Documentation of the pygpc package

Release 2018

Konstantin Weise

Apr 08, 2019

CONTENTS:

CHAPTER

ONE

PYGPC PACKAGE

1.1 Subpackages

1.1.1 pygpc.testfunctions package

Submodules

pygpc.testfunctions.testfunctions module

class pygpc.testfunctions.testfunctions.**BfieldOutsideSphere**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Calculates the B-field outside a sphere, does not depend on conductivity after Jarvas (1987). Dipole in SI units, positions in (mm)

Parameters

- **p["sphere_radius"]** (*float*) – Radius of sphere in (mm)
- **p["dipole_pos"]** (*ndarray of float [3 x 1]*) – Position of dipole in (mm)
- **p["dipole_moment"]** (*ndarray of float [3 x 1]*) – Moment of dipole in (Ams)
- **p["detector_positions"]** (*ndarray of float [n x 3]*) – Position of detectors, must lie outside sphere

Returns **B** – B-fields in detector positions

Return type ndarray of float [1 x 3*N]

Notes

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Franke**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Franke function [1] with 2 parameters. It is often used in regression or interpolation analysis. It is defined in the interval [0, 1] x [0, 1]. Hampton and Doostan used in the framework of BASE-PC [2].

$$y = \frac{3}{4}\exp\left(-\frac{(9x_1-2)^2}{4} - \frac{(9x_2-2)^2}{4}\right) + \frac{3}{4}\exp\left(-\frac{(9x_1+1)^2}{49} - \frac{(9x_2+1)}{10}\right) + \frac{1}{2}\exp\left(-\frac{(9x_1-7)^2}{4} - \frac{(9x_2-3)^2}{4}\right) +$$

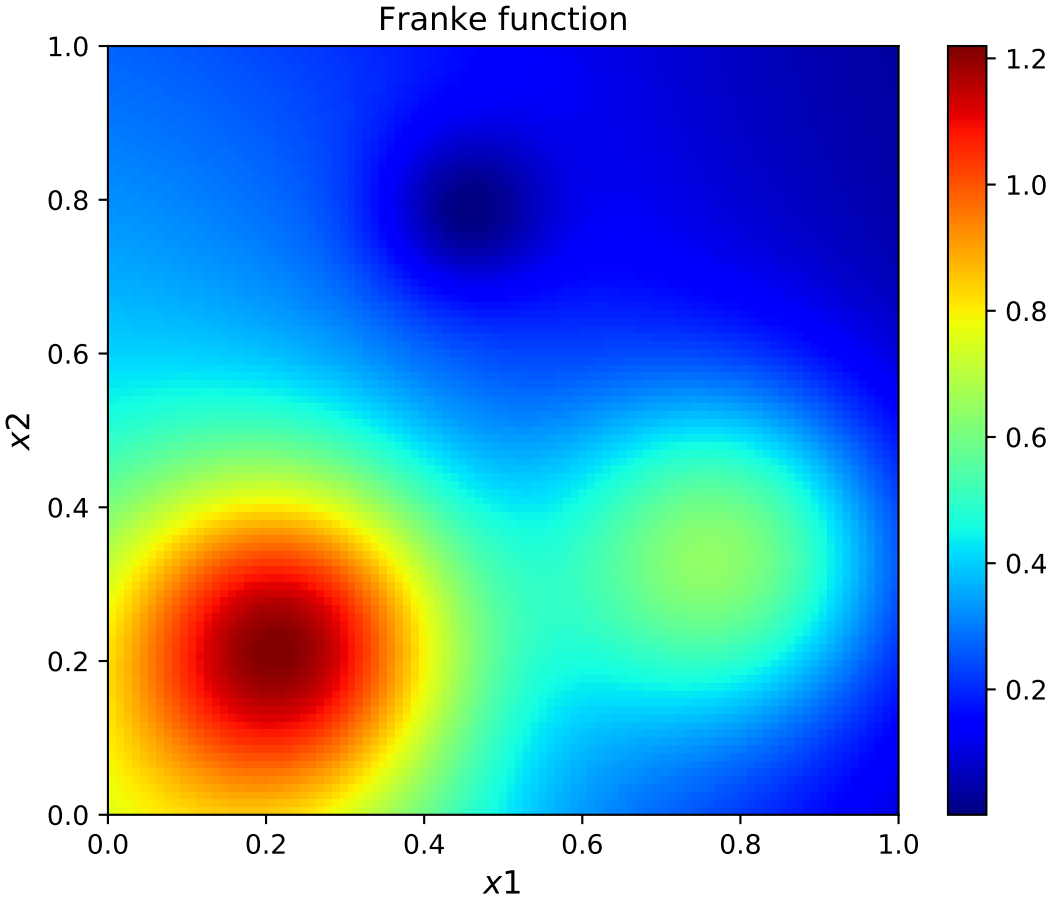
Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter [0, 1]
- **p["x2"]** (*float or ndarray of float [n_grid]*) – Second parameter [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**GFunction**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional g-function used by Saltelli and Sobol (1995) [1].

This test function is used as an integrand for various numerical estimation methods, including sensitivity analysis methods, because it is fairly complex, and its sensitivity indices can be expressed analytically. The exact value of the integral with this function as an integrand is 1. For each index i, a lower value of a_i indicates a higher importance of the input variable xi.

$$\prod_{i=1}^{N} \frac{|4x_i - 2| + a_i}{1 + a_i}$$

The recommended values of a_i by Crestaux et al. (2007) [2] are:

$$a_i = \frac{i-2}{2} \quad \text{for all} \quad i = 1, ..., d$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter [0, 1]
- **p["a"]** (*ndarray of float [N_dims]*) – Importance factors of dimensions

Returns **y** – Output data

Return type ndarray of float [N_input x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

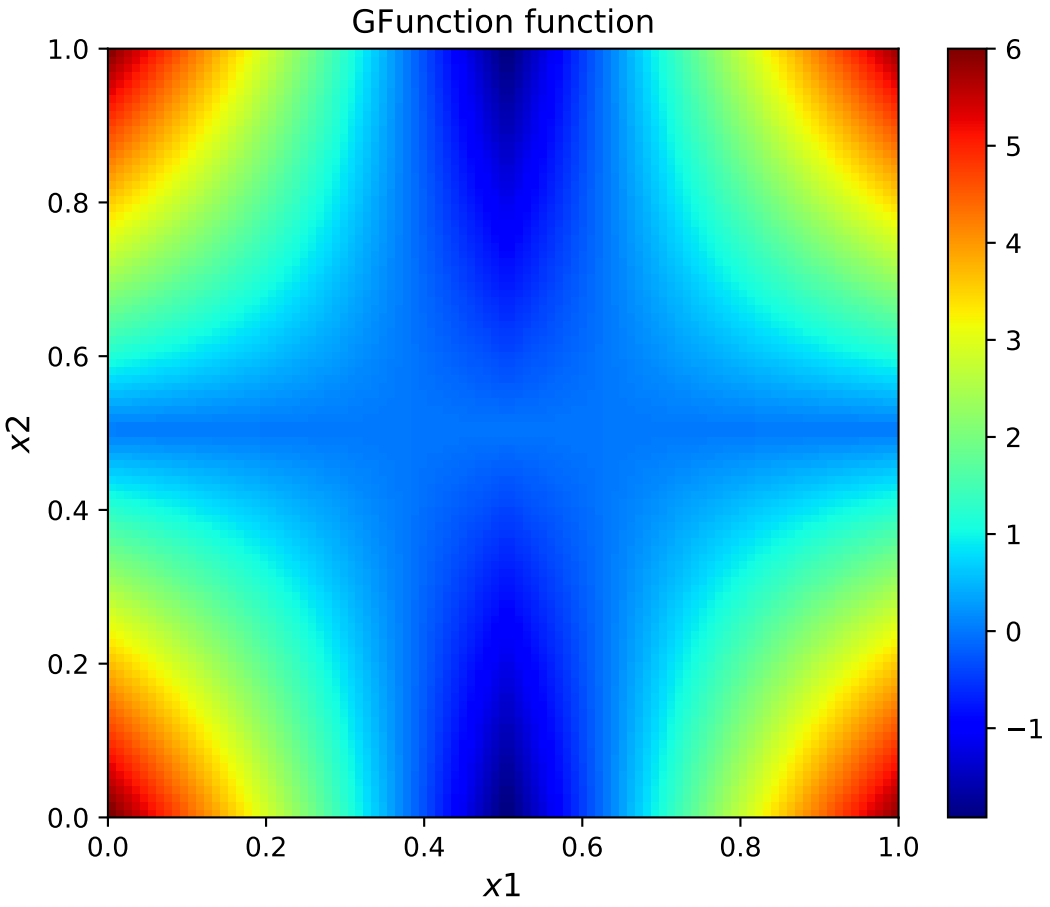
Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**GenzContinuous**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "continuous" Genz function [1]. It is defined in the interval [0, 1] x ... x [0, 1].

$$y = \exp\left(-\sum_{i=1}^{N} a_i |x_i - u_i|\right)$$


GFunction function
1.0
0.8
0.6
0.4
0.2
0.0
x2
0.0
0.2
0.4
0.6
0.8
1.0
x1
6
5
4
3
2
1
0
−1

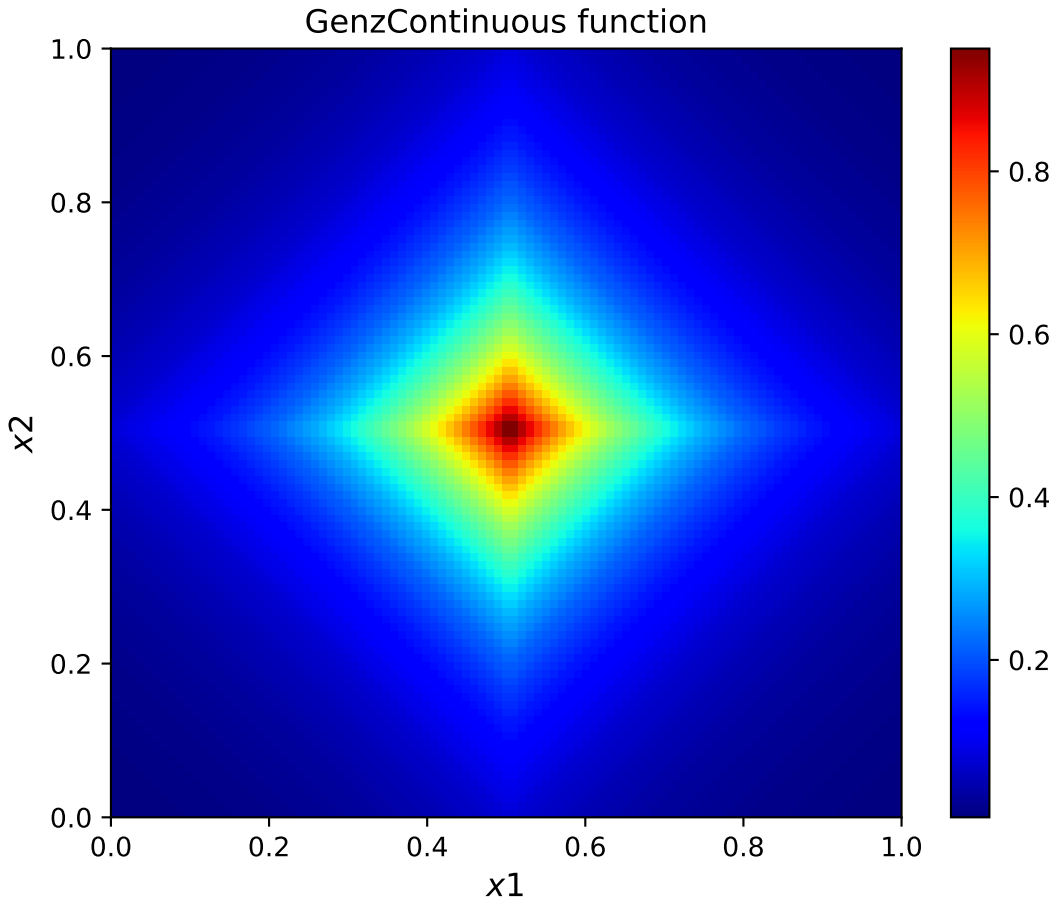
Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**GenzCornerPeak**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "CornerPeak" Genz function [1,2]. It is defined in the interval [0, 1] x ... x [0, 1]. Used by [3] as testfunction.

$$y = \left(1 + \sum_{i=1}^{N} a_i x_i\right)^{-(N+1)}$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

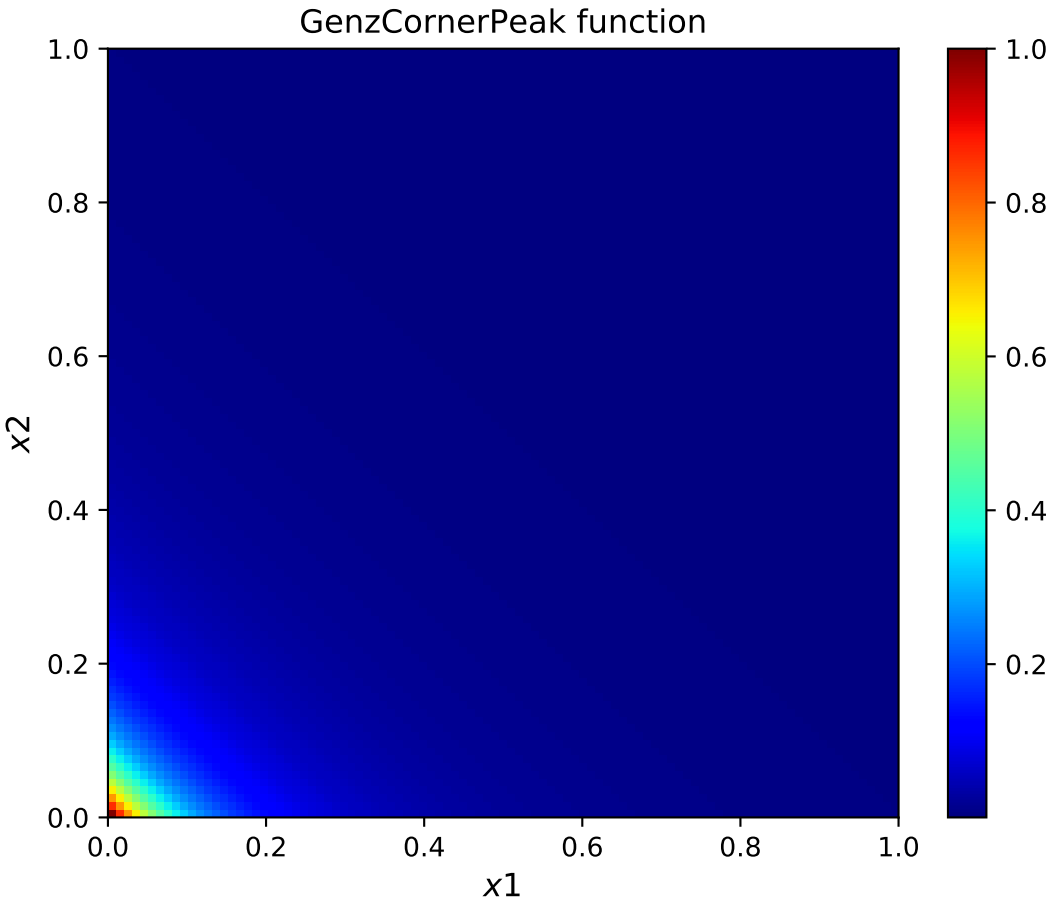
class pygpc.testfunctions.testfunctions.**GenzDiscontinuous**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "Discontinuous" Genz function [1]. It is defined in the interval [0, 1] x ... x [0, 1].

$$y = \exp\left(\sum_{i=1}^{N} a_i x_i\right) \quad \text{if} \quad x_i < u_i \quad \text{else} \quad 0$$

Parameters

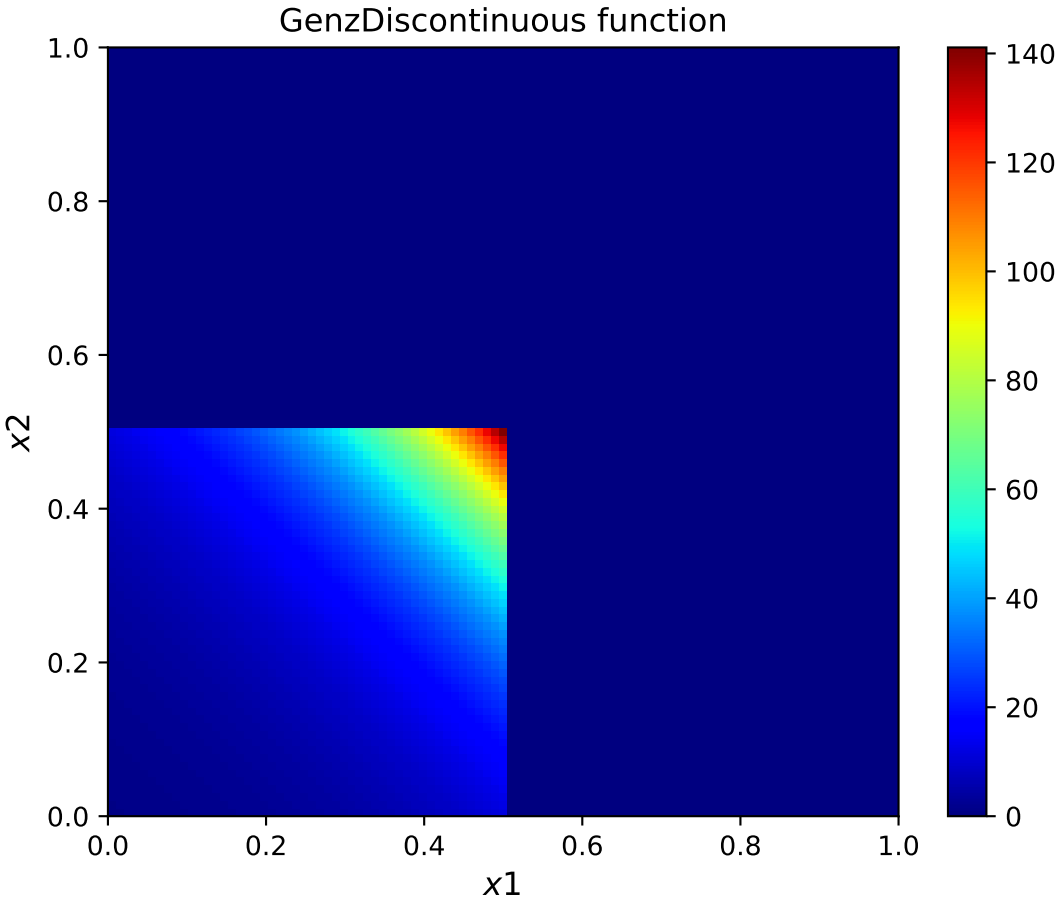
- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]


GenzCornerPeak function
1.0
0.8
0.6
0.4
0.2
0.0
x2
0.0
0.2
0.4
0.6
0.8
1.0
x1
1.0
0.8
0.6
0.4
0.2

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**GenzGaussianPeak**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "GaussianPeak" Genz function [1]. It is defined in the interval [0, 1] x ... x [0, 1].

$$y = \exp\left(-\sum_{i=1}^{N} a_i^2 (x_i - u_i)^2\right)$$

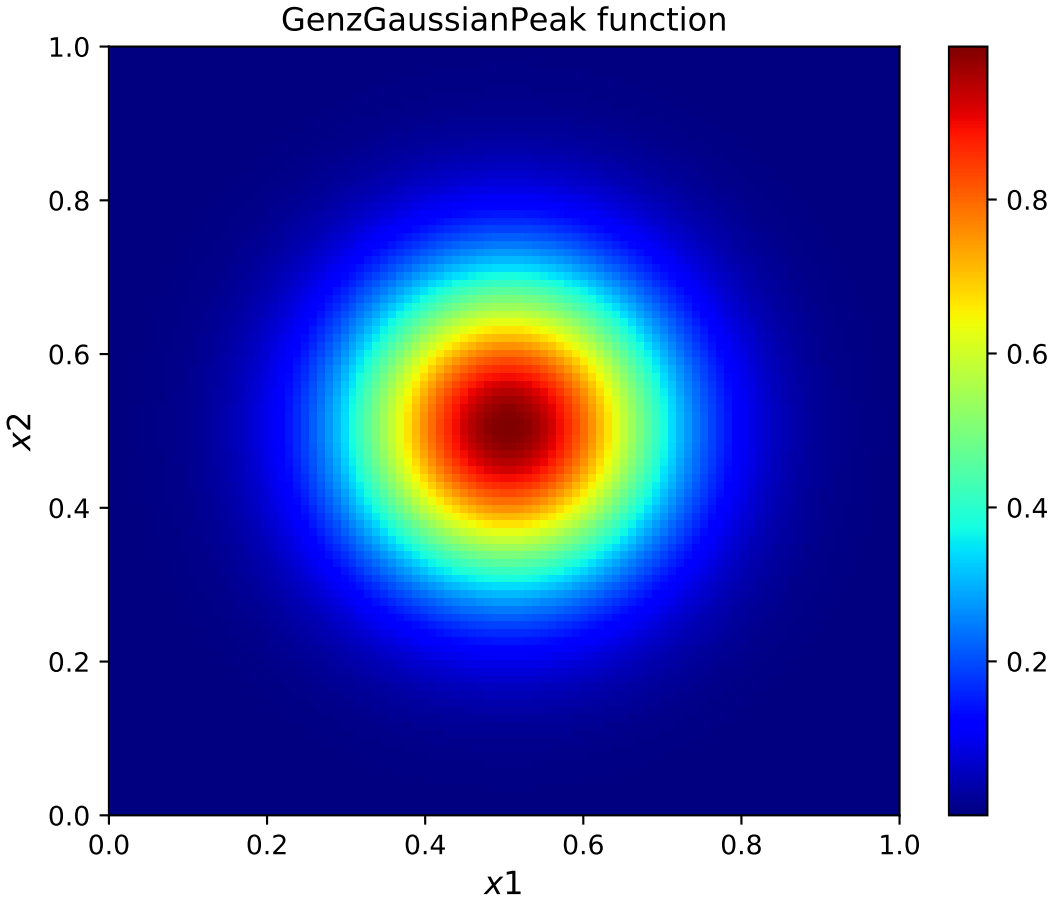
Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**GenzOscillatory**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "Oscillatory" Genz function [1]. It is defined in the interval [0, 1] x ... x [0, 1].

$$y = \cos\left(2\pi u_1 + \sum_{i=1}^{N} a_i x_i\right)$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

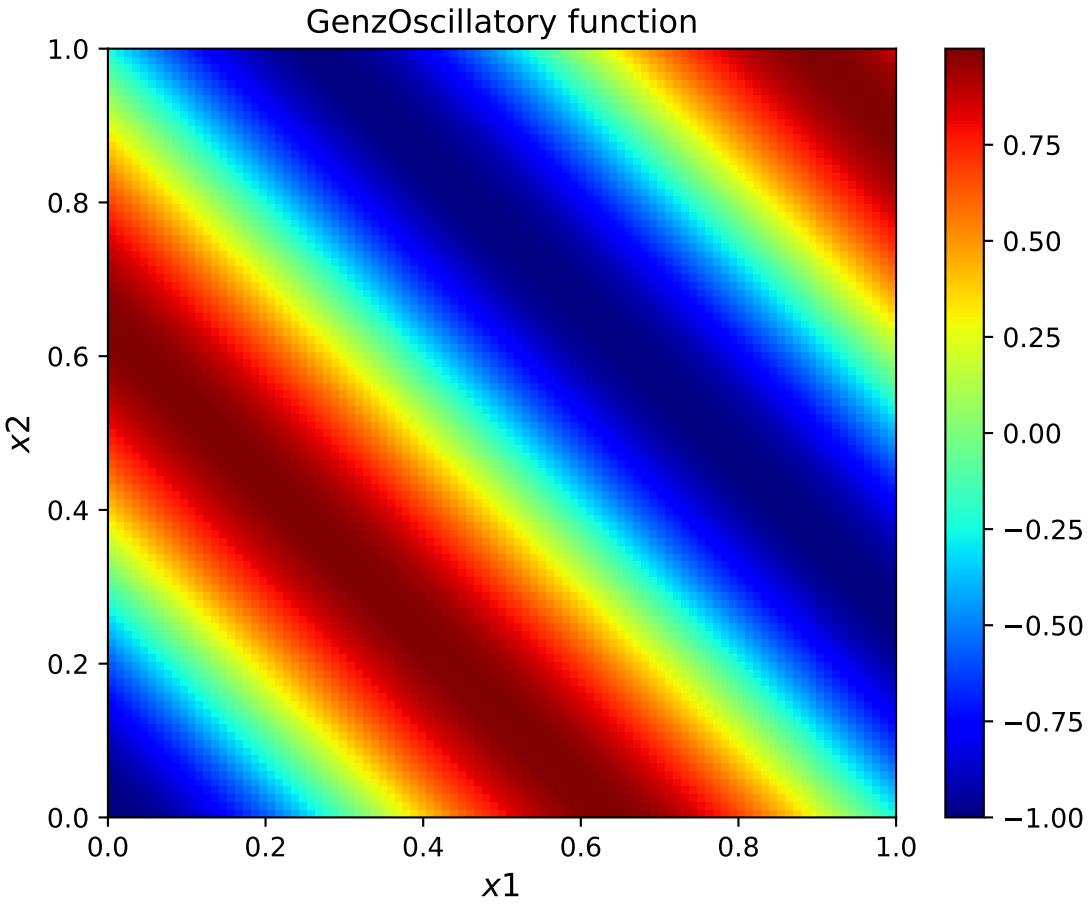
class pygpc.testfunctions.testfunctions.**GenzProductPeak**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "ProductPeak" Genz function [1]. It is defined in the interval [0, 1] x ... x [0, 1].

$$y = \prod_{i=1}^{N} \left(a_i^{-2} + (x_i - u_i)^2\right)^{-1}$$

Parameters

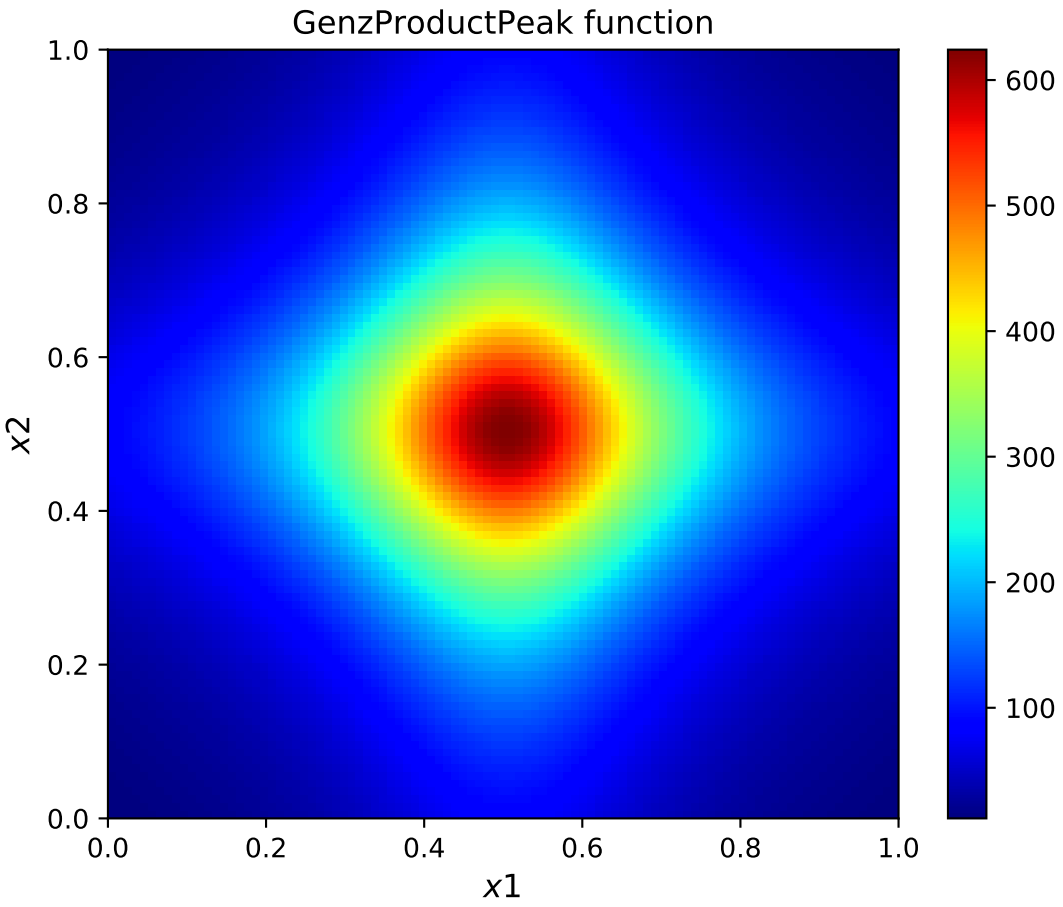
- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]


GenzOscillatory function
1.0
0.8
0.6
0.4
0.2
0.0
x2
0.0
0.2
0.4
0.6
0.8
1.0
x1
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**HyperbolicTangent**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Two-dimensional hyperbolic tangent function [1] to simulate discontinuities. Discontinuity at x1 = 0.

$$y(x_1, x_2) = \tanh(10x_1) + 0.2\sin(10x_1) + 0.3x_2 + 0.1\sin(5x_1)$$

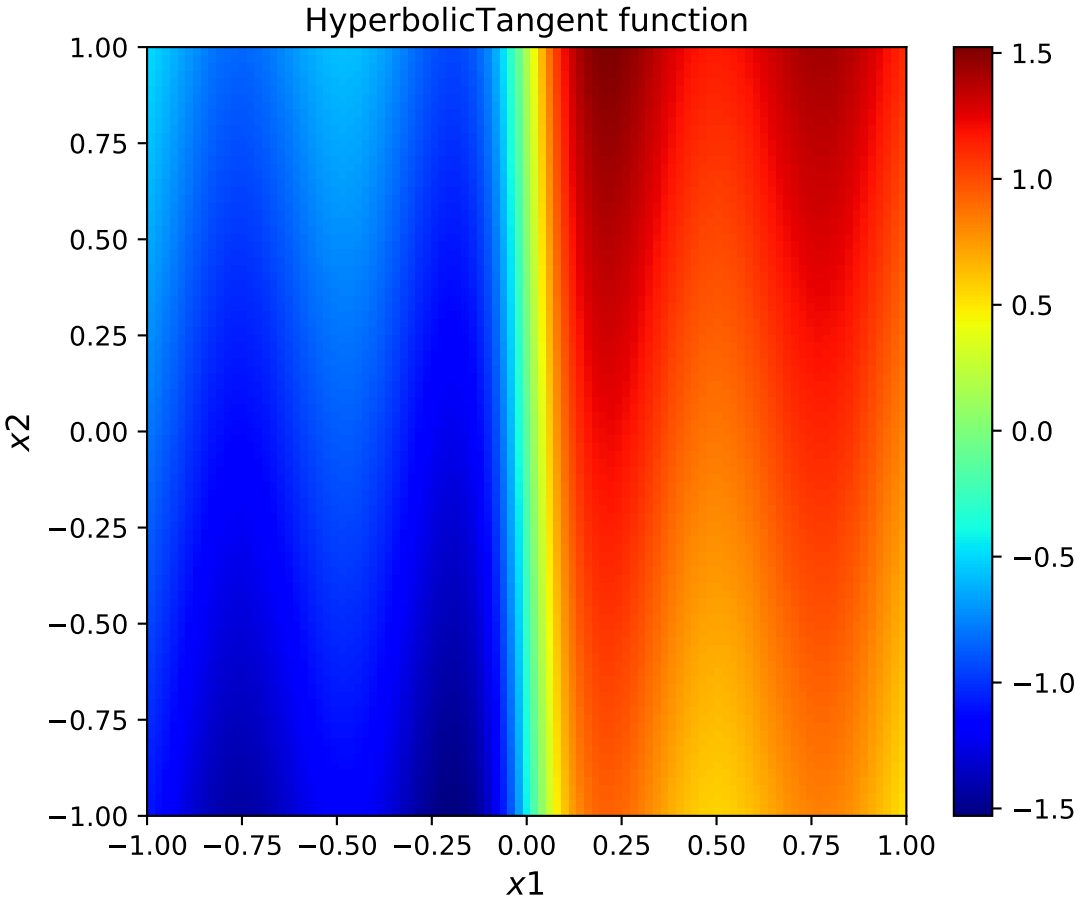
Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – Parameter 1 [-1, 1]
- **p["x2"]** (*float or ndarray of float [n_grid]*) – Parameter 2 [-1, 1]

Returns **y** – Output data

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Ishigami**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

Three-dimensional test function of Ishigami.

The Ishigami function of Ishigami & Homma (1990) [1] is used as an example for uncertainty and sensitivity analysis methods, because it exhibits strong nonlinearity and nonmonotonicity. It also has a peculiar dependence on x3, as described by Sobol' & Levitan (1999) [2]. The values of a and b used by Crestaux et al. (2007) [3] and Marrel et al. (2009) [4] are: a = 7 and b = 0.1.

$$y = \sin(x_1) + a\sin(x_2)^2 + bx_3^4\sin(x_1)$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [-pi, pi]
- **p["x2"]** (*float or ndarray of float [n_grid]*) – Second parameter defined in [-pi, pi]
- **p["x3"]** (*float or ndarray of float [n_grid]*) – Third parameter defined in [-pi, pi]
- **p["a"]** (*float*) – shape parameter (a=7)
- **p["b"]** (*float*) – shape parameter (b=0.1)

Returns **y** – Output data

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Lim2002**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

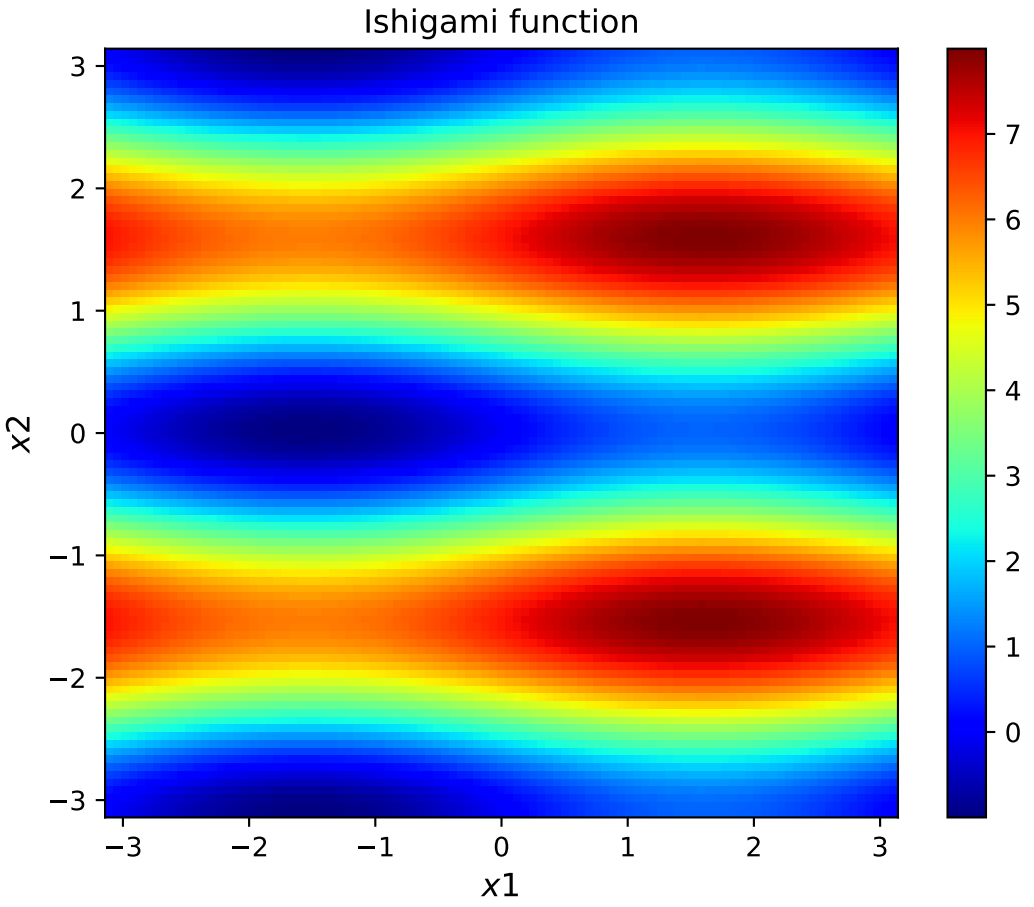
Two-dimensional test function of Lim et al. (2002) [1].

This function is a polynomial in two dimensions, with terms up to degree 5. It is nonlinear, and it is smooth despite being complex, which is common for computer experiment functions.

$$y = 9 + \frac{5}{2}x_1 - \frac{35}{2}x_2 + \frac{5}{2}x_1x_2 + 19x_2^2 - \frac{15}{2}x_1^3 - \frac{5}{2}x_1x_2^2 - \frac{11}{2}x_2^4 + x_1^3x_2^2$$

Parameters

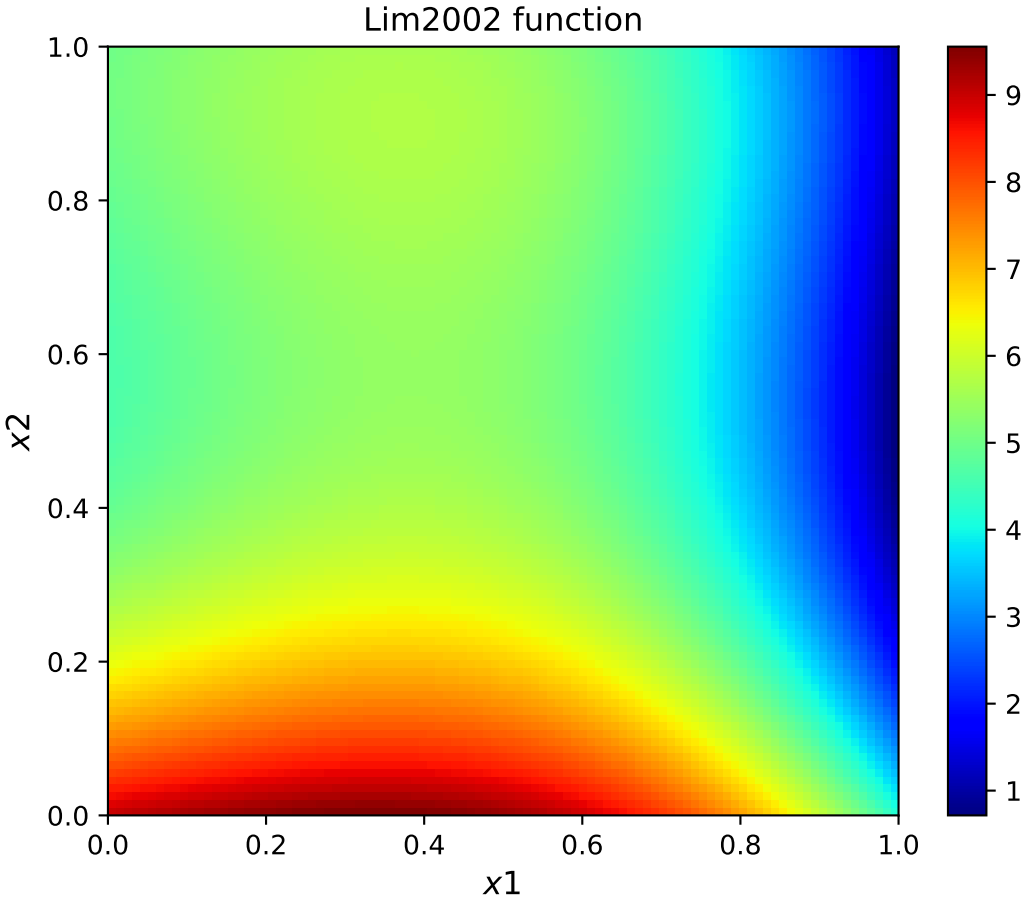
- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["x2"]** (*float or ndarray of float [n_grid]*) – Second parameter defined in [0, 1]


Ishigami function
x2
x1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3
7
6
5
4
3
2
1
0

Returns **y** – Output data

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**ManufactureDecay**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional manufacture decay function [1]. It is defined in the interval [0, 1] x ... x [0, 1]. Hampton and

Doostan used in the framework of BASE-PC [1].

$$y = \exp\left(2 - \sum_{i=1}^{N} x_i \frac{\sin(i+1)}{i+1}\right)$$

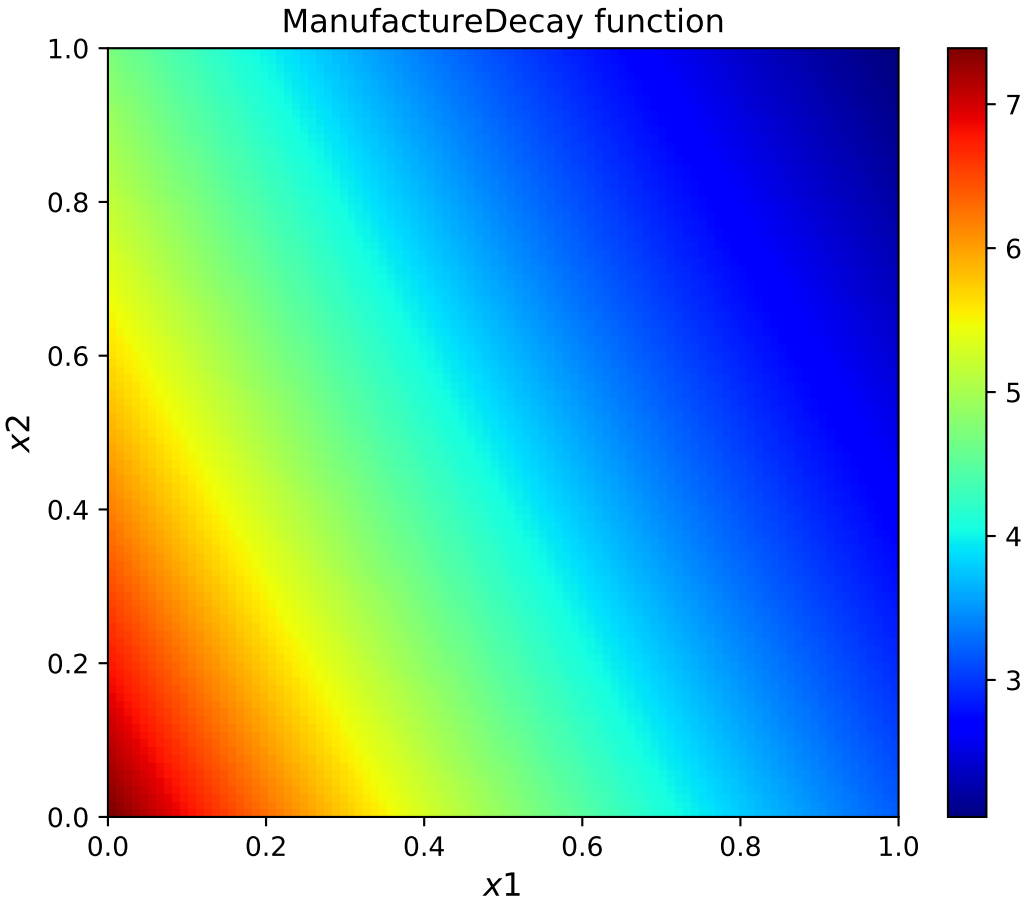
Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in [0, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [0, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in [0, 1]

Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes



simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**MovingParticleFrictionForce**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Differential equation describing a particle moving under the influence of a potential field and of a friction force [1].

$$\frac{d^2x}{dt^2} + f\frac{dx}{dt} = -\frac{35}{2}x^3 + \frac{15}{2}x$$

with:

$$x_1 = x$$

$$x_2 = \frac{dx}{dt}$$

we get a system of two 1st order ODE

$$\frac{dx_1}{dt} = x_2$$

$$\frac{dx_2}{dt} = -\frac{35}{2}x_1^3 + \frac{15}{2}x_1 - fx_2$$

Discontinuity at randomly perturbed initial value x0 = X0 + delta_X * xi = 0.05 - 0.2 * 0.25 and two stable fixed points:

$$x = -\sqrt{15/35}\text{for}\xi < -0.25$$

$$x = +\sqrt{15/35}\text{for}\xi > -0.25$$

xi is uniform distributed [-1, 1]

Mean value: 0.163663 Standard deviation: 0.633865691

Parameters **p["xi"]** (*ndarray of float [1]*) – Pertubation xi of initial value x0 (x0 = X0 + xi) [-1, 1]

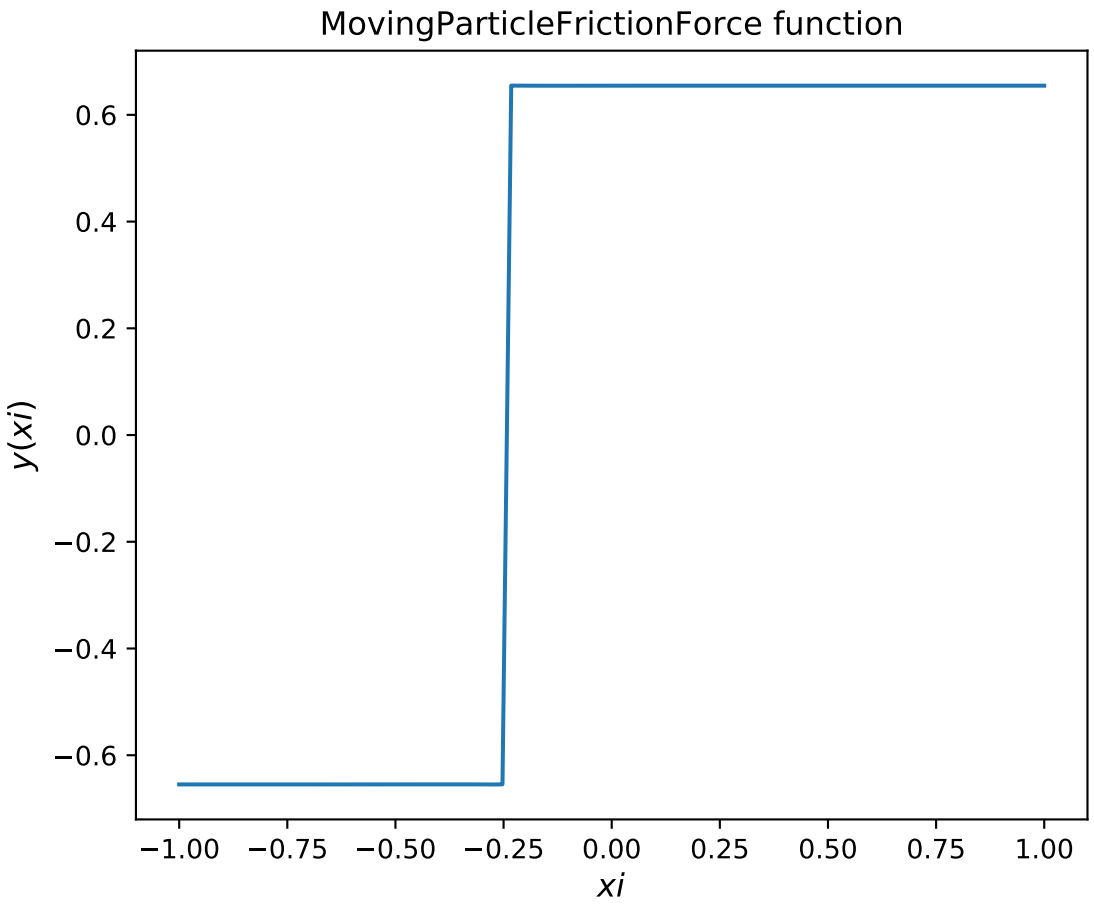
Returns **y** – x(t=10.)

Return type ndarray of float [1 x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier


MovingParticleFrictionForce function
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
y(xi)
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
xi

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**OakleyOhagan2004**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

15-dimensional test function of Oakley and O'Hagan (2004) [1].

This function's a-coefficients are chosen so that 5 of the input variables contribute significantly to the output variance, 5 have a much smaller effect, and the remaining 5 have almost no effect on the output variance.

$$y = \mathbf{a}_1^T \mathbf{x} + \mathbf{a}_2^T \sin(\mathbf{x}) + \mathbf{a}_3^T \cos(\mathbf{x}) + \mathbf{x}^T \mathbf{M} \mathbf{x}$$

The parameter vectors a and matrix M are in /pygpc/pck/data/oakley_ohagan_2004.

Parameters **p["x1...15"]** (*ndarray of float [n_grid]*) – Input data, xi ~ N(mu=0, sigma=1), for all i = 1, 2,. . . , 15.

Returns **y** – Output data

Return type ndarray of float [N_input x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Peaks**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

Two-dimensional peaks function.

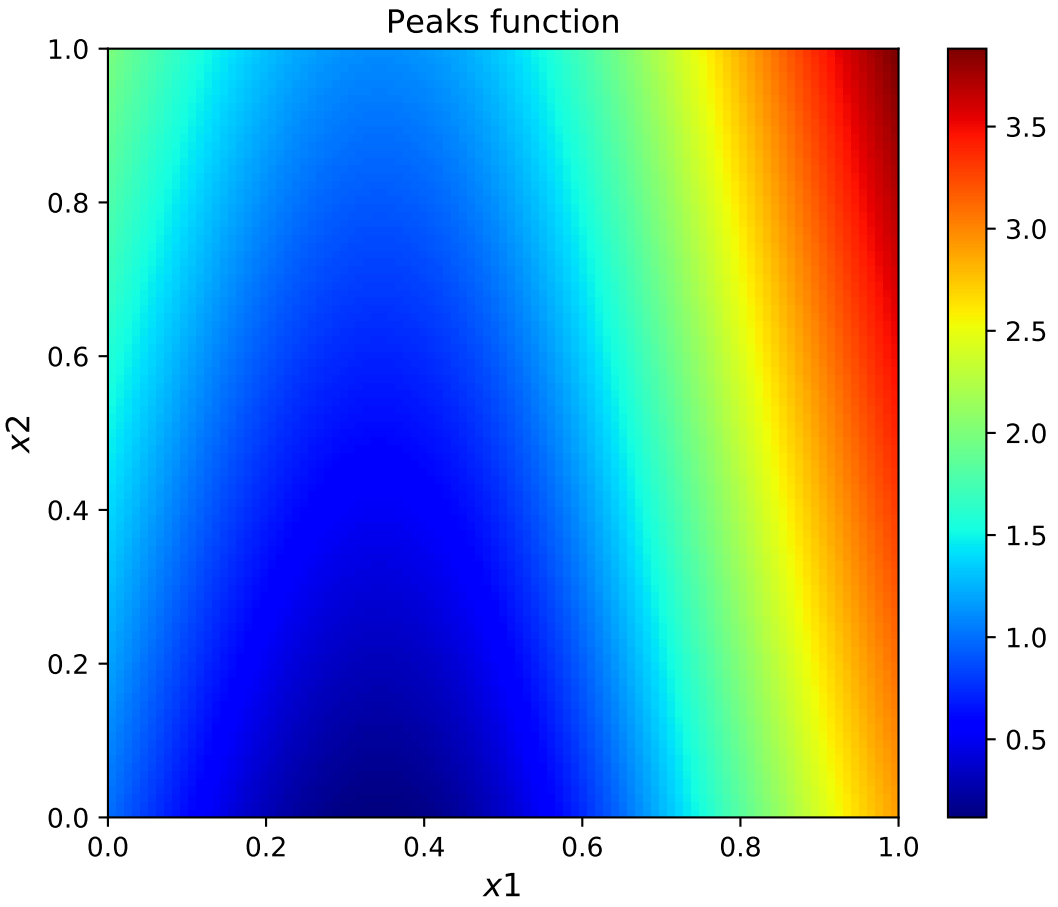
y = Peaks(x)

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – Parameter 1
- **p["x2"]** (*float or ndarray of float [n_grid]*) – Parameter 2
- **p["x3"]** (*float or ndarray of float [n_grid]*) – Parameter 3

Returns

- **y** (*ndarray of float [n_grid x n_out]*) – Output data
- **misc** (*dict or list of dict [n_grid]*) – Additional data, will be saved under its keys in the .hdf5 file during gPC simulations for every grid point


Peaks function
1.0
0.8
0.6
0.4
0.2
0.0
x2
0.0
0.2
0.4
0.6
0.8
1.0
x1
3.5
3.0
2.5
2.0
1.5
1.0
0.5

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**PotentialDipole3Layers**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Calculates the electric potential in a 3-layered sphere caused by a dipole after Ary et al. (1981).

Parameters

- **p["radii"]** (*list [3]*) – Radius of each of the 3 layers (innermost to outermost) in (mm)
- **p["cond_brain_scalp"]** (*float*) – Conductivity of the brain and scalp layers in (S/m)
- **p["cond_skull"]** (*float*) – Conductivity of the skull layer in (S/m)
- **p["dipole_pos"]** (*ndarray of float [3 x 1]*) – Position of the dipole, in (mm)
- **p["dipole_moment"]** (*ndarray of float [3 x 1]*) – Moment of dipole, in (Cm)
- **p["surface_points"]** (*ndarray of float [N x 3]*) – List of positions where the potential should be calculated in (mm)

Returns **potential** – Values of the electric potential, in (V)

Return type ndarray of float [1 x n_out]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**PotentialHomogeneousDipole**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Calculates the surface potential generated by a dipole inside a homogeneous conducting sphere after Yao (2000).

Parameters

- **p["sphere_radius"]** (*float*) – Radius of sphere in (mm)
- **p["conductivity"]** (*float*) – Conductivity of medium in (S/m)
- **p["dipole_pos"]** (*ndarray of float [3 x 1]*) – Position of dipole in (mm)
- **p["dipole_moment"]** (*ndarray of float [3 x 1]*) – Moment of dipole in (Cm)
- **p["detector_positions"]** (*ndarray of float [n x 3]*) – Position of detectors, will be projected into the sphere surface in (mm)

Returns **potential** – Potential at the points

Return type ndarray of float [1 x n_out]

Notes

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Ridge**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional "Ridge" function [1] (and also used as testfunction therein). Typically defined in the interval [-4, 4] x ... x [-4, 4].

$$y = \sum_{i=1}^{N} x_i + 0.25 \left(\sum_{i=1}^{N} x_i \right)^2 + 0.025 \left(\sum_{i=1}^{N} x_i \right)^3$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter defined in e.g. [-4, 4]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in e.g. [-4, 4]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter defined in e.g. [-4, 4]

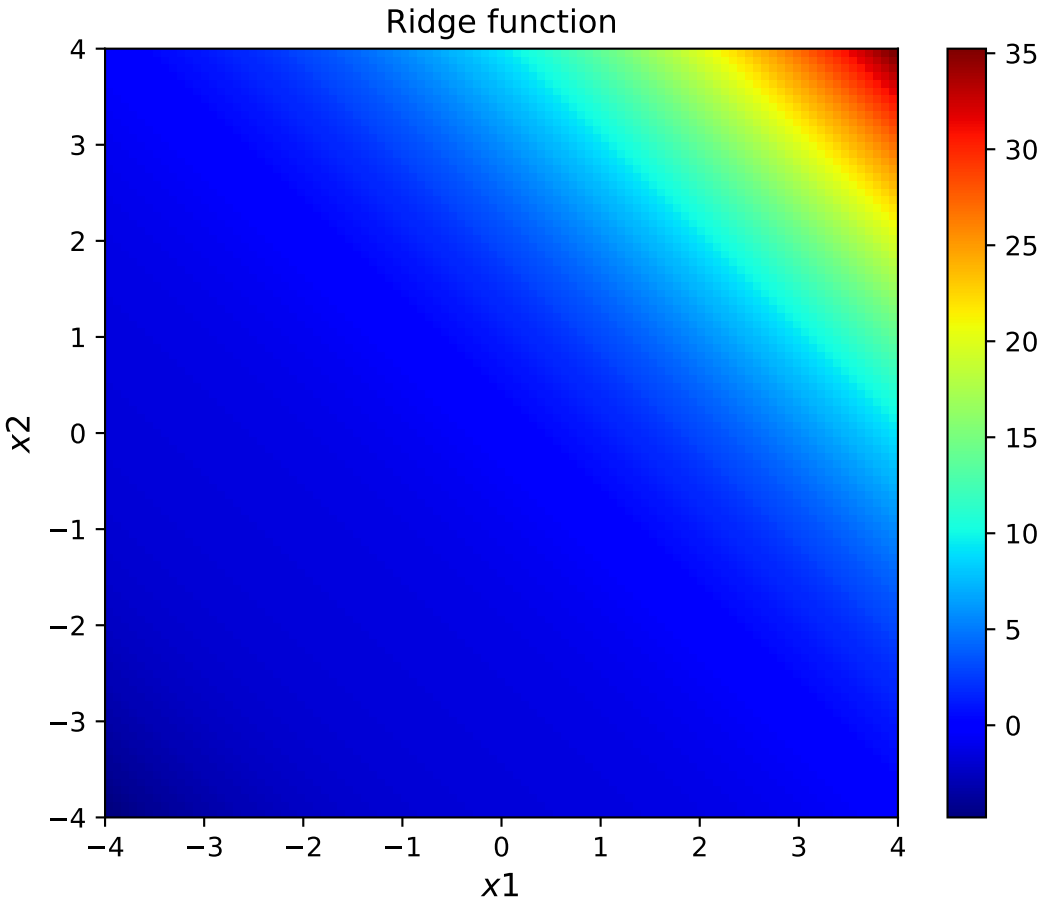
Returns **y** – Output

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.


Ridge function
x2
x1
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4
35
30
25
20
15
10
5
0

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**SphereFun**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

N-dimensional sphere function with zero mean.

$$y = \sum_{i=1}^{N} x_i^2$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – First parameter [-1, 1]
- **p["xi"]** (*float or ndarray of float [n_grid]*) – i-th parameter defined in [-1, 1]
- **p["xN"]** (*float or ndarray of float [n_grid]*) – Nth parameter [-1, 1]

Returns **y** – Output data

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

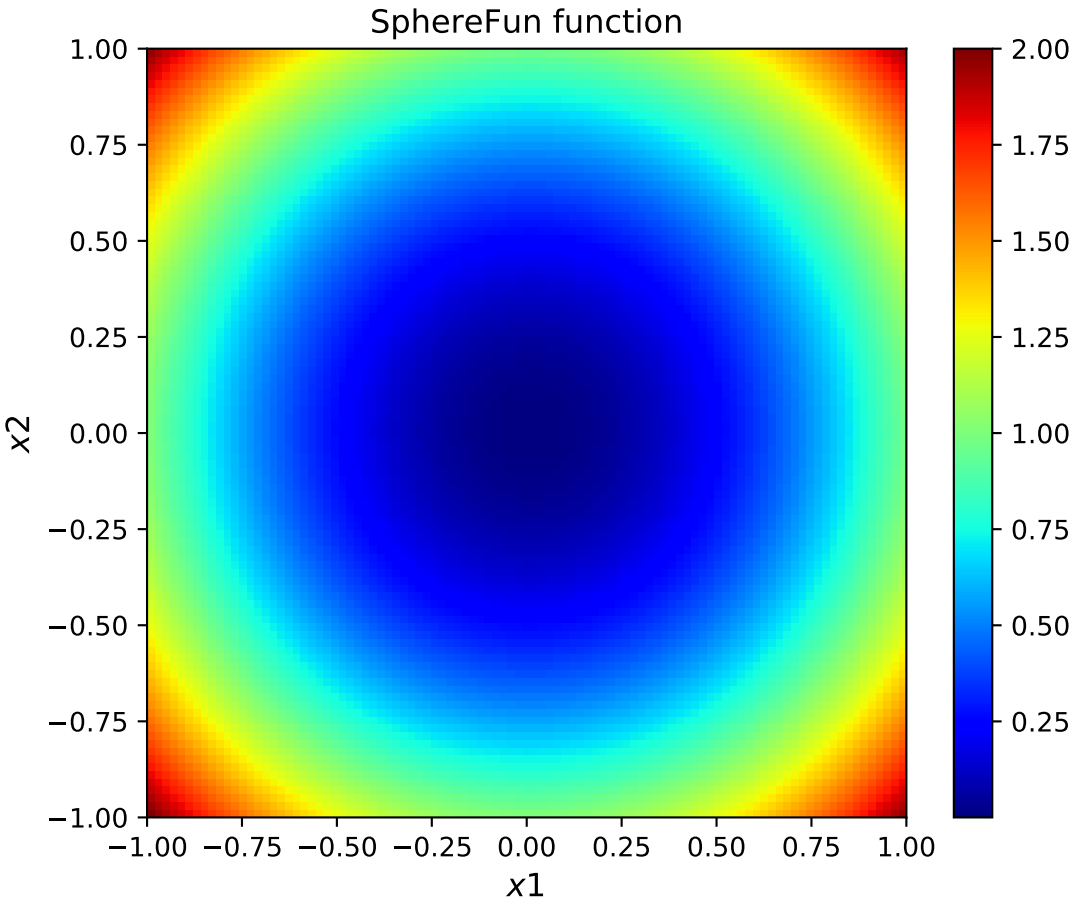
validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**SphereModel**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

Calculates the electric potential in a 3-layered sphere caused by point-like electrodes after Rush and Driscoll (1969) [1].

Parameters

- **p["sigma_1"]** (*float*) – Conductivity of the innermost layer, in (S/m)
- **p["sigma_2"]** (*float*) – Conductivity of the intermediate layer, in (S/m)
- **p["sigma_3"]** (*float*) – Conductivity of the outermost layer, in (S/m)
- **p["radii"]** (*list [3]*) – Radius of each of the 3 layers (innermost to outermost), in (mm)
- **p["anode_pos"]** (*ndarray of float [3 x 1]*) – Position of the anode_pos, in (mm)


SphereFun function
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
x2
−1.00 −0.75 −0.50 −0.25 0.00 0.25 0.50 0.75 1.00
x1
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25

- **p["cathode_pos"]** (*ndarray of float [3 x 1]*) – Position of cathode_pos, in (mm)
- **p["p"]** (*ndarray of float [N x 3]*) – Positions where the potential should be calculated, in (mm)

Returns **potential** – Values of the electric potential, in (V)

Return type ndarray of float [1 x n_out]

Notes

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()

This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**SurfaceCoverageSpecies**(*p*, *context=None*)

Bases: *pygpc.AbstractModel.AbstractModel*

Differential equation describing the time-evolution of the surface coverage rho [0, 1] for a given species [1]. This problem has one or two fixed points according to the value of the recombination rate beta and it exhibits smooth dependence on the other parameters. The statistics of the solution at t=1 are investigated considering uncertainties in the initial coverage rho_0 and in the reaction parameter beta. Additionally uncertainty in the surface absorption rate alpha can be considered to make the problem 3-dimensional. Gamma=0.01 denotes the desorption rate.

$$\frac{d\rho}{dt} = \alpha(1-\rho) - \gamma\rho - \beta(\rho-1)^2\rho$$

Parameters

- **p["rho_0"]** (*ndarray of float [1]*) – Initial value rho(t=0) (uniform distributed [0, 1])
- **p["beta"]** (*ndarray of float [1]*) – Recombination rate (uniform distributed [0, 20])
- **p["alpha"]** (*ndarray of float [1]*) – Surface absorption rate (1 or uniform distributed [0.1, 2])

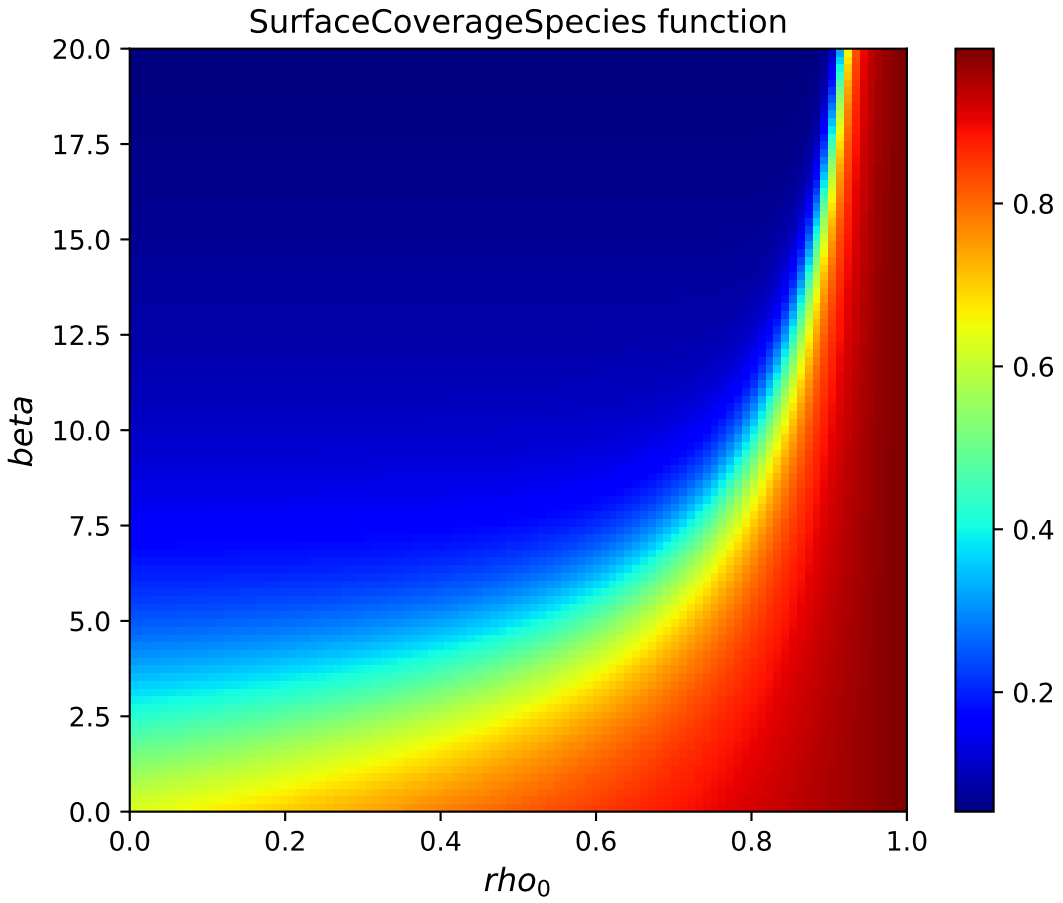
Returns **y** – rho(t->1)

Return type ndarray of float [1 x 1]

Notes

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.


SurfaceCoverageSpecies function
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
beta
0.0
0.2
0.4
0.6
0.8
1.0
rho0
0.8
0.6
0.4
0.2

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**TMSEfieldSphere**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

Calculate the E-field in a sphere caused by external magnetic dipoles after Heller and van Hulsteyn (1992). The results are independent of conductivity.

Parameters

- **p["dipole_pos"]** (*ndarray of float [M x 3]*) – Position of dipoles, must be outside sphere
- **p["dipole_moment"]** (*ndarray of float [m x 3]*) – Moment of dipoles
- **p["didt"]** (*float*) – Variation rate of current in the coil
- **p["positions"]** (*ndarray of float [N x 3]*) – Position where fields should be calculated, must lie inside sphere in (mm)

Returns **E** – E-fields at detector positions

Return type ndarray of float [1 x 3*N]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**Welch1992**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

20-dimensional test function of Welch et al. (1992) [1].

For input variable screening purposes, it can be found that some input variables of this function have a very high effect on the output, compared to other input variables. As Welch et al. (1992) [1] point out, interactions and nonlinear effects make this function challenging.

$$y = \frac{5x_{12}}{1+x_1} + 5(x_4 - x_{20})^2 + x_5 + 40x_{19}^3 + 5x_{19} + 0.05x_2 + 0.08x_3 - 0.03x_6 + 0.03x_7 - 0.09x_9 - 0.01x_{10} - 0.07x_{11} + 0.25x_{13}^2 - 0.04x_{14} + 0.06x_{15} - 0.01x_{17} - 0.03x_{18}$$

Parameters **p["x1...x20"]** (*float*) – Input data, xi ~ U(-0.5, 0.5), for all i = 1,..., 20.

Returns **y** – Output data

Return type ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

class pygpc.testfunctions.testfunctions.**WingWeight**(*p*, *context=None*)
Bases: *pygpc.AbstractModel.AbstractModel*

10-dimensional test function which models a light aircraft wing from Forrester et al. (2008) [1]

$$y = \frac{0.036 x_1^{0.758} x_2^{0.0035} x_3}{\cos(x_4)^2)^{0.6}} x_5^{0.006} x_6^{0.04} \left(\frac{100 x_7}{\cos(x_4)}\right)^{-0.3} (x_8 x_9)^{0.49} + x_1 x_{10}$$

Parameters

- **p["x1"]** (*float or ndarray of float [n_grid]*) – x1(Sw) [150, 200]
- **p["x2"]** (*float or ndarray of float [n_grid]*) – x2(Wfw) [220, 300]
- **p["x3"]** (*float or ndarray of float [n_grid]*) – x3(A) [6, 10]
- **p["x4"]** (*float or ndarray of float [n_grid]*) – x4(Lambda) [-10, 10]
- **p["x5"]** (*float or ndarray of float [n_grid]*) – x5(q) [16, 45]
- **p["x6"]** (*float or ndarray of float [n_grid]*) – x6(lambda) [0.5, 1]
- **p["x7"]** (*float or ndarray of float [n_grid]*) – x7(tc) [0.08, 0.18]
- **p["x8"]** (*float or ndarray of float [n_grid]*) – x8(Nz) [2.5, 6]
- **p["x9"]** (*float or ndarray of float [n_grid]*) – x9(Wdg) [1700, 2500]
- **p["x10"]** (*float or ndarray of float [n_grid]*) – x10(Wp) [0.025, 0.08]

Returns **y** – Output data

Return type float or ndarray of float [n_grid x 1]

Notes

simulate(*process_id=None*)
This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

pygpc.testfunctions.testfunctions.**plot_testfunction**(*testfunction_name*, *parameters*, *constants=None*, *output_idx=0*)

Plot 1D or 2D testfunctions for documentation.

Parameters

- **testfunction_name** (*str*) – Name of testfunction AbstractModel class
- **parameters** (*OrdererdDict*) – Dictionary containing the 1D coordinates as ndarrays, where the testfunction is evaluated (will be tensorized)
- **constants** (*OrderedDict (optional)*) – Dictionary containing the (remaining) parameters treated as constants
- **output_idx** (*int*) – index of output quantity to plot

Returns **<plot>** – Plot showing the QoI of the testfunction in 1D or 2D

Return type matplotlib figure

Module contents

1.2 Submodules

1.3 pygpc.AbstractModel module

class pygpc.AbstractModel.**AbstractModel**(*p*, *context=None*)

Bases: object

Abstract base class for the SimulationWrapper. This base class provides basic functions for serialization/deserialization and printing progress. It cannot be used directly, but a derived class implementing the "simulate" method must be created.

get_seq_number()

increment_ctr()

This functions increments the global counter by 1.

print_progress(*func_time=None*, *read_from_file=False*)

This function prints the progress according to the current context and global_counter.

read_previous_results(*coords*)

This functions reads previous results from the hard disk (if present). When reading from the array containing the results, the current grid-index (i_grid) is considered to maintain the order of the results when the SimulationModels are executed in parallel. If the function evaluated the results in parallel internally, i_grid is a range [i_grid_min, i_grid_max].

Parameters **coords** (*ndarray of float [n_sims x dim]*) – Grid coordinates the simulations are conducted with

Returns

- *None* – if no serialized results could be found or does not fit to grid
- *list* – data at coords

simulate(*process_id=None*)

This abstract method must be implemented by the subclass. It should perform the simulation task depending on the input_values provided to the object on instantiation.

Parameters **process_id** (*int*) – A unique identifier; no two processes of the pool will run concurrently with the same identifier

validate()
This abstract method must be implemented by the subclass. It should perform the validation task depending on the parameters defined in the problem. In cases, the model may not run correctly for some parameter combinations, this function changes the definition of the random parameters and the constants.

write_results(*data_dict*)
This function writes the data to a file on hard disk. When writing the data the current grid-index (i_grid) is considered. The data are written to the row corresponding i_grid in order to maintain the order of the results when the SimulationModels are executed in parallel.

Parameters **data_dict** (*dict of ndarray*) – Dictionary, containing the data to write in an .hdf5 file. The keys are the dataset names.

1.4 pygpc.Algorithm module

class pygpc.Algorithm.**Algorithm**(*problem*, *options*)
Bases: object

Class for GPC algorithms

class pygpc.Algorithm.**RegAdaptive**(*problem*, *options*)
Bases: *pygpc.Algorithm.Algorithm*

Adaptive regression approach based on leave one out cross validation error estimation

run()
Runs adaptive gPC algorithm to solve problem.

Returns

- **gpc** (*GPC object instance*) – GPC object containing all information i.e., Problem, Model, Grid, Basis, RandomParameter instances
- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients
- **res** (*ndarray of float [n_grid x n_out]*) – Simulation results at n_grid points of the n_out output variables

class pygpc.Algorithm.**Static**(*problem*, *options*, *grid*)
Bases: *pygpc.Algorithm.Algorithm*

Static gPC algorithm

run()
Runs static gPC algorithm to solve problem.

Returns

- **gpc** (*GPC object instance*) – GPC object containing all information i.e., Problem, Model, Grid, Basis, RandomParameter instances
- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients
- **res** (*ndarray of float [n_grid x n_out]*) – Simulation results at n_grid points of the n_out output variables

1.5 pygpc.Basis module

class pygpc.Basis.**Basis**

Basis class of gPC

b

Parameter wise basis function objects used in gPC. Multiplying all elements in a row at location xi = (x1, x2, ..., x_dim) yields the global basis function.

Type list of BasisFunction object instances [n_basis x n_dim]

b_gpu

???

Type ???

b_id

Unique IDs of global basis functions

Type list of UUID objects (version 4) [n_basis]

b_norm

Normalization factor of individual basis functions

Type ndarray [n_basis x dim]

b_norm_basis

Normalization factor of global basis functions

Type ndarray [n_basis x 1]

dim

Number of variables

n_basis

Total number of (global) basis function

Type int

extend_basis(*b_added*)

Extend set of basis functions and update gpc matrix (append columns).

Parameters **b_added** (*2D list of BasisFunction instances [n_b_added x dim]*) – Individual BasisFunctions to add

init_b_norm()

Construct array of scaling factors self.b_norm [n_basis x dim] and self.b_norm_basis [n_basis x 1] to normalize basis functions <psi^2> = int(psi^2*p)dx

init_basis_sgpc(*problem*, *order*, *order_max*, *order_max_norm*, *interaction_order*)

Initializes basis functions for standard gPC.

Parameters

- **problem** (*Problem object*) – GPC Problem to analyze
- **order** (*[dim] list of int*) – Maximum individual expansion order Generates individual polynomials also if maximum expansion order in order_max is exceeded
- **order_max** (*int*) – Maximum global expansion order. The maximum expansion order considers the sum of the orders of combined polynomials together with the chosen norm "order_max_norm". Typically this norm is 1 such that the maximum order is the sum of all monomial orders.

- **order_max_norm** (*float*) – Norm for which the maximum global expansion order is defined [0, 1]. Values < 1 decrease the total number of polynomials in the expansion such that interaction terms are penalized more. This truncation scheme is also referred to "hyperbolic polynomial chaos expansion" such that sum(a_i^q)^1/q <= p, where p is order_max and q is order_max_norm (for more details see eq. (27) in [1]).
- **interaction_order** (*int*) – Number of random variables, which can interact with each other All polynomials are ignored, which have an interaction order greater than specified

Notes

Polynomial Index	Dimension 1	Dimension 2	...	Dimension M
Basis 1	[Order D1]	[Order D2]	⋮	[Order M]
Basis 2	[Order D1]	[Order D2]	⋮	[Order M]
⋮	[Order D1]	[Order D2]	⋮	[Order M]
Basis N	[Order D1]	[Order D2]	⋮	[Order M]

Adds Attributes:

b: list of BasisFunction object instances [n_basis x n_dim] Parameter wise basis function objects used in gPC. Multiplying all elements in a row at location xi = (x1, x2, . . . , x_dim) yields the global basis function.

1.6 pygpc.BasisFunction module

class pygpc.BasisFunction.**BasisFunction**(*p*)
Bases: object

Abstract class of basis functions. This base class provides basic properties and methods for the basis functions. It cannot be used directly, but inherits properties and methods to the specific basis function sub classes.

__call__(*x*)
Evaluates basis function for argument x

Parameters **x** (*float or ndarray of float*) – Argument for which the basis function is evaluated

Returns **y** – Function value of basis function at argument x

Return type float or ndarray of float

class pygpc.BasisFunction.**Hermite**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

Hermite basis function used in the orthogonal gPC to model normal distributed random variables.

class pygpc.BasisFunction.**Jacobi**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

Jacobi basis function used in the orthogonal gPC to model beta distributed random variables.

class pygpc.BasisFunction.**Rect**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

Rectangular basis function used in the non-orthogonal gPC.

class pygpc.BasisFunction.**SigmoidDown**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

SigmoidDown (from 0 to 1) basis function used in the non-orthogonal gPC.

class pygpc.BasisFunction.**SigmoidUp**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

SigmoidUp (from 0 to 1) basis function used in the non-orthogonal gPC.

class pygpc.BasisFunction.**StepDown**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

StepDown (from 1 to 0) basis function used in the non-orthogonal gPC.

class pygpc.BasisFunction.**StepUp**(*p*)
Bases: *pygpc.BasisFunction.BasisFunction*

StepUp (from 0 to 1) basis function used in the non-orthogonal gPC.

1.7 pygpc.Computation module

pygpc.Computation.**Computation**(*n_cpu*)
Helper function to initialize the Computation class. n_cpu = 0 : use this if the model is capable of to evaluate several parameterizations in parallel n_cpu = 1 : the model is called in serial for every paramerization. n_cpu > 1 : A multiprocessing.Pool will be opened and n_cpu parameterizations are calculated in parallel

Parameters **n_cpu** (*int*) – Number of CPU cores to use

Returns **obj** – Object instance of Computation class

Return type object instance of Computation class

class pygpc.Computation.**ComputationFuncPar**(*n_cpu*)
Computation sub-class to run the model using a the models internal parallelization

close()
Closes the pool

run(*model*, *problem*, *coords*, *coords_norm=None*, *i_iter=None*, *i_subiter=None*, *fn_results=None*, *print_func_time=False*)
Runs model evaluations for parameter combinations specified in coords array

Parameters

- **model** (*Model object*) – Model object instance of model to investigate (derived from AbstractModel class, implemented by user)
- **problem** (*Problem class instance*) – GPC Problem under investigation, includes the parameters of the model (constant and random)
- **coords** (*ndarray of float [n_sims, n_dim]*) – Set of n_sims parameter combinations to run the model with (only the random parameters!).
- **coords_norm** (*ndarray of float [n_sims, n_dim]*) – Set of n_sims parameter combinations to run the model with (normalized coordinates [-1, 1].
- **i_iter** (*int*) – Index of main-iteration
- **i_subiter** (*int*) – Index of sub-iteration
- **fn_results** (*string, optional, default=None*) – If provided, model evaluations are saved in fn_results.hdf5 file and gpc object in fn_results.pkl file

- **print_func_time** (*bool*) – Print time of single function evaluation

Returns **res** – n_sims simulation results of the n_out output quantities of the model under investigation.

Return type ndarray of float [n_sims x n_out]

class pygpc.Computation.**ComputationPoolMap**(*n_cpu*)

Computation sub-class to run the model using a processing pool for parallelization

close()

Closes the pool

run(*model*, *problem*, *coords*, *coords_norm=None*, *i_iter=None*, *i_subiter=None*, *fn_results=None*, *print_func_time=False*)

Runs model evaluations for parameter combinations specified in coords array

Parameters

- **model** (*Model object*) – Model object instance of model to investigate (derived from AbstractModel class, implemented by user)
- **problem** (*Problem class instance*) – GPC Problem under investigation, includes the parameters of the model (constant and random)
- **coords** (*ndarray of float [n_sims, n_dim]*) – Set of n_sims parameter combinations to run the model with (only the random parameters!).
- **coords_norm** (*ndarray of float [n_sims, n_dim]*) – Set of n_sims parameter combinations to run the model with (normalized coordinates [-1, 1].
- **i_iter** (*int*) – Index of main-iteration
- **i_subiter** (*int*) – Index of sub-iteration
- **fn_results** (*string, optional, default=None*) – If provided, model evaluations are saved in fn_results.hdf5 file and gpc object in fn_results.pkl file
- **print_func_time** (*bool*) – Print time of single function evaluation

Returns **res** – n_sims simulation results of the n_out output quantities of the model under investigation.

Return type ndarray of float [n_sims x n_out]

pygpc.Computation.**compute_cluster**(*algorithms*, *nodes*, *start_scheduler=True*)

Computes Algorithm instances on compute cluster composed of nodes. The first node is also the dispy-scheduler. Afterwards, the dispy-nodes are started on every node. On every node, screen sessions are started with the names "scheduler" and "node", where the scheduler and the nodes are residing, respectively. They can be accessed by "screen -rD scheduler" or "screen -rD node" when connected via ssh to the machines.

Parameters

- **algorithms** (*list of Algorithm instances*) – Algorithm instances initialized with different gPC problems and/or models
- **nodes** (*str or list of str*) – Node names
- **start_scheduler** (*bool*) – Starts a scheduler on the first machine in the nodes list or not. Set this to False if a scheduler is already running somewhere on the cluster.

1.8 pygpc.EGPC module

class pygpc.EGPC.**EGPC**
Bases: *pygpc.GPC.GPC*

get_approximation(*coeffs=None*, *xi=None*, *output_idx=None*)
Calculates the gPC approximation in points with output_idx and normalized parameters xi (interval: [-1, 1]).

pce = EGPC.get_approximation(coeffs=None, xi=None, output_idx=None)

Parameters

- **coeffs** (*[N_coeffs x N_out] np.ndarray, optional, default=None*) – Gpc coefficients
- **xi** (*[1 x dim] np.ndarray, optional, default=None*) – Point in variable space to evaluate local sensitivity in normalized coordinates
- **output_idx** (*[1 x N_out] np.ndarray, optional, default=None*) – Index of output quantities to consider (Default: all outputs).

Returns **pce** – Gpc approximation at normalized coordinates xi.

Return type [N_xi x N_out] np.ndarray

get_global_sens(*coeffs*)
Determine the global derivative based sensitivity coefficients after Xiu (2009) [1].

global_sens = EGPC.get_global_sens(coeffs)

Parameters **coeffs** (*[N_coeffs x N_out] np.ndarray*) – Gpc coefficients

Returns **global_sens** – Global derivative based sensitivity coefficients

Return type [dim x N_out] np.ndarray

Notes

get_local_sens(*coeffs*, *xi*)
Determine the local derivative based sensitivity coefficients in the point of interest xi (normalized coordinates [-1, 1]).

local_sens = EGPC.calc_localsens(coeffs, xi)

Parameters

- **coeffs** (*[N_coeffs x N_out] np.ndarray*) – Gpc coefficients
- **xi** (*[N_coeffs x N_out] np.ndarray*) – Point in variable space to evaluate local sensitivity in (normalized coordinates!)

Returns **local_sens** – Local sensitivity

Return type [dim x N_out] np.ndarray

static get_mean(*coeffs*)
Calculate the expected mean value.

mean = SGPC.get_mean(coeffs)

Parameters **coeffs** (*[N_coeffs x N_out] np.ndarray*) – Gpc coefficients

Returns **mean** – Expected mean value

Return type [1 x N_out] np.ndarray

get_pdf (*coeffs*, *n_samples*, *output_idx=None*)
Determine the estimated pdfs of the output quantities

pdf_x, pdf_y = EGPC.get_pdf(coeffs, N_samples, output_idx=None)

Parameters

- **coeffs** (*[N_coeffs x N_out] np.ndarray*) – Gpc coefficients
- **n_samples** (*int*) – Number of samples used to estimate output pdf
- **output_idx** (*[1 x N_out] np.ndarray, optional, default=None*) – Index of output quantities to consider. If output_idx=None, all output quantities are considered

Returns

- **pdf_x** (*[100 x N_out] np.ndarray*) – x-coordinates of output pdf (output quantity),
- **pdf_y** (*[100 x N_out] np.ndarray*) – y-coordinates of output pdf (probability density of output quantity)

static get_samples (*self*, *coeffs=None*, *n_samples=100*, *output_idx=None*)
Randomly sample the gPC expansion to determine output pdfs in specific points.

xi = EGPC.get_pdf_mc(N_samples, coeffs=None, output_idx=None)

Parameters

- **coeffs** (*[N_coeffs x N_out] np.ndarray, optional, default=None*) – gPC coefficients
- **n_samples** (*int*) – Number of random samples drawn from the respective input pdfs.
- **output_idx** (*[1 x N_out] np.ndarray, optional, default=None*) – Index of output quantities to consider.

Returns

- **xi** (*[N_samples x dim] np.ndarray*) – Generated samples in normalized coordinates.
- **pce** (*[N_samples x N_out] np.ndarray*) – GPC approximation at points xi.

get_sobol_composition (*sobol=None*, *sobol_idx=None*, *sobol_idx_bool=None*)
Determine average ratios of Sobol indices over all output quantities: (i) over all orders and (e.g. 1st: 90%, 2nd: 8%, 3rd: 2%) (ii) for the 1st order indices w.r.t. each random variable. (1st: x1: 50%, x2: 40%)

sobol, sobol_idx, sobol_rel_order_mean, sobol_rel_order_std, sobol_rel_1st_order_mean, sobol_rel_1st_order_std = EGPC.get_sobol_composition(coeffs=None, sobol=None, sobol_idx=None, sobol_idx_bool=None)

Parameters

- **sobol** (*[N_sobol x N_out] np.ndarray*) – Unnormalized sobol_indices
- **sobol_idx** (*list of [N_sobol x dim] np.ndarray*) – Parameter combinations in rows of sobol.
- **sobol_idx_bool** (*list of np.ndarray of bool*) – Boolean mask that determines which multi indices are unique.

Returns

- **sobol_rel_order_mean** (*np.ndarray*) – Average proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,), (over all output quantities)

- **sobol_rel_order_std** (*np.ndarray*) – Standard deviation of the proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,), (over all output quantities)
- **sobol_rel_1st_order_mean** (*np.ndarray*) – Average proportion of the random variables of the 1st order Sobol indices to the total variance, (over all output quantities)
- **sobol_rel_1st_order_std** (*np.ndarray*) – Standard deviation of the proportion of the random variables of the 1st order Sobol indices to the total variance (over all output quantities)

static get_sobol_indices(*self*, *coeffs=None*)

Calculate the available sobol indices.

sobol, sobol_idx = EGPC.get_sobol_indices(coeffs=None)

Parameters **coeffs** (*[N_coeffs x N_out] np.ndarray, optional, default=None*) – Gpc coefficients

Returns

- **sobol** (*[N_sobol x N_out] np.ndarray*) – Unnormalized sobol_indices
- **sobol_idx** (*list of [N_sobol x dim] np.ndarray*) – Parameter combinations in rows of sobol.
- **sobol_idx_bool** (*list of np.ndarray of bool*) – Boolean mask that determines which multi indices are unique.

static get_standard_deviation(*coeffs*)

Calculate the standard deviation.

std = EGPC.get_standard_deviation(coeffs)

Parameters **coeffs** (*np.array of float [N_coeffs x N_out]*) – Gpc coefficients

Returns **std** – Standard deviation

Return type [1 x N_out] np.ndarray

1.9 pygpc.GPC module

class pygpc.GPC.**GPC**(*problem*, *fn_results*)

Bases: object

General gPC base class

problem

GPC Problem under investigation

Type Problem class instance

basis

Basis of the gPC including BasisFunctions

Type Basis class instance

grid

Grid of the derived gPC approximation

Type Grid class instance

gpc_matrix

generalized polynomial chaos matrix

Type [N_samples x N_poly] np.ndarray

gpc_matrix_inv
pseudo inverse of the generalized polynomial chaos matrix

Type [N_poly x N_samples] np.ndarray

nan_elm
Indices of NaN elements of model output

Type ndarray of int

gpc_matrix_coords_id
UUID4() IDs of grid points the gPC matrix derived with

Type list of UUID4()

gpc_matrix_b_id
UUID4() IDs of basis functions the gPC matrix derived with

Type list of UUID4()

solver
Default solver to determine the gPC coefficients (can be chosen during GPC.solve) - 'Moore-Penrose' ... Pseudoinverse of gPC matrix (SGPC.Reg, EGPC) - 'OMP' ... Orthogonal Matching Pursuit, sparse recovery approach (SGPC.Reg, EGPC) - 'NumInt' ... Numerical integration, spectral projection (SGPC.Quad)

Type str

gpu
Flag to execute the calculation on the gpu

Type bool

verbose
boolean value to determine if to print out the progress into the standard output

Type bool

fn_results
If provided, model evaluations are saved in fn_results.hdf5 file and gpc object in fn_results.pkl file

Type string, optional, default=None

n_cpu
Number of threads to use for parallel evaluation of the model function.

Type int, optional, default=1

calc_gpc_matrix(*b*, *x*, *verbose=False*)
Construct the gPC matrix.

gpc_matrix = calc_gpc_matrix(b, x)

Parameters

- **b** (*list of BasisFunction object instances [n_basis x n_dim]*) – Parameter wise basis function objects used in gPC (Basis.b) Multiplying all elements in a row at location xi = (x1, x2, ..., x_dim) yields the global basis function.
- **x** (*ndarray of float [n_x x n_dim]*) – Coordinates of x = (x1, x2, ..., x_dim) where the rows of the gPC matrix are evaluated (normalized [-1, 1])
- **verbose** (*bool*) – boolean value to determine if to print out the progress into the standard output

Returns **gpc_matrix** – GPC matrix where the columns correspond to the basis functions and the rows the to the sample coordinates

Return type ndarray of float [n_x x n_basis]

get_approximation(*coeffs*, *x*, *output_idx=None*)

Calculates the gPC approximation in points with output_idx and normalized parameters xi (interval: [-1, 1]).

pce = GPC.get_approximation(coeffs, x, output_idx=None)

Parameters

- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients for each output variable
- **x** (*ndarray of float [n_x x n_dim]*) – Coordinates of x = (x1, x2, . . . , x_dim) where the rows of the gPC matrix are evaluated (normalized [-1, 1])
- **output_idx** (*ndarray of int, optional, default=None [n_out]*) – Index of output quantities to consider (Default: all).

Returns **pce** – GPC approximation at normalized coordinates x.

Return type ndarray of float [n_x x n_out]

get_pdf(*coeffs*, *n_samples*, *output_idx=None*)

Determine the estimated pdfs of the output quantities

pdf_x, pdf_y = SGPC.get_pdf(coeffs, n_samples, output_idx=None)

Parameters

- **coeffs** (*ndarray of float [n_coeffs x n_out]*) – GPC coefficients
- **n_samples** (*int*) – Number of samples used to estimate output pdfs
- **output_idx** (*ndarray, optional, default=None [1 x n_out]*) – Index of output quantities to consider (if output_idx=None, all output quantities are considered)

Returns

- **pdf_x** (*ndarray of float [100 x n_out]*) – x-coordinates of output pdfs of output quantities
- **pdf_y** (*ndarray of float [100 x n_out]*) – y-coordinates of output pdfs (probability density of output quantity)

get_samples(*coeffs*, *n_samples*, *output_idx=None*)

Randomly sample gPC expansion.

x, pce = SGPC.get_pdf_mc(n_samples, coeffs, output_idx=None)

Parameters

- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients
- **n_samples** (*int*) – Number of random samples drawn from the respective input pdfs.
- **output_idx** (*ndarray of int [1 x n_out] optional, default=None*) – Index of output quantities to consider.

Returns

- **x** (*ndarray of float [n_samples x dim]*) – Generated samples in normalized coordinates [-1, 1].
- **pce** (*ndarray of float [n_samples x n_out]*) – GPC approximation at points x.

init_gpc_matrix()
Sets self.gpc_matrix with given self.basis and self.grid

replace_gpc_matrix_samples(*idx*, *seed=None*)
Replace distinct sample points from the gPC matrix with new ones.

GPC.replace_gpc_matrix_samples(idx, seed=None)

Parameters

- **idx** (*ndarray of int [n_samples]*) – Array of grid indices of grid.coords[idx, :] which are going to be replaced (rows of gPC matrix will be replaced by new ones)
- **seed** (*float, optional, default=None*) – Random seeding point

save_gpc_matrix_hdf5()
Save gPC matrix in .hdf5 file <"fn_results" + ".hdf5"> under the key "gpc_matrix". If a gpc matrix is already present, check for equality and save only appended rows and columns

solve(*sim_results*, *solver=None*, *settings=None*, *gpc_matrix=None*, *verbose=False*)
Determines gPC coefficients

Parameters

- **sim_results** (*[N_grid x N_out] np.ndarray of float*) – results from simulations with N_out output quantities
- **solver** (*str*) – Solver to determine the gPC coefficients - 'Moore-Penrose' ... Pseudoinverse of gPC matrix (SGPC.Reg, EGPC) - 'OMP' ... Orthogonal Matching Pursuit, sparse recovery approach (SGPC.Reg, EGPC) - 'NumInt' ... Numerical integration, spectral projection (SGPC.Quad)
- **settings** (*dict*) – Solver settings - 'Moore-Penrose' ... None - 'OMP' ... {"n_coeffs_sparse": int} Number of gPC coefficients != 0 or "sparsity": float 0...1 - 'NumInt' ... None
- **gpc_matrix** (*ndarray of float [n_grid x n_basis], optional, default: self.gpc_matrix*) – GPC matrix to invert
- **verbose** (*bool*) – boolean value to determine if to print out the progress into the standard output

Returns **coeffs** – gPC coefficients

Return type ndarray of float [n_coeffs x n_out]

update_gpc_matrix()
Update gPC matrix according to existing self.grid and self.basis.

Call this method when self.gpc_matrix does not fit to self.grid and self.basis objects anymore The old gPC matrix with their self.gpc_matrix_b_id and self.gpc_matrix_coords_id is compared to self.basis.b_id and self.grid.coords_id. New rows and columns are computed when differences are found.

1.10 pygpc.Grid module

Functions and classes that provide data and methods for the generation and processing of numerical grids

class pygpc.Grid.**Grid**(*parameters_random*)
Bases: object

Grid class

parameters_random
OrderedDict containing the RandomParameter instances the grids are generated for

Type OrderedDict of RandomParameter instances

_weights
Weights of the grid (all)

Type ndarray of float [n_grid x dim]

_coords
Denormalized coordinates xi

Type ndarray of float [n_grid x dim]

_coords_norm
Normalized [-1, 1] coordinates xi

Type nd array of float [n_grid x dim]

coords_id
Unique IDs of grid points

Type list of UUID objects (version 4) [n_grid]

n_grid
Total number of nodes in grid.

Type int

coords

coords_norm

get_denormalized_coordinates(*coords_norm*)
Denormalize grid from standardized ([-1, 1] except hermite) to original parameter space for simulations.

coords = Grid.get_denormalized_coordinates(coords_norm)

Parameters **coords_norm** (*[N_samples x dim] np.ndarray*) – normalized [-1, 1] coordinates xi

Returns **coords** – Denormalized coordinates xi

Return type [N_samples x dim] np.ndarray

get_normalized_coordinates(*coords*)
Normalize grid from original parameter (except hermite) to standardized ([-1, 1] space for simulations.

coords_norm = Grid.get_normalized_coordinates(coords)

Parameters **coords** (*[N_samples x dim] np.ndarray*) – Denormalized coordinates xi in original parameter space

Returns **coords_norm** – Normalized [-1, 1] coordinates xi

Return type [N_samples x dim] np.ndarray

static get_quadrature_clenshaw_curtis_1d(*n*)
Get the Clenshaw Curtis nodes and weights.

knots, weights = Grid.get_quadrature_clenshaw_curtis_1d(n)

Parameters **n** (*int*) – Number of knots

Returns

- **knots** (*np.ndarray*) – Knots of the grid

- **weights** (*np.ndarray*) – Weights of the grid

static get_quadrature_fejer1_1d(*n*)
Computes the Fejer type 1 nodes and weights.

This method uses a direct approach after Davis and Rabinowitz (2007) [1] and Gautschi (1967) [2]. The paper by Waldvogel (2006) [3] exhibits a more efficient approach using Fourier transforms.

knots, weights = Grid.get_quadrature_fejer1_1d(n)

Parameters **n** (*int*) – Number of knots

Returns

- **knots** (*ndarray*) – Knots of the grid
- **weights** (*ndarray*) – Weights of the grid

Notes

static get_quadrature_fejer2_1d(*n*)
Computes the Fejer type 2 nodes and weights (Clenshaw Curtis without boundary nodes).

This method uses a direct approach after Davis and Rabinowitz (2007) [1] and Gautschi (1967) [2]. The paper by Waldvogel (2006) [3] exhibits a more efficient approach using Fourier transforms.

knots, weights = Grid.get_quadrature_fejer2_1d(n)

Parameters **n** (*int*) – Number of knots

Returns

- **knots** (*np.ndarray*) – Knots of the grid
- **weights** (*np.ndarray*) – Weights of the grid

Notes

static get_quadrature_hermite_1d(*n*)
Get knots and weights of Hermite polynomials (normal distribution).

knots, weights = Grid.get_quadrature_hermite_1d(n)

Parameters **n** (*int*) – number of knots

Returns

- **knots** (*np.ndarray*) – knots of the grid
- **weights** (*np.ndarray*) – weights of the grid

static get_quadrature_jacobi_1d(*n*, *p*, *q*)
Get knots and weights of Jacobi polynomials.

knots, weights = Grid.get_quadrature_jacobi_1d(n, p, q)

Parameters

- **n** (*int*) – Number of knots
- **p** (*float*) – First shape parameter
- **q** (*float*) – Second shape parameter

Returns

- **knots** (*np.ndarray*) – Knots of the grid
- **weights** (*np.ndarray*) – Weights of the grid

static get_quadrature_patterson_1d(*n*)
Computes the nested Gauss-Patterson nodes and weights for n = 1,3,7,15,31 nodes.

knots, weights = Grid.get_quadrature_patterson_1d(n)

Parameters **n** (*int*) – Number of knots (possible values: 1, 3, 7, 15, 31)

Returns

- **knots** (*np.ndarray*) – Knots of the grid
- **weights** (*np.ndarray*) – Weights of the grid

weights

class pygpc.Grid.**RandomGrid**(*parameters_random*, *options*)
Bases: *pygpc.Grid.Grid*

RandomGrid object

RandomGrid(parameters_random, options)

n_grid
Number of random samples to generate

Type int

seed
Seeding point to replicate random grids

Type float

extend_random_grid(*n_grid_new*, *seed=None*)
Add sample points according to input pdfs to grid (old points are kept).

extend_random_grid(n_grid_new, seed=None):

Parameters

- **n_grid_new** (*float*) – Total number of grid points in extended random grid (old points are kept) (n_grid_add = n_grid_new - n_grid_old)
- **seed** (*float, optional, default=None*) – Random seeding point

class pygpc.Grid.**SparseGrid**(*parameters_random*, *options*)
Bases: *pygpc.Grid.Grid*

SparseGrid object instance.

Grid.SparseGrid(parameters_random, options)

grid_type
specify type of quadrature used to construct sparse grid ('jacobi', 'hermite', 'cc', 'fejer2')

Type [N_vars] list of str

level
number of levels in each dimension

Type [N_vars] list of int

level_max
global combined level maximum

Type int

level_sequence
list containing the levels

Type list of int

interaction_order
interaction order of parameters and grid, i.e. the grid points are lying between this number of dimensions

Type int

order_sequence_type
type of order sequence ('lin', 'exp') common: 'exp'

Type str

order_sequence
list containing the polynomial order of the levels

Type list of int

make_grid
boolean value to determine if to generate grid during initialization

Type boolean

verbose
boolean value to determine if to print out the progress into the standard output

Type bool

calc_coords_weights()
Determine coords and weights of sparse grid by generating, merging and subtracting sub-grids.

calc_grid()
Calculate a cubature lookup table for knots and weights.

dl_k, dl_w = calc_grid()

Returns

- **dl_k** (*list of list of float*) – Cubature lookup table for knots
- **dl_w** (*list of list of float*) – Cubature lookup table for weights

calc_l_level()
Calculate the l-level needed for the Fejer grid type 2.

l_level = calc_l_level()

Returns **l_level** – Multi indices filtered by level capacity and interaction order

Return type np.ndarray

calc_multi_indices()
Calculate the multi index list needed for the calculation of the SparseGrid.

calc_tensor_products()
Calculate the tensor products of the knots and the weights.

dll_k, dll_w = calc_tensor_products()

Returns

- **dll_k** (*np.ndarray*) – Tensor product of knots
- **dll_w** (*np.ndarray*) – Tensor product of weights

class pygpc.Grid.**TensorGrid**(*parameters_random*, *options*)

Bases: *pygpc.Grid.Grid*

Generate TensorGrid object instance.

TensorGrid(random_parameters, parameters):

grid_type
Type of quadrature used to construct tensor grid ('jacobi', 'hermite', 'clenshaw_curtis', 'fejer2')

Type [N_vars] list of str

knots_dim_list
Knots of grid in each dimension

Type [dim] list of np.ndarray

weights_dim_list
Weights of grid in each dimension

Type [dim] list of np.ndarray

1.11 pygpc.Problem module

class pygpc.Problem.**Problem**(*model*, *parameters*)

Data wrapper for the gpc problem containing the model to investigate and the associated parameters.

Notes

Add Attributes:

random_vars: [dim] list of str String labels of the random variables

N_out: int Number of output coefficients

dim: int Number of uncertain parameters to process

pdf_type: [dim] list of str Type of pdf 'beta' or 'norm'

pdf_shape: list of list of float Shape parameters of pdfs beta-dist: [[], ... [alpha, beta], ..., []] normal-dist: [[], ... [mean, std], ..., []]

pdf_limits: list of list of float upper and lower bounds of random variables beta-dist: [[], ... [min, max], ..., []] normal-dist: [[], ... [0, 0], ..., []] (not used)

Examples

Setup model and specify parameters of gPC problem

```
>>> import pygpc
>>> from collections import OrderedDict
>>>
>>> # Define model
>>> model = pygpc.testfunctions.SphereModel
>>>
>>> # Define Problem
>>> parameters = OrderedDict()  # we must use an ordered dict form the start,␣
↪otherwise the order will be mixed
```

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```
>>> parameters["R"] = [80, 90, 100]
↪  # constant parameter
>>> parameters["phi_electrode"] = 15
↪  #       "
>>> parameters["N_points"] = 201
↪  #       "
>>> parameters["sigma_1"] = pygpc.RandomParameter.Beta(pdf_shape=[5, 5], pdf_
↪limits=[0.15, 0.45])  # random variable
>>> parameters["sigma_2"] = pygpc.RandomParameter.Beta(pdf_shape=[1, 3], pdf_
↪limits=[0.01, 0.02])  #       "
>>> parameters["sigma_3"] = pygpc.RandomParameter.Norm(pdf_shape=[2, 2])
↪                  #       "
>>> problem = pygpc.Problem(model, parameters)
```

validate()

Verifies the problem, by testing if the parameters including the random variables are defined appropriate. In cases, the model may not run correctly for some parameter combinations, the user may change the definition of the random parameters or the constants in model.validate.

calls model.validate

overwrites parameters

1.12 pygpc.RandomParameter module

class pygpc.RandomParameter.**Beta**(*pdf_shape*, *pdf_limits*)

Bases: *pygpc.RandomParameter.RandomParameter*

Beta distributed random variable sub-class

Probability density function:

init_basis_function(*order*)

Initializes Jacobi BasisFunction of Beta RandomParameter

Parameters **order** (*int*) – Order of basis function

pdf(*x*)

Calculate the probability density function of the beta distributed random variable.

pdf = Beta.pdf(x)

Parameters **x** (*ndarray of float [n_x]*) – Values of random variable

Returns **pdf** – Probability density at values x

Return type ndarray of float [n_x]

pdf_norm(*x*)

Calculate the probability density function of the normalized beta distributed random variable in interval [-1, 1].

pdf = Beta.pdf_norm(x)

Parameters **x** (*ndarray of float [n_x]*) – Values of random variable

Returns **pdf** – Probability density at values x

Return type ndarray of float [n_x]

class pygpc.RandomParameter.**Norm**(*pdf_shape*)

Bases: *pygpc.RandomParameter.RandomParameter*

Normal distributed random variable sub-class

Probability density function

$$pdf = \frac{1}{\sqrt{2\pi\sigma^2}} \exp - \frac{(x-\mu)^2}{2\sigma^2}$$

static init_basis_function(*order*)

Initializes Hermite BasisFunction of Norm RandomParameter

Parameters **order** (*int*) – Order of basis function

pdf(*x*)

Calculate the probability density function of the normal distributed random variable.

pdf = Norm.pdf(x)

Parameters **x** (*ndarray of float [n_x]*) – Values of random variable

Returns **pdf** – Probability density

Return type ndarray of float [n_x]

static pdf_norm(*x*)

Calculate the probability density function of the normalized normal distributed random variable (zero mean, std 1).

pdf = Norm.pdf_norm(x)

Parameters **x** (*ndarray of float [n_x]*) – Values of random variable

Returns **pdf** – Probability density

Return type ndarray of float [n_x]

class pygpc.RandomParameter.**RandomParameter**(*pdf_type=None*, *pdf_shape=None*, *pdf_limits=None*)

Bases: object

RandomParameter class

pdf_type

Distribution type of random variable ('beta', 'norm')

Type str

pdf_shape

Shape parameters of beta distributed random variable [p, q]

Type list of float [2]

pdf_limits

Lower and upper bounds of random variable [min, max]

Type list of float [2]

mean

Mean value

Type float

std

Standard deviation

Type float

var
Variance

Type float

1.13 pygpc.SGPC module

class pygpc.SGPC.**Quad**(*problem*, *order*, *order_max*, *order_max_norm*, *interaction_order*, *fn_results=None*)
Bases: *pygpc.SGPC.SGPC*

Quadrature SGPC sub-class

class pygpc.SGPC.**Reg**(*problem*, *order*, *order_max*, *order_max_norm*, *interaction_order*, *fn_results=None*)
Bases: *pygpc.SGPC.SGPC*

Regression gPC subclass

Reg(problem, order, order_max, interaction_order, fn_results=None)

relative_error_loocv
relative error of the leave-one-out-cross-validation

Type list of float

solver
Solver to determine the gPC coefficients - 'Moore-Penrose' ... Pseudoinverse of gPC matrix (SGPC.Reg, EGPC) - 'OMP' ... Orthogonal Matching Pursuit, sparse recovery approach (SGPC.Reg, EGPC) - 'NumInt' ... Numerical integration, spectral projection (SGPC.Quad)

Type str

settings
Solver settings - 'Moore-Penrose' ... None - 'OMP' ... {"n_coeffs_sparse": int} Number of gPC coefficients != 0 - 'NumInt' ... None

Type dict

loocv(*sim_results*, *coeffs*)
Perform leave-one-out cross validation of gPC approximation and add error value to self.relative_error_loocv. The loocv error is calculated analytically after eq. (35) in [1] but omitting the "1 - " term, i.e. it corresponds to 1 - Q^2.

relative_error_loocv = SGPC.loocv(sim_results, coeffs)

$$\epsilon_{LOOCV} = \frac{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{y(\xi_i)-\hat{y}(\xi_i)}{1-h_i}\right)^2}{\frac{1}{N-1}\sum_{i=1}^{N}\left(y(\xi_i)-\bar{y}\right)^2}$$

with

$$\mathbf{h} = \mathrm{diag}(\mathbf{\Psi}(\mathbf{\Psi}^T\mathbf{\Psi})^{-1}\mathbf{\Psi}^T)$$

Parameters

- **sim_results** (*ndarray of float [n_grid x n_out]*) – Results from n_grid simulations with n_out output quantities
- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients

Returns **relative_error_loocv** – Relative mean error of leave one out cross validation

Return type float

Notes

class pygpc.SGPC.**SGPC**(*problem*, *order*, *order_max*, *order_max_norm*, *interaction_order*, *fn_results=None*)

Bases: *pygpc.GPC.GPC*

Sub-class for standard gPC (SGPC)

order
Maximum individual expansion order [order_1, order_2, . . . , order_dim]. Generates individual polynomials also if maximum expansion order in order_max is exceeded

Type list of int [dim]

order_max
Maximum global expansion order. The maximum expansion order considers the sum of the orders of combined polynomials together with the chosen norm "order_max_norm". Typically this norm is 1 such that the maximum order is the sum of all monomial orders.

Type int

order_max_norm
Norm for which the maximum global expansion order is defined [0, 1]. Values < 1 decrease the total number of polynomials in the expansion such that interaction terms are penalized more. This truncation scheme is also referred to "hyperbolic polynomial chaos expansion" such that sum(a_i^q)^1/q <= p, where p is order_max and q is order_max_norm (for more details see eq. (27) in [1]).

Type float

interaction_order
Number of random variables, which can interact with each other. All polynomials are ignored, which have an interaction order greater than the specified

Type int

interaction_order_current
Number of random variables, which can interact with each other. All polynomials are ignored, which have an interaction order greater than the specified Current interaction order counter (only used in case of adaptive algorithms)

Type int

fn_results
If provided, model evaluations are saved in fn_results.hdf5 file and gpc object in fn_results.pkl file

Type string, optional, default=None

static get_extracted_sobol_order(*sobol*, *sobol_idx_bool*, *order=1*)
Extract Sobol indices with specified order from Sobol data.

sobol_1st, sobol_idx_1st = SGPC.get_extracted_sobol_order(sobol, sobol_idx, order=1)

Parameters

- **sobol** (*ndarray of float [n_sobol x n_out]*) – Sobol indices of n_out output quantities
- **sobol_idx_bool** (*list of ndarray of bool*) – Boolean mask which contains unique multi indices.

- **order** (*int, optional, default=1*) – Sobol index order to extract

Returns

- **sobol_n_order** (*ndarray of float [n_out]*) – n-th order Sobol indices of n_out output quantities
- **sobol_idx_n_order** (*ndarray of int*) – Parameter label indices belonging to n-th order Sobol indices

get_global_sens (*coeffs*)

Determine the global derivative based sensitivity coefficients after Xiu (2009) [1].

global_sens = SGPC.get_global_sens(coeffs)

Parameters **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients

Returns **global_sens** – Global derivative based sensitivity coefficients

Return type ndarray [dim x n_out]

Notes

get_local_sens (*coeffs*, *x*)

Determine the local derivative based sensitivity coefficients in the point of interest x (normalized coordinates [-1, 1]).

local_sens = SGPC.calc_localsens(coeffs, x)

Parameters

- **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients
- **x** (*ndarray of float [n_basis x n_out]*) – Point in variable space to evaluate local sensitivity in (normalized coordinates [-1, 1])

Returns **local_sens** – Local sensitivity of output quantities in point x

Return type ndarray [dim x n_out]

static get_mean (*coeffs*)

Calculate the expected mean value.

mean = SGPC.get_mean(coeffs)

Parameters **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients

Returns **mean** – Expected value of output quantities

Return type ndarray of float [1 x n_out]

get_sobol_composition (*sobol*, *sobol_idx_bool*)

Determine average ratios of Sobol indices over all output quantities: (i) over all orders and (e.g. 1st: 90%, 2nd: 8%, 3rd: 2%) (ii) for the 1st order indices w.r.t. each random variable. (1st: x1: 50%, x2: 40%)

sobol, sobol_idx, sobol_rel_order_mean, sobol_rel_order_std, sobol_rel_1st_order_mean, sobol_rel_1st_order_std = SGPC.get_sobol_composition(coeffs, sobol, sobol_idx, sobol_idx_bool)

Parameters

- **sobol** (*ndarray of float [n_sobol x n_out]*) – Unnormalized sobol_indices
- **sobol_idx_bool** (*list of ndarray of bool*) – Boolean mask which contains unique multi indices.

Returns

- **sobol_rel_order_mean** (*ndarray of float [n_out]*) – Average proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,), (over all output quantities)
- **sobol_rel_order_std** (*ndarray of float [n_out]*) – Standard deviation of the proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,), (over all output quantities)
- **sobol_rel_1st_order_mean** (*ndarray of float [n_out]*) – Average proportion of the random variables of the 1st order Sobol indices to the total variance, (over all output quantities)
- **sobol_rel_1st_order_std** (*ndarray of float [n_out]*) – Standard deviation of the proportion of the random variables of the 1st order Sobol indices to the total variance (over all output quantities)
- **sobol_rel_2nd_order_mean** (*ndarray of float [n_out]*) – Average proportion of the random variables of the 2nd order Sobol indices to the total variance, (over all output quantities)
- **sobol_rel_2nd_order_std** (*ndarray of float [n_out]*) – Standard deviation of the proportion of the random variables of the 2nd order Sobol indices to the total variance (over all output quantities)

get_sobol_indices(*coeffs*)

Calculate the available sobol indices.

sobol, sobol_idx = SGPC.get_sobol_indices(coeffs)

Parameters **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients

Returns

- **sobol** (*ndarray of float [n_sobol x n_out]*) – Unnormalized Sobol indices
- **sobol_idx** (*list of ndarray of int [n_sobol x (n_sobol_included)]*) – Parameter combinations in rows of sobol.
- **sobol_idx_bool** (*ndarray of bool [n_sobol x dim]*) – Boolean mask which contains unique multi indices.

static get_standard_deviation(*coeffs*)

Calculate the standard deviation.

std = SGPC.get_standard_deviation(coeffs)

Parameters **coeffs** (*ndarray of float [n_basis x n_out]*) – GPC coefficients

Returns **std** – Standard deviation of output quantities

Return type ndarray of float [1 x n_out]

1.14 pygpc.Test module

class pygpc.Test.**Franke**

Bases: *pygpc.Test.Test*

Franke test function

class pygpc.Test.**GFunction**(*dim=2*)

Bases: *pygpc.Test.Test*

GFunction test function

class pygpc.Test.**GenzContinuous**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzContinuous test function

class pygpc.Test.**GenzCornerPeak**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzCornerPeak test function

class pygpc.Test.**GenzDiscontinuous**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzDiscontinuous test function

class pygpc.Test.**GenzGaussianPeak**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzGaussianPeak test function

class pygpc.Test.**GenzOscillatory**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzOscillatory test function

class pygpc.Test.**GenzProductPeak**(*dim=2*)
Bases: *pygpc.Test.Test*

GenzProductPeak test function

class pygpc.Test.**HyperbolicTangent**
Bases: *pygpc.Test.Test*

HyperbolicTangent test function

class pygpc.Test.**Ishigami**(*dim=2*)
Bases: *pygpc.Test.Test*

Ishigami test function

class pygpc.Test.**Lim2002**
Bases: *pygpc.Test.Test*

Lim2002 test function

class pygpc.Test.**ManufactureDecay**(*dim=2*)
Bases: *pygpc.Test.Test*

ManufactureDecay test function

class pygpc.Test.**MovingParticleFrictionForce**
Bases: *pygpc.Test.Test*

MovingParticleFrictionForce test function

class pygpc.Test.**OakleyOhagan2004**
Bases: *pygpc.Test.Test*

OakleyOhagan2004 test function

class pygpc.Test.**Peaks**
Bases: *pygpc.Test.Test*

Peaks test function

class pygpc.Test.**Ridge**(*dim=2*)
Bases: *pygpc.Test.Test*

Ridge test function

class pygpc.Test.**SphereFun**(*dim=2*)
Bases: *pygpc.Test.Test*

SphereFun test function

class pygpc.Test.**SurfaceCoverageSpecies**(*dim*)
Bases: *pygpc.Test.Test*

SurfaceCoverageSpecies test function

class pygpc.Test.**Test**(*dim*)
Bases: object

Test function objects

class pygpc.Test.**Welch1992**
Bases: *pygpc.Test.Test*

Welch1992 test function

class pygpc.Test.**WingWeight**
Bases: *pygpc.Test.Test*

WingWeight test function

1.15 pygpc.TestBench module

class pygpc.TestBench.**TestBench**(*algorithm*, *problem*, *options*, *n_cpu*)
Bases: object

TestBench for gPC algorithms

run()
Run algorithms with test problems and save results

class pygpc.TestBench.**TestBenchContinuous**(*algorithm*, *options*, *n_cpu=1*)
Bases: *pygpc.TestBench.TestBench*

class pygpc.TestBench.**TestBenchContinuousND**(*algorithm*, *options*, *dims*, *n_cpu=1*)
Bases: *pygpc.TestBench.TestBench*

class pygpc.TestBench.**TestBenchDiscontinuous**(*algorithm*, *options*, *n_cpu=1*)
Bases: *pygpc.TestBench.TestBench*

class pygpc.TestBench.**TestBenchDiscontinuousND**(*algorithm*, *options*, *dims*, *n_cpu=1*)
Bases: *pygpc.TestBench.TestBench*

pygpc.TestBench.**run_test**(*algorithm*)

1.16 pygpc.Visualization module

Functions and classes that provide visualisation functionalities

class pygpc.Visualization.**Visualization**(*dims=(10, 10)*)

Creates a new visualization in a new window. Any added sub-charts will be added to this window.

Visualisation(dims=(10, 10))

Visualisation.**figure_number**

Number of figures that have been created

Type int, begin=0

Visualisation.**horizontal_padding**

Horizontal padding of plot

Type float, default=0.4

Visualisation.**font_size_label**

Font size of title

Type int, default=12

Visualisation.**font_size_label**

Font size of label

Type int, default=12

Visualisation.**graph_lind_width**

Line width of graph

Type int, default 2

fig

Handle of figure created by matplotlib.pyplot

Type mpl.figure

Parameters **dims** (*list of int, optional, default=(10,10)*) – Size of the newly created window

add_heat_map(*title*, *labels*, *grid_points*, *data_points*, *v_lim=(None*, *None)*, *x_lim=None*, *y_lim=None*, *colormap=None*)

Draw a 2D heatmap into the current figure.

add_heat_map(title, labels, grid_points, data_points, v_lim=(None, None), x_lim=None, y_lim=None, colormap=None)

Parameters

- **title** (*str*) – Title of the graph
- **labels** (*{str:str} dict*) – {'x': name of x-axis, 'y': name of y-axis}
- **grid_points** (*list of ndarray of float [2]*) – Arrays of the x and y positions of the grid points e.g.: [np.array(x_points), np.array(y_points)]
- **data_points** (*np.ndarray of the data points that are placed into the grid*) –
- **x_lim** (*list of float [2], optional, default=None*) – x-limits for the function argument or value
- **y_lim** (*list of float [2], optional, default=None*) – y-limits for the function argument or value
- **v_lim** (*list of float [2], optional, default=(None,None)*) – Limits of the color scale

- **colormap** (*str, optional, default=None*) – The colormap to use

add_line_plot(*title*, *labels*, *data*, *x_lim=None*, *y_lim=None*)

Draw a 1D line graph into the current figure.

add_line_plot(title, labels, data, x_lim=None, y_lim=None)

Parameters

- **title** (*str*) – Title of the graph
- **labels** (*{str:str} dict*) – {'x': name of x-axis, 'y': name of y-axis}
- **x_lim** (*list of float [2], optional, default=None*) – x-limits for the function argument or value
- **y_lim** (*list of float [2], optional, default=None*) – y-limits for the function argument or value
- **data** (*ndarray of float*) – Data that should be plotted

static add_scatter_plot(*shape*, *plot_size*, *color_sequence*, *colormap=None*, *v_lim=(None*, *None)*)

Draw a scatter plot onto the current chart.

add_scatter_plot(shape, plot_size, color_sequence, colormap=None, v_lim=(None, None))

Parameters

- **shape** (*{str: np.ndarray} dict*) – {'x': positions on x-axis, 'y': positions on y-axis}
- **plot_size** (*ndarray of float*) – The marker size in the squared number of points
- **color_sequence** (*str or list of str*) – Marker colors
- **colormap** (*str, optional, default=None*) – The colormap to use
- **v_lim** (*list of float [2], optional, default=(None,None)*) – Limits of the color scale

create_new_chart(*layout_id=None*)

Add a new subplot to the current visualization, so that multiple graphs can be overlaid onto one chart (e.g. scatterplot over heatmap).

create_new_chart(layout_id=None)

Parameters **layout_id** (*(3-digit) int, optional, default=None*) – Denoting the position of the graph in figure (xyn : 'x'=width, 'y'=height of grid, 'n'=position within grid)

static create_sub_plot(*title*, *labels*, *x_lim*, *y_lim*)

Set the title, labels and the axis limits of a plot.

create_sub_plot(title, labels, x_lim, y_lim)

Parameters

- **title** (*str*) – Title of the plot
- **labels** (*{str:str} dict*) – {'x': name of x-axis, 'y': name of y-axis}
- **x_lim** (*list of float [2]*) – x-limits for the function argument or value
- **y_lim** (*list of float [2]*) – y-limits for the function argument or value

figure_number = 0

font_size_label = 12

font_size_title = 12

graph_line_width = 2

horizontal_padding = 0.4

static show()
Show plots.

pygpc.Visualization.**b2rcw**(*cmin_input*, *cmax_input*)
Blue, white, and red color map. This function is designed to generate a blue to red colormap. The color of the colorbar is from blue to white and then to red, corresponding to the data values from negative to zero to positive, respectively. The color white always corresponds to value zero. The brightness of blue and red will change according to your setting, so that the brightness of the color corresponded to the color of his opposite number.

Parameters

- **cmin_input** (*float*) – Minimum value of data
- **cmax_input** (*float*) – Maximum value of data

Returns **newmap** – Colormap

Return type ndarray of float [N_RGB x 3]

Examples

```
>>> b2rcw_cmap_1 = make_cmap(b2rcw(-3, 6)) # is from light blue to deep red
>>> b2rcw_cmap_2 = make_cmap(b2rcw(-3, 3)) # is from deep blue to deep red
```

pygpc.Visualization.**make_cmap**(*colors*, *position=None*, *bit=False*)
make_cmap takes a list of tuples which contain RGB values. The RGB values may either be in 8-bit [0 to 255] (in which bit must be set to True when called) or arithmetic [0 to 1] (default). make_cmap returns a cmap with equally spaced colors. Arrange your tuples so that the first color is the lowest value for the colorbar and the last is the highest.

Parameters

- **colors** (*list of 3-tuples [n_rgb]*) – RGB values. The RGB values may either be in 8-bit [0 to 255] (in which bit must be set to True when called) or arithmetic [0 to 1] (default).
- **position** (*ndarray of float [n_rgb], optional, default=None*) – Contains values from 0 to 1 to dictate the location of each color.
- **bit** (*boolean, optional, default=False*) – Defines if colors are in 8-bit [0 to 255] (True) or arithmetic [0 to 1] (False)

Returns **cmap** – Colormap

Return type mpl.colors instance

pygpc.Visualization.**plot_2d_grid**(*coords*, *weights=None*, *fn_plot=None*)
Plot 2D grid and save it as fn_plot.pdf

Parameters

- **coords** (*ndarray of float [n_grid, 2]*) – Grid points
- **weights** (*ndarray of float [n_grid], optional, default=None*) – Integration weights

- **fn_plot** (*str*) – Filename of plot so save (.pdf)

Returns Plot of grid-points

Return type <file> .pdf file

pygpc.Visualization.**plot_beta_pdf_fit**(*data*, *a_beta*, *b_beta*, *p_beta*, *q_beta*, *a_uni=None*, *b_uni=None*, *interactive=True*, *fn_plot=None*, *xlabel='x'*, *ylabel='$p(x)$'*)

Plot data, fitted beta pdf (and corresponding uniform) distribution

Parameters

- **data** (*ndarray of float*) – Data to fit beta distribution on
- **a_beta** (*float*) – Lower limit of beta distribution
- **b_beta** (*float*) – Upper limit of beta distribution
- **p_beta** (*float*) – First shape parameter of beta distribution
- **q_beta** (*float*) – Second shape parameter of beta distribution
- **a_uni** (*float (optional)*) – Lower limit of uniform distribution
- **b_uni** (*float (optional)*) – Upper limit of uniform distribution
- **interactive** (*bool, default = True*) – Show plot (True/False)
- **fn_plot** – Filename of plot so save (as .png and .pdf)
- **xlabel** (*str (optional)*) – Label of x-axis
- **ylabel** (*str (optional)*) – Label of y-axis

Returns Plots

Return type <file> .png and .pdf files

pygpc.Visualization.**plot_sobol_indices**(*sobol_rel_order_mean*, *sobol_rel_1st_order_mean*, *fn_plot*, *random_vars*)

Plot the Sobol indices into different sub-plots.

plot_sobol_indices(sobol_rel_order_mean, sobol_rel_1st_order_mean, fn_plot, random_vars)

Parameters

- **sobol_rel_order_mean** (*ndarray of float [n_sobol]*) – Average proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,) over all output quantities
- **sobol_rel_1st_order_mean** (*ndarray of float [dim]*) – Average proportion of the random variables of the 1st order Sobol indices to the total variance over all output quantities
- **fn_plot** (*str*) – Filename of plot
- **random_vars** (*[dim] list of str*) – String labels of the random variables

1.17 pygpc.Worker module

pygpc.Worker.**init**(*queue*)

This is a wrapper script to be called by the 'multiprocessing.map' function to calculate the model functions in parallel.

This function will be called upon initialization of the process. It sets a global variable denoting the ID of this process that can be read by any function of this process

Parameters **queue** (*multiprocessing.Queue*) – the queue object that manages the unique IDs of the process pool

pygpc.Worker.**run**(*obj*)

This is the main worker function of the process. Methods of the provided object will be called here.

Parameters **obj** (*any callable object*) –

The object that

a) handles the simulation work

b) reading previous results

c) writing the calculated result fields

d) printing global process

1.18 pygpc.io module

Functions that provide input and output functionality

pygpc.io.**iprint**(*message*, *verbose=True*, *tab=None*)

Function that prints out a message over the python logging module

iprint(message, verbose=True)

Parameters

- **message** (*string*) – String to print in standard output
- **verbose** (*bool, optional, default=True*) – Determines if string is printed out
- **tab** (*int*) – Number of tabs before message

pygpc.io.**read_data_hdf5**(*fname*, *loc*)

Read data from .hdf5 file (e.g. coeffs, mean, std, . . .).

load_data_hdf5(fname, loc)

Parameters

- **fname** (*str*) – path to input file
- **loc** (*str*) – location (folder and name) in hdf5 file (e.g. data/phi)

Returns **data** – Loaded data from .hdf5 file

Return type ndarray of float

pygpc.io.**read_gpc_pkl**(*fname*)

Read gPC object including information about input pdfs, polynomials, grid etc.

object = read_gpc_obj(fname)

Parameters **fname** (*str*) – path to input file

Returns **obj** – GPC object containing instances of Basis, Problem and Model.

Return type GPC Object

pygpc.io.**read_sobol_idx_txt**(*fname*)
Read sobol_idx list from file.

read_sobol_idx_txt(fname)

Parameters **fname** (*str*) – Path to input file

Returns **sobol_idx** – List of parameter label indices belonging to Sobol indices

Return type [N_sobol] list of np.array

pygpc.io.**wprint**(*message*, *verbose=True*, *tab=None*)
Function that prints out a warning message over the python logging module

wprint(message, verbose=True)

Parameters

- **message** (*string*) – String to print in standard output
- **verbose** (*bool, optional, default=True*) – Determines if string is printed out
- **tab** (*int*) – Number of tabs before message

pygpc.io.**write_data_hdf5**(*data*, *fname*, *loc*)
Write quantity of interest in .hdf5 file (e.g. coeffs, mean, std, ...).

write_data_hdf5(data, fname, loc)

Parameters

- **data** (*np.ndarray*) – data to save
- **fname** (*str*) – path to output file
- **loc** (*str*) – location (folder and name) in hdf5 file (e.g. data/phi)

pygpc.io.**write_data_txt**(*data*, *fname*)
Write data (quantity of interest) in .txt file (e.g. coeffs, mean, std, ...).

write_data_txt(data, fname)

Parameters

- **data** (*ndarray of float*) – Data to save
- **fname** (*str*) – Path to output file

Returns **<file>** – File containing the data (tab delimited)

Return type txt file

pygpc.io.**write_gpc_pkl**(*obj*, *fname*)
Write gPC object including information about the Basis, Problem and Model as pickle file.

write_gpc_obj(obj, fname)

Parameters

- **obj** (GPC *or derived class*) – Class instance containing the gPC information
- **fname** (*str*) – path to output file

Returns **<file>** – File containing the GPC object

Return type pkl file

pygpc.io.**write_log_sobol**(*fname*, *random_vars*, *sobol_rel_order_mean*, *sobol_rel_1st_order_mean*, *sobol_extracted_idx_1st*)
Write average ratios of Sobol indices into logfile.

Parameters

- **fname** (*str*) – Path of logfile
- **random_vars** (*list of str*) – Labels of random variables
- **sobol_rel_order_mean** (*np.ndarray*) – Average proportion of the Sobol indices of the different order to the total variance (1st, 2nd, etc..,). (over all output quantities)
- **sobol_rel_1st_order_mean** (*np.ndarray*) – Average proportion of the random variables of the 1st order Sobol indices to the total variance. (over all output quantities)
- **sobol_extracted_idx_1st** (*list of int [N_sobol_1st]*) – Indices of extracted 1st order Sobol indices corresponding to SGPC.random_vars.

Returns **<File>** – Logfile containing information about the average ratios of 1st order Sobol indices w.r.t. the total variance

Return type txt file

pygpc.io.**write_sobol_idx_txt**(*sobol_idx*, *fname*)

Write sobol_idx list in file.

write_sobol_idx_txt(sobol_idx, filename)

Parameters

- **sobol_idx** (*[N_sobol] list of np.ndarray*) – List of parameter label indices belonging to Sobol indices
- **fname** (*str*) – Path to output file

Returns **<file>** – File containing the sobol index list.

Return type txt file

1.19 pygpc.misc module

Functions and classes that provide data and methods with general usage in the pygpc package

pygpc.misc.**display_fancy_bar**(*text*, *i*, *n_i*, *more_text=None*)

Display a simple progress bar. Call in each iteration and start with i=1.

Parameters

- **text** (*str*) – Text to display in front of actual iteration
- **i** (*str or int*) – Actual iteration
- **n_i** (*int*) – Total number of iterations
- **more_text** (*str, optional, default=None*) – Text that is displayed on an extra line above the bar.

Examples

fancy_bar('Run',7,10): Run 07 from 10 [==================================] 70%

fancy_bar(Run,9,10,'Some more text'): Some more text Run 09 from 10 [==] 90%

pygpc.misc.**get_all_combinations**(*array*, *number_elements*)

Compute all k-tuples (e_1, e_2, ..., e_k) of combinations of the set of elements of the input array where e_n+1 > e_n. combinations = get_all_combinations(array, number_elements) :param array: Array to perform the combinatorial problem with :type array: np.ndarray :param number_elements: Number of elements in tuple :type number_elements: int

Returns **combinations** – Array of combination vectors

Return type np.ndarray

pygpc.misc.**get_array_unique_rows**(*array*)

Compute unique rows of 2D array and delete rows that are redundant.

unique = get_array_unique_rows(array)

Parameters **array** (*ndarray of float*) – Matrix with k redundant rows

Returns **unique** – Matrix without k redundant rows

Return type ndarray of float

pygpc.misc.**get_beta_pdf_fit**(*data*, *beta_tolerance=0*, *uni_interval=0*, *fn_plot=None*)

Fit data to a beta distribution in the interval [a, b].

beta_parameters, moments, p_value, uni_parameters = get_beta_pdf_fit(data, beta_tolerance=0, uni_interval=0)

Parameters

- **data** (*ndarray of float*) – Data to fit beta distribution on
- **beta_tolerance** (*float, optional, default=0*) – Tolerance interval to calculate the bounds of beta distribution from observed data, e.g. 0.2 (+-20% tolerance on observed max and min value)
- **uni_interval** (*float, optional, default=0*) – uniform distribution interval defined as fraction of beta distribution interval (e.g. 0.95 (95%))
- **fn_plot** (*str*) – Filename of plot so save (.pdf and .png)

Returns

- **beta_parameters** (*list of float [4]*) – Two shape parameters and lower and upper limit [p, q, a, b]
- **moments** (*list of float [4]*) – Mean and std of raw data and fitted beta distribution [data_mean, data_std, beta_mean, beta_std]
- **p_value** (*float*) – p-value of the Kolmogorov Smirnov test
- **uni_parameters** (*list of float [2]*) – Lower and upper limits of uniform distribution [a, b]

pygpc.misc.**get_cartesian_product**(*array_list*)

Generate a cartesian product of input arrays (all combinations).

cartesian_product = get_cartesian_product(array_list)

Parameters **array_list** (*list of 1D ndarray of float*) – Arrays to compute the cartesian product with

Returns **cartesian_product** – Array containing the cartesian products (all combinations of input vectors) (M, len(arrays))

Return type ndarray of float

Examples

```
>>> import pygpc
>>> out = pygpc.get_cartesian_product(([1, 2, 3], [4, 5], [6, 7]))
>>> out
```

pygpc.misc.**get_list_multi_delete**(*input_list*, *index*)

Delete multiple entries from list.

input_list = get_list_multi_delete(input_list, index)

Parameters

- **input_list** (*list*) – Simple list
- **index** (*list of integer*) – List of indices to delete

Returns **input_list** – Input list without entries specified in index

Return type list

pygpc.misc.**get_multi_indices_max_order**(*dim*, *order_max*, *order_max_norm=1.0*)

Computes all multi-indices with a maximum overall order of max_order.

multi_indices = get_multi_indices_max_order(length, max_order)

Parameters

- **dim** (*int*) – Number of random parameters (length of multi-index tuples)
- **order_max** (*int*) – Maximum global expansion order. The maximum expansion order considers the sum of the orders of combined polynomials together with the chosen norm "order_max_norm". Typically this norm is 1 such that the maximum order is the sum of all monomial orders.
- **order_max_norm** (*float*) – Norm for which the maximum global expansion order is defined [0, 1]. Values < 1 decrease the total number of polynomials in the expansion such that interaction terms are penalized more. sum(a_i^q)^1/q <= p, where p is order_max and q is order_max_norm (for more details see eq (11) in [1]).

Returns **multi_indices** – Multi-indices for a maximum order gPC assuming a certain order norm.

Return type np.ndarray [n_basis x dim]

pygpc.misc.**get_normalized_rms_deviation**(*array*, *array_ref*, *x_axis=False*)

Determine the normalized root mean square deviation between input data and reference data in [%].

normalized_rms = get_normalized_rms(array, array_ref)

Parameters

- **array** (*np.ndarray*) – input data [(x), y0, y1, y2 ...]
- **array_ref** (*np.ndarray*) – reference data [(x_ref), y0_ref, y1_ref, y2_ref ...] if array_ref is 1D, all sizes have to match
- **x_axis** (*boolean, optional, default=False*) – If True, the first column of array and array_ref is interpreted as the x-axis, where the data points are evaluated. If False, the data points are assumed to be at the same location.

Returns **normalized_rms** – Normalized root mean square deviation between the columns of array and array_ref

Return type ndarray of float [array.shape[1]]

pygpc.misc.**get_num_coeffs**(*order*, *dim*)

Calculate the number of gPC coefficients by the maximum order and the number of random variables.

num_coeffs = (order+dim)! / (order! * dim!)

num_coeffs = get_num_coeffs(order , dim)

Parameters

- **order** (*int*) – Maximum order of expansion
- **dim** (*int*) – Number of random variables

Returns **num_coeffs** – Number of gPC coefficients and polynomials

Return type int

pygpc.misc.**get_num_coeffs_sparse**(*order_dim_max*, *order_glob_max*, *order_inter_max*, *dim*, *order_glob_max_norm=1*)

Calculate the number of gPC coefficients for a specific maximum order in each dimension "order_dim_max", global maximum order "order_glob_max" and the interaction order "order_inter_max".

num_coeffs_sparse = get_num_coeffs_sparse(order_dim_max, order_glob_max, order_inter_max, dim)

Parameters

- **order_dim_max** (*ndarray of int or list of int [dim]*) – Maximum order in each dimension
- **order_glob_max** (*int*) – Maximum global order of interacting polynomials
- **order_inter_max** (*int*) – Interaction order
- **dim** (*int*) – Number of random variables
- **order_glob_max_norm** (*float*) – Norm, which defines how the orders are accumulated to derive the total order (default: 1-norm). Values smaller than one restrict higher orders and shrink the basis.

Returns **num_coeffs_sparse** – Number of gPC coefficients and polynomials

Return type int

pygpc.misc.**get_pdf_beta**(*x*, *p*, *q*, *a*, *b*)

Calculate the probability density function of the beta distribution in the interval [a, b].

pdf = (gamma(p)*gamma(q)/gamma(p+q).*(b-a)(p+q-1))**(-1) *** (x-a)**(p-1) * (b-x)**(q-1);

pdf = get_pdf_beta(x, p, q, a, b)

Parameters

- **x** (*ndarray of float*) – Values of random variable
- **a** (*float*) – lower boundary
- **b** (*float*) – upper boundary
- **p** (*float*) – First shape parameter defining the distribution
- **q** (*float*) – Second shape parameter defining the distribution

Returns **pdf** – Probability density

Return type ndarray of float

pygpc.misc.**get_rotation_matrix**(*theta*)
Generate rotation matrix from euler angles.

rotation_matrix = get_rotation_matrix(theta)

Parameters **theta** (*list of float [3]*) – Euler angles

Returns **rotation_matrix** – Rotation matrix computed from euler angles

Return type ndarray of float [3, 3]

pygpc.misc.**list2dict**(*l*)
Transform list of dicts with same keys to dict of list

Parameters **l** (*list of dict*) – List containing dictionaries with same keys

Returns **d** – Dictionary containing the entries in a list

Return type dict of lists

pygpc.misc.**mutual_coherence**(*array*)
Calculate the mutual coherence of a matrix A. It can also be referred as the cosine of the smallest angle between two columns.

mutual_coherence = mutual_coherence(array)

Parameters **array** (*ndarray of float*) – Input matrix

Returns **mutual_coherence** – Mutual coherence

Return type float

pygpc.misc.**sample_sphere**(*n_points*, *r*)
Creates n_points evenly spread in a sphere of radius r.

Parameters

- **n_points** (*int*) – Number of points to be spread, must be odd
- **r** (*float*) – Radius of sphere

Returns **points** – Evenly spread points in a unit sphere

Return type ndarray of float [N x 3]

pygpc.misc.**wrap_function**(*fn*, *x*, *args*)
Function wrapper to call anonymous function with variable number of arguments (tuple).

wrap_function(fn, x, args)

Parameters

- **fn** (*function*) – anonymous function to call
- **x** (*tuple*) – parameters of function
- **args** (*tuple*) – arguments of function

Returns **function_wrapper** – wrapped function

Return type function

1.20 pygpc.postprocessing module

pygpc.postprocessing.**get_sensitivities_hdf5**(*fn_gpc*, *output_idx=False*, *calc_sobol=True*, *calc_global_sens=False*, *calc_pdf=False*)

Post-processes the gPC expansion and adds mean, standard deviation, relative standard deviation, variance, Sobol indices, global derivative based sensitivity coefficients and probability density functions of output quantities to .hdf5 file of gPC.

Parameters

- **fn_gpc** (*str*) – Filename of gPC .pkl object and corresponding .hdf5 results file (without file extension) (e.g. . . . /foo/gpc)
- **output_idx** (*nparray of int*) – Indices of output quantities (QOIs) to consider in postprocessing (default: all)
- **calc_sobol** (*bool*) – Calculate Sobol indices (default: True)
- **calc_global_sens** (*bool*) – Calculate global derivative based sensitivities (default: False)
- **calc_pdf** (*bool*) – Calculate probability density functions of output quantities (default: False)

Returns **<File>** – Adds datasets "sens/. . . " to the gPC .hdf5 file

Return type hdf5

Example

The content of .hdf5 files can be shown using the tool HDFView (https://support.hdfgroup.org/products/java/hdfview/)

:: sens I—/mean [n_qoi] Mean of QOIs I—/std [n_qoi] Standard deviation of QOIs I—/rstd [n_qoi] Relative standard deviation of QOIs I—/var [n_qoi] Variance of QOIs I—/sobol [n_sobol x n_qoi] Sobol indices (all available orders) I—/sobol_idx_bool [n_sobol x n_dim] Corresponding parameter (combinations) of Sobol indices I—/global_sens [n_dim x n_qoi] Global derivative based sensitivity coefficients I—/pdf_x [100 x n_qoi] x-axis values of output PDFs I—/pdf_y [100 x n_qoi] y-axis values of output PDFs

1.21 pygpc.validation module

pygpc.validation.**validate_gpc_mc**(*gpc*, *coeffs*, *n_samples=10000.0*, *output_idx=0*, *n_cpu=1*, *fn_out=None*)

Compares gPC approximation with original model function. Evaluates both at "n_samples" sampling points and evaluates the root mean square deviation. It also computes the pdf at the output quantity with output_idx and saves the plot as fn_pdf.png and fn_pdf.pdf.

Parameters

- **gpc** (*GPC object instance*) – GPC object containing all information i.e., Problem, Model, Grid, Basis, RandomParameter instances
- **coeffs** (*ndarray of float [n_coeffs x n_out]*) – GPC coefficients
- **n_samples** (*int*) – Number of samples to validate the gPC approximation
- **output_idx** (*ndarray, optional, default=None [1 x n_out]*) – Index of output quantities to consider (if output_idx=None, all output quantities are considered)

- **ncpu** (*int, optional, default=1*) – Number of CPU cores to use (parallel function evaluations) to evaluate original model function
- **fn_out** (*str*) – Filename of validation results and pdf plot comparing original vs gPC model

Returns

- **nrmsd** (*ndarray of float [n_out]*) – Normalized root mean square deviation for all output quantities between gPC and original model
- **<file>** (*.hdf5 file*) – Data file containing the sampling points, the results and the pdfs of the original and the gpc approximation
- **<file>** (*.pdf file*) – Plot showing the pdfs of the original and the gpc approximation

pygpc.validation.**validate_gpc_plot**(*gpc*, *coeffs*, *random_vars*, *n_grid=None*, *coords=None*, *output_idx=0*, *data_original=None*, *fn_out=None*, *n_cpu=1*)

Compares gPC approximation with original model function. Evaluates both at n_grid (x n_grid) sampling points and calculate the difference between two solutions at the output quantity with output_idx and saves the plot as *_QOI_idx_<output_idx>.png/pdf. Also generates one .hdf5 results file with the evaluation results.

Parameters

- **gpc** (*GPC object instance*) – GPC object containing all information i.e., Problem, Model, Grid, Basis, RandomParameter instances
- **coeffs** (*ndarray of float [n_coeffs x n_out]*) – GPC coefficients
- **random_vars** (*str or list of str [2]*) – Names of the random variables, the analysis is performed for one or max. two random variables
- **n_grid** (*int or list of int [2], optional*) – Number of samples in each dimension to compare the gPC approximation with the original model function. A cartesian grid is generated based on the limits of the specified random_vars
- **coords** (*ndarray of float [n_coords x n_dim]*) – Parameter combinations for the random_vars the comparison is conducted with
- **output_idx** (*int or list of int, optional, default=0*) – Indices of output quantity to consider
- **data_original** (*ndarray of float [n_coords x n_out], optional, default: None*) – If available, data of original model function at grid
- **fn_out** (*str*) – Filename of plot comparing original vs gPC model (*_QOI_idx_<output_idx>.png is added)
- **n_cpu** (*int, default=1*) – Number of CPU cores to use to calculate results of original model on grid.

Returns

- **<file>** (*.hdf5 file*) – Data file containing the grid points and the results of the original and the gpc approximation
- **<file>** (*.png and .pdf file*) – Plot comparing original vs gPC model

1.22 Module contents

A package that provides submodules to perform polynomial chaos uncertainty analysis on complex dynamic systems.

CHAPTER

TWO

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PYTHON MODULE INDEX

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