
matk Documentation

Release 0

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Contents:

class `matk.matk` (***kwargs*)

Class for Model Analysis ToolKit (MATK) module

add_obs (*name, **kwargs*)

Add observation to problem

Parameters

- **name** (*str*) – Name of observation
- **kwargs** – keyword arguments passed to observation class

add_par (*name, **kwargs*)

Add parameter to problem

Parameters

- **name** (*str*) – Name of parameter
- **kwargs** – keyword arguments passed to parameter class

add_sampleset (*name, samples, responses=None, indices=None, index_start=1*)

Add sample set to problem

Parameters

- **name** (*str*) – Name of sample set
- **samples** (*list(fl64), ndarray(fl64)*) – Matrix of parameter samples with `npar` columns in order of [p.name for p in `matkobj.parlist`]
- **responses** (*list(fl64), ndarray(fl64)*) – Matrix of associated responses with `nobs` columns in order of [o.name for o in `matkobj.obslist`] if observation exists (existence of observations is not required)
- **indices** (*list(int), ndarray(int)*) – Sample indices to use when creating working directories and output files

calibrate (*workdir=None, reuse_dirs=False, report_fit=True*)

Calibrate MATK model

Parameters

- **workdir** (*str*) – Name of directory where model will be run. It will be created if it does not exist
- **reuse_dirs** (*bool*) – If True and `workdir` exists, the model will reuse the directory
- **report_fit** (*bool*) – If True, parameter statistics and correlations are printed to the screen

Returns `lmfit` minimizer object

forward (*pardict=None, workdir=None, reuse_dirs=False*)

Run MATK model using current values

Parameters

- **pardict** (*dict*) – Dictionary of parameter values keyed by parameter names
- **workdir** (*str*) – Name of directory where model will be run. It will be created if it does not exist
- **reuse_dirs** (*bool*) – If True and `workdir` exists, the model will reuse the directory

Returns `int` – 0: Successful run, 1: `workdir` exists

get_obs_names ()
Get observation names

get_obs_values ()
Get observation values

get_par_dist_pars ()
Get parameters needed by parameter distributions

get_par_dists ()
Get parameter probabilistic distributions

get_par_maxs ()
Get parameter lower bounds

get_par_mins ()
Get parameter lower bounds

get_par_names ()
Get parameter names

get_par_nvals ()
Get parameter nvals (number of values for parameter studies)

get_par_values ()
Get parameter values

get_residuals ()
Get least squares values

get_sims ()
Get the current simulated values :returns: list(float) – simulated values in order of matk.obslist

make_workdir (*workdir=None, reuse_dirs=False*)
Create a working directory

Parameters

- **workdir** (*str*) – Name of directory where model will be run. It will be created if it does not exist
- **reuse_dirs** (*bool*) – If True and workdir exists, the model will reuse the directory

Returns int – 0: Successful run, 1: workdir exists

model None

Python function that runs model

model_args None

Tuple of extra arguments to MATK model expected to come after parameter dictionary

model_kwargs None

Dictionary of extra keyword arguments to MATK model expected to come after parameter dictionary and model_args

n_cpus None

Set number of cpus to use for concurrent model evaluations

parameters_file None

Set the name of the parameters_file for parallel runs

results_file None

Set the name of the results_file for parallel runs

run_samples (*name=None, ncpus=1, templatedir=None, workdir_base=None, save=True, reuse_dirs=False*)

Run model using values in samples for parameter values If samples are not specified, LHS samples are produced

Parameters

- **name** – Name of MATK sample set object
- **ncpus** (*int*) – number of cpus to use to run models concurrently
- **templatedir** (*str*) – Name of folder including files needed to run model (e.g. template files, instruction files, executables, etc.)
- **workdir_base** (*str*) – Base name for model run folders, run index is appended to workdir_base
- **save** (*bool*) – If True, model files and folders will not be deleted during parallel model execution
- **reuse_dirs** (*bool*) – Will use existing directories if True, will return an error if False and directory exists

Returns tuple(ndarray(fl64), ndarray(fl64)) - (Matrix of responses from sampled model runs siz rows by npar columns, Parameter samples, same as input samples if provided)

save_sampleset (*outfile, sampleset*)

Save sampleset to file

Parameters

- **outfile** (*str*) – Name of file where sampleset will be written
- **sampleset** (*str*) – Sampleset name

seed None

Set the seed for random sampling

set_lhs_samples (*name, siz=None, noCorrRestr=False, corrmatrix=None, seed=None, index_start=1*)

Draw lhs samples of parameter values from scipy.stats module distribution

Parameters

- **name** (*str*) – Name of sample set to be created
- **siz** (*int*) – Number of samples to generate, ignored if samples are provided
- **noCorrRestr** (*bool*) – If True, correlation structure is not enforced on sample, use if siz is less than number of parameters
- **corrmatrix** (*matrix*) – Correlation matrix
- **seed** (*int*) – Random seed to allow replication of samples
- **index_start** – Starting value for sample indices

Type int

Returns matrix – Parameter samples

set_obs_values (**args, **kwargs*)

Set simulated values using a dictionary or keyword arguments

set_par_values (**args, **kwargs*)

Set parameters using values in first argument

set_parstudy_samples (*name*, **args*, ***kwargs*)

Generate parameter study samples

Parameters

- **name** (*str*) – Name of sample set to be created
- **outfile** (*str*) – Name of file where samples will be written. If outfile=None, no file is written.
- ***args** – Number of values for each parameter. The order is expected to match order of matk.parlist (e.g. [p.name for p in matk.parlist])
- ****kwargs** – keyword arguments where keyword is the parameter name and argument is the number of desired values

Returns ndarray(fl64) – Array of samples

templatedir None

Set the name of the templatedir for parallel runs

workdir None

Set the base name for parallel working directories

workdir_base None

Set the base name for parallel working directories

workdir_index None

Set the working directory index for parallel runs

class matk.**Parameter** (*name*, ***kwargs*)

MATK parameter class

dist None

Probabilistic distribution of parameter belonging to scipy.stats module

dist_pars None

Distribution parameters required by self.dist (e.g. if dist == uniform, dist_pars = (min,max-min))

expr None

Mathematical expression to use to evaluate value

max None

Parameter upper bound

mean None

Parameter mean

min None

Parameter lower bound

name None

Parameter name

nvals None

Number of values the paramter will take for parameter studies

offset None

Offset to add to parameter

scale None

Scale factor to multiply parameter by

std None

Parameter st. dev.

value None

Parameter value

vary None

Boolean indicating whether or not to vary parameter

class `matk.Observation` (*name*, ***kwargs*)

MATK observation class

name None

Observation name

residual None

Observation value minus simulated value

sim None

Simulated value generated by MATK model

value None

Observation value

weight None

Weight to apply to simulated values

class `matk.SampleSet` (*name*, *samples*, *index_start=1*, ***kwargs*)

MATK samples class - Stores information related to a sample including parameter samples, associated responses, and sample indices

corr (*type='pearson'*, *plot=False*)

Calculate correlation coefficients of parameters and responses

Parameters **type** (*str*) – Type of correlation coefficient (pearson by default, spearman also available)

Returns `ndarray(fl64)` – Correlation coefficients

index_start None

Starting integer value for sample indices

indices None

Array of sample indices

name None

Sample set name

obsnames None

Array of observation names

parnames None

Array of parameter names

responses None

Ndarray of sample set responses, rows are samples, columns are responses associated with observations in order of `MATKobject.obslist`

samples None

Ndarray of parameter samples, rows are samples, columns are parameters in order of `MATKobject.parlist`

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