Property and Method List for SNOBFit Object (snobfitclass)

In this document you will find a list of available properties and methods of the SNOBFit object created by snobfitclass.

Properties

Below is a list of properties of the object. To get a list of properties from the MATLAB command line, type:

```
snobfit_metadata = ?snobfitclass.snobclass;
snobfit_properties = reshape({snobfit_metadata.PropertyList.Name},
size(snobfit_metadata.PropertyList))
```

There are some properties of the SNOBFit object that you can change and others that only the object itself can change. The properties that you can change are:

Property Name	Description	Type
name	The name that your experiment should be saved under	string
fcn	The name of the function that you want to minimise, it should return the value of your lead property	string
constraintFcn	The name of the function that calculates your constrained properties; this property is required only for a constrained optimisation	string
linked	This property is mainly relevant for flow reactors, where you may need to control the relative and total flow rates of two reagent streams (see *defining_an_optimisation.md*). If two of your input parameters are linked, set to true	boolean (true or false)
constrained	If you are running a contrained optimisation, set to true	boolean
continuing	If you are continuing a previous optimisation (can be inititialised by creating a SNOBFit object with the same name as a previous optimisation)	boolean
combo	If you are running a constrained optimisation, in which you first search for a feasible point by minimising the penalty function P calculated from the constraint functions	boolean
ncall	The maximum number of function evaluations before termination	integer
termination	The termination criteria for the optimisation, can be set to *n_runs* (default), *minimised*, or *no_change*	string
filepath	The file path that specifies where the optimisation results will be saved	string
x_lower	The lower bounds on your input parameters	*n*-x-1 array
x_upper	The upper bounds on your input parameters	*n*-x-1 array
xyMin	The overall minimum of two linked input parameters	float
xyMax	The overall maximum of two linked input parameters	float

Property Name	Description	Type
minRatio	The minimum ratio between two linked input parameters	float
maxRatio	The maximum ratio between two linked input parameters	float
zMin	The minimum of an optional third input parameter when using two linked input parameters	float
zMax	The maximum of an optional third input parameter when using two linked input parameters	float
F_upper	Upper limits on the constrained properties	*n_constraints*-x-1 array
F_lower	Lower limits on the constraint properties	*n_constraints*-x-1 array
sigma	Maximum permitted deviations from preferred upper and lower bounds of properties	*n_constraints*-x-1 array
sigmaUpper	Maximum permitted deviations from preferred upper bounds of properties	*n_constraints*-x-1 array
sigmaLower	Maximum permitted deviation from preferred lower bounds of properties	*n_constraints*-x-1 array
nreq	The number of points to request from the SNOBFit algorithm	integer
npoint	The number of random points used to initialise the optimisation	integer
p	Defines the ratio between local and global minimisers recommended by the SNOBFit algorithm (defaults to 0.4)	float, between 0 and 1
fglob	The expected function minimum for your lead property (defaults to 0)	float
threshold	The threshold from the expected function minimum. The optimisation will terminate when the function value is smaller than fglob + threshold	float
nCallNoChange	The SNOBFit algorithm terminates if nCallNoChange successive function evaluations lead to no reduction in the lowest function value, use with *no_change* termination criterion	float
minCalls	The minimum number of function evaluations to run before termination, use with *no_change* termination criterion	float
repeatBest	If true, re-evaluates the lead property function at the best point (xbest) at the end of the optimisation	boolean
plot_delay	Delay in seconds between each function evaluation, can aid with plotting during optimisation	integer

The properties that only the SNOBFit object can change are:

Property Name	Description	Type
x	The values of the input parameters that have been investigated already	*ncall0*-x-*n* array
f	The values of the lead property for points that have already been evaluated	*ncall0*-x-*1* array
F	The values of the constrained properties for points that have already been evaluated	*nreq*-x-*n_constraints* array
fm	The values of the constrained merit function for points that have already been evaluated	*nreq*-x-*1* array

Property Name	Description	Type
xVirt	The transformed values of input parameters, when two input parameters are linked together	*nreq*-x-*n* array
n	The number of input parameters, the dimension of the optimisation	integer
ncall0	The number of function evaluations during the optimisation	integer
status	The status of the optimisation	string
minimised	True if the optimisation has found a minimum, false if not	boolean
xbest	The input parameters at the best result found during the optimisation	*1*-x-*n* array
fbest	The value of your lead property at the best result found during the optimisation	float
xcon	The input parameters at the best feasible result found during a constrained optimisation	*1*-x-*n* array
fcon	The value of your lead property at the best feasible result found during a constrained optimisation	float
f0	The value of your lead property at an initial feasible point, used in the constrained merit function	float
Delta	A scaling parameter used in the constrained merit function (see our article or original SNOBFit paper)	float
next	The input parameters recommended by the latest call to the SNOBFit algorithm	*nreq*-x-*n* array
fbestHistory	A store of the lead property value at the best result found after each call to the SNOBFit algorithm, used for *no_change* termination criterion	*n_snobfit_calls*-x-1 array
valuesToPass	A store of values to be passed between an objected function and the constraint function, can be accessed by a MATLAB function	*nreq*-x-*m* array, *m* depends on what values you are passing
trapezoid	The corners of the trapezoidal input parameter bounds defined by two linked input parameters	2-x-4 array
created	The date and time that the SNOBFit object was created	
conStart	The function evaluation number that the constrained portion of a combined optimisation started at	integer

Methods

Below is a list of methods and a description of what they can do. You can access most of them, but you should avoid using the second set of methods listed.

These are the methods that you may safely use yourself:

Method Name	Description
startExp	Begins the optimisation. If you have not set up your optimisation properly, it will throw errors saying what you have forgotten to do
saveExp	Saves the results and a summary of your optimistion
plotBounds	Plots an outline of the input parameter bounds

These are the methods that the *startExp* method calls; you should not need to use these yourself:

Method Name	Description
runsnob	Runs an unconstrained SNOBFit optimisation
runconstrained	Runs a constrained SNOBFit optimisation
runcombo	Runs a combined SNOBFit optimisation - a constrained optimisation initialised by an unconstrained optimisation of the constrained properties
defaults	Sets default values for SNOBFit object properties when a particular function name is set.