



UQpy - Uncertainty Quantification with Python

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Version 1.1.0
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Contents

1	Overview	3
2	Installing UQpy	6
2.1	Manual Installation	6
2.2	Developer Installation	6
3	License	7
4	UQpy Modules, Classes, & Functions	8
4.1	SampleMethods Module	9
4.1.1	UQpy.SampleMethods.MCS	9
4.1.2	UQpy.SampleMethods.LHS	12
4.1.3	UQpy.SampleMethods.STS	15
4.1.4	UQpy.SampleMethods.Strata	18
4.1.5	UQpy.SampleMethods.MCMC	20
4.1.6	UQpy.SampleMethods.Correlate	25
4.1.7	UQpy.SampleMethods.Decorrelate	28
4.1.8	UQpy.SampleMethods.Nataf	31
4.1.9	UQpy.SampleMethods.InvNataf	36
4.2	Surrogates Module	40
4.2.1	UQpy.Surrogates.SROM	41
4.2.2	UQpy.Surrogates.Kriging (Coming in V2.0)	45
4.3	Reliability Module	45
4.3.1	UQpy.Reliability.SubsetSimulation	45
4.3.2	UQpy.Reliability.TaylorSeries (Coming in V2.0)	51
4.4	Inference Module	52
4.4.1	InfoModelSelection (Coming in V2.0)	52
4.4.2	BayesModelSelection (Coming in V2.0)	52
4.4.3	BayesParameterEstimation (Coming in V2.0)	52
4.5	StochasticProcess Module (Coming in V2.0)	52
4.5.1	UQpy.StochasticProcess.SRM (Coming in V2.0)	53
4.5.2	UQpy.StochasticProcess.BSRM (Coming in V2.0)	54
4.5.3	UQpy.StochasticProcess.KLE (Coming in V2.0)	56
4.5.4	UQpy.StochasticProcess.Translation (Coming in V2.0)	57
4.5.5	UQpy.StochasticProcess.InverseTranslation (Coming in V2.0)	58
4.6	RunModel Module	60

4.6.1	RunModel with direct Python communications (<code>model_type = 'python'</code>)	63
4.6.2	RunModel with file passing communications (<code>model_type</code> <code>= None</code>)	66
4.6.3	Files and scripts used by RunModel	71
4.6.4	Template scripts for common software applications . .	74
5	Support Modules	75
5.1	Distributions Module	75
5.2	Utilities Module	80
6	Adding new classes to UQpy	81

1 Overview

UQpy (Uncertainty Quantification with Python) is a general purpose Python toolbox for modeling uncertainty in the simulation of physical and mathematical systems. The code is organized as a set of modules centered around core capabilities in Uncertainty Quantification (UQ) as illustrated in Figure 1. The modules are distinct, but are designed to be easily extensible (new capabilities can be easily added and integrated into the code, see Section 6) and to easily call one another.

The UQpy workflow is simple. Each module, as illustrated in Figure 1, contains a set of classes that perform various operations in UQ. A list of the current capabilities for each module is provided in Table 1. A list of ex-

Table 1: Current UQpy capabilities organized by Module and Class structure.

Module	Class	Description	Version
SampleMethods	MCS	Monte Carlo Sampling	1.1.0
	LHS	Latin Hypercube Sampling	1.1.0
	STS	Stratified Sampling	1.1.0
	MCMC	Markov Chain Monte Carlo	1.1.0
	Correlate	Induces correlation	1.1.0
	Decorrelate	Removes correlation	1.1.0
	Nataf	Nataf transformation	1.1.0
	InvNataf	Inverse Nataf transformation	1.1.0
Surrogates	SROM	Stochastic Reduced Order Model	1.0.0
Reliability	SubsetSimulation	Subset Simulation	1.0.0

pending capabilities that are currently in development is provided in Table 2.

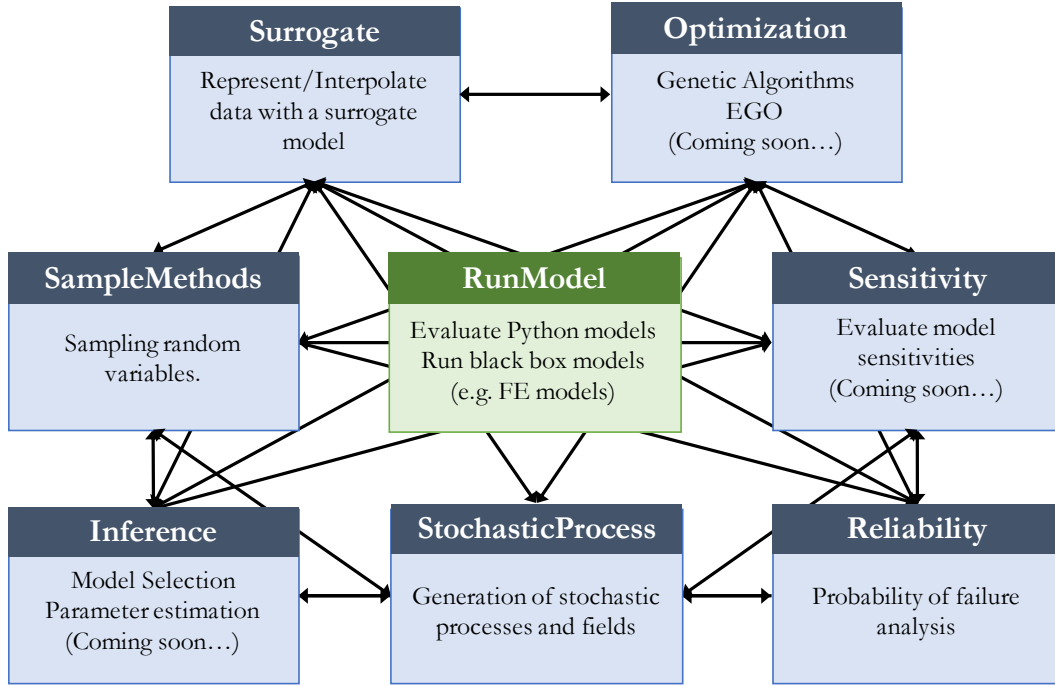


Figure 1: UQpy modules and their basic architecture.

13 Modules and Classes in **UQpy** are invoked using standard Python conventions.
14 Because each module is organized into a set of classes, it is straightforward
15 to add a new capability to **UQpy** by simply writing a new class into the ap-
16 propriate module (although some care should be taken to ensure consistency
17 in input/output naming and data type conventions). Moreover, because of
18 its module-class structure, the various classes can easily invoke one-another
19 and can be combined in any way the user desires. A simple example of this
20 is that the **SubsetSimulation** class in the **Reliability** module invokes the
21 **MCMC** class from the **SampleMethods** module.

22 The various classes and modules interface in a straightforward manner
23 with computational models of physical or mathematical systems through the
24 **RunModel** module shown in the center of the chart in Figure 1. The **RunModel**
25 module allows **UQpy** to serve not just as a useful tool for performing UQ oper-
26 ations, but also as the driver for a complete uncertainty study - including pre-
27 processing operations, submission and execution of computational model eval-
28 uations, and monitoring and post-processing of results. Thus, it is amenable to
29 performing adaptivity UQ analyses. The **RunModel** module, detailed in Section
30 4.6, is designed to interface with any user-defined third-party computational

Table 2: Future UQpy capabilities organized by Module and Class structure.

Module	Class	Description	Version
SampleMethods	LSS	Latinized Stratified Sampling	2.0.0
	PSS	Partially Stratified Sampling	2.0.0
	LPSS	Latinized Partially Stratified Sampling	2.0.0
	IS	Importance Sampling	2.0.0
	RSS	Refined Stratified Sampling	3.0.0
	GE-RSS	Gradient Enhance Refined Stratified Sampling	3.0.0
	LRSS	Latinized Refined Stratified Sampling	3.0.0
	SparseGrid	Sparse Grid Cubature Sampling	3.0.0
	QMC	Quasi Monte Carlo	3.0.0
	Simplex	Simplex Sampling	3.0.0
	Composition	Composition Sampling Method	2.0.0
	ASGC	Adaptive Sparse Grid Collocation	3.0.0
	SCAMR	Stochastic Collocation with Adaptive Mesh Refinement	3.0.0
	PCE	Polynomial Chaos Surrogate	3.0.0
Surrogates	Kriging	Gaussian Process/Kriging Surrogate	2.0.0
	MMK	Multimodel Kriging Surrogate	2.0.0
	ANN	Artificial Neural Network Surrogate	3.0.0
	SSC	Simplex Stochastic Collocation	3.0.0
	VSSC	Variance-based Simplex Stochastic Collocation	3.0.0
	Grassmann	Grassmann Manifold Projection Surrogate	3.0.0
	TaylorSeries	Taylor Series for First Order Reliability Method and/or Second Order Reliability Method	2.0.0
	TRS	Targeted Random Sampling	3.0.0
	SESS	Surrogate Enhance Stochastic Search	3.0.0
	AK-MCS	Adaptive Kriging Monte Carlo Simulation	2.0.0
	InfoModelSelection	Information Theoretic Model Selection	2.0.0
Inference	BayesModelSelection	Bayesian Model Selection	2.0.0
	BayesParameter	Bayesian Parameter Estimation	2.0.0
	KDE	Kernel Density Estimation	2.0.0
Optimization	EGO	Efficient Global Optimization	2.0.0
	GA	Genetic Algorithms	3.0.0
Sensitivity	Sobol	Sobol Indices	2.0.0
	PCESobol	Polynomial Chaos Sobol Indices	3.0.0

31 model (either through user-defined shell scripts or a Python script) or directly
32 with a Python model.

33 2 Installing UQpy

34 UQpy is written in the Python 3 programming language and requires a Python
35 interpreter 3.6+ installed on your computer. UQpy is distributed through the
36 Python Package Index, PyPI, and can be installed using a simple pip command
37 on the terminal as follows:

```
38     pip install UQpy
```

40 Upon installation, the UQpy software modules are installed in the site-
41 packages directory of the user's Python installation. For example, within the
42 user's Python (version 3.6) installation, the installed modules can be found at:

```
43     ./lib/python3.6/site-packages/UQpy
```

45 UQpy can be uninstalled in a similar manner using pip:

```
46     pip uninstall UQpy
```

47 2.1 Manual Installation

48 Alternatively, UQpy can be installed from GitHub directly by typing the fol-
49 lowing commands in the terminal:

```
50     git clone https://github.com/SURGroup/UQpy.git
```

```
51     cd UQpy/
```

```
52     python setup.py install
```

53 Direct installation from GitHub is equivalent to pip installation.

54 UQpy can be uninstalled using pip as:

```
55     pip uninstall UQpy
```

56 2.2 Developer Installation

57 Users interested in developing new capabilities in UQpy may install it as a
58 developer. This is achieved by typing the following commands in the terminal:

```
59     git clone https://github.com/SURGroup/UQpy.git
```

60 `cd UQpy/`

61 `python setup.py develop`

62 Installing as a developer allows the user to maintain a local copy of **UQpy**
63 (located in a directory of the user's choosing) that can be edited – with changes
64 being recognized by the **UQpy** “installation”. Installing as a developer does not
65 install the software directly to site-packages as in the installation procedures
66 above. Instead, developer installation creates an ‘egg-link’ (**UQpy.egg-link**)
67 in the site-packages that directs **UQpy** calls to the user's local, editable copy of
68 the software. For more details, see the following link:

69 `http://setuptools.readthedocs.io/en/latest/setuptools.html#`
70 `development-mode`

71 **3 License**

72 **UQpy** is distributed under the MIT license.

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75
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91 ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN
92 ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM,
93 OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE
94 OR OTHER DEALINGS IN THE SOFTWARE.

95 4 UQpy Modules, Classes, & Functions

96 UQpy is structured in eight core modules (see Figure 1), each centered around
97 specific functionalities. The modules are as follows:

- 98 1. **Distributions:** This module contains a set of supported distributions
99 and their functions (pdf, cdf, moments, random numbers, fit, inverse cdf,
100 log-pdf).
- 101 2. **SampleMethods:** This module contains a set of classes and functions to
102 draw samples from random variables. These samples may be randomly
103 drawn, as in Monte Carlo sampling, or they may be deterministically
104 drawn as in sparse-grid or quasi-Monte Carlo sampling.
- 105 3. **Inference:** (Coming in Version 2.0.0) This module contains a set of
106 classes and functions to conduct probabilistic inference. The module
107 contains methods that are based on Bayesian, frequentist, likelihood,
108 and information theories.
- 109 4. **Reliability:** This module contains a set of classes and functions de-
110 signed specifically to estimate rare event probabilities and probability of
111 failure.
- 112 5. **Surrogate:** This module contains a set of classes and functions for build-
113 ing surrogate models, meta-models, or emulators.
- 114 6. **Sensitivity:** (Coming in Version 2.0.0) This module contains a set of
115 classes and functions for performing global and local sensitivity analysis.
- 116 7. **Optimization:** (Coming in Version 2.0.0) This module contains a set of
117 classes and functions to perform optimization for stochastic problems.
- 118 8. **StochasticProcess:** (Coming in Version 2.0.0) This module contains
119 a set of classes and functions for the simulation of stochastic processes
120 and fields.
- 121 9. **RunModel:** This module contains a set of classes and functions that allows
122 UQpy to initiate simulations using Python or third-party computational
123 solvers, and monitor and post-process simulation results.

124 The following sections detail the classes and functions in each module with
125 reference to examples that illustrate their use.

126 4.1 SampleMethods Module

127 The **SampleMethods** module consists of classes and functions to draw samples
128 from random variables, to induce or remove correlation from samples and to
129 transform the samples. It is imported in a python script using the following
130 command:

```
131 from UQpy import SampleMethods
```

132 The **SampleMethods** module has the following classes, each corresponding to
133 a different sampling method:

Class	Method
MCS	Monte Carlo Sampling
LHS	Latin Hypercube Sampling
STS	Stratified Sampling
134 MCMC	Markov Chain Monte Carlo
Correlate	Induces correlation
Decorrelate	Removes correlation
Nataf	Nataf transformation
InvNataf	Inverse Nataf transformation

135 Each class can be imported individually into a python script. For example,
136 the **MCMC** class can be imported to a script using the following command:

```
137 from UQpy.SampleMethods import MCMC
```

138 The following subsections describe each class, their respective inputs and at-
139 tributes, and their use.

140 4.1.1 UQpy.SampleMethods.MCS

141 **MCS** is a class for Monte Carlo Sampling – random sampling from independent
142 random variables having user specified distributions. The **MCS** class is imported
143 using the following command:

```
144 from UQpy.SampleMethods import MCS
```

145 The attributes of the **MCS** class are listed below:

MCS Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
dist_name	Input	★	
dist_params	Input	★	
nsamples	Input	★	
samplesU01	Output		
samples	Output		

A brief description of each attribute can be found in the table below:

MCS Class Attributes			
Attribute	Type	Options	Default
dimension	<i>integer</i>		<code>dimension = len(dist_name)</code>
dist_name	<i>function/string list</i>	See Distributions Module or User-defined function	
dist_params	<i>ndarray list</i>		
nsamples	<i>integer</i>		None
samplesU01	<i>ndarray</i>		
samples	<i>ndarray</i>		

Detailed Description of MCS Class Attributes:

Input Attributes:

- **dimension:**

A scalar integer value defining the dimension of the random variables.

- **dist_name:**

Defines the name of the distribution for each random variable.

`dist_name` may be a string, a function, or a list of strings/functions.

If `dist_name[i]` is a string, the distribution is matched with one of the available functions in the `Distributions` module (see Sec. 5.1) or the ‘custom_dist.py’ (again see Sec. 5.1).

if `dist_name[i]` is a function, it must be defined in the user’s Python script and passed directly as a function.

167 `dist_name` can contain an arbitrary combination of strings and functions.
 168

169 If `dist_name` is a string or function (or a list of length one) and
 170 `dimension > 1`, then `dist_name` is converted into a list of length
 171 `dimension` with each variable having the distribution.
 172

173 `dist_name` must be specified. There is no default value.

174 • **dist_params:**
 175 Specifies the parameters for each distribution in `dist_name`.
 176

177 Each set of parameters is defined as a numpy array. `dist_params` is a
 178 list of arrays, with each item in the list corresponding to the associated
 179 random variable.
 180

181 If `dist_params` is an array (or a list of length one), then `dist_params`
 182 is converted to a list of length `dimension` with each variable having the
 183 same parameters.
 184

185 `dist_params` must be specified. There is no default value.

186 • **nsamples:**
 187 Specifies the number of samples to be generated.
 188

189 `nsamples` must be specified. There is no default value.

190 *Output Attributes:*

191 • **samplesU01:**
 192 A numpy array of dimension `nsamples × dimension` containing the sam-
 193 ples generated uniformly on the hypercube $[0, 1]^{\text{dimension}}$.

194 • **samples:**
 195 A numpy array of dimension `nsamples × dimension` containing the sam-
 196 ples following the specified distribution.

197 **Examples:**
 198 An example illustrating the use of the `MCS` class is provided in the following
 199 Jupyter script.

- MCS.ipynb:
In this example, 1000 2-dimensional samples are drawn from a normal distribution.

4.1.2 UQpy.SampleMethods.LHS

LHS is a class for Latin hypercube sampling. The LHS class is imported using the following command:

```
from UQpy.SampleMethods import LHS
```

The attributes of the LHS class are listed below:

LHS Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
dist_name	Input	★	
dist_params	Input	★	
lhs_criterion	Input		★
lhs_metric	Input		★
lhs_iter	Input		★
nsamples	Input	★	
samplesU01	Output		
samples	Output		

A brief description of each attribute can be found in the table below:

LHS Class Attributes			
Attribute	Type	Options	Default
dimensions	<i>integer</i>		<code>dimension = len(dist_name)</code>
dist_name	<i>function/string list</i>	See Distributions Module or User-defined function	
dist_params	<i>ndarray list</i>		
lhs_criterion	<i>string</i>	'random' 'centered' 'maximin' 'correlate'	'random'
lhs_metric	<i>string</i>	'braycurtis', 'canberra', 'chebyshev' 'cityblock', 'correlation', 'cosine' 'dice', 'euclidean', 'hamming' 'jaccard', 'kulsinski', 'mahalanobis' 'matching', 'minkowski', 'rogerstanimoto' 'russellrao', 'seuclidean', 'sokalmichener' 'sokalsneath', 'sqeuclidean', 'yule'	'euclidean'
lhs_iter	<i>integer</i>		<code>iterations = 100</code>
nsamples	<i>integer</i>		<code>None</code>
samplesU01	<i>ndarray</i>		
samples	<i>ndarray</i>		

212 **Detailed Description of LHS Class Attributes:**

213

214 *Input Attributes:*

215 • **dimension:**

216 A scalar integer value defining the dimension of the random variables.

217 • **dist_name:**

218 Defines the distributions for each random variable.

219

220 **dist_name** may be a string, a function, or a list of strings/functions.

221

222 If **dist_name[i]** is a string, the distribution is matched with with one
223 of the available functions in the **Distributions** module (see Sec. 5.1)
224 or the ‘custom_dist.py’ (again see Sec. 5.1).

225

226 if **dist_name[i]** is a function, it must be defined in the user’s Python
227 script and passed directly as a function.

228

229 **dist_name** can contain an arbitrary combination of strings and functions.

230

231 If **dist_name** is a string or function (or a list of length one) and
232 **dimension** > 1, then **dist_name** is converted into a list of length
233 **dimension** with each variable having the same distribution.

234

235 **dist_name** must be specified. There is no default value.

236 • **dist_params:**

237 Specifies the parameters for each distribution in **dist_name**.

238

239 Each set of parameters is defined as a numpy array. **dist_params** is a
240 list of arrays, with each item in the list corresponding to the associated
241 random variable.

242

243 If **dist_params** is an array (or a list of length one), then **dist_params**
244 is converted to a list of length **dimension** with each variable having the
245 same parameters.

246

247 `dist_params` must be specified. There is no default value.

248 • **lhs_criterion:**
 249 Design criterion for the Latin hypercube samples. The different choices
 250 available are given below:

- 251 – ‘random’: Samples are drawn randomly in the Latin hypercube
 252 strata.
- 253 – ‘centered’: Samples are centered in the Latin hypercube strata.
- 254 – ‘maximin’: The minimum distance between the sample points is
 255 maximized.
- 256 – ‘correlate’: The correlation among the sample points is minimized.

257 • **lhs_metric:**
 258 Specifies the distance metric to be used in the case of ‘maximin’
 259 criterion. The choices are the available distance metrics in `scipy`.
 260

261 Only required in the case of `lhs_criterion = ‘maximin’`.

262 • **lhs_iter:**
 263 Specifies the number of iterations to be run for deciding the design in the
 264 case of `lhs_criterion = ‘maximin’` and `lhs_criterion = ‘correlate’`.

265 • **nsamples:**
 266 Specifies the number of samples to be generated.
 267

268 `nsamples` must be specified. There is no default value.

269 *Output Attributes:*

270 • **samplesU01:**
 271 A numpy array of dimension `nsamples × dimension` containing the sam-
 272 ples generated uniformly on the hypercube $[0, 1]^{\text{dimension}}$.

273 • **samples:**
 274 A numpy array of dimension `nsamples × dimension` containing the sam-
 275 ples following the specified distribution.

276 **Examples:**

277 An example illustrating the use of the `LHS` class is provided in the following
 278 Jupyter script.

- LHS.ipynb:
In this example, 5 2-dimensional samples are drawn using Latin hypercube sampling with different `lhs_criterion` to illustrate its use.

4.1.3 UQpy.SampleMethods.STS

STS is a class for stratified sampling. The STS class is imported using the following command:

```
from UQpy.SampleMethods import STS
```

The attributes of the STS class are listed below:

STS Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
dist_name	Input	★	
dist_params	Input	★	
sts_design	Input		★
input_file	Input		★
samples	Output		
samplesU01	Output		
strata	Input		

A brief description of each attribute can be found in the table below:

STS Class Attributes			
Attribute	Type	Options	Default
dimension	<i>integer</i>		<code>dimension = len(sts_design)</code>
dist_name	<i>function/string list</i>	See Distributions Module or User-defined function	
dist_params	<i>ndarray list</i>		
sts_design	<i>int list</i>		None
input_file	<i>string</i>		None
samples	<i>ndarray</i>		
samplesU01	<i>ndarray</i>		
strata	<i>class object</i>	See <code>UQpy.SampleMethods.Strata</code>	

Detailed Description of STS Class Attributes:

Input Attributes:

- **dimension:**
A scalar integer value defining the dimension of the random variables.

296 • **dist_name:**
 297 Defines the distributions for each random variable.
 298
 299 **dist_name** may be a string, a function, or a list of strings/functions.
 300
 301 If **dist_name[i]** is a string, the distribution is matched with one of the
 302 available functions in the **Distributions** module (see Sec. 5.1) or the
 303 ‘custom_dist.py’ (again see Sec. 5.1).
 304
 305 if **dist_name[i]** is a function, it must be defined in the user’s Python
 306 script and passed directly as a function.
 307
 308 **dist_name** can contain an arbitrary combination of strings and functions.
 309
 310 If **dist_name** is a string or function (or a list of length one) and
 311 **dimension > 1**, then **dist_name** is converted into a list of length
 312 **dimension** with each variable having the same distribution.
 313
 314 **dist_name** must be specified. There is no default value.

315 • **dist_params:**
 316 Specifies the parameters for each distribution in **dist_name**.
 317
 318 Each set of parameters is defined as a numpy array. **dist_params** is a
 319 list of arrays, with each item in the list corresponding to the associated
 320 random variable.
 321
 322 If **dist_params** is an array (or a list of length one), then **dist_params**
 323 is converted to a list of length **dimension** with each variable having the
 324 same parameters.
 325
 326 **dist_params** must be specified. There is no default value.

327 • **sts_design:**
 328 Specifies the number of strata in each dimension.
 329

330 `sts_design` specifies a stratification that breaks every dimension equally
331 into a specified number of strata of the same size. For more complex
332 strata geometries, the strata boundaries can be explicitly defined through
333 a text input file. See `input_file` and the corresponding documentation
334 in Section 4.1.4.

335 STS places one sample in each stratum so the total number of samples
336 drawn by STS is the product of the components of `sts_design`.

337

338 Example: `sts_design = [2, 4, 3]` specifies a three-dimensional strat-
339 ified design with two strata in the first dimension, four strata in the
340 second dimension, and three strata in the third dimension for a total of
341 $2 \times 4 \times 3 = 24$ samples.

342 • **input_file:**

343 Specifies the file path of for a text file defining a stratification. See
344 Section 4.1.4

345 *Output Attributes:*

346 • **samples:**

347 The generated samples. The samples are returned as a numpy array.

348 • **samplesU01:**

349 The untransformed samples drawn from the unit hypercube with dimen-
350 sion `dimension`.

351 • **strata:**

352 A class object that defines the strata on the unit hypercube with dimen-
353 sion `dimension`.

354 **Examples:**

355 Two examples illustrating the use of the STS class are provided in the following
356 Jupyter scripts.

357 • **STS_Example1.ipynb:**

358 In this example, 25 samples are drawn from an exponential distribution
359 using stratified sampling with the strata specified using the `sts_design`
360 input for a regular, equal probability stratification.

361 • **STS_Example2.ipynb:**

362 In this example, 6 samples are drawn from an exponential distribution
363 using stratified sampling with the strata specified using an `input_file`
364 ('strata.txt') to create an irregular stratification with unequal probability
365 strata.

366 4.1.4 UQpy.SampleMethods.Strata

367 The **Strata** class is a supporting class for stratified sampling and its variants.
 368 The class defines a rectilinear stratification of the unit hypercube. Strata are
 369 defined by specifying an origin as the coordinates of the stratum corner nearest
 370 to the origin and a stratum width for each dimension.
 371 The attributes of the **STS** class are listed below:

Strata Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
nstrata	Input		★
input_file	Input		★
origins	Output		
widths	Output		
weights	Input		

373 A brief description of each attribute can be found in the table below:

Strata Class Attributes			
Attribute	Type	Options	Default
nstrata	<i>int list</i>		None
input_file	<i>string</i>		None
origins	<i>ndarray</i>		
widths	<i>ndarray</i>		
weights	<i>ndarray</i>		

375 Detailed Description of Strata Class Attributes:

376

377 *Input Attributes:*

- 378 • **nstrata:**
 379 Specifies the number of strata in each dimension. This is equivalent
 380 to **sts.design** from the **STS** class. For additional details, see **STS**
 381 documentation in Section 4.1.3.

382

383 When calling the **Strata** class, the user must provide either **nstrata** or
 384 a text file defining the strata specified through **input_file**.

- 385 • **input_file:**
 386 Specifies the file path of for a text file defining a stratification.

387

388 When calling the **Strata** class, the user must provide either **nstrata** or
389 a text file defining the strata specified through **input_file**.

390

391 *File format:* This file must be a space delimited text file having
392 $2 \times \text{dimension}$ columns and the number of rows equal to the number
393 of strata. The first **dimension** columns correspond to the coordinates
394 in each dimension of the stratum origin. Columns **dimension+1** to
395 $2 \times \text{dimension}$ correspond to the stratum widths in each dimension.

396 For example, to specify stratification with two 2-dimensional strata, the
397 text file might contain the following:

398

```
399 0.0 0.0 0.5 1.0  
400 0.5 0.0 0.5 1.0
```

401

402 The first stratum (row 1) has origin (0.0, 0.0) and has width 0.5 in
403 dimension 1 and width 1.0 in dimension 2. The second stratum (row
404 2) has origin (0.5, 0.0) and has width 0.5 in dimension 1 and width
405 1.0 in dimension 2.

406

407 When manually assigning the strata definitions, the user must be careful
408 to ensure that the stratification fills the space without overlap. That is,
409 each strata that the user defines must be disjoint and the total volume
410 of the strata must be equal to one (i.e. it must fill the unit hypercube).

411 An example **input_file** can be found in 'STS_Example2' in the provided
412 example Jupyter scripts.

413 *Output Attributes:*

- 414 • **origins:**
415 Specifies the coordinates of the origin of each stratum.
- 416 • **widths:**
417 Specifies the width in each dimension of each stratum.
- 418 • **weights:**
419 The volume of each stratum ($= \text{prod}(\text{widths})$ for each stratum), **weights**
420 are the probabilities assigned to each sample in a stratified sample design.

421 4.1.5 UQpy.SampleMethods.MCMC

422 The MCMC class is imported using the following command:

423 `from UQpy.SampleMethods import MCMC`

424 The attributes of the MCMC class are listed below:

MCMC Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
pdf_proposal_type	Input		★
pdf_proposal_scale	Input		★
pdf_target_type	Input		★
pdf_target	Input	★	
pdf_target_params	Input		★
algorithm	Input		★
jump	Input		★
nsamples	Input	★	
seed	Input		★
nburn	Input		★
samples	Output		

426 A brief description of each attribute can be found in the table below:

MCMC Class Attributes			
Attribute	Type	Options	Default
dimension	<i>integer</i>		dimension = 1
algorithm	<i>string</i>	'MH' 'MMH' 'Stretch'	'MMH'
pdf_proposal_type	<i>string</i>	'Normal' 'Uniform'	'Uniform'
pdf_proposal_scale	<i>float</i> <i>float list</i>		if algorithm = 'MMH' or 'MH': pdf_proposal_scale = [1,1,...,1] if algorithm='Stretch': pdf_proposal_scale = 2
pdf_target_type	<i>string</i>	'marginal.pdf' 'joint.pdf'	if algorithm = 'MMH': pdf_target_type = 'marginal.pdf' if algorithm='Stretch': pdf_target_type = 'joint.pdf'
pdf_target	<i>function</i> <i>string</i>		Normal(0 , I)
pdf_target_params	<i>float</i> <i>float list</i>		None
jump	<i>integer</i>		1
nsamples	<i>integer</i>		None
seed	<i>ndarray</i> <i>ndarray list</i>		array(0,0,...,0) size = 1 × dimension
nburn	<i>integer</i>		0
samples	<i>ndarray</i>		

Detailed Description of MCMC Class Attributes:

Input Attributes:

- **dimension:**
A scalar integer value defining the dimension of the random variables.
- **algorithm:**
Specifies the algorithm used to generate samples. **UQpy** currently supports three commonly used algorithms.
 - 'MH':
Metropolis-Hastings algorithm. For a description of the algorithm, see [5, 4, 1].
 - 'MMH':
Component-wise modified Metropolis-Hastings algorithm. For a description of the algorithm, see [1].
 - 'Stretch':
Affine invariant ensemble sampler employing “stretch” moves. For a description of the algorithm, see [2].

445 • `pdf_proposal_type`:
 446 Type of proposal density function. This option is only invoked when
 447 `algorithm = 'MH'` or `'MMH'`. `UQpy` currently supports two types of
 448 proposal densities:

- 449 – ‘Normal’:
 450 The proposal density is specified as a normal distribution with mean
 451 value equal to the current state of the Markov Chain and standard
 452 deviation specified by `pdf_proposal_scale`. That is, a new candi-
 453 date sample is generated as
 454 $x_{i+1} \sim N(x_i, \text{pdf_proposal_scale})$.
- 455 – ‘Uniform’:
 456 The proposal density is specified as a uniform distribution with cen-
 457 tered at the current state of the Markov Chain with width equal to
 458 `pdf_proposal_scale`. That is, a new candidate sample is generated
 459 as
 460 $x_{i+1} \sim U(x_i - \text{pdf_proposal_scale}/2, x_i + \text{pdf_proposal_scale}/2)$.

461 When `dimension > 1`, `pdf_proposal_type` may be specified as a string
 462 or a list of strings assigned to each dimension. When `pdf_proposal_type`
 463 is specified as a string, the same proposal type is specified for all dimen-
 464 sions.

465 • `pdf_proposal_scale`:
 466 Sets the scale of the proposal probability density. The scale
 467 of the proposal density depends on both the MCMC algorithm
 468 employed (`algorithm`) and the type of proposal density specified
 469 (`pdf_proposal_type`).

- 470 – For `algorithm = 'MH'` or `'MMH'`, this defines either the standard
 471 deviation of a normal proposal density or the width of a uniform
 472 density. See `pdf_proposal_type` above.
- 473 – For `algorithm = 'Stretch'`, this sets the scale of the stretch density
 474 $g(z) = \frac{1}{\sqrt{z}}, \sim z \in [1/\text{pdf_proposal_scale}, \text{pdf_proposal_scale}]$.
 475 See [2].

476 When `dimension > 1`, `pdf_proposal_scale` may be specified as
 477 a scalar or a list of values assigned to each dimension. When
 478 `pdf_proposal_scale` is specified as a scalar, the same scale is specified
 479 for all dimensions.

480 • `pdf_target_type`:
 481 [Use only with `algorithm = 'MMH'`]
 482

483 MCMC algorithms use acceptance-rejection based on a ratio of the target
 484 probability densities between the current state and the proposed state. In
 485 the 'MH' algorithm and the 'Stretch' algorithm, the ratio of probabilities
 486 is computed using the target joint pdf. For the 'MMH' algorithm with
 487 independent random variables, acceptance/rejection can be computed
 488 based on the ratio of the marginals for each dimension. This variable
 489 specifies whether to use a ratio of target joint pdf's or a ratio of target
 490 marginal pdf's in the acceptance-rejection step for each dimension of the
 491 'MMH' algorithm. This option is not used for the 'MH' and 'Stretch'
 492 algorithms.

- 493 – 'joint_pdf':
 494 Compute the acceptance-rejection using the ratio of the target joint
 495 pdf's. [Always use when random variables are dependent.]
- 496 – 'marginal_pdf':
 497 Compute the acceptance-rejection using the ratio of target marginal
 498 pdf's in each dimension. [Only use when random variables are in-
 499 dependent.]

500 • `pdf_target`:
 501 Specifies the target probability density function from which to draw
 502 MCMC samples (i.e. the stationary distribution of the Markov chain).
 503 `pdf_target` must be passed into `MCMC` as a function. In `UQpy`, this can
 504 be achieved in two ways:

- 505 – Direct function definition:
 506 The easiest way to define `pdf_target` is to create a function in the
 507 python script that calls `MCMC`. When the function is directly defined,
 508 `pdf_target` is specified directly using the function name (not as a
 509 string).
- 510 – Definition through 'custom_pdf.py':
 511 If the function is to be called frequently by the user or may need to
 512 be shared among python scripts in a project, the user may define the
 513 function in a python script 'custom_pdf.py' that resides in the user's
 514 working directory. When this is the case, `pdf_target` is specified by
 515 a string that corresponds to the function name in 'custom_pdf.py'.
 516 See Section 5.1 for a detailed description of 'custom_pdf.py'.

517 In both cases, the function must be defined to accept two parameters:

- 518 1. The point at which to compute the pdf,
- 519 2. A list of parameters of the pdf specified through
- 520 `pdf_target_params`

521 If the pdf does not have any user-defined parameters, the user still must

522 define the function to accept a parameter list.

523

524 When `dimension > 1` and `pdf_target_type = 'marginal_pdf'`,

525 `pdf_target` may be specified as a string/function or a list of

526 strings/functions assigned to each dimension. When specified as a

527 string/function, the same marginal pdf is specified for all dimensions.

- 528 • `pdf_target_params`:
529 Parameters of the target pdf to be passed into the function defined by
- 530 `pdf_target`.
- 531 • `jump`
532 Specifies the number of samples between accepted states of the Markov
- 533 chain. Setting `jump = 1` corresponds to accepting every state. Setting
- 534 `jump = n` corresponds skipping $n - 1$ states between accepted states of
- 535 the chain.
- 536 • `nsamples`
537 Specifies the number of samples to be generated (not including skipped
- 538 states of the chain). `nsamples` must be specified. There is no default
- 539 value.
- 540 • `seed`
541 Specifies the initial state of the Markov chain.
- 542
- 543 For `algorithm = 'MMH'` or `'MH'`, this is a numpy array of zeros with
- 544 size $1 \times \text{dimension}$.
- 545
- 546 For `algorithm = 'Stretch'`, this is a list of n_s points, each defined as
- 547 numpy arrays with size $1 \times \text{dimension}$, where n_s is the size of the en-
- 548 semble being propagated. [2]. The default value in the table above is
- 549 not valid for `algorithm = 'Stretch'`.

- **nburn**
Specifies the number of samples at the start of the chain to be discarded as “burn-in.” This option is only applicable for `algorithm=‘MMH’` and `‘MH’`

Output Attributes:

- **samples:**
The only output of the **MCMC** class are the generated samples. The samples are returned as a numpy array of dimension `nsamples × dimension`.

Examples:

Two examples illustrating the use of the **MCMC** class are provided in the following Jupyter scripts.

- **MCMC_Example1.ipynb:**
In this example, the three MCMC algorithms are used to generate 1000 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is defined as a function directly in the script.
- **MCMC_Example2.ipynb:**
In this example, the three MCMC algorithms are used to generate 1000 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is defined as a function in the ‘custom_pdf.py’ script.

4.1.6 `UQpy.SampleMethods.Correlate`

Correlate is a class for inducing correlation in independent standard normal random variables. This is done using the standard Cholesy method as follows. Let **C** denote the symmetric positive definite correlation matrix and **X** denote the `nsamples × dimension` array of independent standard normal samples. Perform the Cholesky decomposition such that:

$$\mathbf{C} = \mathbf{U}\mathbf{U}^T \quad (1)$$

where **U** is a lower-triangular matrix. The `nsamples × dimension` array, **Y** of correlated standard normal samples possessing correlation **C** is determined by:

$$\mathbf{Y}^T = \mathbf{U}\mathbf{X}^T \quad (2)$$

The **Correlate** class is imported using the following command:

```
from UQpy.SampleMethods import Correlate
```

The attributes of the **Correlate** class are listed below:

Correlate Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
input_samples	Input	★	
corr_norm	Input	★	
dimension	Input	★	★
samples_uncorr	Output		
samples	Output		

A brief description of each attribute can be found in the table below:

Correlate Class Attributes			
Attribute*	Type	Options	Default
input_samples	<i>ndarray/object</i>	SampleMethods object or User-defined array	
corr_norm	<i>ndarray</i>	User-defined array	
dimension	<i>integer</i>	Inherited from SampleMethods object or User-defined scalar	
samples_uncorr	<i>ndarray</i>		
samples	<i>ndarray</i>		

* Note: If `input_samples` is a `SampleMethods` object, the `Correlate` object will inherit all attributes of that object.

Detailed Description of Correlate Class Attributes:

Input Attributes:

- **input_samples:**
Contains the independent standard normal random samples on which to impose correlation.

`input_samples` can be an object (instance of a `SampleMethods` class) or an array.

If `input_samples` is an instance of a `SampleMethods` class, then the `Correlate` class inherits all of its attributes and the correlation is induced on the samples contained in the attribute `input_samples.samples`.

595 If `input_samples` is a `numpy` array, then the correlation is induced
 596 directly on `input_samples`. The number of samples is given by
 597 `nsamples=input_samples.shape[0]`.
 598

- 599 • **corr_norm:**
 600 A `numpy` array containing the correlation matrix **C** for the random
 601 variables.
 602
 603 `corr_norm` must be a symmetric positive definite array of size
 604 `dimension × dimension` and satisfy:
 605 $\text{corr_norm}[i, j] = 1$ for $i = j$.
 606 $0 < \text{corr_norm}[i, j] < 1$ for $i \neq j$.
 607 $\text{corr_norm}[i, j] = \text{corr_norm}[j, i]$
- 608 • **dimension:**
 609 A scalar integer value defining the dimension of the random variables.
 610
 611 If `input_samples` is a `SampleMethods` object then `dimension`
 612 is not required since `input_samples` already has the attribute
 613 `input_samples.dimension`.
 614
 615 If `input_samples` is a `numpy` array, `dimension` must be specified.

616 *Output Attributes:*

- 617 • **samples_uncorr:**
 618 A `numpy` array of dimension `nsamples × dimension` containing the orig-
 619 inal uncorrelated standard normal samples.
 620 If `input_samples` is an array then `samples_uncorr=input_samples`.
 621
 622 if `input_samples` is a `SampleMethods` object, then
 623 `samples_uncorr=input_samples.samples`.
- 624 • **samples:**
 625 A `numpy` array of dimension `nsamples × dimension` containing the cor-
 626 related standard normal samples with correlation defined in `corr_norm`.

627 **Examples:**

628 An example illustrating the use of the `Correlate` class is provided in the
 629 following Jupyter script.

630 • `Correlate.ipynb`:

631 In this example, 1000 2-dimensional standard normal samples are corre-
 632 lated according to a specified correlation matrix. The input samples are
 633 specified using both the `MCS` class and as a `numpy` array generated using
 634 `scipy.stats`.

635 4.1.7 `UQpy.SampleMethods.Decorrelate`

`Decorrelate` is a class for removing correlation from a `nsamples×dimension` array, **Y**, of standard normal random samples with correlation matrix **C**. This is performed by simply inverting the expression in Eq. (2) as:

$$\mathbf{X}^T = \mathbf{U}^{-1}\mathbf{Y}^T \quad (3)$$

636 to obtain the `nsamples×dimension` array, **X**, of uncorrelated standard
 637 normal samples.

638

639 The `Decorrelate` class is imported using the following command:

640 `from UQpy.SampleMethods import Decorrelate`

641 The attributes of the `Decorrelate` class are listed below:

642

Decorrelate Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
<code>input_samples</code>	Input	★	
<code>corr_norm</code>	Input	★	
<code>dimension</code>	Input	★	★
<code>samples_corr</code>	Output		
<code>samples</code>	Output		

643 A brief description of each attribute can be found in the table below:

644

Decorrelate Class Attributes			
Attribute*	Type	Options	Default
input_samples	<i>ndarray/object</i>	Object of class Correlate or User-defined array	
corr_norm	<i>ndarray</i>	Inherited from Correlate object or User-defined array	
dimension	<i>integer</i>	Inherited from Correlate object or User-defined scalar	
samples_corr	<i>ndarray</i>		
samples	<i>ndarray</i>		

* Note: If **input_samples** is a **Correlate** object, the **Decorrelate** object will inherit all attributes of that object.

Detailed Description of Decorrelate Class Attributes:

Input Attributes:

- **input_samples:**

Contains the correlated standard normal samples whose correlation will be removed.

input_samples can be an object (instance of the **Correlate** class) or a **numpy** array.

If **input_samples** is an instance of **Correlate**, then the **Decorrelate** class inherits all of its attributes and the decorrelation is performed on the attribute **input_samples.samples**.

If **input_samples** is a **numpy** array, then the decorrelation is performed directly on **input_samples**. The number of samples is given by **nsamples=input_samples.shape[0]**.

- **corr_norm:**

A **numpy** array containing the correlation matrix **C** for the random variables.

671 If `input_samples` is an object of the `Correlate` class, then `corr_norm`
672 is inherited this class.

673

674 If `input_samples` is a numpy array, then `corr_norm` must be specified.

675

676 `corr_norm` must be a symmetric positive definite array of size
677 `dimension × dimension` and satisfy:

678 $\text{corr_norm}[i, j] = 1$ for $i = j$.

679 $0 < \text{corr_norm}[i, j] < 1$ for $i \neq j$.

680 $\text{corr_norm}[i, j] = \text{corr_norm}[j, i]$

681 • **dimension:**

682 A scalar integer value defining the dimension of the random variables.

683

684 If `input_samples` is a `Correlate` object then `dimension` may not
685 be required since `input_samples` may already have the attribute
686 `input_samples.dimension`.

687

688 If `input_samples` is a numpy array, `dimension` must be specified.

689 *Output Attributes:*

690 • **samples_corr:**

691 A numpy array of dimension `nsamples × dimension` containing the
692 original correlated samples.

693

694 If `input_samples` is an array then `samples_corr=input_samples`
695 and if `input_samples` is an object of the `Correlate` class then
696 `samples_corr=input_samples.samples`.

697 • **samples:**

698 A numpy array of dimension `nsamples × dimension` containing the un-
699 correlated standard normal samples.

700 **Examples:**

701 An example illustrating the use of the `Decorrelate` class is provided in the
702 following Jupyter script.

703 • Decorrelate.ipynb:
 704 In this example, 1000 2-dimensional correlated standard normal samples
 705 are generated using the `Correlate` class and using the `scipy.stats`
 706 package. The samples from each are decorrelate using the `Decorrelate`
 707 class.

708 4.1.8 UQpy.SampleMethods.Nataf

`Nataf` is a class for transforming standard normal random samples to a prescribed non-Gaussian distribution using the Nataf transform as follows. Let \mathbf{X} denote an n -dimensional standard normal random vector and let $F_i(y), i = 1, \dots, n$ be the marginal cumulative distribution functions of the n non-Gaussian random variables. The non-Gaussian random vector, \mathbf{Y} , following $F_i(y)$ is defined component-wise through the transformation:

$$Y_i = F_i^{-1}(\Phi(X_i)) \quad (4)$$

709 where $\Phi(x)$ is the standard normal cumulative distribution function.

710

When the random vector X has correlated components possessing correlation matrix \mathbf{C} and correlation coefficients ρ_{ij} between components X_i and X_j , the transformation in Eq. (4) causes a so-called *correlation distortion* such that the correlation coefficient between the non-Gaussian variables Y_i and Y_j , denoted ξ_{ij} is not equal to the correlation between the Gaussian variables ($\rho_{ij} \neq \xi_{ij}$). The non-Gaussian correlation coefficient, ξ_{ij} , can be determined from the Gaussian correlation coefficient, ρ_{ij} , through the following integral:

$$\xi_{ij} = \frac{1}{\sigma_{Y_i} \sigma_{Y_j}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (F_i^{-1}(\Phi(x_i)) - \mu_{Y_i}) (F_j^{-1}(\Phi(x_j)) - \mu_{Y_j}) \phi(x_i, x_j; \rho_{ij}) dx_i dx_j \quad (5)$$

711 The `Nataf` class is imported using the following command:

712 `from UQpy.SampleMethods import Nataf`

713 The attributes of the `Nataf` class are listed below:

Nataf Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
input_samples	Input		★
corr_norm	Input	★	
dist_name	Input	★	
dist_params	Input	★	
dimension	Input	★	★
samplesN01	Output		
samples	Output		
corr	Output		
jacobian	Output		

A brief description of each attribute can be found in the table below:

Nataf Class Attributes			
Attribute	Type	Options	Default
input_samples	<i>ndarray/object</i>	SampleMethods object or User-defined array	None
corr_norm	<i>ndarray</i>	Inherited from SampleMethods object or User-defined array	Identity Matrix $I_{\text{dimension}}$
dimension	<i>integer</i>	Inherited from SampleMethods object or User-defined integer	
dist_name	<i>function/string list</i>	name attribute from Distributions class See Section 5.1	
dist_params	<i>ndarray list</i>	See Section 5.1	
samplesN01	<i>ndarray</i>		
samples	<i>ndarray</i>		
corr	<i>ndarray</i>		
jacobian	<i>ndarray list</i>		

Detailed Description of Nataf Class Attributes:

Input Attributes:

- **input_samples:**

Contains the samples to be transformed. The samples need to be standard normal samples i.e $\sim N(0, 1)$.

input_samples can be a SampleMethods object or a $\text{nsamples} \times \text{dimension}$ numpy array. The Nataf transformation is applied to the samplesN01 object. Depending on the type of input_samples, samplesN01 is assigned as follows:

729 – If `input_samples` is a `SampleMethods` object, then the `Nataf`
730 class inherits all the attributes of that object and `samplesN01 =`
731 `input_samples.samples`
732

733 – If `input_samples` is an array, then `samplesN01 = input_samples`.
734

735 If `input_samples` is not provided, then `Nataf` calculates the correlation
736 distortion of the standard normal correlation matrix `corr_norm` from
737 Eq. (5).
738

739 The default value of `input_samples` is `None`.
740

741 • **dimension:**
742 A scalar integer value defining the dimension of the random variables.
743

744 If `input_samples` is a `SampleMethods` object, then `dimension` may
745 not be required since `input_samples` may already have the attribute
746 `input_samples.dimension`.
747

748 If `input_samples` is a numpy array, `dimension` must be specified.

749 • **corr_norm:**
750 A numpy array containing the correlation matrix **C** for the standard
751 normal random variables.
752

753 `corr_norm` must be a symmetric positive definite array of size
754 `dimension × dimension` and satisfy:

755 `corr_norm[i, j] = 1` for `i = j`.
756 `0 < corr_norm[i, j] < 1` for `i ≠ j`.
757 `corr_norm[i, j] = corr_norm[j, i]`

758 If `input_samples` is an object of type `Correlate` then `corr_norm` is
759 inherited from this object.
760

761 The default value of `corr_norm` is the `dimension × dimension` identity
762 matrix **I_{dimension}**.
763

764 • **dist_name:**
765 Specifies the name of the marginal distribution that each transformed
766 random variable.
767
768 **dist_name** may be a string or a list of strings of length **dimension**.
769
770 For each dimension **i**, **dist_name[i]** must be a string specifying a
771 distribution defined in the **Distributions** module (see Sec. 5.1). To
772 use a custom distribution, set **dist_name[i] = 'custom_dist'** to use the
773 custom distribution assignment option in the **Distributions** module
774 (again, see Sec. 5.1).
775
776 If **dist_name** is a string (or a list of length one) and **dimension > 1**,
777 then **dist_name** is converted into a list of length **dimension** with each
778 component having identical distribution name.
779
780 **dist_name** must be specified. There is no default value.
781
781 • **dist_params:**
782 Specifies the parameters for each marginal distribution in **dist_name** as
783 defined in the **Distributions** module (see Sec. 5.1).
784
785 Each set of parameters is defined as a **numpy** array. **dist_params** is a
786 list of arrays, with each item in the list corresponding to the associated
787 random variable.
788
789 If **dist_params** is an array (or a list of length one), then **dist_params**
790 is converted to a list of length **dimension** with each component having
791 the same parameters.
792
793 **dist_params** must be specified. There is no default value.
794 *Output Attributes:*
795
795 • **samplesN01:**
796 A **numpy** array of dimension **nsamples × dimension** containing the
797 correlated or uncorrelated standard normal samples that have been
798 transformed.
799

800 If `input_samples = None`, `samplesN01` is not returned.
801

802 If `input_samples` is a `SampleMethods` object, then `samplesN01`
803 `= SampleMethods.samples`. If `input_samples` is an array then
804 `samplesN01 = input_samples`.
805

- 806 • **samples:**
807 A numpy array of dimension `nsamples × dimension` containing the
808 correlated or uncorrelated transformed samples following the prescribed
809 distribution.
810

811 If `input_samples = None`, `samples` is not returned.
812

- 813 • **corr:**
814 A numpy array containing the transformed/distorted correlation matrix.
815

816 If `corr_norm = None` or `corr_norm = I`, where **I** is the identity matrix,
817 then `corr = corr_norm = I`.
818

- 819 • **jacobian:**
820 A list of numpy arrays containing the Jacobian of the transformation
821 evaluated at each sample.
822

823 **Examples:**
824 Three examples illustrating the use of the `Nataf` class are provided in the
825 following Jupyter scripts.

- 826 • **Nataf - Example 1.ipynb:**
827 In this example, the `Nataf` class is used in order to transform 1000
828 samples of 2 uncorrelated standard normal variables to a lognormal and
829 a gamma distribution. The example illustrates the transformation for
830 samples drawn using the `MCS` class and for samples specified as a **numpy**
831 array.
- 832 • **Nataf - Example 2.ipynb:**
833 In this example, the `Nataf` class is used in order to transform 1000
834 samples of 2 correlated standard normal variables to a lognormal and

835 a gamma distribution. The example illustrates the transformation for
 836 samples drawn using the `MCS` class and correlated using the `Correlate`
 837 class and for samples specified as a `numpy` array.

- 838 • Nataf - Example 3.ipynb:
 839 In this example, the `Nataf` class is used to calculate the correlation
 840 distortion for the transformation of two correlated random variables from
 841 a standard normal to a lognormal distribution.

842 4.1.9 `UQpy.SampleMethods.InvNataf`

843 `InvNataf` is a class for transforming non-Gaussian random variables to equiv-
 844 alent standard normal space. The `InvNataf` class is imported using the fol-
 845 lowing command:

```
846 from UQpy.SampleMethods import InvNataf
```

847 The attributes of the `InvNataf` class are listed below:

InvNataf Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
<code>input_samples</code>	Input	★	★
<code>dimension</code>	Input	★	★
<code>corr</code>	Input	★	
848 <code>dist_name</code>	Input	★	★
<code>dist_params</code>	Input	★	★
<code>samplesNG</code>	Output		
<code>samples</code>	Output		
<code>corr_norm</code>	Output		
<code>jacobian</code>	Output		

849 A brief description of each attribute can be found in the table below:

InvNataf Class Attributes			
Attribute	Type	Options	Default
input_samples	<i>ndarray/object</i>	Attribute of class MCS, LHS, STS, Correlate, Nataf or User-defined array	None
corr	<i>ndarray</i>	Attribute of class Nataf or User-defined array	
dimension	<i>integer</i>	Attribute of class MCS, LHS, STS, Correlate, Nataf or User-defined scalar	
dist_name	<i>function/string list</i>	See Distributions Module or User-defined function	
dist_params	<i>ndarray list</i>		
samplesNG	<i>ndarray</i>		
samples	<i>ndarray</i>		
corr_norm	<i>ndarray</i>		
jacobian	<i>ndarray list</i>		

Detailed Description of InvNataf Class Attributes:

Input Attributes:

- **input_samples:**

Contains the samples to be transformed to standard normal samples.

`input_samples` can be an object of type MCS, LHS, STS, Correlate, Nataf or a numpy array.

If `input_samples` is an object of type MCS, LHS, STS, Correlate, Nataf, then the `InvNataf` class inherits all the attributes of the class and the transformation is performed to the attribute `.samples` of the class.

If `input_samples` is an array then the transformation is performed directly to the `input_samples`. The number of samples is given by `nsamples=input_samples.shape[0]`.

If `input_samples` is not provided then class `InvNataf` calculates the correlation matrix `corr_norm` in the standard normal space.

The default value of `input_samples` is None.

874 • **dimension:**
875 A scalar integer value defining the dimension of the random variables.

876 • **corr:**
877 A numpy array showing the correlation coefficients between the
878 non-Gaussian random variables.

879
880 **corr** must be an array of size **dimension** \times **dimension** and satisfy:
881

882 $\text{corr}[i, j] = 1$ for $i = j$.
883 $\text{corr}[i, j] < 1$ for $i \neq j$.
884

885 if **input_samples** is an object of type **Nataf** then **corr** is an attribute
886 of this class.
887

888 if **input_samples** is an object of type **MCS**, **LHS**, **STS** then **corr** is set
889 to be the identity matrix **I_dimension**.
890

891 • **dist_name:**
892 Defines the name of the marginal distribution that each standard
893 normal random variable will be transformed to.

894
895 **dist_name** may be a string, a function, or a list of strings/functions.
896

897 If **dist_name[i]** is a string, the distribution is matched with one of the
898 available functions in the **Distributions** module (see Sec. 5.1) or the
899 ‘custom_dist.py’ (again see Sec. 5.1).
900

901 if **dist_name[i]** is a function, it must be defined in the user’s Python
902 script and passed directly as a function.
903

904 **dist_name** can contain an arbitrary combination of strings and functions.
905

906 If **dist_name** is a string or function (or a list of length one) and
907 **dimension** > 1 , then **dist_name** is converted into a list of length

908 `dimension` with each variable having the distribution.
 909

910 if `data` is not an object of type `MCS`, `LHS`, `STS`, `Nataf` then `dist_name`
 911 must be specified. There is no default value.

912 • `dist_params`:
 913 Specifies the parameters for each marginal distribution in `dist_name`.
 914

915 Each set of parameters is defined as a numpy array. `dist_params` is a
 916 list of arrays, with each item in the list corresponding to the associated
 917 random variable.
 918

919 If `dist_params` is an array (or a list of length one), then `dist_params`
 920 is converted to a list of length `dimension` with each variable having the
 921 same parameters.
 922

923 if `input_samples` is not an object of type `MCS`, `LHS`, `STS`, `Nataf` then
 924 `dist_params` must be specified. There is no default value.

925 *Output Attributes:*

926 • `samplesNG`:
 927 A numpy array of dimension `nsamples` \times `dimension` containing the
 928 correlated or uncorrelated non-Gaussian samples. It is an output of the
 929 class only if `data` is not `None`.
 930

931 If `input_samples` is an object of type `MCS`, `LHS`, `STS`, `Correlate`,
 932 `Nataf` then `samplesNG` `.samples`. If `input_samples` is an array then
 933 `samplesNG=input_samples`.
 934

935 • `samples`:
 936 A numpy array of dimension `nsamples` \times `dimension` containing the
 937 correlated or uncorrelated standard normal samples. It is an output of
 938 the class only if `input_samples` is not `None`.
 939

940 • `corr_norm`:
 941 A numpy array containing the correlation matrix in the standard

942 normal space.

943

944 if `data` is an object of type `MCS`, `LHS`, `STS`, `Correlate` then `corr =`
945 `corr_norm = I_dimension`.

946

947 • **jacobian:**
948 A list containing the jacobian of the transformation for each sample as
949 an numpy array.

950

951 **Examples:**

952 An example illustrating the use of the `Correlate` class is provided in the
953 following Jupyter script.

- 954 • **InvNataf - Example 1.ipynb:**
955 In this example, `InvNataf` class is used in order to transform 2 correlated
956 lognormal variables to two standard normal random variables.
- 957 • **InvNataf - Example 2.ipynb:**
958 In this example, `Nataf` class is used to perform the Iterative Translation
959 Approximation Method (ITAM) [6] to estimate the underlying Gaussian
960 correlation from known values of the correlation for lognormal random
961 variables.

962 **4.2 Surrogates Module**

963 The `Surrogates` module consists of classes and functions to build simplified
964 mathematical expressions to interpolate data and serve as a meta-model, sur-
965rogate model, or emulator. It is imported in a python script using the following
966 command:

967 **from** `UQpy` **import** `Surrogates`

968 The `Surrogates` module has the following classes, each corresponding to a
969 different surrogate model form:

Class	Method
<code>SRM</code>	Stochastic Reduced Order Model

970

971 4.2.1 UQpy.Surrogates.SROM

972 SROM takes a set of samples and attributes of a distribution and optimizes the
 973 sample probability weights according to the method of Stochastic Reduced
 974 Order Models as defined by Grigoriu [3]. The SROM class is imported using the
 975 following command:

976 `from UQpy.Surrogates import SROM`

977 The attributes of the SROM class are listed below:

SROM Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
samples	Input	★	
cdf_target	Input	★	
cdf_target_params	Input	★	
properties	Input		★
978 moments	Input	★	
correlation	Input		★
weights_error	Input		★
weights_distribution	Input		★
weights_moments	Input		★
weights_correlation	Input		★
sample_weights	Output		

979 A brief description of each attribute can be found in the table below:

SROM Class Attributes			
Attribute	Type	Options	Default
samples	<i>ndarray</i>		None
cdf_target	<i>function/string list</i>		None
cdf_target_params	<i>ndarray list</i>		None
properties	<i>boolean list</i>	True False	[True, True, True, False]
981 moments	<i>ndarray list</i>		None
correlation	<i>ndarray</i>		Identity matrix
weights_error	<i>list</i>		[1, 0.2, 0]
weights_distribution	<i>ndarray list</i>		Array of ones with size of samples
weights_moments	<i>ndarray list</i>		$\frac{1}{\text{moments}^2}$
weights_correlation	<i>ndarray list</i>		
sample_weights	<i>ndarray</i>		

982 **Detailed Description of SROM Class Attributes:**

983

984 *Input Attributes:*

985 • **samples:**

986 An array or list containing the samples from which to build the Stochastic
987 Reduced Order Model.

988 • **cdf_target:**

989 A list of functions or strings specifying the Cumulative Distribution
990 Functions (CDFs) of the random variables.

991

992 If `cdf_target[i]` is a string, the distribution is matched with its
993 corresponding `cdf (cdf)` in the `Distributions` module (see Sec. 5.1) or
994 the `cdf` defined by ‘`custom_dist.py`’ (again see Sec. 5.1).

995

996 if `cdf_target[i]` is a function, it must be defined in the user’s Python
997 script and passed directly as a function.

998

999 `cdf_target` can contain an arbitrary combination of strings and
1000 functions.

1001

1002 When `dimension > 1`, `cdf_target` may be specified as a string/function
1003 or a list of strings/functions assigned to each dimension. When specified
1004 as a string/function, the same `cdf` is specified for all dimensions.

1005 • **cdf_target_params:**

1006 A list of parameters corresponding to each random variable where the
1007 parameters for each random variable are assigned as a numpy array..

1008

1009 Example: `cdf_target = ['Gamma']` and `cdf_target_params =`
1010 `[np.array([2, 1, 3])]` , where the random variables have gamma
1011 distribution with shape, shift and scale parameters equal to 2, 1 and 3
1012 respectively.

1013 • **properties:**

1014 A boolean list specifying which properties of the distribution are to be
1015 included in the objective function. The list is of size 4 with the items of
1016 the list defined as follows:

1017 1. *it CDF*: Minimize error in the match to the cumulative distribution
1018 function.

1019 2. *it mean*: Minimize error in the first-order moments about the origin.

1020 3. *variance*: Minimize error in the second-order moments about the
1021 origin.

1022 4. *correlation*: Minimize error in correlation.

1023 ‘True’ includes the corresponding property in the objection function and
1024 ‘False’ excludes it.

1025 • **moments**:
1026 A list of numpy arrays specifying the first and second-order moments
1027 about the origin for each random variable. **SROM** supports the following
1028 size of **moments** array:

1029 – Array of size $1 \times \text{dimension}$: If error in either, but not both, first
1030 or second-order moments is included in **SROM**.

1031 – Array of size $2 \times \text{dimension}$: If error in both first and second-
1032 order moments are included in the **SROM**. The first row contains
1033 first-order moments and the second row contains the second-order
1034 moments.

1035 • **correlation**:
1036 An array specifying the correlations among the random variables. It is
1037 defined such that size of array is $\text{dimension} \times \text{dimension}$.

1038 • **weights_error**:
1039 **SROM** generates **sample_weights** which minimize the error between the
1040 cdf, moments, and correlation of the samples and the probability model.
1041 **weights_error** specifies weights assigned to each property in the objec-
1042 tive function as outlined in [3]. It is a list of size 3 with the items defined
1043 as follows:

1044 – *Item 1*: Weight assigned to the cumulative distribution function.

1045 – *Item 2*: Weight assigned to the first and second marginal moments.

1046 – *Item 3*: Weight assigned to the correlation matrix.

1047 Default values are set as in [3].

1048 • **weights_distribution:**
1049 A list of arrays containing weights defining the error in distribution at
1050 each sample of the random variables. **SROM** supports the following options
1051 for **weights_distribution**:

- 1052 – **None**: Default value is defined as an array of the same size as
1053 **samples** with each value equal to 1. For default value, See [3].
- 1054 – Array of size $1 \times \text{dimension}$: Equal weights are assigned to all
1055 samples in same dimension.
- 1056 – Arbitrary array of the same size as **samples**: User specifies all
1057 weights explicitly.

1058 • **weights_moments:**
1059 A list of arrays containing weights defining the error in moments in each
1060 dimension. **SROM** supports the following options for **weights_moments**:

- 1061 – **None**: Default value is defined as array of the same size as **moments**
1062 with each value equal to the reciprocal of the square of **moments**.
1063 For default value, see [3].
- 1064 – Array of size $1 \times \text{dimension}$: Equal weights are assigned to both
1065 moments in same dimension.
- 1066 – Array of size same as **moments**: User specifies all weights explicitly.

1067 • **weights_correlation:**
1068 A list of arrays containing the weights defining the error in correlation
1069 among random variables. It is define such that the size of the array is
1070 the same as **correlation**. For default value, See [3].

1071 *Output Attributes:*

- 1072 • **sample_weights:**
1073 The generated **SROM** weights corresponding to **samples**. The samples
1074 are returned as a numpy array with each sampling having a correspond-
1075 ing weight.

1076 **Examples:**
1077 Two examples illustrating the use of the **SROM** class are provided in the follow-
1078 ing Jupyter scripts.

- 1079 • **SROM.Example1.ipynb:**
1080 In this example, the **STS** is used to generate 16 samples from a two-
1081 dimensional Gamma pdf. The Gamma pdf is defined as a function di-
1082 rectly in the script. Then, **SROM** is used to obtain sample weights.

1083 • `SROM.Example2.ipynb`:
 1084 In this example, sample weights are compared when `SROM` is called using
 1085 default values for `weights_distribution` and `weights_moments` and
 1086 when `SROM` is called with user-defined values for `weights_distribution`
 1087 and `weights_moments`.

1088 4.2.2 `UQpy.Surrogates.Kriging` (Coming in V2.0)

1089 4.3 Reliability Module

1090 The `Reliability` module consists of classes and functions to provide
 1091 simulation-based estimates of probability of failure from a given user-defined
 1092 computational model and failure criterion. It is imported in a python script
 1093 using the following command:

```
1094 from UQpy import Reliability
```

1095 The `Reliability` module has the following classes, each corresponding to a
 1096 method for probability of failure estimation:

	Class	Method
1097	<code>SubsetSimulation</code>	Subset Simulation
	<code>TaylorSeries</code>	FORM/SORM

1098 Each class can be imported individually into a python script. For example,
 1099 the `SubsetSimulation` and the `TaylorSeries` classes can be imported to a
 1100 script using the following commands:

```
1101 from UQpy.SampleMethods import SubsetSimulation
```

```
1102 from UQpy.SampleMethods import TaylorSeries
```

1103 The following subsections describe each class, their respective inputs and at-
 1104 tributes, and their use.

1105 4.3.1 `UQpy.Reliability.SubsetSimulation`

1106 The `SubsetSimulation` class is imported using the following command:

```
1107 from UQpy.Reliability import SubsetSimulation
```

1108 The attributes of the `SubsetSimulation` class are listed below:

1109

SubsetSimulation Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
nsamples_init	Input		★
nsamples_ss	Input	★	
p_cond	Input		★
algorithm	Input		★
pdf_target_type	Input		★
pdf_target	Input	★	
pdf_target_params	Input		★
pdf_proposal_type	Input		★
pdf_proposal_scale	Input		★
model_type	Input		★
model_script	Input	★	
input_script	Input		★
output_script	Input		★
samples	Output		
g	Output		
g_level	Output		
pf	Output		

1110 A brief description of each attribute can be found in the table below:

1111

SubsetSimulation Class Attributes			
Attribute	Type	Options	Default
dimension	<i>integer</i>		dimension = 1
samples_init	<i>nparray</i>		None
nsamples_ss	<i>integer</i>		None
p_cond	<i>float</i>	$0 < \text{p_cond} < 1$	p_cond = 0.1
algorithm	<i>string</i>	'MMH' 'Stretch'	'MMH'
pdf_target_type	<i>string</i>	'marginal_pdf' 'joint_pdf'	'marginal_pdf'
pdf_target	<i>function</i> <i>string</i>		Normal(0, I)
pdf_target_params	<i>float</i> <i>float list</i>		None
pdf_proposal_type	<i>string</i>	'Normal' 'Uniform'	'Uniform'
pdf_proposal_scale	<i>float</i> <i>float list</i>		algorithm = 'MMH' or 'MH' [1,1,...,1] algorithm='Stretch' 2
model_type	<i>string</i>	See UQpy.RunModel	See UQpy.RunModel
model_script	<i>string</i>	See UQpy.RunModel	See UQpy.RunModel
input_script	<i>string</i>	See UQpy.RunModel	See UQpy.RunModel
output_script	<i>string</i>	See UQpy.RunModel	See UQpy.RunModel
samples	<i>nparray list</i>		
g	<i>nparray list</i>		
g_level	<i>list</i>		
pf	<i>float</i>		

Detailed Description of SubsetSimulation Class Attributes:

Input Attributes:

- **dimension:**

A scalar integer value defining the dimension of the random variables.

- **samples_init**

Specifies the initial samples for subset/level 0. The size of the array **samples_init** must be **nsamples_ss**×**dimension**. These samples can be generated in any way the user chooses.

If **samples_init** is not specified, the subset/level 0 samples are drawn internally in **SubsetSimulation** using the component-wise Modified Metropolis-Hastings algorithm.

1126 • **nsamples_ss**
1127 Specifies the number of samples to be generated in each conditional level
1128 (i.e. per subset). **nsamples_ss** must be specified. There is no default
1129 value.

1130 • **p_cond**
1131 Specifies the conditional probability for each subset.
1132

1133 The current implementation does not allow for variable conditional
1134 probabilities (i.e. setting different conditional probabilities for each
1135 level).
1136

1137 The current implementation does not allow for the conditional proba-
1138 bilities to be defined implicitly by instead specifying the intermediate
1139 failure domains explicitly.

1140 • **algorithm:**
1141 Specifies the MCMC algorithm used to generate samples in each condi-
1142 tional level. **SubsetSimulation** currently supports two commonly-used
1143 algorithms.

1144 – ‘MMH’:
1145 Component-wise modified Metropolis-Hastings algorithm. For a
1146 description of the algorithm, see [1].

1147 – ‘Stretch’:
1148 Affine invariant ensemble sampler employing “stretch” moves. For
1149 a description of the algorithm, see [2].

1150 **SubsetSimulation** currently does not support the conventional
1151 Metropolis-Hastings algorithm.

1152 • **pdf_target_type:**
1153 This is used for Markov Chain Monte Carlo (MCMC) sampling from
1154 the conditional probability densities in subset simulation. For details,
1155 the user is referred to documentation for **UQpy.SampleMethods.MCMC** in
1156 Section 4.1.5

1157 • **pdf_target:**
1158 This is used for Markov Chain Monte Carlo (MCMC) sampling from
1159 the conditional probability densities in subset simulation. For details,

1160 the user is referred to documentation for `UQpy.SampleMethods.MCMC` in
 1161 Section 4.1.5

- 1162 • `pdf_target_params`:
 1163 This is used for Markov Chain Monte Carlo (MCMC) sampling from
 1164 the conditional probability densities in subset simulation. For details,
 1165 the user is referred to documentation for `UQpy.SampleMethods.MCMC` in
 1166 Section 4.1.5
- 1167 • `pdf_proposal_type`:
 1168 This is used for Markov Chain Monte Carlo (MCMC) sampling from
 1169 the conditional probability densities in subset simulation. For details,
 1170 the user is referred to documentation for `UQpy.SampleMethods.MCMC` in
 1171 Section 4.1.5
- 1172 • `pdf_proposal_scale`:
 1173 This is used for Markov Chain Monte Carlo (MCMC) sampling from
 1174 the conditional probability densities in subset simulation. For details,
 1175 the user is referred to documentation for `UQpy.SampleMethods.MCMC` in
 1176 Section 4.1.5
- 1177 • `model_type`
 1178 This is used to evaluate the model at each sample point using the
 1179 `RunModel` class. For details, the user is referred to documentation for
 1180 `UQpy.RunModel` in Section 4.6.
- 1181 • `model_script`
 1182 This is used to evaluate the model at each sample point using the
 1183 `RunModel` class. For details, the user is referred to documentation for
 1184 `UQpy.RunModel` in Section 4.6.
 1185

1186 Note that a computational model must be specified using `model_script`.
 1187 Without this model, `SubsetSimulation` cannot run.

- 1188 • `input_script`
 1189 This is used to evaluate the model at each sample point using the
 1190 `RunModel` class. For details, the user is referred to documentation for
 1191 `UQpy.RunModel` in Section 4.6.
- 1192 • `output_script`
 1193 This is used to evaluate the model at each sample point using the

1194 `RunModel` class. For details, the user is referred to documentation for
1195 `UQpy.RunModel` in Section 4.6.

1196 *Output Attributes:*

1197 • **samples:**
1198 Contains the sample values from each conditional level as a list of
1199 numpy arrays.

1200
1201 Each item of the list is a numpy array containing the sam-
1202 ples from the corresponding conditional level. For example,
1203 `SubsetSimulation.samples[0]` contains a numpy array of dimension
1204 `nsamples_ss × dimension` with the samples from conditional level 0 (i.e.
1205 the initial sample set).

1206 • **g**
1207 Returns the scalar values of the performance function evaluated by the
1208 computational model at each point in **samples**. **g** is structured in the
1209 same manner as **samples** (a *numpy array list*) with each entry equal to
1210 the performance function evaluation of the corresponding sample.

1211
1212 By convention, failure of a given sample `sample[i][j]` is defined by
1213 `g[i][j] < 0`, where *i* indexes the conditional level and *j* indexes the
1214 sample number. For use with `SubsetSimulation`, the user's compu-
1215 tational model must return a scalar value that follows this convention.
1216 The value is passed from `RunModel` into `SubsetSimulation` through the
1217 attribute `RunModel.model_eval.QOI` as detailed in Section 4.6.

1218 • **g_level**
1219 Specifies the value of the performance function for each conditional level.
1220 **g_level** is structured as a list with each entry of the list equal to the value
1221 of the corresponding performance function at the respective conditional
1222 level. For example, `g_level[3]` corresponds to the performance function
1223 value that defines the third subset.

1224 Note that **g_level** is implicitly defined by the **samples** and **p_cond**. `UQpy`
1225 currently does not support the direct assignment of conditional perfor-
1226 mance levels.

1227 • **pf**
1228 Probability of failure estimate from subset simulation

1229 **SubsetSimulation Examples:**

1230 Two examples illustrating the use of the **MCMC** class are provided in the follow-
1231 ing Jupyter scripts.

1232 • **MCMC_Example1.ipynb:**

1233 In this example, the three MCMC algorithms are used to generate 1000
1234 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is
1235 defined as a function directly in the script.

1236 • **MCMC_Example2.ipynb:**

1237 In this example, the three MCMC algorithms are used to generate 1000
1238 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is
1239 defined as a function in the 'custom_pdf.py' script.

1240 **4.3.2 UQpy.Reliability.TaylorSeries (Coming in V2.0)**

1241 The **FORM** class is imported using the following command:

1242 `from UQpy.Reliability import TaylorSeries`

1243 The attributes of the **SubsetSimulation** class are listed below:

1244

SubsetSimulation Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
nsamples_init	Input		★
nsamples_ss	Input	★	
p_cond	Input		★
algorithm	Input		★
pdf_target_type	Input		★
pdf_target	Input	★	
pdf_target_params	Input		★
pdf_proposal_type	Input		★
pdf_proposal_scale	Input		★
model_type	Input		★
model_script	Input	★	
input_script	Input		★
output_script	Input		★
samples	Output		
g	Output		
g_level	Output		
pf	Output		

1245 4.4 Inference Module

1246 4.4.1 InfoModelSelection (Coming in V2.0)

1247 Information-theoretic model selection coming soon...

1248 4.4.2 BayesModelSelection (Coming in V2.0)

1249 Bayesian model selection coming soon...

1250 4.4.3 BayesParameterEstimation (Coming in V2.0)

1251 Bayesian parameter estimation coming soon...

1252 4.5 StochasticProcess Module (Coming in V2.0)

1253 The `StochasticProcess` module consists of classes and functions to generate
1254 samples of Stochastic Processes from Power Spectrum, Bispectrums and Auto-
1255 correlation Functions. The generated Stochastic Processes can be transformed
1256 into other random variables. We can import the module into a Python script
1257 with the following command

```
1258 from UQpy import StochasticProcess
```

1259 The `StochasticProcess` module has the following classes, each corresponding
1260 to a different method:

1261	Class	Method
	SRM	Spectral Representation Method
	BSRM	Bispectral Representation Method
	KLE	Karhunen Louve Expansion
	Translate	Translate Gaussian into Non-Gaussian
	Inverse_Translate	Translates Non-Gaussian into Gaussian

1262 Each class can be imported individually into a python script. For example,
1263 the `SRM` class can be imported to a script using the following command:

```
1264 from UQpy.StochasticProcess import SRM
```

1265 The following subsections describe each class, their respective inputs and at-
1266 tributes, and their use.

1267 4.5.1 UQpy.StochasticProcess.SRM (Coming in V2.0)

1268 **SRM** is a class for generating Stochastic Processes by Spectral Representation
 1269 Method from a prescribed Power Spectral Density Function. The **SRM** class is
 1270 imported using the following command:

1271 `from UQpy.StochasticProcess import SRM`

1272 The attributes of the **SRM** class are listed below:

SRM Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
nsamples	Input	★	
S	Input	★	
dw	Input	★	
nt	Input	★	
nw	Input	★	
case	Input	★	
g	Input	★	
samples	Output		

1274 Description of SRM Class Attributes:

1275

1276 *Input Attributes:*

- 1277 • **nsamples:**
 1278 A scalar integer value defining the the number of samples of the Stochas-
 1279 tic Process to be generated.
- 1280 • **S:**
 1281 A numpy array defining the Power Spectral Density to be used for
 1282 generation of the Stochastic Processes.
- 1283
- 1284 • **dw:**
 1285 The length of the frequency discretisation to be used for the generation
 1286 of the Stochastic Processes.
- 1287
- 1288 • **nt:**
 1289 Specifies the number of time discretisations of the generated Stochastic
 1290 Processes.
- 1291

- 1292 • **nw:**
1293 Specifies the number of frequency discretisations of the Power Spectrum.
1294
- 1295 • **case:**
1296 A String specifying if it is a univariate or multivariate Stochastic
1297 Process. Acceptable values are 'uni' for one variable case and 'multi'
1298 for multi variable case.
1299
- 1300 • **g:**
1301 A numpy array defining the Cross Power Spectral Density. It is only
1302 used in the 'multi' case.
1303

1304 *Output Attributes:*

- 1305 • **samples:**
1306 A numpy array of samples following the Power Spectral Density.

1307 **Examples:**
1308 A bunch of example files illustrating the use of the **SRM** class are provided:

- 1309 • **SRM_1D_1V.ipynb:**
1310 In this example, one-dimensional uni-variate Stochastic Processes are
1311 generated.
- 1312 • **SRM_1D_mV.ipynb:**
1313 In this example, one-dimensional multi-variate Stochastic Processes are
1314 generated.
- 1315 • **SRM_nD_1V.ipynb:**
1316 In this example, n-dimensional uni-variate Stochastic Processes are gen-
1317 erated.
- 1318 • **SRM_nD_mV.ipynb:**
1319 In this example, n-dimensional multi-variate Stochastic Processes are
1320 generated.

1321 4.5.2 **UQpy.StochasticProcess.BSRM** (Coming in V2.0)

1322 **BSRM** is a class for generating Stochastic Processes by BiSpectral Representa-
1323 tion Method from a prescribed Power Spectral Density Function and a Bis-
1324 spectral Density Function. The **BSRM** class is imported using the following
1325 command:

1326 `from UQpy.StochasticProcess import BSRM`

1327 The attributes of the BSRM class are listed below:

1328

BSRM Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
<code>nsamples</code>	Input	★	
<code>S</code>	Input	★	
<code>B</code>	Input	★	
<code>dt</code>	Input	★	
<code>dw</code>	Input	★	
<code>nt</code>	Input	★	
<code>nw</code>	Input	★	
<code>samples</code>	Output		

1329 **Description of BSRM Class Attributes:**

1330

1331 *Input Attributes:*

- 1332 • **nsamples:**
1333 A scalar integer value defining the the number of samples of the Stochastic
1334 Process to be generated.
- 1335 • **S:**
1336 A numpy array defining the Power Spectral Density to be used for
1337 generation of the Stochastic Processes.
- 1338
- 1339 • **B:**
1340 A numpy array defining the BiSpectral Density to be used for generation
1341 of the Stochastic Processes.
- 1342
- 1343 • **dt:**
1344 The length of the time discretisation to be used for the generation of
1345 the Stochastic Processes.
- 1346
- 1347 • **dw:**
1348 The length of the frequency discretisation to be used for the generation
1349 of the Stochastic Processes.
- 1350

- 1351 • **nt:**
1352 Specifies the number of time discretisations of the generated Stochastic
1353 Processes.
1354
- 1355 • **nw:**
1356 Specifies the number of frequency discretisations of the Power Spectrum.
1357

1358 *Output Attributes:*

- 1359 • **samples:**
1360 A numpy array of samples generated by the BiSpectral Representation
1361 Method.

1362 **Examples:**

1363 Example files illustrating the use of the **BSRM** class have been provided:

- 1364 • **BSRM_1D.ipynb:**
1365 In this example, one-dimensional Stochastic Processes are generated by
1366 BSRM method.
- 1367 • **BSRM_nD.ipynb:**
1368 In this example, n-dimensional Stochastic Processes are generated by
1369 BSRM method.

1370 4.5.3 **UQpy.StochasticProcess.KLE** (Coming in V2.0)

1371 **KLE** is a class for generating Stochastic Processes by Karhunen Louve Expan-
1372 sion from a prescribed Autocorrelation Function. The **BSRM** class is imported
1373 using the following command:

```
1374 from UQpy.StochasticProcess import KLE
```

1375 The attributes of the **KLE** class are listed below:

KLE Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
nsamples	Input	★	
R	Input	★	
samples	Output		

1377 **Description of KLE Class Attributes:**

1378

1379 *Input Attributes:*

- 1380 • **nsamples:**
1381 A scalar integer value defining the the number of samples of the Stochas-
1382 tic Process to be generated.
- 1383 • **R:**
1384 A numpy array defining the Autocorrelation Function to be used for
1385 generation of the Stochastic Processes.

1386

1387 *Output Attributes:*

- 1388 • **samples:**
1389 A numpy array of samples generated by the Karhunen Louve Expansion.

1390 **Examples:**

1391 An example files illustrating the use of the KLE class have been provided:

- 1392 • **KLE.ipynb:**
1393 In this example, Stochastic Processes are generated by Karhunen Louve
1394 Expansion method.

1395 **4.5.4 UQpy.StochasticProcess.Translation (Coming in V2.0)**

1396 **Translate** is a class for translating Gaussian Stochastic Processes to Non-
1397 Gaussian Stochastic Processes. This class returns the non-Gaussian samples
1398 along with the distorted Aurocorrelated Function. The **Translate** class is
1399 imported using the following command:

1400 `from UQpy.StochasticProcess import Translate`

1401 The attributes of the **Translate** class are listed below:

Translate Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
samples_g	Input	★	
R_g	Input	★	
marginal	Input	★	
params	Input	★	
samples_ng	Output		
R_ng	Output		

1402

1403 **Description of Translate Class Attributes:**

1404

1405 *Input Attributes:*

- 1406 • **samples_g:**
1407 Numpy array of Gaussian samples to be translated into specified non-
1408 Gaussian samples.
- 1409 • **R_g:**
1410 Numpy array providing the Autocorrelation Function of the Gaussian
1411 Stochastic Processes.
1412
- 1413 • **marginal:**
1414 The name of the marginal distribution to which to be translated. It
1415 must follow the format discussed in the Distributions module.(Examples
1416 Jupyter script may be referred for further coherence)
- 1417 • **params:**
1418 The parameters of the marginal distribution to which to be translated. It
1419 must follow the format discussed in the Distributions module.(Examples
1420 Jupyter script may be referred for further coherence)

1421 *Output Attributes:*

- 1422 • **samples_ng:**
1423 Numpy array of the translated Non-Gaussian samples.
- 1424 • **R_ng:**
1425 Numpy array of the distorted Non-Gaussian Autocorrelation Function.

1426 **Examples:**

1427 An example files illustrating the use of the **Translate** class have been provided:

- 1428 • **Translate.ipynb:**
1429 In this example, a Gaussian Stochastic Process has been translated into
1430 a Uniform[0, 1] process.

1431 **4.5.5 UQpy.StochasticProcess.InverseTranslation (Coming in V2.0)**

1432 **Inverse_Translate** is a class for translating Non-Gaussian Stochastic Pro-
1433 cesses back to Standard Gaussian Stochastic Processes. This class returns the
1434 non-Gaussian samples along with the distorted Aurocorrelated Function. The
1435 **Translate** class is imported using the following command:

1436 `from UQpy.StochasticProcess import InverseTranslation`

1437 The attributes of the `Translate` class are listed below:

Translate Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
<code>samples_ng</code>	Input	★	
<code>R_ng</code>	Input	★	
<code>marginal</code>	Input	★	
<code>params</code>	Input	★	
<code>samples</code>	Output		

1439 **Description of BSRM Class Attributes:**

1440

1441 *Input Attributes:*

- 1442 • **samples_g:**
1443 Numpy array of non-Gaussian samples to be translated into standard
1444 Gaussian samples.
- 1445 • **R_ng:**
1446 Numpy array providing the Autocorrelation Function of the non-
1447 Gaussian Stochastic Processes.
- 1448
- 1449 • **marginal:**
1450 The name of the marginal distribution the Stochastic Process currently
1451 follows. It must follow the format discussed in the Distributions mod-
1452 ule.(Examples Jupyter script may be referred for further coherence)
- 1453 • **params:**
1454 The parameters of the marginal distribution the Stochastic Process cur-
1455 rently follows. It must follow the format discussed in the Distributions
1456 module.(Examples Jupyter script may be referred for further coherence)

1457 *Output Attributes:*

- 1458 • **samples_g:**
1459 Numpy array of the standard Gaussian samples.
- 1460 • **R_ng:**
1461 Numpy array of the Gaussian Autocorrelation Function.

1462 **Examples:**

1463 An example files illustrating the use of the `Inverse_Translate` class have been
1464 provided:

1465 • `Inverse_Translate.ipynb`:

1466 In this example, a non-Gaussian Stochastic Process is translated into a
1467 standard Gaussian Stochastic Process.

1468 4.6 RunModel Module

1469 The `RunModel` module is how `UQpy` calls user-defined computational mod-
1470 els and collects the results from the output of those simulations. Using the
1471 `RunModel` module requires the user to be familiar with either shell scripting or
1472 python scripting. The `RunModel` module consists of a single class, also called
1473 `RunModel`, that can be imported using the following command:

```
1474 from UQpy.RunModel import RunModel
```

1475 The attributes of the `RunModel` class are listed below:

RunModel Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input		★
samples	Input		★
model_type	Input		★
1476 model_script	Input	★	
input_script	Input		★
output_script	Input		★
cpu	Input		★
model_eval	Output		

1477 A brief description of each attribute can be found in the table below:

RunModel Class Attributes			
Attribute	Type	Options	Default
<code>dimension</code>	<i>integer</i>		<code>dimension = 1</code>
<code>samples</code>	<i>nparray</i>		None
<code>model_type</code>	<i>string</i>	'python' None	None
<code>model_script</code>	<i>string</i>	Must be '.py' or '.sh'	
<code>input_script</code>	<i>string</i>	Must be '.py' or '.sh'	
<code>output_script</code>	<i>string</i>	Must be '.py' or '.sh'	
<code>cpu</code>	<i>integer</i>	<code>cpu < # of available CPUs</code>	<code>cpu = 1</code>
<code>model_eval</code>	<i>class object</i>	RunPythonModel RunSerial RunParallel	

Detailed Description of RunModel Class Attributes:

Input Attributes:

- **dimension:**

A scalar integer value defining the dimension of the random variables.

- **samples**

Specifies the sample points at which to evaluate the model.

If **samples** is not specified, **RunModel** will search the working directory for a file called 'UQpy_Samples.txt'. Creating this text file allows an alternate way of defining samples for the **RunModel** class that does not require the samples to be generated by **UQpy**. Formatting specifications for 'UQpy_Samples.txt' are given in Section 4.6.3.

- **model_type**

Specifies the type of model that will be evaluated.

If **model_type** = 'python', then the model is either a user-defined Python model (i.e. a solver written in Python) or the model is a third-party model with both pre- and post-processing handled by a single Python script. Using a Python model or a Python script to invoke the model allows **UQpy** to handle message passing internally in Python. This mode of operation requires the definition of only one script, defined by **model_script**, which must be a .py file. For more details, see Section 4.6.1.

1503 If `model_type = None`, then the model is called through a series of either
 1504 shell or Python scripts. This is a more general framework that relies on
 1505 text files to pass `samples` into the model input file and to retrieve the
 1506 model quantity of interest (defined by `RunModel.model_eval.QOI`). This
 1507 mode of operation requires the user to define three scripts:

- 1508 1. `input_script`: This user-defined script (which may be a `.sh` or `.py`
 1509 file), reads a text file of samples generated from `UQpy` in a specified
 1510 format (see Section 4.6.2) and generates input files for the compu-
 1511 tational model.
- 1512 2. `model_script`: This user-defined script (which may be a `.sh` or `.py`
 1513 file), calls the computational model and initiates the simulations.
- 1514 3. `output_script`: This user-defined script (which may be a `.sh` or `.py`
 1515 file), reads an output file from the computational model, extracts
 1516 the desired quantity of interest, and prints the value(s) of this quan-
 1517 tity of interest to a text file of specified format (see Section 4.6.2)
 1518 that `UQpy` reads.

- 1519 • `model_script`
 1520 Specifies the user-defined script used to call the computational model.
 1521 If `model_type = None`, `model_script` may be either a `.py` or `.sh` file. If
 1522 `model_type = 'python'`, `model_script` must be a `.py` file.
- 1523 • `input_script`:
 1524 Only used with `model_type = None`.
 1525
 1526 Specifies the user-defined script used to read a text file containing a
 1527 sample value with specified format and create an input file for the com-
 1528 putational model. May be a `.sh` or `.py` file. See Section 4.6.2.
- 1529 • `output_script`:
 1530 Only used with `model_type = None`.
 1531
 1532 Specifies the user-defined script used to read a model output file, extract
 1533 the quantity of interest, and create a text file containing the quantity of
 1534 interest in a specified format that can be ready by `UQpy`. May be a `.sh`
 1535 or `.py` file. See Section 4.6.2.
- 1536 • `cpu`:
 1537 Specifies the number of CPUs over which to distribute the simulations.

1538 This number must be less than the number of available CPUs on the
1539 computer performing the simulations.

1540 *Output Attributes:*

1541 • **model_eval:**

1542 This is an instance of one of three classes used to call the computational
1543 model.

1544

1545 If `model_type = 'python'`, `model_eval` is an instance of the
1546 `RunPythonModel` class defined in the Python `model_script`. See
1547 Section 4.6.1.

1548

1549 If `model_type = None`, `model_eval` is an instance either the `RunSerial`
1550 or `RunParallel` class, depending on whether the user specified serial
1551 (`cpu = 1`) or parallel (`cpu > 1`) computing. See Section 4.6.2.

1552 **RunModel Workflows**

1553

1554 There are two general workflows for the `RunModel` class. In the first, a model
1555 is defined or called through python scripts, which allows all sample passing
1556 to be performed internally and therefore has less computational “overhead.”
1557 In the second workflow, samples and solutions are passed between `UQpy` and
1558 a third-party solver through text files. The following sections detail these two
1559 workflows.

1560 4.6.1 `RunModel` with direct Python communications (`model_type = 'python'`)

1561 The fastest, simplest, and preferred way to run a model using `UQpy` is by
1562 linking `UQpy` to a Python script that calls or runs the model. This link occurs
1563 by calling the `RunModel` class, setting `model_type = 'python'`, and pointing
1564 it to the user-defined Python script that will execute the model. `RunModel` is
1565 pointed to the Python script by defining the input parameter `model_script`
1566 as a string having the name of the Python script (note this file must be a
1567 .py file). More details on defining `model_script` can be found in Section ??.
1568 Figure 2 shows a general flow-chart for the `RunModel` class invoking a Python
1569 script to run simulations.

1570 `UQpy` calls the Python script defined by `model_script` through the class
1571 `RunPythonModel`, which must be present in `model_script` and is defined as
1572 follows:

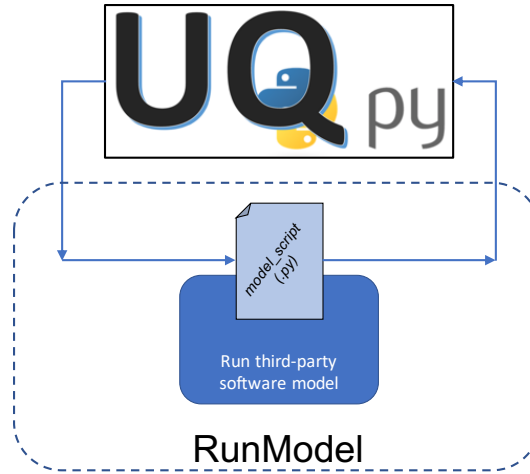


Figure 2: General workflow for running a model from a python script (`model.type = 'python'`) using the `RunModel` class of `UQpy`.

```

1573     class RunPythonModel:
1574
1575         def __init__(self, samples=None, dimension=None):
1576
1577             self.samples = samples
1578             self.dimension = dimension
1579             self.QOI = list()

```

1580 The `RunPythonModel` class in `model_script` must accept, as input, a set
1581 of samples and the dimension of the samples and return, as output, a list
1582 containing the quantity of interest (`self.QOI`) computed for each sample.
1583 The attributes of the `RunPythonModel` are described below. Beyond these
1584 minimal requirements, the user has complete freedom to perform whatever
1585 operations she/he desires. That is, `model_script` may be used directly to
1586 perform some operations on the samples (e.g. solve a set of differential
1587 equations having parameters defined by the samples) or to pass the samples
1588 to input files and call a third-party model (e.g. Matlab, Abaqus, or a custom
1589 simulation code).

1590

1591 The attributes of the `RunPythonModel` class are listed below:

1592

RunPythonModel Class Attribute Definitions			
Attribute	Input/Output	Required	Optional
dimension	Input	★	
samples	Input	★	
QOI	Output	★	

1593 A brief description of each attribute can be found in the table below:

1594

RunPythonModel Class Attributes			
Attribute	Type	Options	Default
dimension	<i>integer</i>		
samples	<i>nparray</i>		
QOI	<i>list</i>		

1595 Detailed Description of RunPythonModel Class Attributes:

1596

1597 *Input Attributes:*

1598

- **dimension:**

1599

A scalar integer value defining the dimension of the random variables.

1600

- **samples**

1601

Specifies the sample points at which to evaluate the model.

1602 *Output Attributes:*

1603

- **QOI:**

1604

A list containing the quantity of interest returned from the model. Each item of the list corresponds to an associated sample value and may be of arbitrary data type.

1607 Examples:

1608

An example illustrating the use of the `RunModel` class with `model_type = 'python'` is provided in the following Jupyter script.

1609

1610

- **Run_Python_Model.ipynb:**

1611

In this example, the component-wise modified Metropolis-Hasting algorithm for MCMC is used to generate 15 (approximately) independent samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is defined as a function directly in the script. The samples are then passed to a Python model (`python_model.py`) that evaluates the sum of the components of each sample and returns the sum as the quantity of interest (`x.model_eval.QOI`).

1612

1613

1614

1615

1616

1617

Running a model in Python is strongly preferred both from the perspective of flexibility for the user, but also because it alleviates the burden of file passing as a means of communication between `UQpy` and model input/output. This is the topic of the next section.

4.6.2 `RunModel` with file passing communications (`model_type = None`)

The `RunModel` class supports an alternate means of running a model for users who prefer shell scripting or who prefer a more prescriptive workflow. This alternate means of running uses a set of scripts and text files to pass information from `UQpy` to a third-party model and return the results. This method of running the model supports both serial computation and parallel processing across multiple cores. It does not currently support distributed processing across multiple nodes in an HPC.

Figure 3 illustrates this workflow, which follows a three-step process:

1. Convert text files of `UQpy` samples to model input files.
2. Run the computational model.
3. Convert model output from each simulation to text files that can be read by `UQpy`.

This three step process is detailed in the following.

Step 1: For each sample value, `UQpy` generates a text file called ‘`UQpy_run_n.txt`’ where `n` indexes the sample number as illustrated in Figure 4. The user must pass the name of a shell or Python script (as a string through `input_script`) that reads ‘`UQpy_run_n.txt`’ and inserts the samples into an input file for the computational model. For specification of the formatting of ‘`UQpy_run_n.txt`’, see Section 4.6.3. An example `input_script` is provided in the example ‘`Matlab_Model_Serial.ipynb`’ provided below.

Step 2: For each sample value, a model input file is generated in step 1. `UQpy` then calls the user-defined `model_script` to run the computational model as illustrated in Figure 5. `RunModel` loops over all samples to run the model for each generated input file. This can be done either serially or in parallel over multiple processors. See description below.

Step 3: For each simulation, an output file is generated. The user-defined `output_script` is used to post-process these outputs, extract the desired

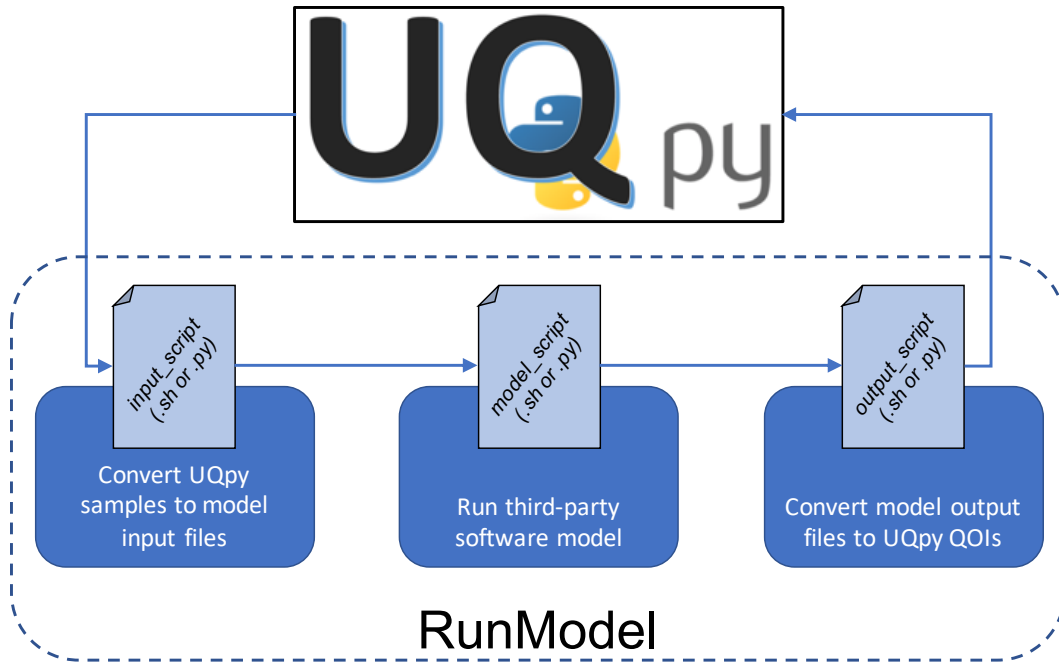


Figure 3: General workflow for running a third-party model with UQpy with samples and solutions passed through text files (`model_type = None`).

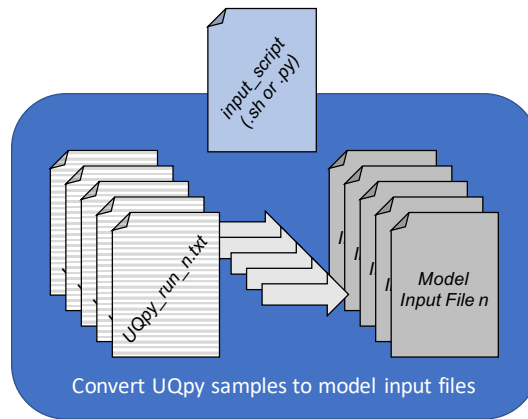


Figure 4: The user-defined `input_script` is used to read UQpy samples from text files defined as ‘UQpy_run_n.txt’ and create model input files.

1653 quantity of interest, and write this quantity of interest to a text file named
 1654 ‘UQpy_eval_n.txt’ where, again `n` indexes over the sample number as
 1655 illustrated in Figure 6. For formatting specifications of ‘UQpy_eval_n.txt’, see

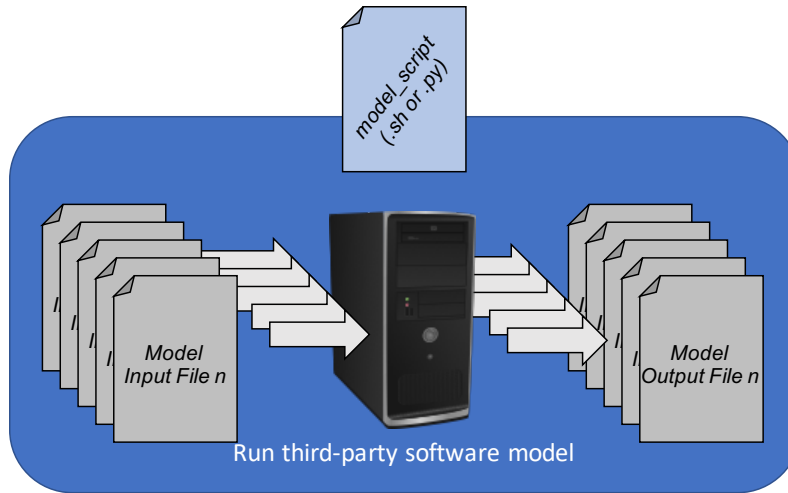


Figure 5: The user-defined `model_script` is used to run a third party software model using the model input files generated by the `input_script`. UQpy runs the model in a loop to evaluate all samples.

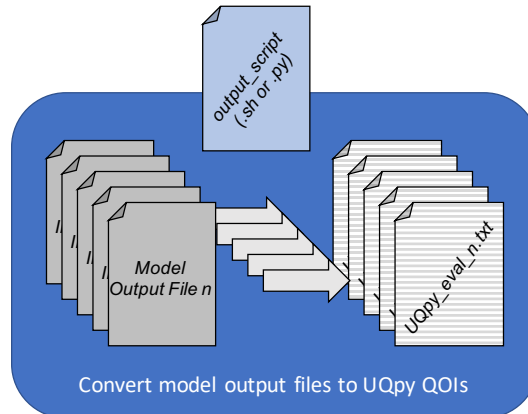


Figure 6: The user-defined `output_script` is used to post-process model results, extract a quantity of interest, and write that quantity of interest to 'UQpy_eval.n.txt' which can be read by UQpy.

1656 Section 4.6.3.

1657

1658 **RunSerial and RunParallel**

1659 Depending on the number of CPUs the user specifies via the `cpu` attribute,
 1660 the model will either be run serially or in parallel across the specified number
 1661 of CPUs by invoking the `RunSerial` and `RunParallel` sub-classes respectively.

1662
1663 When `cpu = 1`, the model is run by calling `RunSerial`, setting the instance
1664 of this class as `model_eval`, and returning the quantities of interest for the
1665 solution as `model_eval.QOI`.

1666
1667 When `cpu > 1`, the model is run by calling `RunParallel`, setting the instance
1668 of this class as `model_eval`, and returning the quantities of interest for
1669 the solution as `model_eval.QOI`. Given N samples, `RunParallel` bundles
1670 the N calculations into $\lfloor N/\text{cpu} \rfloor + \text{mod}\{N/\text{cpu}\}$ calculations on the first
1671 $\text{mod}\{N/\text{cpu}\}$ CPUs and $\lfloor N/\text{cpu} \rfloor$ calculations on all remaining CPUs.

1672 1673 **Directory structure during model evaluation**

1674
1675 To execute `RunModel`, the working directory must contain the necessary
1676 scripts (defined by `model_script`, `input_script`, and `output_script`) along
1677 with any other files necessary for model evaluation. These may include, among
1678 other things, a template model input file (to be edited by `input_script` to
1679 input sample values), compiled executable files for third-party software that
1680 runs locally, and/or 'UQpy_samples.txt' if samples are not being generated
1681 by `UQpy`. To avoid cluttering the working directory, the first step in model
1682 evaluation using `RunModel` is to create a new directory called 'tmp' and copy
1683 all files into this directory as illustrated in Figure 7.

1684 From the 'tmp' directory, the appropriate class `RunSerial` or `RunParallel`
1685 is executed. The first step in either process is to generate, from the samples
1686 (defined either by `RunModel.samples` or 'UQpy_Samples.txt'), a single text file
1687 'UQpy_run_n.txt' where n indexes the sample number, for each sample value.
1688 These are the files that are read by `input_script`. The model evaluation
1689 process then proceeds as illustrated in Figures 3 - 6, ending with the quantities
1690 of interest returned in text files 'UQpy_eval_n.txt' and also saved internally
1691 within `RunModel` as `RunModel.model_eval.QOI`.

1692 The final step is to clean up the working directory. As illustrated in
1693 Figure 8, the input files are returned to the original working directory, all
1694 output files 'UQpy_eval_n.txt' are moved to a new directory 'UQpyOut', and
1695 the 'tmp' directory is removed.

1696 1697 **Examples:**

1698 Two examples illustrating the use of the `RunModel` class with `model_type =`
1699 `None` are provided that run a simple Matlab model from two-dimensional
1700 input in the following Jupyter scripts.

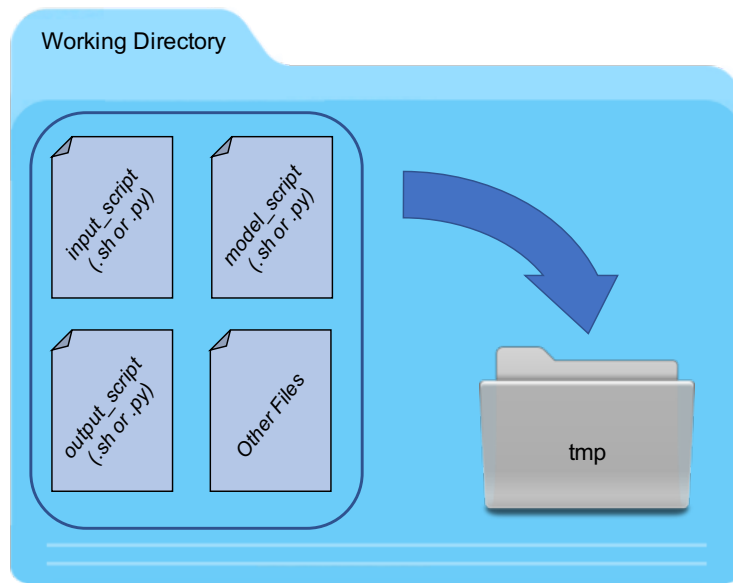


Figure 7: The first step in executing `RunModel` is to copy all files into a temporary subdirectory of the working directory called ‘tmp’ where all computations will be performed.

- 1701 • `Run_Serial_Matlab_Model.ipynb`:
1702 In this example, the component-wise modified Metropolis-Hasting algo-
1703 rithm for MCMC is used to generate 15 (approximately) independent
1704 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is
1705 defined as a function directly in the script. The samples are then saved
1706 as a text file ‘UQpy_Samples.txt’ to illustrate that `RunModel` can read
1707 samples from a text file. A simple Matlab model ‘matlab_model.m’ is
1708 included that evaluates the sum of the components of each sample and
1709 returns them as the quantity of interest (`x.model_eval.QOI`) and
1710 saves each sum as a text file ‘UQpy_eval_n’, $n = 1, \dots, 15$ in the folder
1711 ‘UQpyOut’. The `RunModel` class is run serially, `cpu = 1`, meaning that
1712 all 15 Matlab calculations are performed sequentially. Finally, the re-
1713 sulting data structures are printed to illustrate how UQpy saves model
1714 output.
- 1715 • `Run_Parallel_Matlab_Model.ipynb`:
1716 In this example, the component-wise modified Metropolis-Hasting algo-
1717 rithm for MCMC is used to generate 15 (approximately) independent

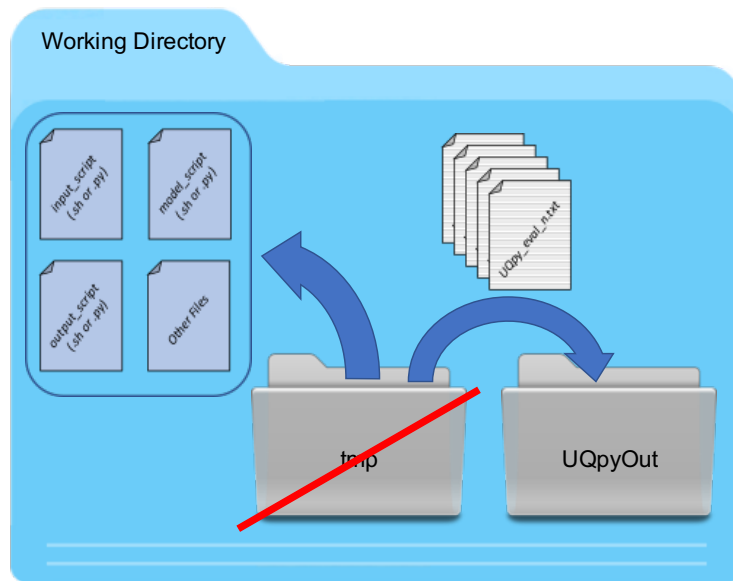


Figure 8: Final cleanup of the working director is the last step of model evaluation using `RunModel`. In the process, the input files are returned to the original working directory, all output files ‘UQpy_eval_n.txt’ are moved to a directory ‘UQpyOut’, and the ‘tmp’ directory is removed.

1718 samples from a two-dimensional Rosenbrock pdf. The Rosenbrock pdf is
 1719 defined as a function directly in the script. The samples are passed di-
 1720 rectly into the `RunModel` class. A simple Matlab model ‘matlab_model.m’
 1721 is included that evaluates the sum of the components of each sample and
 1722 returns them as the as the quantity of interest (`x.model_eval.QOI`) and
 1723 saves each sum as a text file ‘UQpy_eval_n’, $n = 1, \dots, 15$ in the folder
 1724 ‘UQpyOut’. The `RunModel` class is run in parallel over four CPUs, `cpu`
 1725 `= 4`. The 15 Matlab calculations bundled into groups of 4, 4, 4, and 3
 1726 calculations and each group is performed sequentially over one assigned
 1727 CPUs. Finally, the resulting data structures are printed to illustrated
 1728 how `UQpy` saves model output.

1729 4.6.3 Files and scripts used by `RunModel`

1730 As discussed in the sections above and illustrated in the examples, the
 1731 `RunModel` class utilizes a number of files and scripts in order to execute the
 1732 computational model. This section is intended to provide a closer look at

1733 each of these files, their structure, and when/if they are required.

1734 • ‘UQpy_Samples.txt’:

1735 This user-defined text file allows the user to pass samples into the
1736 `RunModel` class without drawing new samples from `UQpy`. Examples of
1737 when this file may be used include, but are not limited to, the following
1738 cases:

- 1739 – The user generates a set of samples using another package (not
1740 `UQpy`), but still wishes to use `UQpy` as the driver to run the model.
- 1741 – The user wishes to retain the same set of samples when evaluating
1742 a model that changes in some way. For example, running models
1743 of different mesh resolution with the same input values.

1744 *File Format:* ‘UQpy_Samples.txt’ is an ASCII formatted text file
1745 having one sample per line with whitespace delimiters separating each
1746 component of the samples.

1747

1748 ‘UQpy_Samples.txt’ can be used with `model_type = None` and
1749 `model_type = ‘python’`.

1750 • ‘UQpy_run_n.txt’:

1751 Each ‘UQpy_run_n.txt’ (where n indexes the sample number) is a `UQpy`
1752 defined ASCII text file containing a single sample. While the user is
1753 not required to generate this file, it is important that the user know its
1754 format as the user-defined `input_script` must read this file and place
1755 its sample values into the model input file.

1756

1757 *File Format:* ‘UQpy_run_n.txt’ is an ASCII formatted text file having
1758 one sample with whitespace delimiters separating each component of
1759 the sample.

1760

1761 These files are generated only when using `RunModel` with `model_type =`
1762 `None`.

1763 • ‘UQpy_eval_n.txt’:

1764 Each ‘UQpy_eval_n.txt’ (where n indexes the sample number) is a user-
1765 created ASCII text file containing a single quantity of interest generated
1766 from post-processing the model output file from the nth simulation. The

1767 user must generate this file using `output_script` so it is important that
 1768 the user know its format.

1769 *File Format:* ‘UQpy_eval.n.txt’ is an ASCII formatted text file having
 1770 one quantity of interest with whitespace delimiters separating each
 1771 component of the quantity of interest (if it is vector-valued). If the
 1772 quantity of interest is matrix-valued or tensor-valued, it currently must
 1773 be unpacked into a vector for saving in ‘UQpy_eval.n.txt’. This will
 1774 change in the future.

1775

1776 These files need to be generated only when using `RunModel` with
 1777 `model_type = None`.

1778 • `input_script`: `input_script` is a script that reads each sample in
 1779 ‘UQpy_run.n.txt’ and places the values in the appropriate location in
 1780 the model input file.

1781 *File Format:* `input_script` must be a python script (.py) or shell script
 1782 (.sh).

1783 `input_script` is used only when using `RunModel` with `model_type =`
 1784 `None`.

1785 • `model_script`: `model_script` is the user-defined script that runs the
 1786 computational model. It can be employed in two different ways depend-
 1787 ing on the assignment of `model_type`.

1788 – `model_type = None`: `model_script` is responsible only for
 1789 initializing the computational model.

1790

1791 *File Format:* `model_script` must be a python script (.py) or shell
 1792 script (.sh).

1793 – `model_type = ‘python’`: `model_script` may contain the
 1794 computational model itself. In such case, the samples that are
 1795 passed into `Runmodel` are input directly into the python solver.
 1796 `model_script` may also call an external solver. In this case,
 1797 `model_script` must also place the sample values in the model input
 1798 file and post-process the model output to generate `model_eval.QOI`.

1799

1800 *File Format:* `model_script` must be a python script (.py) contain-
 1801 ing the `RunPythonModel` class as discussed in Section 4.6.1.

1802 • `output_script` `output_script` is the user-defined script that
1803 post-processes the model output to extract the user-specified quantity
1804 of interest and write this quantity of interest to the ‘UQpy_eval.n.txt’
1805 files.

1806

1807 *File Format:* `model_script` must be a python script (.py) or shell script
1808 (.sh).

1809 `output_script` is used only when using `RunModel` with `model_type =`
1810 `None`.

1811 • **Model Input file** The model input file is a user-defined file that is also
1812 specific to the model application. The model input file is typically a
1813 standard format file that defines all deterministic parameters, geometry,
1814 material, properties, etc. of the computational model. This file should
1815 also have place-holders for the input of sample values generated by UQpy.
1816 In the future, these place-holders will be standardized, but as yet they
1817 are not.

1818 • **Executable Software** Often, the working directory will contain an exe-
1819 cutable software program. When this software is user-defined (as may be
1820 the case for custom solvers), the executable program may need to reside
1821 in the current working directory.

1822 4.6.4 Template scripts for common software applications

1823 • Matlab
1824 Coming soon...

1825 • Abaqus
1826 Coming soon...

1827 • OpenSEAS
1828 Coming soon...

1829 • OpenFOAM
1830 Coming soon...

1831 • FEAP
1832 Coming soon...

1833 • SAFIR
1834 Coming soon...

1835 5 Support Modules

1836 The modules detailed in Section 4 form the core of UQpy and its primary capa-
 1837 bilities. In support of these primary modules are two additional modules that
 1838 provide capabilities that are generally used throughout the primary modules.
 1839 These two support modules are described herein.

1840 5.1 Distributions Module

1841 The `Distributions` module performs probability distribution related opera-
 1842 tions. This includes functions for computing probability densities, cumulative
 1843 distributions and their inverses, moments, the logarithms of the probability
 1844 densities as well as parameter estimates for generic data for common distribu-
 1845 tion types.

1846 The `Distributions` module is imported in a Python script using the fol-
 1847 lowing command:

```
1848 from UQpy import Distributions
```

1849 The `Distributions` module contains a single class, the `Distribution`
 1850 class, possessing the following attributes:

Distribution Class Attribute Definitions			
Attribute	Input/Output	Type	Required
<code>name</code>	Input	<i>string</i>	*
<code>params</code>	Input	<i>list</i>	*
<code>pdf</code>	Output	<i>function</i>	
1851 <code>rvs</code>	Output	<i>function</i>	
<code>cdf</code>	Output	<i>function</i>	
<code>icdf</code>	Output	<i>function</i>	
<code>log_pdf</code>	Output	<i>function</i>	
<code>fit</code>	Output	<i>function</i>	
<code>moments</code>	Output	<i>function</i>	

1852 With the exception of the custom distribution, the `Distribution` class simply
 1853 repackages certain distributions from the `scipy.stats` package in a way that
 1854 is convenient to use within UQpy. A brief description of each attribute of the
 1855 `Distribution` class can be found in the table below:

Distribution Class Attributes			
Attribute	Type	Options	Default
name	<i>string</i>	See list below.	
params	<i>list</i>		
pdf	<i>function</i>		
rvs	<i>function</i>		
cdf	<i>function</i>		
icdf	<i>function</i>		
log_pdf	<i>function</i>		
fit	<i>function</i>		
moments	<i>function</i>		

Detailed Description of Distribution Class Attributes:

Input Attributes:

- **name:**

A string designating the distribution name. Available distributions are shown in the table below.

name must be specified. **Distribution** does not have a default distribution type.

- **params:**

Defines the parameters of the distribution for each random variable as a list. Parameters for all available distributions are shown in the table below. Generally, the parameters adhere to the defined parameters in **Scipy.stats**.

params must be specified. There are no default parameter values for any distribution.

Output Attributes:

- **pdf:**

A function that returns the probability density function at a specified value or values x . Note that the parameters of the distribution must be passed into the **pdf** function.

The function is called as follows:

```
Distribution.pdf(x,params)
```

1882 • **rvs**:
1883 A function that draws random samples from the specified distribution.
1884 Note that the parameters of the distribution must be passed into the
1885 **rvs** function and the number of samples (**nsamples**) must be specified.
1886

1887 The function is called as follows:

1888 `Distribution.rvs(params, nsamples)`

1889 • **cdf**:
1890 A function that returns the cumulative distribution function at a
1891 specified value x . Note that the parameters of the distribution must be
1892 passed into the **cdf** function.
1893

1894 The function is called as follows:

1895 `Distribution.cdf(x,params)`

1896 • **icdf**:
1897 A function that returns the inverse cumulative distribution function at
1898 a specified value or values $x \in [0, 1]$. Note that the parameters of the
1899 distribution must be passed into the **icdf** function.
1900

1901 The function is called as follows:

1902 `Distribution.icdf(x,params)`

1903 • **log_pdf**:
1904 A function that returns the logarithm of the probability density
1905 function at a specified value or values x . Note that the parameters of
1906 the distribution must be passed into the **log_pdf** function.
1907

1908 The function is called as follows:

1909 `Distribution.log_pdf(x,params)`

1910 • **fit**:
1911 A function that fits the parameters of the specified distribution to
1912 user-specified data y . Note that the parameters of the distribution that
1913 are returned follow the conventions of **scipy.stats**, which for some
1914 distributions may be inconsistent with the parameters specified in **UQpy**.
1915

1916 The function is called as follows:

1917 `Distribution.fit(y)`

1918 • **moments:**

1919 A function that returns the mean, variance, skewness, and kurtosis, of
1920 a specified distribution. Note that the parameters of the distribution
1921 must be passed into the **moments** function.

1922

1923 The function is called as follows:

1924 `Distribution.moments(params)`

1925

1926

Available Distributions in UQpy		
Distribution	Name	Parameters
Beta	‘beta’	$[a, b]$ $a, b > 0, (a < b) \in \mathbb{R}$ Fixed: $loc = 0, scale = 1$
Binomial	‘binomial’	$[n, p]$ $n \in \mathbb{N}_0, p \in [0, 1]$
Cauchy	‘cauchy’	$[loc, scale]$ $loc, scale > 0$
Chi-Squared	‘chisquare’	$[df, loc, scale]$
Exponential	‘exponential’	$[loc, scale]$
Gamma	‘gamma’	$[a, loc, scale]$ $a > 0$
Generalized Extreme Value	‘genextreme’	$[c, loc, scale]$
Inverse Gaussian	‘inv_gauss’	$[\mu, loc, scale]$
Laplace	‘laplace’	$[loc, scale]$ $scale > 0$
Levy	‘levy’	$[loc, scale]$ $scale > 0$
Logistic	‘logistic’	$[loc, scale]$ $scale > 0$
Lognormal	‘lognormal’	$[\sigma, \mu]$ $s = \sigma, scale = \exp(\mu)$ $\sigma > 0$
Maxwell-Boltzmann	‘maxwell’	$[loc, scale]$ $scale > 0$
Normal (Gaussian)	‘normal’ or ‘gaussian’	$[\mu, \sigma]$ $loc = \mu, scale = \sigma$ $\sigma > 0$
Pareto	‘pareto’	$[b, loc, scale]$ $b, scale > 0$
Rayleigh	‘rayleigh’	$[loc, scale]$ $scale > 0$
Uniform	‘uniform’	$[a, b]$ $loc = a, scale = b - a$ $b > a$

1927 Custom Distributions:

1928 Other distributions can be easily added by defining the appropriate functions
 1929 in `custom_dist.py`. These functions are those listed in the “Distribution

1930 Class Attributes” table above.

1931

1932 **Description of custom_dist.py**

1933 The script `custom_dist.py` allows the user to define a custom probability
1934 distribution function. In the script, the user may define functions that
1935 compute the pdf, cdf, inverse cdf, or log_pdf at a specified value for the
1936 distribution as well as functions to generate samples, fits the distribution
1937 parameters, and returns the moments of the distribution. For compatibility
1938 with UQpy, the name of each function, `func_name`, must be specified as
1939 `pdf`, `cdf`, `icdf`, `log_pdf`, `fit` or `moments` in accordance with the conven-
1940 tions of the `Distribution` class. Each function is required to take inputs
1941 as prescribed above in the list of *Output Attributes* for the `Distribution` class.

1942

1943 **Examples:**

1944 An example illustrating the use of the `Distribution` class with a built-in
1945 distribution is provided in the following Jupyter script.

- 1946 • `Distributions.ipynb`:

1947 In this example, we explore the use of the `Distribution` class with a
1948 lognormal distribution.

1949 An example illustrating the use of the `Distribution` class with a custom
1950 distribution provided through `custom_dist.py` is provided in the following
1951 Jupyter script.

- 1952 • `Custom_Distribution.ipynb`:

1953 In this example, we explore the use of the `Distribution` class with a
1954 custom Weibull distribution.

1955 **5.2 Utilities Module**

1956 The `Utilities` module contains functionality for all the supporting methods
1957 in UQpy. It is imported in a python script using the following command:

```
1958 from UQpy import Utilities
```

1959 The `Utilities` module consists of various `functions`, each used for different
1960 purposes and can be called as:

```
1961 from UQpy.Utilities import function
```

1962 A list of the available functions that can be found in `Utilities` with a short
1963 description and the class in which is used is presented next.

1964

List of available functions in module <code>Utilities</code>	
Name	Description
<code>transform_ng_to_g</code>	Transform non-Gaussian to Gaussian rvs
<code>transform_g_to_ng</code>	Transform Gaussian to non-Gaussian rvs
<code>itam</code>	Iterative Translation Approximation Method
<code>run_corr</code>	Correlates standard normal variables
<code>run_decorr</code>	Decorrelates standard normal variables
<code>correlation_distortion</code>	Evaluate the modified correlation matrix
<code>bi_variate_normal_pdf</code>	Evaluate the values of the bi-variate normal pdf
<code>_get_a_plus</code>	A supporting function for the <code>nearest_pd</code> function
<code>_get_ps</code>	A supporting function for the <code>nearest_pd</code> function
<code>_get_pu</code>	A supporting function for the <code>nearest_pd</code> function
<code>nearest_psd</code>	Compute the nearest positive semi definite matrix
<code>nearest_pd</code>	Find the nearest positive-definite matrix
<code>estimate_psd</code>	Estimate the Power Spectrum given an ensemble of samples
<code>s_to_r</code>	Transform the power spectrum to an autocorrelation function
<code>r_to_s</code>	Transform the autocorrelation function to a power spectrum
<code>is_pd</code>	Returns true when input is positive-definite.

1965

1966

6 Adding new classes to UQpy

1967 Adding new capabilities to UQpy is as simple as adding a new class to the
 1968 appropriate module and importing the necessary packages into the module.
 1969 Further details will be provided in the future as UQpy coding practices are
 1970 formally established.

1971

References

- 1972 [1] Siu-Kui Au and James L. Beck. Estimation of small failure probabilities in
 1973 high dimensions by subset simulation. *Probabilistic Engineering Mechanics*,
 1974 16(4):263–277, oct 2001.
- 1975 [2] Jonathan Goodman and Jonathan Weare. Ensemble samplers with affine
 1976 invariance. *Communications in applied mathematics and computational*
 1977 *science*, 5(1):65–80, 2010.
- 1978 [3] M. Grigoriu. Reduced order models for random functions. Application to
 1979 stochastic problems. *Applied Mathematical Modelling*, 33(1):161–175, 2009.

- 1980 [4] W K Hastings. Monte Carlo Sampling Methods Using Markov Chains and
1981 Their Applications. *Biometrika*, 57(1):97–109, 1970.
- 1982 [5] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth,
1983 Augusta H. Teller, and Edward Teller. Equation of State Calculations by
1984 Fast Computing Machines. *The Journal of Chemical Physics*, 21(6):1087,
1985 1953.
- 1986 [6] M.D. Shields, G. Deodatis, and P. Bocchini. A simple and efficient method-
1987 ology to approximate a general non-gaussian stationary stochastic process
1988 by a translation process. *Probabilistic Engineering Mechanics*, 26(4):511 –
1989 519, 2011.