

plotPropertyMultiStarts plots the result of the multi-start optimization stored in properties.

Functions

- mlhsInnerSubst< matlabtypesubstitute, fh > [plotPropertyMultiStarts](#) (matlabtypesubstitute properties, matlabtypesubstitute varargin)
plotPropertyMultiStarts plots the result of the multi-start optimization stored in properties.

6.17.1 Detailed Description

plotPropertyMultiStarts plots the result of the multi-start optimization stored in properties.

6.17.2 Function Documentation

6.17.2.1 mlhsInnerSubst< matlabtypesubstitute, fh > [plotPropertyMultiStarts](#) (matlabtypesubstitute *properties*, matlabtypesubstitute *varargin*)

plotPropertyMultiStarts plots the result of the multi-start optimization stored in properties.

USAGE

fh = plotPropertyMultiStarts(properties) fh = plotPropertyMultiStarts(properties,fh) fh = plotPropertyMultiStarts(properties,fh,options)

History

- 2015/03/03 Jan Hasenauer

Parameters

<i>properties</i>	property struct containing information about properties and log-posterior.
<i>varargin</i>	<div>1 plotPropertyMultiStarts (..., fh, options)</div> <div>Required Parameters for varargin:</div>
Generated by Doxygen	<div>• fh handle of figure in which profile likelihood is plotted. If no figure handle is provided, a new figure is opened.</div> <div>• options options of plotting as instance of PestoPlottingOptions</div>

Return values

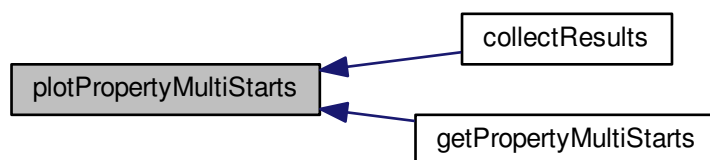
<i>fh</i>	figure handle
-----------	---------------

Required fields of properties:

Definition at line 17 of file plotPropertyMultiStarts.m.

Referenced by collectResults(), and getPropertyMultiStarts().

Here is the caller graph for this function:



6.18 plotPropertyProfiles.m File Reference

[plotPropertyProfiles.m](#) visualizes profile likelihood of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

Functions

- mlhsInnerSubst< matlabtypesubstitute, fh > [plotPropertyProfiles](#) (matlabtypesubstitute properties, matlabtypesubstitute varargin)

[plotPropertyProfiles.m](#) visualizes profile likelihood of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

6.18.1 Detailed Description

[plotPropertyProfiles.m](#) visualizes profile likelihood of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

6.18.2 Function Documentation

6.18.2.1 `mlhsInnerSubst < matlabtypesubstitute, fh > plotPropertyProfiles (matlabtypesubstitute properties,
matlabtypesubstitute varargin)`

[plotPropertyProfiles.m](#) visualizes profile likelihood of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

USAGE

```
fh = plotPropertyProfiles(properties) fh = plotPropertyProfiles(properties,type) fh = plotPropertyProfiles(properties,type,fh) fh = plotPropertyProfiles(properties,type,fh,I) fh = plotPropertyProfiles(properties,type,fh,I,options)
```

History

- 2015/03/02 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>properties</i>	property struct containing information about properties and results of optimization (.MS) and uncertainty analysis (.P and .S).
<i>varargin</i>	<pre>1 plotPropertyProfiles (..., type, fh, I, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D or 2D • fh handle of figure. If no figure handle is provided, a new figure is opened. • I index of properties which are updated. If no index is provided all properties are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

<i>fh</i>	figure handle
-----------	---------------

Definition at line 17 of file `plotPropertyProfiles.m`.

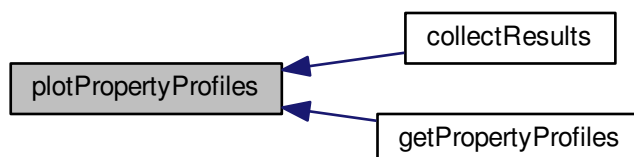
References `plotPropertyUncertainty()`.

Referenced by `collectResults()`, and `getPropertyProfiles()`.

Here is the call graph for this function:



Here is the caller graph for this function:



6.19 plotPropertySamples.m File Reference

[plotPropertySamples.m](#) visualizes samples of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotPropertySamples` (matlabtypesubstitute properties, matlabtypesubstitute varargin)

[plotPropertySamples.m](#) visualizes samples of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

6.19.1 Detailed Description

[plotPropertySamples.m](#) visualizes samples of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

6.19.2 Function Documentation

6.19.2.1 `mlhsInnerSubst < matlabtypesubstitute, fh > plotPropertySamples (matlabtypesubstitute properties,
matlabtypesubstitute varargin)`

[plotPropertySamples.m](#) visualizes samples of model properties. Note: This routine provides an interface for [plotPropertyUncertainty.m](#).

USAGE

```
fh = plotPropertySamples(properties) fh = plotPropertySamples(properties,type) fh = plotPropertySamples(properties,type,fh) fh = plotPropertySamples(properties,type,fh,I) fh = plotPropertySamples(properties,type,fh,I,options)
```

History

- 2015/04/01 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>properties</i>	property struct containing information about properties and results of optimization (.MS) and uncertainty analysis (.P and .S).
<i>varargin</i>	<pre>1 plotPropertySamples (..., type, fh, I, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D or 2D • fh handle of figure. If no figure handle is provided, a new figure is opened. • I index of properties which are updated. If no index is provided all properties are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

<i>fh</i>	figure handle
-----------	---------------

Definition at line 17 of file `plotPropertySamples.m`.

References `plotPropertyUncertainty()`.

Referenced by `getPropertySamples()`.

Here is the call graph for this function:



Here is the caller graph for this function:



6.20 plotPropertyUncertainty.m File Reference

[plotPropertyUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in properties.

Functions

- `mlhsInnerSubst< matlabtypesubstitute, fh > plotPropertyUncertainty` (`matlabtypesubstitute properties`, `matlabtypesubstitute varargin`)
[plotPropertyUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in properties.

6.20.1 Detailed Description

[plotPropertyUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in properties.

6.20.2 Function Documentation

- 6.20.2.1 `mlhsInnerSubst< matlabtypesubstitute, fh > plotPropertyUncertainty` (`matlabtypesubstitute properties`, `matlabtypesubstitute varargin`)

[plotPropertyUncertainty.m](#) visualizes profile likelihood and MCMC samples stored in properties.

USAGE

`fh = plotPropertyUncertainty(properties,type)` `fh = plotPropertyUncertainty(properties,type,fh)` `fh = plotPropertyUncertainty(properties,type,fh,l)` `fh = plotPropertyUncertainty(properties,type,fh,l,options)`

History

- 2012/05/31 Jan Hasenauer
- 2014/06/20 Jan Hasenauer
- 2016/10/10 Daniel Weindl

Parameters

<i>properties</i>	properties struct.
<i>varargin</i>	<pre>1 plotPropertyUncertainty (..., type, fh, I, options)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • type string indicating the type of visualization: 1D • fh handle of figure. If no figure handle is provided, a new figure is opened. • I index of properties which are updated. If no index is provided all parameters are updated. • options options of plotting as instance of PestoPlottingOptions

Return values

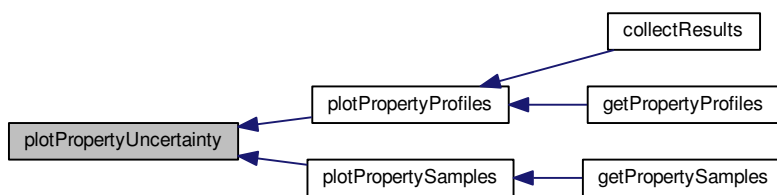
<i>fh</i>	figure handle
-----------	---------------

Required fields of properties:

Definition at line 17 of file plotPropertyUncertainty.m.

Referenced by plotPropertyProfiles(), and plotPropertySamples().

Here is the caller graph for this function:



6.21 runPestoTests.m File Reference

runPestoTests Run a set of PESTO unit tests

Functions

- noret::substitute [runPestoTests](#) ()
runPestoTests Run a set of PESTO unit tests

6.21.1 Detailed Description

`runPestoTests` Run a set of PESTO unit tests

6.22 testGradient.m File Reference

`testGradient.m` calculates finite difference approximations to the gradient to check an analytical version.

Functions

- `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, g >,mlhsInnerSubst< matlabtypesubstitute, g_fd_↔
f >,mlhsInnerSubst< matlabtypesubstitute, g_fd_b >,mlhsInnerSubst< matlabtypesubstitute, g_fd_c > >
testGradient (matlabtypesubstitute varargin)
testGradient.m calculates finite difference approximations to the gradient to check an analytical version.`

6.22.1 Detailed Description

`testGradient.m` calculates finite difference approximations to the gradient to check an analytical version.

6.22.2 Function Documentation

- 6.22.2.1 `mlhsSubst< mlhsInnerSubst< matlabtypesubstitute, g >,mlhsInnerSubst< matlabtypesubstitute, g_fd_f
>,mlhsInnerSubst< matlabtypesubstitute, g_fd_b >,mlhsInnerSubst< matlabtypesubstitute, g_fd_c > >
testGradient (matlabtypesubstitute varargin)`

`testGradient.m` calculates finite difference approximations to the gradient to check an analytical version.

backward differences: $g_fd_f = (f(\theta + \epsilon \cdot e_i) - f(\theta)) / \epsilon$

forward differences: $g_fd_b = (f(\theta) - f(\theta - \epsilon \cdot e_i)) / \epsilon$

central differences: $g_fd_c = (f(\theta + \epsilon \cdot e_i) - f(\theta - \epsilon \cdot e_i)) / (2 \cdot \epsilon)$

in order to work with tensors of order n the gradient must be returned as tensor of order $n+1$ where the $n+1$ th tensor dimension indexes the parameters with respect to which the differentiation was carried out

USAGE

`[...] = testGradient(theta,fun,eps,il,ig) [g,g_fd_f,g_fd_b,g_fd_c] = testGradient(...)`

History

- 2014/06/11 Jan Hasenauer
- 2015/01/16 Fabian Froehlich
- 2015/04/03 Jan Hasenauer
- 2015/07/28 Fabian Froehlich

Parameters

<i>varargin</i>	<pre>1 testGradient (theta, fun, eps, il, ig)</pre> <p><i>Required Parameters for varargin:</i></p> <ul style="list-style-type: none"> • theta parameter vector at which gradient is evaluated. • fun function of theta for which gradients are checked. • eps epsilon used for finite difference approximation of gradient (eps = 1e-4). • il argout index/fieldname at which function values are returned (default = 1). • ig argout index/fieldname at which gradient values are returned (default = 2).
-----------------	--

Return values

<i>g</i>	gradient computed by f
<i>g_fd↔ _f</i>	backward differences
<i>g_fd↔ _b</i>	forward differences
<i>g_fd↔ _c</i>	central differences

Definition at line 17 of file testGradient.m.

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