PEtab

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Data format

CHAPTER 1

PEtab data format specification

This document explains the PEtab data format.

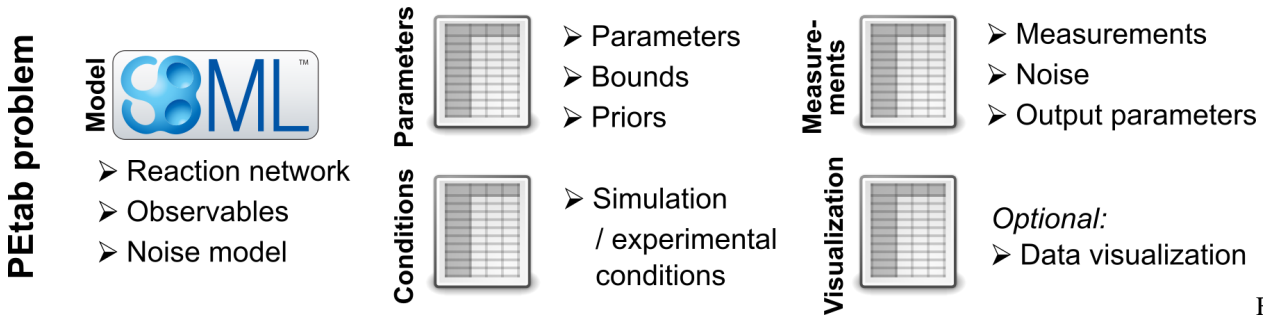
1.1 Purpose

Providing a standardized way for specifying parameter estimation problems in systems biology, especially for the case of Ordinary Differential Equation (ODE) models.

1.2 Overview

The PEtab data format specifies a parameter estimation problem using a number of text-based files (Systems Biology Markup Language (SBML) and Tab-Separated Values (TSV)), i.e.

- An SBML model [SBML]
- A measurement file to fit the model to [TSV]
- A condition file specifying model inputs and condition-specific parameters [TSV]
- A parameter file specifying optimization parameters and related information [TSV]
- (optional) A simulation file, which has the same format as the measurement file, but contains model simulations [TSV]
- (optional) A visualization file, which contains specifications how the data and/or simulations should be plotted by the visualization routines [TSV]



Files constituting a PEtab problem

The following sections will describe the minimum requirements of those components in the core standard, which should provide all information for defining the parameter estimation problem.

Extensions of this format (e.g. additional columns in the measurement table) are possible and intended. However, those columns should provide extra information for example for plotting, or for more efficient parameter estimation, but they should not affect the optimization problem as such. Some optional extensions are described in the last section, "Extensions", of this document.

General remarks

- All model entities column and row names are case-sensitive
- Fields in "[]" in the second row are optional and may be left empty.

1.3 SBML model definition

The model must be specified as valid SBML. Since parameter estimation is beyond the scope of SBML, there exists no standard way to specify observables (model outputs) and respective noise models. Therefore, we use the following convention.

1.3.1 Observables

In the SBML model, observables are specified as `AssignmentRules` assigning to parameters with `ids` starting with `observable_` followed by the `observableId` as in the corresponding column of the *measurement table* (see below).

E.g.

```
observable_pErk = observableParameter1_pErk + observableParameter2_pErk*pErk
```

where `observableParameter1_pErk` would be an offset, and `observableParameter2_pErk` a scaling parameter for the observable `pErk`. The observable parameter names have the structure: `observableParameter${indexOfObservableParameter}_${observableId}` to facilitate automatic recognition. The specific values or parameters are assigned in the *measurement table*.

1.3.2 Noise model

Measurement noise can be specified as a numerical value in the `noiseParameters` column of the *measurement table* (see below), which will default to a Gaussian noise model with standard deviation as provided in `noiseParameters`.

Alternatively, more complex noise models can be specified for each observable, using additional `AssignmentRules`. Those noise model rules assign to `sigma_${observableId}` parameters. A noise model which accounts for relative and absolute contributions could, e.g., be defined as

```
sigma_pErk = noiseParameter1_pErk + noiseParameter2_pErk*pErk
```

with `noiseParameter1_pErk` denoting the absolute and `noiseParameter2_pErk` the relative contribution for the observable `pErk`. The noise parameter names have the structure: `noiseParameter${indexOfNoiseParameter}_${observableId}` to facilitate automatic recognition. The specific values or parameters are assigned in the *measurement table*.

Any parameters named `noiseParameter${1..n}` *must* be overwritten in the `noiseParameters` column of the measurement file (see below).

1.4 Condition table

The condition table specifies parameters or *constant* species for specific simulation condition (generally corresponding to different experimental conditions).

This is specified as tab-separated value file with condition-specific species/parameters in the following way:

Row names are condition names as referenced in the measurement table below. Column names are global parameter IDs or IDs of constant species as given in the SBML model. These parameters will override any parameter values specified in the model. `parameterOrStateId`s and `conditionId`s must be unique.

Row- and column-ordering are arbitrary, although specifying `parameterId` first may improve human readability. The `conditionName` column is optional. Additional columns are *not* allowed.

Note 1: Instead of adding additional columns to the condition table, they can easily be added to a separate file, since every row of the condition table has `parameterId` as unique key.

1.5 Measurement table

A tab-separated values files containing all measurements to be used for model training or validation.

Expected to have the following named columns in any (but preferably this) order:

(wrapped for readability)

Additional (non-standard) columns may be added. If the additional plotting functionality of PEtab should be used, such columns could be

where `datasetId` is a necessary column to use particular plotting functionality, and `replicateId` is optional, which can be used to group replicates and plot error bars.

1.5.1 Detailed field description

- `observableId` [STRING, NOT NULL, REFERENCES(sbml.observableID)]

  Observable ID with a matching parameter in the SBML model with ID `observable_${observableId}`

- `preequilibrationConditionId` [STRING OR NULL, REFERENCES(conditionsTable.conditionID)]

  The `conditionId` to be used for preequilibration. E.g. for drug treatments the model would be preequilibrated with the no-drug condition. Empty for no preequlibration.

- `simulationConditionId` [STRING, NOT NULL, REFERENCES(conditionsTable.conditionID)]

  `conditionId` as provided in the condition table, specifying the condition-specific parameters used for simulation.

- `measurement` [NUMERIC, NOT NULL]

  The measured value in the same units/scale as the model output.

- `time` [NUMERIC OR STRING, NOT NULL]

  Time point of the measurement in the time unit specified in the SBML model, numeric value or `inf` (lower-case) for steady-state measurements.

- `observableParameters` [STRING OR NULL]

  This field allows overriding or introducing condition-specific versions of parameters defined in the model. The model can define observables (see above) containing place-holder parameters which can be replaced by condition-specific dynamic or constant parameters. Placeholder parameters must be named `observableParameter${n}_${observableId}` with `n` ranging from 1 (not 0) to the number of placeholders for the given observable, without gaps. If the observable specified under `observableId` contains no placeholders, this field must be empty. If it contains `n > 0` placeholders, this field must hold `n` semicolon-separated numeric values or parameter names. No trailing semicolon must be added.

  Different lines for the same `observableId` may specify different parameters. This may be used to account for condition-specific or batch-specific parameters. This will translate into an extended optimization parameter vector.

  All placeholders defined in the model must be overwritten here. If there are not placeholders in the model, this column may be omitted.

- `noiseParameters` [STRING]

  The measurement standard deviation or `NaN` if the corresponding sigma is a model parameter.

  Numeric values or parameter names are allowed. Same rules apply as for `observableParameters` in the previous point.

- `observableTransformation` [STRING]

  Transformation of the observable and measurement for computing the objective function. `lin`, `log` or `log10`. Defaults to 'lin'. The measurements and model outputs are both assumed to be provided in linear space.

- `noiseDistribution` [STRING: 'normal' or 'laplace']

  Assumed Noise distribution for the given measurement. Only normally or Laplace distributed noise is currently allowed. Defaults to `normal`. If `normal`, the specified `noiseParameters` will be interpreted as standard deviation (*not* variance).

- `datasetId` [STRING, optional]

  The datasetId is used to group certain measurements to datasets. This is typically the case for data points which belong to the same observable, the same simulation and preequilibration condition, the same noise model, the same observable tranformation and the same observable parameters. This grouping makes it possible to use the plotting routines which are provided in the PEtab repository.

- `replicateId` [STRING, optional]

  The replicateId can be used to discern replicates with the same datasetId, which is helpful for plotting e.g. error bars.

1.6 Parameter table

A tab-separated value text file containing information on model parameters.

This table must include the following parameters:

- Named parameter overrides introduced in the *conditions table*
- Named parameter overrides introduced in the *measurement table*

and must not include

- placeholder parameters (see `observableParameters` and `noiseParameters` above)
- parameters included as column names in the *condition table*

One row per parameter with arbitrary order of rows and columns:

Additional columns may be added.

1.6.1 Detailed field description:

- `parameterId` [STRING, NOT NULL, REFERENCES(sbml.parameterId)]

  The `parameterId` of the parameter described in this row. This has be identical to the parameter IDs specified in the SBML model or in the `observableParameters` or `noiseParameters` column of the measurement table (see above).

  There must exist one line for each parameterId specified in the SBML model (except for placeholder parameter, see above) or the `observableParameters` or `noiseParameters` column of the measurement table.

- `parameterName` [STRING, OPTIONAL]

  Parameter name to be used e.g. for plotting etc. Can be chosen freely. May or may not coincide with the SBML parameter name.

- `parameterScale` [lin|log|log10]

  Scale of the parameter. The parameters and boundaries and the nominal parameter value in the following fields are expected to be given in this scale.

- `lowerBound` [NUMERIC]

  Lower bound of the parameter used for optimization. Optional, if `estimate==0`. Must be provided in linear space, independent of `parameterScale`.

- `upperBound` [NUMERIC]

  Upper bound of the parameter used for optimization. Optional, if `estimate==0`. Must be provided in linear space, independent of `parameterScale`.

- `nominalValue` [NUMERIC]

  Some parameter value to be used if the parameter is not subject to estimation (see `estimate` below). Must be provided in linear space, independent of `parameterScale`. Optional, unless `estimate==0`.

- `estimate` [BOOL 0|1]

  1 or 0, depending on, if the parameter is estimated (1) or set to a fixed value(0) (see `nominalValue`).

- `priorType`

Type of prior, which is used for sampling of initial points for a possible optimization and for the objective function. Priors which are only used for sampling of initial starting points or only for optimization should be specified in the additional columns `initializationPriorType` or `objectivePriorType`, respectively.

Possible prior types are (see also Extensions):

- *uniform*: flat prior on linear parameters
- *normal*: Gaussian prior on linear parameters
- *laplace*: Laplace prior on linear parameters
- *logNormal*: exponentiated Gaussian prior on linear parameters
- *logLaplace*: exponentiated Laplace prior on linear parameters
- *parameterScaleUniform* (default): Flat prior on original parameter scale (equivalent to "no prior")
- *parameterScaleNormal*: Gaussian prior on original parameter scale
- *parameterScaleLaplace*: Laplace prior on original parameter scale

- `priorParameters`

Parameters for prior specified in `priorType`, separated by a semicolon. Accordingly, there are optional columns for priors which should be used for initial point sampling or optimization only. (i.e., `initializationPriorParameters` and `objectivePriorParameters`, respectively). So far, only numeric values will be supported, no parameter names. Parameters for the different prior types are:

- uniform: lower bound; upper bound
- normal: mean; standard deviation (**not** variance)
- laplace: location; scale
- logNormal: parameters of corresp. normal distribution (see: normal)
- logLaplace: parameters of corresp. Laplace distribution (see: laplace)
- parameterScaleUniform: lower bound; upper bound
- parameterScaleNormal: mean; standard deviation (**not** variance)
- parameterScaleLaplace: location; scale

1.6.2 Additional optional columns

Extra columns:

- `hierarchicalOptimization` (optional)

hierarchicalOptimization: 1 if parameter is optimized using hierarchical optimization approach, 0 otherwise.

- `initializationPriorType` (optional)

Prior types used for sampling of initial points for optimization. Uses the entries from `priorType` as default, but will overwrite those, if something else is specified here. For more detailed documentation, see `priorType`.

- `initializationPriorParameters` (optional)

Prior parameters used for sampling of initial points for optimization. Uses the entries from `priorParameters` as default, but will overwrite those, if something else is specified here. For more detailed documentation, see `priorParameters`.

- `objectivePriorType` (optional)

  Prior types used for the objective function during optimization or sampling. Uses the entries from `priorType` as default, but will overwrite those, if something else is specified here. For more detailed documentation, see `priorType`.

- `objectivePriorParameters` (optional)

  Prior parameters used for the objective function during optimization. Uses the entries from `priorParameters` as default, but will overwrite those, if something else is specified here. For more detailed documentation, see `priorParameters`.

1.7 Visualization table

A tab-separated value file containing the specification of the visualization routines which come with the PEtab repository. Plots are in general collections of different datasets as specified using their `datasetId` (if provided) inside the measurement table.

Expected to have the following columns in any (but preferably this) order:

(wrapped for readability)

(wrapped for readability)

1.7.1 Detailed field description:

- `plotId` [STRING, NOT NULL]

  An ID which corresponds to a specific plot. All datasets with the same plotId will be plotted into the same axes object.

- `plotName` [STRING]

  A name for the specific plot.

- `plotTypeSimulation` [STRING]

  The type of the corresponding plot, can be `LinePlot` or `BarPlot`. Default is `LinePlot`.

- `plotTypeData`

  The type how replicates should be handled, can be `MeanAndSD`, `MeanAndSEM`, `replicate` (for plotting all replicates separately), or `provided` (if numeric values for the noise level are provided in the measurement table). Default is `MeanAndSD`.

- `datasetId` [STRING, NOT NULL, REFERENCES(measurementTable.datasetId)]

The datasets, which should be grouped into one plot.

- `xValues` [STRING]

The independent variable, which will be plotted on the x-axis. Can be `time` (default, for time resolved data), or it can be `parameterOrStateId` for dose-response plots. The corresponding numeric values will be shown on the x-axis.

- `xOffset` [NUMERIC]

Possible data-offsets for the independent variable (default is `0`).

- `xLabel` [STRING]

Label for the x-axis.

- `xScale` [STRING]

  Scale of the independent variable, can be `lin`, `log`, or `log10`.

- `yValues` [observableId, REFERENCES(measurementTable.observableId)]

  The observable which should be plotted on the y-axis.

- `yOffset` [NUMERIC]

  Possible data-offsets for the observable (default is `0`).

- `yLabel` [STRING]

  Label for the y-axis.

- `yScale` [STRING]

  Scale of the observable, can be `lin`, `log`, or `log10`.

- `legendEntry` [STRING]

  The name that should be displayed for the corresponding dataset in the legend and which defaults to `datasetId`.

1.7.2 Extensions

Additional columns, such as `Color`, etc. may be specified.

1.8 YAML file for grouping files

To link the SBML model, measurement table, condition table, etc. in an unambiguous way, we use a YAML file.

This file also allows specifying a PEtab version (as the format is not unlikely to change in the future).

Furthermore, this can be used to describe parameter estimation problems comprising multiple models (more details below).

The format is described in the schema ../petab/petab_schema.yaml, which allows for easy validation.

1.8.1 Parameter estimation problems combining multiple models

Parameter estimation problems can comprise multiple models. For now, PEtab allows to specify multiple SBML models with corresponding condition and measurement tables, and one joint parameter table. This means that the parameter namespace is global. Therefore, parameters with the same ID in different models will be considered identical.

CHAPTER 2

API Reference

petab	PEtab exports
petab.composite_problem	PEtab problems consisting of multiple models
petab.core	PEtab core functions (or functions that don't fit anywhere else)
petab.conditions	Functions operating on the PEtab condition table
petab.lint	Integrity checks and tests for specific features used
petab.measurements	Functions operating on the PEtab measurement table
petab.parameter_mapping	Functions related to mapping parameter from model to parameter estimation problem
petab.parameters	Functions operating on the PEtab parameter table
petab.problem	PEtab Problem class
petab.sampling	Functions related to parameter sampling
petab.sbml	Functions for interacting with SBML models
petab.yaml	Code regarding the PEtab YAML config files
petab.visualize.data_overview	Functions for creating an overview report of a PEtab problem
petab.visualize.helper_functions	This file should contain the functions, which PEtab internally needs for plotting, but which are not meant to be used by non-developers and should hence not be directly visible/usable when using import *petab.visualize*
petab.visualize.plot_data_and_simulation(...)	Main function for plotting data and simulations.
petab.visualize.plotting_config	

2.1 petab

PEtab exports

2.2 petab.composite_problem

PEtab problems consisting of multiple models

Classes

CompositeProblem(parameter_df, problems)	Representation of a PEtab problem consisting of multiple models

class petab.composite_problem.**CompositeProblem**(*parameter_df: pandas.core.frame.DataFrame = None*, *problems: List[petab.problem.Problem] = None*)

Bases: object

Representation of a PEtab problem consisting of multiple models

problems
List petab.Problems

parameter_df
PEtab parameter DataFrame

static from_yaml(*yaml_config: Union[Dict[KT, VT], str]*) → petab.composite_problem.CompositeProblem
Create from YAML file

Factory method to create a CompositeProblem instance from a PEtab YAML config file

Parameters **yaml_config** – PEtab configuration as dictionary or YAML file name

2.3 petab.core

PEtab core functions (or functions that don't fit anywhere else)

Functions

flatten_timepoint_specific_output_overrides(...)	Flatten timepoint-specific output parameter overrides.
get_notnull_columns(df, candidates)	Return list of df-columns in candidates which are not all null/nan.
get_observable_id(parameter_id)	Get PEtab observable ID from PEtab-style sigma or observable *AssignmentRule*-target parameter_id.
parameter_is_offset_parameter(parameter, formula)	Check if is offset parameter.
parameter_is_scaling_parameter(parameter, ...)	Check if is scaling parameter.

petab.core.**flatten_timepoint_specific_output_overrides**(*petab_problem: petab.problem.Problem*) → None

Flatten timepoint-specific output parameter overrides.

If the PEtab problem definition has timepoint-specific *observableParameters* or *noiseParameters* for the same observable, replace those by replicating the respective observable.

This is a helper function for some tools which may not support such timepoint-specific mappings. The measurement table is modified in place.

Parameters **petab_problem** – PEtab problem to work on

petab.core.**get_notnull_columns**(*df: pandas.core.frame.DataFrame, candidates: Iterable[T_co]*)
Return list of df-columns in candidates which are not all null/nan.

The output can e.g. be used as input for pandas.DataFrame.groupby.

Parameters

- **df** – Dataframe
- **candidates** – Columns of df to consider

petab.core.**get_observable_id**(*parameter_id: str*) → str
Get PEtab observable ID from PEtab-style sigma or observable *AssignmentRule*-target parameter_id.

e.g. for 'observable_obs1' -> 'obs1', for 'sigma_obs1' -> 'obs1'

Parameters **parameter_id** – Some parameter ID

Returns Observable ID

petab.core.**parameter_is_offset_parameter**(*parameter: str*, *formula: str*) → bool
Check if is offset parameter.

Parameters

- **parameter** – Some identifier.
- **formula** – Some sympy-compatible formula.

Returns True if parameter parameter is an offset parameter with positive sign in formula formula.

petab.core.**parameter_is_scaling_parameter**(*parameter: str*, *formula: str*) → bool
Check if is scaling parameter.

Parameters

- **parameter** – Some identifier.
- **formula** – Some sympy-compatible formula.

Returns

True if parameter parameter is a scaling parameter in formula formula.

2.4 petab.conditions

Functions operating on the PEtab condition table

Functions

create_condition_df(parameter_ids, condition_ids)	Create empty condition DataFrame
get_condition_df(condition_file_name)	Read the provided condition file into a `pandas.Dataframe`

petab.conditions.**create_condition_df**(*parameter_ids: Iterable[str], condition_ids: Optional[Iterable[str]] = None*) → pandas.core.frame.DataFrame

Create empty condition DataFrame

Parameters

- **parameter_ids** – the columns
- **condition_ids** – the rows

Returns A `pandas.DataFrame` with empty given rows and columns and all nan values

petab.conditions.**get_condition_df**(*condition_file_name: str*) → pandas.core.frame.DataFrame

Read the provided condition file into a `pandas.Dataframe`

Conditions are rows, parameters are columns, conditionId is index.

Parameters **condition_file_name** – File name of PEtab condition file

2.5 petab.lint

Integrity checks and tests for specific features used

Functions

assert_all_parameters_present_in_parameter_df(...)	Ensure all required parameters are contained in the parameter table with no additional ones
assert_measured_observables_present_in_model(...)	Check if all observables in measurement files have been specified in the model
assert_model_parameters_in_condition_or_parameter_table(...)	Model parameters that are targets of AssignmentRule must not be present in parameter table or in condition table columns.
assert_no_leading_trailing_whitespace(...)	Check that there is no trailing whitespace in elements of Iterable
assert_noise_distributions_valid(measurement_df)	Check whether there are not multiple noise distributions for an observable, and that the names are correct.
assert_parameter_bounds_are_numeric(parameter_df)	Check if all entries in the lowerBound and upperBound columns of the parameter table are numeric.
assert_parameter_estimate_is_boolean(...)	Check if all entries in the estimate column of the parameter table are 0 or 1.
assert_parameter_id_is_string(parameter_df)	Check if all entries in the parameterId column of the parameter table are string and not empty.
assert_parameter_id_is_unique(parameter_df)	Check if the parameterId column of the parameter table is unique.

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assert_parameter_scale_is_valid(parameter_df)	Check if all entries in the parameterScale column of the parameter table are 'lin' for linear, 'log' for natural logarithm or 'log10' for base 10 logarithm.
check_condition_df(df, sbml_model)	Run sanity checks on PEtab condition table
check_measurement_df(df)	Run sanity checks on PEtab measurement table
check_parameter_bounds(parameter_df)	Check if all entries in the lowerBound are smaller than upperBound column in the parameter table and that bounds are positive for parameterScale log|log10.
check_parameter_df(df, sbml_model, ...)	Run sanity checks on PEtab parameter table
condition_table_is_parameter_free(condition_df)	Check if all entries in the condition table are numeric (no parameter IDs)
lint_problem(problem)	Run PEtab validation on problem
measurement_table_has_observable_parameter_mapping(df)	Are there any numbers to override observable parameters?
measurement_table_has_timepoint_specific_mapping(df)	Are there time point or replicate specific parameter assignments in the measurement table.

petab.lint.**_check_df**(*df: pandas.core.frame.DataFrame, req_cols: Iterable[T_co], name: str*) → None

Check if given columns are present in DataFrame

Parameters

- **df** – Dataframe to check
- **req_cols** – Column names which have to be present
- **name** – Name of the DataFrame to be included in error message

Raises `AssertionError` – if a column is missing

petab.lint.**assert_all_parameters_present_in_parameter_df**(*parameter_df: pandas.core.frame.DataFrame, sbml_model: libsbml.Model, measurement_df: pandas.core.frame.DataFrame, condition_df: pandas.core.frame.DataFrame*) → None

Ensure all required parameters are contained in the parameter table with no additional ones

Parameters

- **parameter_df** – PEtab parameter DataFrame
- **sbml_model** – PEtab SBML Model
- **measurement_df** – PEtab measurement table
- **condition_df** – PEtab condition table

Raises `AssertionError` – in case of problems

petab.lint.**assert_measured_observables_present_in_model**(*measurement_df: pandas.core.frame.DataFrame, sbml_model: libsbml.Model*) → None

Check if all observables in measurement files have been specified in the model

Parameters

- **sbml_model** – PEtab SBML Model
- **measurement_df** – PEtab measurement table

Raises AssertionError – in case of problems

petab.lint.**assert_model_parameters_in_condition_or_parameter_table**(*sbml_model: libsbml.Model*, *condition_df: pandas.core.frame.DataFrame*, *parameter_df: pandas.core.frame.DataFrame*) → None

Model parameters that are targets of AssignmentRule must not be present in parameter table or in condition table columns. Other parameters must only be present in either in parameter table or condition table columns. Check that.

Parameters

- **parameter_df** – PEtab parameter DataFrame
- **sbml_model** – PEtab SBML Model
- **condition_df** – PEtab condition table

Raises AssertionError – in case of problems

petab.lint.**assert_no_leading_trailing_whitespace**(*names_list: Iterable[str], name: str*) → None

Check that there is no trailing whitespace in elements of Iterable

Parameters

- **names_list** – strings to check for whitespace
- **name** – name of *names_list* for error messages

Raises AssertionError – if there is trailing whitespace

petab.lint.**assert_noise_distributions_valid**(*measurement_df: pandas.core.frame.DataFrame*) → None

Check whether there are not multiple noise distributions for an observable, and that the names are correct.

Parameters **measurement_df** – PEtab measurement table

Raises AssertionError – in case of problems

petab.lint.**assert_parameter_bounds_are_numeric**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if all entries in the lowerBound and upperBound columns of the parameter table are numeric.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**assert_parameter_estimate_is_boolean**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if all entries in the estimate column of the parameter table are 0 or 1.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**assert_parameter_id_is_string**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if all entries in the parameterId column of the parameter table are string and not empty.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**assert_parameter_id_is_unique**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if the parameterId column of the parameter table is unique.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**assert_parameter_scale_is_valid**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if all entries in the parameterScale column of the parameter table are 'lin' for linear, 'log' for natural logarithm or 'log10' for base 10 logarithm.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**check_condition_df**(*df: pandas.core.frame.DataFrame, sbml_model: Optional[libsbml.Model]*) → None

Run sanity checks on PEtab condition table

Parameters

- **df** – PEtab condition DataFrame
- **sbml_model** – SBML Model for additional checking of parameter IDs

Raises AssertionError – in case of problems

petab.lint.**check_measurement_df**(*df: pandas.core.frame.DataFrame*) → None

Run sanity checks on PEtab measurement table

Parameters **df** – PEtab measurement DataFrame

Raises AssertionError – in case of problems

petab.lint.**check_parameter_bounds**(*parameter_df: pandas.core.frame.DataFrame*) → None

Check if all entries in the lowerBound are smaller than upperBound column in the parameter table and that bounds are positive for parameterScale log|log10.

Parameters **parameter_df** – PEtab parameter DataFrame

Raises AssertionError – in case of problems

petab.lint.**check_parameter_df**(*df: pandas.core.frame.DataFrame, sbml_model: Optional[libsbml.Model], measurement_df: Optional[pandas.core.frame.DataFrame], condition_df: Optional[pandas.core.frame.DataFrame]*) → None

Run sanity checks on PEtab parameter table

Parameters

- **df** – PEtab condition DataFrame
- **sbml_model** – SBML Model for additional checking of parameter IDs

- **measurement_df** – PEtab measurement table for additional checks
- **condition_df** – PEtab condition table for additional checks

Raises `AssertionError` – in case of problems

petab.lint.**condition_table_is_parameter_free**(*condition_df: pandas.core.frame.DataFrame*) → bool

Check if all entries in the condition table are numeric (no parameter IDs)

Parameters **condition_df** – PEtab condition table

Returns True if there are no parameter overrides in the condition table, False otherweise.

petab.lint.**lint_problem**(*problem: petab.problem.Problem*) → bool

Run PEtab validation on problem

Parameters **problem** – PEtab problem to check

Returns True is errors occurred, False otherwise

petab.lint.**measurement_table_has_observable_parameter_numeric_overrides**(*measurement_df: pandas.core.frame.DataFrame*) → bool

Are there any numbers to override observable parameters?

Parameters **measurement_df** – PEtab measurement table

Returns True if there any numbers to override observable parameters, False otherwise.

petab.lint.**measurement_table_has_timepoint_specific_mappings**(*measurement_df: pandas.core.frame.DataFrame*) → bool

Are there time-point or replicate specific parameter assignments in the measurement table.

Parameters **measurement_df** – PEtab measurement table

Returns True if there are time-point or replicate specific parameter assignments in the measurement table, False otherwise.

2.6 petab.measurements

Functions operating on the PEtab measurement table

Functions

assert_overrides_match_parameter_count(...)	Ensure that number of parameters in the observable definition matches the number of overrides in `measurement_df`
concat_measurements(measurement_tables, str]])	Concatenate measurement tables
create_measurement_df()	Create empty measurement dataframe
get_measurement_df(measurement_file_name)	Read the provided measurement file into a `pandas.Dataframe`.

Continued on next page

Table 6 – continued from previous page

get_measurement_parameter_ids(measurement_df)	Return list of ID of parameters which occur in measurement table as observable or noise parameter overrides.
get_noise_distributions(measurement_df)	Returns dictionary of cost definitions per observable, if specified.
get_placeholders(formula_string, ...)	Get placeholder variables in noise or observable definition for the given observable ID.
get_rows_for_condition(measurement_df, ...)	Extract rows in *measurement_df* for *condition* according to 'preequilibrationConditionId' and 'simulationConditionId' in *condition*.
get_simulation_conditions(measurement_df)	Create a table of separate simulation conditions.
measurements_have_replicates(measurement_df)	Tests whether the measurements come with replicates
split_parameter_replacement_list(...)	Split values in observableParameters and noiseParameters in measurement table.

petab.measurements.**assert_overrides_match_parameter_count**(*measurement_df: pandas.core.frame.DataFrame, observables: Dict[str, str], noise: Dict[str, str]*) → None

Ensure that number of parameters in the observable definition matches the number of overrides in `measurement_df`

Parameters

- **measurement_df** – PEtab measurement table
- **observables** – dict: obsId => {obsFormula}
- **noise** – dict: obsId => {obsFormula}

petab.measurements.**concat_measurements**(*measurement_tables: Iterable[Union[pandas.core.frame.DataFrame, str]]*) → pandas.core.frame.DataFrame

Concatenate measurement tables

Parameters **measurement_tables** – Iterable of measurement tables to join, as DataFrame or filename.

petab.measurements.**create_measurement_df**() → pandas.core.frame.DataFrame

Create empty measurement dataframe

Returns Created DataFrame

petab.measurements.**get_measurement_df**(*measurement_file_name: str*) → pandas.core.frame.DataFrame

Read the provided measurement file into a `pandas.Dataframe`.

Parameters **measurement_file_name** – Name of file to read from

Returns Measurement DataFrame

petab.measurements.**get_measurement_parameter_ids**(*measurement_df: pandas.core.frame.DataFrame*) → List[str]

Return list of ID of parameters which occur in measurement table as observable or noise parameter overrides.

Parameters **measurement_df** – PEtab measurement DataFrame

Returns List of parameter IDs

petab.measurements.**get_noise_distributions**(*measurement_df: pandas.core.frame.DataFrame*) → dict

Returns dictionary of cost definitions per observable, if specified.

Looks through all parameters satisfying *sbml_parameter_is_cost* and return as dictionary.

Parameters **measurement_df** – PEtab measurement table

Returns Dictionary with *observableId => cost definition*

petab.measurements.**get_placeholders**(*formula_string: str*, *observable_id: str*, *override_type: str*) → Set[str]

Get placeholder variables in noise or observable definition for the given observable ID.

Parameters

- **formula_string** – observable formula (typically from SBML model)
- **observable_id** – ID of current observable
- **override_type** – 'observable' or 'noise', depending on whether *formula* is for observable or for noise model

Returns (Un-ordered) set of placeholder parameter IDs

petab.measurements.**get_rows_for_condition**(*measurement_df: pandas.core.frame.DataFrame*, *condition: Union[pandas.core.frame.DataFrame, Dict[KT, VT]]*) → pandas.core.frame.DataFrame

Extract rows in *measurement_df* for *condition* according to 'preequilibrationConditionId' and 'simulationConditionId' in *condition*.

Parameters

- **measurement_df** – PEtab measurement DataFrame
- **condition** – DataFrame with single row and columns 'preequilibrationConditionId' and 'simulationConditionId'. Or dictionary with those keys.

Returns The subselection of rows in `measurement_df` for the condition `condition`.

petab.measurements.**get_simulation_conditions**(*measurement_df: pandas.core.frame.DataFrame*) → pandas.core.frame.DataFrame

Create a table of separate simulation conditions. A simulation condition is a specific combination of simulationConditionId and preequilibrationConditionId.

Parameters **measurement_df** – PEtab measurement table

Returns Dataframe with columns 'simulationConditionId' and 'preequilibrationConditionId'. All-NULL columns will be omitted.

petab.measurements.**measurements_have_replicates**(*measurement_df: pandas.core.frame.DataFrame*) → bool

Tests whether the measurements come with replicates

Parameters **measurement_df** – Measurement table

Returns `True` if there are replicates, `False` otherwise

petab.measurements.**split_parameter_replacement_list**(*list_string: Union[str, numbers.Number], delim: str = ';'*) → List[Union[str, float]]

Split values in observableParameters and noiseParameters in measurement table.

Parameters

- **list_string** – delim-separated stringified list
- **delim** – delimiter

Returns List of split values. Numeric values converted to float.

2.7 petab.parameter_mapping

Functions related to mapping parameter from model to parameter estimation problem

Functions

fill_in_nominal_values(mapping, Union[str, ...)	Replace non-estimated parameters in mapping list for a given condition by `nominalValues` provided in parameter table.
get_optimization_to_simulation_parameter_mapping(...)	Create list of mapping dicts from PEtab-problem to SBML parameters.
get_optimization_to_simulation_scale_mapping(...)	Get parameter scale mapping for all conditions
get_parameter_mapping_for_condition(...)	Create dictionary of mappings from PEtab-problem to SBML parameters for the given condition.
get_scale_mapping_for_condition(...)	Get parameter scale mapping for the given condition.
handle_missing_overrides(...)	Find all observable parameters and noise parameters that were not mapped and set their mapping to np.nan.
merge_preeq_and_sim_pars(parameter_mappings, ...)	Merge preequilibration and simulation parameters and scales for a list of conditions while checking for compatibility.
merge_preeq_and_sim_pars_condition(...)	Merge preequilibration and simulation parameters and scales for a single condition while checking for compatibility.

petab.parameter_mapping.**_apply_dynamic_parameter_overrides**(*mapping: Dict[str, Union[str, numbers.Number]], condition_id: str, condition_df: pandas.core.frame.DataFrame*) → None

Apply dynamic parameter overrides from condition table (in-place).

Parameters

- **mapping** – see get_parameter_mapping_for_condition
- **condition_id** – ID of condition to work on
- **condition_df** – PEtab condition table

petab.parameter_mapping.**_apply_output_parameter_overrides**(*mapping: Dict[str, Union[str, numbers.Number]], cur_measurement_df: pandas.core.frame.DataFrame*) → None

Apply output parameter overrides to the parameter mapping dict for a given condition as defined in the measurement table (`observableParameter`, `noiseParameters`).

Parameters

- **mapping** – parameter mapping dict as obtained from `get_parameter_mapping_for_condition`
- **cur_measurement_df** – Subset of the measurement table for the current condition

petab.parameter_mapping.**_apply_overrides_for_observable**(*mapping: Dict[str, Union[str, numbers.Number]], observable_id: str, override_type: str, overrides: List[str]*) → None

Apply parameter-overrides for observables and noises to mapping matrix.

Parameters

- **mapping** – mapping dict to which to apply overrides
- **observable_id** – observable ID
- **override_type** – 'observable' or 'noise'
- **overrides** – list of overrides for noise or observable parameters

petab.parameter_mapping.**_perform_mapping_checks**(*measurement_df: pandas.core.frame.DataFrame*) → None

Check for PEtab features which we can't account for during parameter mapping.

petab.parameter_mapping.**fill_in_nominal_values**(*mapping: Dict[str, Union[str, numbers.Number]], parameter_df: pandas.core.frame.DataFrame*) → None

Replace non-estimated parameters in mapping list for a given condition by `nominalValues` provided in parameter table.

Parameters

- **mapping** – mapping dict obtained from get_parameter_mapping_for_condition
- **parameter_df** – PEtab parameter table

petab.parameter_mapping.**get_optimization_to_simulation_parameter_mapping**(*condition_df: pandas.core.frame.DataFrame*, *measurement_df: pandas.core.frame.DataFrame*, *parameter_df: Optional[pandas.core.frame.* = *None*, *sbml_model: Optional[libsbml.Model]* = *None*, *simulation_conditions: Optional[pandas.core.frame.* = *None*, *warn_unmapped: Optional[bool]* = *True*) → List[Tuple[Dict[str, Union[str, numbers.Number]], Dict[str, Union[str, numbers.Number]]]]

Create list of mapping dicts from PEtab-problem to SBML parameters.

Parameters

- **measurement_df, parameter_df** (*condition_df,*) – The dataframes in the PEtab format.
- **sbml_model** – The sbml model with observables and noise specified according to the PEtab format.
- **simulation_conditions** – Table of simulation conditions as created by `petab.get_simulation_conditions`.
- **warn_unmapped** – If `True`, log warning regarding unmapped parameters

Returns The length of the returned array is n_conditions, each entry is a tuple of two dicts of length n_par_sim, listing the optimization parameters or constants to be mapped to the simulation parameters, first for preequilibration (empty if no preequilibration condition is specified), second for simulation. `NaN` is used where no mapping exists.

petab.parameter_mapping.**get_optimization_to_simulation_scale_mapping**(*parameter_df: pandas.core.frame.DataFrame, mapping_par_opt_to_par_sim: List[Tuple[Dict[str, Union[str, numbers.Number]], Dict[str, Union[str, numbers.Number]]]], measurement_df: pandas.core.frame.DataFrame, simulation_conditions: Optional[pandas.core.frame.DataF = None*) → List[Tuple[Dict[str, str], Dict[str, str]]]

Get parameter scale mapping for all conditions

Parameters

- **parameter_df** – PEtab parameter DataFrame
- **mapping_par_opt_to_par_sim** – Parameter mapping as obtained from `get_optimization_to_simulation_parameter_mapping`
- **measurement_df** – PEtab measurement DataFrame
- **simulation_conditions** – Result of `petab.measurements.get_simulation_conditions` to avoid reevaluation.

Returns List of tuples with mapping dictionaries.

petab.parameter_mapping.**get_parameter_mapping_for_condition**(*condition_id: str*, *is_preeq: bool*, *cur_measurement_df: pandas.core.frame.DataFrame*, *condition_df: pandas.core.frame.DataFrame*, *parameter_df: pandas.core.frame.DataFrame = None*, *sbml_model: libsbml.Model = None*, *warn_unmapped: bool = True*) → Dict[str, Union[str, numbers.Number]]

Create dictionary of mappings from PEtab-problem to SBML parameters for the given condition.

Parameters

- **condition_id** – Condition ID for which to perform mapping
- **is_preeq** – If `True`, output parameters will not be mapped
- **cur_measurement_df** – Measurement sub-table for current condition
- **condition_df** – PEtab condition DataFrame
- **parameter_df** – PEtab parameter DataFrame
- **sbml_model** – The sbml model with observables and noise specified according to the PEtab format.
- **warn_unmapped** – If `True`, log warning regarding unmapped parameters

Returns Dictionary of parameter IDs with mapped parameters IDs to be estimated or filled in values in case of non-estimated parameters. NaN is used where no mapping exists.

petab.parameter_mapping.**get_scale_mapping_for_condition**(*parameter_df: pandas.core.frame.DataFrame*, *mapping_par_opt_to_par_sim: Dict[str, Union[str, numbers.Number]]*) → Dict[str, str]

Get parameter scale mapping for the given condition.

Parameters

- **parameter_df** – PEtab parameter table
- **mapping_par_opt_to_par_sim** – Mapping as obtained from `get_parameter_mapping_for_condition`

Returns parameterId => parameterScale

Return type Mapping dictionary

petab.parameter_mapping.**handle_missing_overrides**(*mapping_par_opt_to_par_sim: Dict[str, Union[str, numbers.Number]]*, *warn: bool = True*, *condition_id: str = None*) → None

Find all observable parameters and noise parameters that were not mapped and set their mapping to np.nan.

Assumes that parameters matching "(noiselobservable)Parameter[0-9]+_" were all supposed to be overwritten.

Parameters

- **mapping_par_opt_to_par_sim** – Output of get_parameter_mapping_for_condition
- **warn** – If True, log warning regarding unmapped parameters
- **condition_id** – Optional condition ID for more informative output

petab.parameter_mapping.**merge_preeq_and_sim_pars**(*parameter_mappings: Iterable[Tuple[Dict[str, Union[str, numbers.Number]], Dict[str, Union[str, numbers.Number]]]], scale_mappings: Iterable[Tuple[Dict[str, str], Dict[str, str]]]*) → Tuple[List[Tuple[Dict[str, Union[str, numbers.Number]], Dict[str, Union[str, numbers.Number]]]], List[Tuple[Dict[str, str], Dict[str, str]]]]

Merge preequilibration and simulation parameters and scales for a list of conditions while checking for compatibility.

Parameters

- **parameter_mappings** – As returned by petab.get_optimization_to_simulation_parameter_mapping
- **scale_mappings** – As returned by petab.get_optimization_to_simulation_scale_mapping.

Returns The parameter and scale simulation mappings, modified and checked.

petab.parameter_mapping.**merge_preeq_and_sim_pars_condition**(*condition_map_preeq: Dict[str, Union[str, numbers.Number]], condition_map_sim: Dict[str, Union[str, numbers.Number]], condition_scale_map_preeq: Dict[str, str], condition_scale_map_sim: Dict[str, str], condition: Any*) → None

Merge preequilibration and simulation parameters and scales for a single condition while checking for compatibility.

This function is meant for the case where we cannot have different parameters (and scales) for preequilibration and simulation. Therefore, merge both and ensure matching scales and parameters. `condition_map_sim` and `condition_scale_map_sim` will ne modified in place.

Parameters

- **condition_map_sim**(*condition_map_preeq,*) – Parameter mapping as obtained from *get_parameter_mapping_for_condition*
- **condition_scale_map_sim** (*condition_scale_map_preeq,*) – Parameter scale mapping as obtained from *get_get_scale_mapping_for_condition*

- **condition** – Condition identifier for more informative error messages

2.8 petab.parameters

Functions operating on the PEtab parameter table

Functions

create_parameter_df(sbml_model, ...)	Create a new PEtab parameter table
get_optimization_parameters(parameter_df)	Get list of optimization parameter ids from parameter dataframe.
get_parameter_df(parameter_file_name)	Read the provided parameter file into a `pandas.Dataframe`.
get_priors_from_df(parameter_df)	Create list with information about the parameter priors
get_required_parameters_for_parameter_table(...)	Get set of parameters which need to go into the parameter table
map_scale(parameters, scale_strs)	As scale(), but for Iterables
parameter_id_is_valid(parameter_id)	Check whether parameter_id is a valid PEtab parameter ID
scale(parameter, scale_str)	Scale parameter according to scale_str

petab.parameters.**create_parameter_df**(*sbml_model: libsbml.Model*, *condition_df: pandas.core.frame.DataFrame*, *measurement_df: pandas.core.frame.DataFrame*, *parameter_scale: str = 'log10'*, *lower_bound: Iterable[T_co] = None*, *upper_bound: Iterable[T_co] = None*) → pandas.core.frame.DataFrame

Create a new PEtab parameter table

All table entries can be provided as string or list-like with length matching the number of parameters

Parameters

- **sbml_model** – SBML Model
- **condition_df** – PEtab condition DataFrame
- **measurement_df** – PEtab measurement DataFrame
- **parameter_scale** – parameter scaling
- **lower_bound** – lower bound for parameter value
- **upper_bound** – upper bound for parameter value

Returns The created parameter DataFrame

petab.parameters.**get_optimization_parameters**(*parameter_df: pandas.core.frame.DataFrame*) → List[str]

Get list of optimization parameter ids from parameter dataframe.

Parameters **parameter_df** – PEtab parameter DataFrame

Returns List of parameter IDs in the parameter table

petab.parameters.**get_parameter_df**(*parameter_file_name: str*) → pandas.core.frame.DataFrame

Read the provided parameter file into a `pandas.Dataframe`.

Parameters **parameter_file_name** – Name of the file to read from.

Returns Parameter DataFrame

petab.parameters.**get_priors_from_df**(*parameter_df: pandas.core.frame.DataFrame*) → List[Tuple]

Create list with information about the parameter priors

Parameters **parameter_df** – PEtab parameter table

Returns List with prior information.

petab.parameters.**get_required_parameters_for_parameter_table**(*sbml_model: libsbml.Model*, *condition_df: pandas.core.frame.DataFrame*, *measurement_df: pandas.core.frame.DataFrame*) → Set[str]

Get set of parameters which need to go into the parameter table

Parameters

- **sbml_model** – PEtab SBML model
- **condition_df** – PEtab condition table
- **measurement_df** – PEtab measurement table

Returns Set of parameter IDs which PEtab requires to be present in the parameter table

petab.parameters.**map_scale**(*parameters: Iterable[numbers.Number], scale_strs: Iterable[str]*) → Iterable[numbers.Number]

As scale(), but for Iterables

petab.parameters.**parameter_id_is_valid**(*parameter_id: str*) → bool

Check whether parameter_id is a valid PEtab parameter ID

This should pretty much correspond to what is allowed for SBML identifiers.

TODO(#179) improve checking

Parameters **parameter_id** – Parameter ID to validate

Returns `True` if valid, `False` otherwise

petab.parameters.**scale**(*parameter: numbers.Number*, *scale_str: str*) → numbers.Number

Scale parameter according to scale_str

Parameters

- **parameter** – Parameter to be scaled
- **scale_str** – One of 'lin' (synonymous with ''), 'log', 'log10'

2.9 petab.problem

PEtab Problem class

Functions

get_default_condition_file_name(model_name, ...)	Get file name according to proposed convention
get_default_measurement_file_name(...)	Get file name according to proposed convention
get_default_parameter_file_name(model_name, ...)	Get file name according to proposed convention
get_default_sbml_file_name(model_name, folder)	Get file name according to proposed convention

Classes

Problem(sbml_model, sbml_reader, ...)	PEtab parameter estimation problem as defined by

class petab.problem.**Problem**(*sbml_model: libsbml.Model = None*, *sbml_reader: libsbml.SBMLReader = None*, *sbml_document: libsbml.SBMLDocument = None*, *condition_df: pandas.core.frame.DataFrame = None*, *measurement_df: pandas.core.frame.DataFrame = None*, *parameter_df: pandas.core.frame.DataFrame = None*)

Bases: object

PEtab parameter estimation problem as defined by

- SBML model
- condition table
- measurement table
- parameter table

condition_df
PEtab condition table

measurement_df
PEtab measurement table

parameter_df
PEtab parameter table

sbml_reader
Stored to keep object alive.

sbml_document
Stored to keep object alive.

sbml_model
PEtab SBML model

create_parameter_df(**args*, ***kwargs*)
Create a new PEtab parameter table

See create_parameter_df

static from_files(*sbml_file: str = None*, *condition_file: str = None*, *measurement_file: str = None*, *parameter_file: str = None*) → petab.problem.Problem
Factory method to load model and tables from files.

Parameters

- **sbml_file** – PEtab SBML model
- **condition_file** – PEtab condition table
- **measurement_file** – PEtab measurement table
- **parameter_file** – PEtab parameter table

static from_folder(*folder: str*, *model_name: str = None*) → petab.problem.Problem
Factory method to use the standard folder structure and file names, i.e.

```
${model_name}/
  +-- experimentalCondition_${model_name}.tsv
  +-- measurementData_${model_name}.tsv
  +-- model_${model_name}.xml
  +-- parameters_${model_name}.tsv
```

Parameters

- **folder** – Path to the directory in which the files are located.
- **model_name** – If specified, overrides the model component in the file names. Defaults to the last component of `folder`.

static from_yaml(*yaml_config: Union[Dict[KT, VT], str]*) → petab.problem.Problem
Factory method to load model and tables as specified by YAML file.

Parameters **yaml_config** – PEtab configuration as dictionary or YAML file name

get_dynamic_simulation_parameters()
See *get_model_parameters*

get_noise_distributions()
See *get_noise_distributions*.

get_observables(*remove: bool = False*)
Returns dictionary of observables definitions See *assignment_rules_to_dict* for details.

get_optimization_parameters()
Return list of optimization parameter IDs.

See get_optimization_parameters.

get_optimization_to_simulation_parameter_mapping(*warn_unmapped: bool = True*)
See get_simulation_to_optimization_parameter_mapping.

get_sigmas(*remove: bool = False*)
Return dictionary of observableId => sigma as defined in the SBML model. This does not include parameter mappings defined in the measurement table.

get_simulation_conditions_from_measurement_df()
See petab.get_simulation_conditions

lb
Parameter table lower bounds

lb_scaled
Parameter table lower bounds with applied parameter scaling

sample_parameter_startpoints(*n_starts: int = 100*)
Create starting points for optimization

See sample_parameter_startpoints

ub
Parameter table upper bounds

ub_scaled
Parameter table upper bounds with applied parameter scaling

x_fixed_indices
Parameter table non-estimated parameter indices

x_fixed_vals
Nominal values for parameter table non-estimated parameters

x_ids
Parameter table parameter IDs

x_nominal
Parameter table nominal values

x_nominal_scaled
Parameter table nominal values with applied parameter scaling

petab.problem.**get_default_condition_file_name**(*model_name: str*, *folder: str = ''*)
Get file name according to proposed convention

petab.problem.**get_default_measurement_file_name**(*model_name: str*, *folder: str = ''*)
Get file name according to proposed convention

petab.problem.**get_default_parameter_file_name**(*model_name: str*, *folder: str = ''*)
Get file name according to proposed convention

petab.problem.**get_default_sbml_file_name**(*model_name: str*, *folder: str = ''*)
Get file name according to proposed convention

2.10 petab.sampling

Functions related to parameter sampling

Functions

sample_from_prior(prior, list, str, list], ...)	Creates samples for one parameter based on prior
sample_parameter_startpoints(parameter_df, ...)	Create numpy.array with starting points for an optimization

petab.sampling.**sample_from_prior**(*prior: Tuple[str, list, str, list]*, *n_starts: int*) → numpy.array
Creates samples for one parameter based on prior

Parameters

- **prior** – A tuple as obtained from petab.parameter.get_priors_from_df
- **n_starts** – Number of samples

Returns Array with sampled values

petab.sampling.**sample_parameter_startpoints**(*parameter_df: pandas.core.frame.DataFrame*, *n_starts: int = 100*, *seed: int = None*) → numpy.array
Create numpy.array with starting points for an optimization

Parameters

- **parameter_df** – PEtab parameter DataFrame
- **n_starts** – Number of points to be sampled
- **seed** – Random number generator seed (see numpy.random.seed)

Returns Array of sampled starting points with dimensions n_optimization_parameters x n_startpoints

2.11 petab.sbml

Functions for interacting with SBML models

Functions

add_global_parameter(sbml_model, ...)	Add new global parameter to SBML model
add_model_output(sbml_model, observable_id, ...)	Add PEtab-style output to model
add_model_output_sigma(sbml_model, ...)	Add PEtab-style sigma for the given observable id
add_model_output_with_sigma(sbml_model, ...)	Add PEtab-style output and corresponding sigma with single (newly created) parameter
assignment_rules_to_dict(sbml_model[, ...])	Turn assignment rules into dictionary.
create_assigment_rule(sbml_model, ...)	Create SBML AssignmentRule
get_model_parameters(sbml_model)	Return list of SBML model parameter IDs which are not AssignmentRule targets for observables or sigmas
get_observables(sbml_model, remove)	Get observables defined in SBML model according to PEtab format.
get_sigmas(sbml_model, remove)	Get sigmas defined in SBML model according to PEtab format.
globalize_parameters(sbml_model, ...)	Turn all local parameters into global parameters with the same properties
is_sbml_consistent(sbml_document, check_units)	Check for SBML validity / consistency
log_sbml_errors(sbml_document[, ...])	Log libsbml errors
sbml_parameter_is_observable(sbml_parameter)	Returns whether the `libsbml.Parameter` `sbml_parameter` matches the defined observable format.
sbml_parameter_is_sigma(sbml_parameter)	Returns whether the `libsbml.Parameter` `sbml_parameter` matches the defined sigma format.

petab.sbml.**add_global_parameter**(*sbml_model: libsbml.Model*, *parameter_id: str*, *parameter_name: str = None*, *constant: bool = False*, *units: str = 'dimensionless'*, *value: float = 0.0*) → libsbml.Parameter

Add new global parameter to SBML model

Parameters

- **sbml_model** – SBML model
- **parameter_id** – ID of the new parameter

- **parameter_name** – Name of the new parameter
- **constant** – Is parameter constant?
- **units** – SBML unit ID
- **value** – parameter value

Returns The created parameter

petab.sbml.**add_model_output**(*sbml_model: libsbml.Model*, *observable_id: str*, *formula: str*, *observable_name: str = None*) → None

Add PEtab-style output to model

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add output to
- **formula** – Formula string for model output
- **observable_id** – ID without "observable_" prefix
- **observable_name** – Any observable name

petab.sbml.**add_model_output_sigma**(*sbml_model: libsbml.Model*, *observable_id: str*, *formula: str*) → None

Add PEtab-style sigma for the given observable id

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add to
- **observable_id** – Observable id for which to add sigma
- **formula** – Formula for sigma

petab.sbml.**add_model_output_with_sigma**(*sbml_model: libsbml.Model*, *observable_id: str*, *observable_formula: str*, *observable_name: str = None*) → None

Add PEtab-style output and corresponding sigma with single (newly created) parameter

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add output to
- **observable_formula** – Formula string for model output
- **observable_id** – ID without "observable_" prefix
- **observable_name** – Any name

petab.sbml.**assignment_rules_to_dict**(*sbml_model: libsbml.Model*, *filter_function=<function <lambda>>*, *remove: bool = False*) → Dict[str, Dict[str, Any]]

Turn assignment rules into dictionary.

Parameters

- **sbml_model** – a sbml model instance.
- **filter_function** – callback function taking assignment variable as input and returning True/False to indicate if the respective rule should be turned into an observable.

- **remove** – Remove the all matching assignment rules from the model

Returns

```
{
    assigneeId:
    {
        'name': assigneeName,
        'formula': formulaString
    }
}
```

petab.sbml.**create_assigment_rule**(*sbml_model: libsbml.Model*, *assignee_id: str*, *formula: str*, *rule_id: str = None*, *rule_name: str = None*) → libsbml.AssignmentRule

Create SBML AssignmentRule

Parameters

- **sbml_model** – Model to add output to
- **assignee_id** – Target of assignment
- **formula** – Formula string for model output
- **rule_id** – SBML id for created rule
- **rule_name** – SBML name for created rule

Returns The created `AssignmentRule`

petab.sbml.**get_model_parameters**(*sbml_model: libsbml.Model*) → List[str]

Return list of SBML model parameter IDs which are not AssignmentRule targets for observables or sigmas

petab.sbml.**get_observables**(*sbml_model: libsbml.Model*, *remove: bool = False*) → dict

Get observables defined in SBML model according to PEtab format.

Returns Dictionary of observable definitions. See *assignment_rules_to_dict* for details.

petab.sbml.**get_sigmas**(*sbml_model: libsbml.Model*, *remove: bool = False*) → dict

Get sigmas defined in SBML model according to PEtab format.

Returns

Dictionary of sigma definitions.

Keys are observable IDs, for values see *assignment_rules_to_dict* for details.

petab.sbml.**globalize_parameters**(*sbml_model: libsbml.Model*, *prepend_reaction_id: bool = False*) → None

Turn all local parameters into global parameters with the same properties

Local parameters are currently ignored by other PEtab functions. Use this function to convert them to global parameters. There may exist local parameters with identical IDs within different kinetic laws. This is not checked here. If in doubt that local parameter IDs are unique, enable *prepend_reaction_id* to create global parameters named ${reaction_id}_${local_parameter_id}.

Parameters

- **sbml_model** – The SBML model to operate on
- **prepend_reaction_id** – Prepend reaction id of local parameter when creating global parameters

petab.sbml.**is_sbml_consistent**(*sbml_document: libsbml.SBMLDocument*, *check_units: bool = False*) → bool

Check for SBML validity / consistency

Parameters

- **sbml_document** – SBML document to check
- **check_units** – Also check for unit-related issues

Returns False if problems were detected, otherwise True

petab.sbml.**log_sbml_errors**(*sbml_document: libsbml.SBMLDocument*, *minimum_severity=1*) → None

Log libsbml errors

Parameters

- **sbml_document** – SBML document to check
- **minimum_severity** – Minimum severity level to report (see libsbml)

petab.sbml.**sbml_parameter_is_observable**(*sbml_parameter: libsbml.Parameter*) → bool

Returns whether the `libsbml.Parameter` `sbml_parameter` matches the defined observable format.

petab.sbml.**sbml_parameter_is_sigma**(*sbml_parameter: libsbml.Parameter*) → bool

Returns whether the `libsbml.Parameter` `sbml_parameter` matches the defined sigma format.

2.12 petab.yaml

Code regarding the PEtab YAML config files

Functions

add_constructor
add_implicit_resolver
add_multi_constructor
add_multi_representer
add_path_resolver
add_representer
compose
compose_all
dump
dump_all
emit
full_load
full_load_all
load
load_all
load_warning
parse
safe_dump
safe_dump_all
safe_load
safe_load_all

Continued on next page

Table 13 – continued from previous page

scan	
serialize	
serialize_all	
unsafe_load	
unsafe_load_all	
warnings	Python part of the warnings subsystem.

Classes

YAMLObject
YAMLObjectMetaclass

Exceptions

YAMLLoadWarning

petab.yaml.**assert_single_condition_and_sbml_file**(*problem_config: Dict[KT, VT]*) → None

Check that there is only a single condition file and a single SBML file specified.

Parameters **problem_config** – Dictionary as defined in the YAML schema inside the *problems* list.

Raises NotImplementedError – If multiple condition or SBML files specified.

petab.yaml.**is_composite_problem**(*yaml_config: Union[Dict[KT, VT], str]*) → bool

Does this YAML file comprise multiple models?

Parameters **yaml_config** – PEtab configuration as dictionary or YAML file name

petab.yaml.**load_yaml**(*yaml_config: Union[Dict[KT, VT], str]*) → Dict[KT, VT]

Load YAML

Convenience function to allow for providing YAML inputs either as filename or as dictionary.

Parameters **yaml_config** – PEtab YAML config as filename or dict.

Returns The unmodified dictionary if yaml_config was dictionary. Otherwise the parsed the YAML file.

petab.yaml.**validate**(*yaml_config: Union[Dict[KT, VT], str], path_prefix: Optional[str] = None*)

Validate syntax and semantics of PEtab config YAML

Parameters

- **yaml_config** – PEtab YAML config as filename or dict.
- **path_prefix** – Base location for relative paths. Defaults to location of YAML file if a filename was provided for yaml_config or the current working directory.

petab.yaml.**validate_yaml_semantics**(*yaml_config: Union[Dict[KT, VT], str], path_prefix: Optional[str] = None*)

Validate PEtab YAML file semantics

Check for existence of files. Assumes valid syntax.

Version number and contents of referenced files are not yet checked.

Parameters

- **yaml_config** – PEtab YAML config as filename or dict.
- **path_prefix** – Base location for relative paths. Defaults to location of YAML file if a filename was provided for `yaml_config` or the current working directory.

Raises `AssertionError` – in case of problems

`petab.yaml.`**validate_yaml_syntax**(*yaml_config: Union[Dict[KT, VT], str], schema: Union[None, Dict[KT, VT], str] = None*)

Validate PEtab YAML file syntax

Parameters

- **yaml_config** – PEtab YAML file to validate, as file name or dictionary
- **schema** – Custom schema for validation

Raises see jsonschema.validate

2.13 petab.visualize.data_overview

Functions for creating an overview report of a PEtab problem

Functions

create_report(problem, model_name)	Create an HTML overview data / model overview report
get_data_per_observable(measurement_df)	Get table with number of data points per observable and condition
main()	

`petab.visualize.data_overview.`**create_report**(*problem: petab.problem.Problem, model_name: str*) → None

Create an HTML overview data / model overview report

Parameters

- **problem** – PEtab problem
- **model_name** – Name of the model, used for file name for report

`petab.visualize.data_overview.`**get_data_per_observable**(*measurement_df: pandas.core.frame.DataFrame*) → pandas.core.frame.DataFrame

Get table with number of data points per observable and condition

Parameters **measurement_df** – PEtab measurement data frame

2.14 petab.visualize.helper_functions

This file should contain the functions, which PEtab internally needs for plotting, but which are not meant to be used by non-developers and should hence not be directly visible/usable when using import *petab.visualize*

Functions

check_vis_spec_consistency(dataset_id_list, ...)	Helper function for plotting data and simulations, which check the visualization setting, if no visualization specification file is provided.
create_dataset_id_list(simcond_id_list, ...)	
create_figure(uni_plot_ids)	Helper function for plotting data and simulations, open figure and axes
get_data_to_plot(vis_spec, m_data, ...)	group the data, which should be plotted and save it in pd.dataframe called 'ms'.
get_default_vis_specs(exp_data, exp_conditions)	Helper function for plotting data and simulations, which creates a default visualization table.
handle_dataset_plot(i_visu_spec, ind_plot, ...)	
import_from_files(data_file_path, ...)	Helper function for plotting data and simulations, which imports data from PEtab files.

petab.visualize.helper_functions.**check_vis_spec_consistency**(*dataset_id_list*, *sim_cond_id_list*, *sim_cond_num_list*, *observable_id_list*, *observable_num_list*, *exp_data*)

Helper function for plotting data and simulations, which check the visualization setting, if no visualization specification file is provided.

For documentation, see main function plot_data_and_simulation()

petab.visualize.helper_functions.**create_figure**(*uni_plot_ids*)

Helper function for plotting data and simulations, open figure and axes

Parameters **uni_plot_ids** (*ndarray*) – Array with unique plot indices

Returns

- **fig** (*Figure object of the created plot.*)
- **ax** (*Axis object of the created plot.*)
- **num_row** (*int, number of subplot rows*)
- **num_col** (*int, number of subplot columns*)

petab.visualize.helper_functions.**get_data_to_plot**(*vis_spec: pandas.core.frame.DataFrame*, *m_data: pandas.core.frame.DataFrame*, *simulation_data: pandas.core.frame.DataFrame*, *condition_ids: numpy.ndarray*, *i_visu_spec: int*, *col_id: str*)

group the data, which should be plotted and save it in pd.dataframe called 'ms'.

Parameters

- **vis_spec** – pandas data frame, contains defined data format (visualization file)
- **m_data** – pandas data frame, contains defined data format (measurement file)

- **simulation_data** – pandas data frame, contains defined data format (simulation file)
- **condition_ids** – numpy array, containing all unique condition IDs which should be plotted in one figure (can be found in measurementData file, column simulationConditionId)
- **i_visu_spec** – int, current index (row number) of row which should be plotted in visualizationSpecification file
- **col_id** – str, the name of the column in visualization file, whose entries should be unique (depends on condition in column independentVariableName)

Returns pandas.DataFrame containing the data which should be plotted (Mean and Std)

Return type data_to_plot

petab.visualize.helper_functions.**get_default_vis_specs**(*exp_data*, *exp_conditions*, *dataset_id_list=None*, *sim_cond_id_list=None*, *sim_cond_num_list=None*, *observable_id_list=None*, *observable_num_list=None*, *plotted_noise='MeanAndSD'*)

Helper function for plotting data and simulations, which creates a default visualization table.

For documentation, see main function plot_data_and_simulation()

petab.visualize.helper_functions.**import_from_files**(*data_file_path*, *condition_file_path*, *visualization_file_path*, *simulation_file_path*, *dataset_id_list*, *sim_cond_id_list*, *sim_cond_num_list*, *observable_id_list*, *observable_num_list*, *plotted_noise*)

Helper function for plotting data and simulations, which imports data from PEtab files.

For documentation, see main function plot_data_and_simulation()

2.15 petab.visualize.plot_data_and_simulation

petab.visualize.**plot_data_and_simulation**(*data_file_path: str*, *condition_file_path: str*, *visualization_file_path: str = ''*, *simulation_file_path: str = ''*, *dataset_id_list=None*, *sim_cond_id_list=None*, *sim_cond_num_list=None*, *observable_id_list=None*, *observable_num_list=None*, *plotted_noise: str = 'MeanAndSD'*)

Main function for plotting data and simulations.

What exactly should be plotted is specified in a visualizationSpecification.tsv file.

Also, the data, simulations and conditions have to be defined in a specific format (see "doc/documentation_data_format.md").

Parameters

- **data_file_path** (*str*) – Path to the data file.
- **condition_file_path** (*str*) – Path to the condition file.

- **visualization_file_path** (*str (optional)*) – Path to the visualization specification file.
- **simulation_file_path** (*str (optional)*) – Path to the simulation output data file.
- **dataset_id_list** (*list (optional)*) – A list of lists. Each sublist corresponds to a plot, each subplot contains the datasetIds for this plot. Only to be used if no visualization file was available.
- **sim_cond_id_list** (*list (optional)*) – A list of lists. Each sublist corresponds to a plot, each subplot contains the simulationConditionIds for this plot. Only to be used if no visualization file was available.
- **sim_cond_num_list** (*list (optional)*) – A list of lists. Each sublist corresponds to a plot, each subplot contains the numbers corresponding to the simulationConditionIds for this plot. Only to be used if no visualization file was available.
- **observable_id_list** (*list (optional)*) – A list of lists. Each sublist corresponds to a plot, each subplot contains the observableIds for this plot. Only to be used if no visualization file was available.
- **observable_num_list** (*list (optional)*) – A list of lists. Each sublist corresponds to a plot, each subplot contains the numbers corresponding to the observableIds for this plot. Only to be used if no visualization file was available.
- **plotted_noise** (*str (optional)*) – String indicating how noise should be visualized: ['MeanAndSD' (default), 'MeanAndSEM', 'replicate', 'provided']

Returns ax

Return type Axis object of the created plot.

2.16 petab.visualize.plotting_config

Functions

plot_lowlevel(vis_spec, ax, axx, axy, ...)	plotting routine / preparations: set properties of figure and plot the data with given specifications (lineplot with errorbars, or barplot)

petab.visualize.plotting_config.**plot_lowlevel**(*vis_spec: pandas.core.frame.DataFrame*, *ax: numpy.ndarray*, *axx: int*, *axy: int*, *conditions: pandas.core.series.Series*, *ms: pandas.core.frame.DataFrame*, *ind_plot: pandas.core.series.Series*, *i_visu_spec: int*, *plot_sim: bool*)

plotting routine / preparations: set properties of figure and plot the data with given specifications (lineplot with errorbars, or barplot)

Parameters

- **vis_spec** – pandas data frame, contains defined data format (visualization file)
- **ax** – np.ndarray, matplotlib.Axes
- **axx** – int, subplot axis indices for x

- **axy** – int, subplot axis indices for y
- **conditions** – pd.Series, Values on x-axis
- **ms** – pd.DataFrame, containing measurement data which should be plotted
- **ind_plot** – pd.Series, boolean vector, with size: len(rows in visualization file) x 1 with 'True' entries for rows which should be plotted
- **i_visu_spec** – int64, current index (row number) of row which should be plotted in visualizationSpecification file
- **plot_sim** – bool, tells whether or not simulated data should be plotted as well

Returns ax

Return type matplotlib.Axes

CHAPTER 3

PEtab changelog

3.1 0.0.2

Bugfix release

- Fix `petablint` error
- Fix minor issues in `petab.visualize`

3.2 0.0.1

Data format:

- Update format and documentation with respect to data and parameter scales (#169)
- Define YAML schema for grouping PEtab files, also allowing for more complex combinations of files (#183)

Library:

- Refactor library. Reorganize `petab.core` functions.
- Fix visualization w/o condition names #142
- Extend validator
- Removed deprecated functions petab.Problem.get_constant_parameters and petab.sbml.constant_species_to_parameters
- Minor fixes and extensions

3.3 0.0.0a17

Data format: *No changes*

Library:

- Extended visualization support
- Add helper function and test case to deal with timepoint-specific parameters flatten_timepoint_specific_output_overrides (#128) (Closes #125)
- Fix get_noise_distributions: so far we got 'normal' everywhere due to wrong grouping (#147)
- Fix create_parameter_df: Exclude rule targets (#149)
- Verify condition table column names occur as model parameters (Closes #150) (#151)
- More informative error messages in case of wrongly set observable and noise parameters (Closes #118) (#155)
- Update doc for copasi import and github installation (#158)
- Extend validator to check if all required parameters are present in parameter table (Closes #43) (#159)
- Setup documentation for RTD (#161)
- Handle None in petab.core.split_parameter_replacement_list (Closes #121)
- Fix(lint) correct handling of optional columns. Check before access.
- Remove obsolete generate_experiment_id.py (Closes #111) #166

3.4 0.0.0a16 and earlier

See git history

CHAPTER 4

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```
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CHAPTER 5

PEtab logo license

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Logo

CHAPTER 6

Indices and tables

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Python Module Index

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