

OpenTURNS Developer training: first steps

Trainer : Régis LEBRUN
Airbus
regis.lebrun@airbus.com

Developers training



OpenTURNS: first steps

1 Navigation in the source code

2 Library development

3 Module development

Navigation in the source code

The Uniform distribution

- Locate the class within the library source code;
- Follow its inheritance graph in order to explore the Bridge pattern;
- Locate the associated regression test;
- Execute the test;
- Locate its SWIG interface file and its associated Python module;
- Execute the associated python test.

Library development 1/9

Projects

- ① (*) **InverseDistanceWeightingInterpolation** as a specialization of **EvaluationImplementation** (see `lib/src/Base/Func`). Given a set of data $(x_i, y_i)_{i=1, \dots, N}$ in $\mathbb{R}^n \times \mathbb{R}^p$, the IDW interpolation is defined by:

$$\forall x \in \mathbb{R}^n, u(x) = \begin{cases} \frac{\sum_{i=1}^N w_i(x) y_i}{\sum_{i=1}^N w_i(x)} & \text{if } \forall i, d(x, x_i) > 0 \\ y_i & \text{if } \exists i, d(x, x_i) = 0 \end{cases} \quad (1)$$

where $w_i(x) = \frac{1}{d(x, x_i)^p}$ and $p > 0$ a given smoothness parameter.

The distance d can be the Euclidean distance, the 1-norm or the sup norm.

- ② (**) **DiscreteIntegralCompound** as a specialization of **DiscreteDistribution** (see `lib/src/Uncertainty/Distribution`). Given the discrete distribution of a random variable N and the common discrete distribution of a sequence of iid integral valued random variables (X_i) , compute the distribution of the integral valued discrete random variable Y defined by:

$$Y = \sum_{i=1}^N X_i \quad (2)$$

Library development 2/9

Projects

Its generating function $\phi_Y(z) = \mathbb{E}[z^Y]$ is given by:

$$\forall z \in \mathbb{C}, \phi_Y(z) = \phi_N(\phi_X(z)) \quad (3)$$

and thanks to Poisson's summation formula for discrete distributions, we have for $0 < r < 1$ and $m \in \mathbb{N}^*$:

$$\forall n \in \{0, \dots, m-1\}, p_Y(n) = \frac{1}{mr^n} \sum_{k=0}^{m-1} \phi_Y\left(re^{\frac{2i\pi k}{m}}\right) e^{-\frac{2i\pi kn}{m}} - e_d \quad (4)$$

where $0 \leq e_d \leq r^m$ is the approximation error. For a given $\epsilon > 0$ and $m \in \mathbb{N}^*$, set $r = \sqrt[m]{\epsilon}$ and compute the FFT $(\omega_0, \dots, \omega_{m-1})$ of the complex vector $(\phi_Y(re^{\frac{2i\pi k}{m}}), \dots, \phi_Y(re^{\frac{2i\pi k}{m}}))$. Then, the distribution is equal to the UserDefined distribution with locations $\{0, \dots, m-1\}$ and probabilities $\left(p_i = \frac{\Re(\omega_i)}{mr^i}\right)_{i=0, \dots, m-1}$.

Library development 3/9

Projects

- ③ (*) **ClenshawCurtis** integration algorithm as a specialization of **IntegrationAlgorithmImplementation** (see `lib/src/Base/Algo`). This integration algorithm allows to compute integrals of the form:

$$\begin{aligned} I(f) &= \int_a^b f(t) dt \\ &= \frac{b-a}{2} \int_{-1}^1 f\left(a + \frac{b-a}{2}(1+x)\right) dx \\ &\simeq \frac{b-a}{2} \sum_{k=0}^n w_k f\left(a + \frac{b-a}{2}(1+x_k)\right) \end{aligned}$$

where $x_k = \cos \theta_k$, $\theta_k = \frac{k\pi}{n}$ and w_k is given by:

$$w_k = \frac{c_k}{n} \left(1 - \sum_{j=1}^{\lfloor n/2 \rfloor} \frac{b_j}{4j^2 - 1} \cos(2j\theta_k) \right) \quad (5)$$

Library development 4/9

Projects

where the coefficients b_j and c_k are given by:

$$b_j = \begin{cases} 1 & j = n/2 \\ 2 & j < n/2 \end{cases} \quad c_k = \begin{cases} 1 & k = 0[n] \\ 2 & k \neq 0[n] \end{cases} \quad (6)$$

for $k = 0, \dots, n$. An efficient FFT-based implementation of the computation of the weights and nodes is given in `fc1encurt.m`, another one (**) in `1311.0445.pdf`.

- ④ (*) **Fejer1** integration algorithm as a specialization of **IntegrationAlgorithmImplementation** (see `lib/src/Base/Algo`). This integration algorithm is based on the nodes $x_k = \cos \theta_{k+1/2}$ and weights:

$$w_k^{f1} = \frac{2}{n} \left(1 - 2 \sum_{j=1}^{\lfloor n/2 \rfloor} \frac{1}{4j^2 - 1} \cos(j\theta_{2k+1}) \right) \quad (7)$$

for $k = 0, \dots, n-1$. There also exist fast implementations based on FFT or modified moments, see the references for Clenshaw Curtis.

Library development 5/9

Projects

- ⑤ (*) **Fejer2** integration algorithm as a specialization of **IntegrationAlgorithmImplementation** (see `lib/src/Base/Algo`). This integration algorithm is based on the nodes $x_k = \cos \theta_k$ and weights:

$$w_k^{f2} = \frac{4}{n+1} \sin \theta_{k+1} \sum_{j=1}^{\lfloor n/2 \rfloor} \frac{\sin((2j-1)\theta_k)}{2j-1} \quad (8)$$

for $k = 0, \dots, n-1$. There also exist fast implementations based on FFT or modified moments, see the references for Clenshaw Curtis.

- ⑥ (**) **ClenshawCurtisProductExperiment** as a specialization of **WeightedExperiment**: same algorithm as for **ClenshawCurtis** but with adaptation to any weight function.
- ⑦ (*) **Marshall101kinCopula** as a specialization of **CopulaImplementation** (see `lib/src/Uncertainty/Distribution`). This copula is defined by:

$$\forall (u, v) \in [0, 1]^2, C(u, v) = \begin{cases} u^{1-\alpha} v & \text{for } u^\alpha \geq v^\beta \\ uv^{1-\beta} & \text{for } u^\alpha < v^\beta \end{cases} \quad (9)$$

where $0 < \alpha, \beta < 1$.

Library development 6/9

Projects

- 8 (*) **GumbelCopula** as a specialization of `ExtremeValueCopula` (see `lib/src/Uncertainty/Distribution`). This copula already exists, but not as an extreme value copula. It is defined by its Pickand function:

$$\forall t \in [0, 1], A(t) = [t^\theta + (1 - t)^\theta]^{1/\theta} \quad (10)$$

where $\theta \geq 1$.

- 9 (*) **GalambosCopula** as a specialization of `ExtremeValueCopula` (see `lib/src/Uncertainty/Distribution`). This copula is defined by its Pickand function:

$$\forall t \in [0, 1], A(t) = 1 - [t^{-\theta} + (1 - t)^{-\theta}]^{-1/\theta} \quad (11)$$

where $\theta \geq 0$.

- 10 (*) **TawnCopula** as a specialization of `ExtremeValueCopula` (see `lib/src/Uncertainty/Distribution`). This copula is defined by its Pickand function:

$$\forall t \in [0, 1], A(t) = (1 - \psi_1)(1 - t) + (1 - \psi_2)t + [\{\psi_1 t\}^{1/\theta} + \{\psi_2(1 - t)\}^{1/\theta}]^\theta \quad (12)$$

Library development 7/9

Projects

- ❶ (*) **JoeCopula** as a specialization of `ExtremeValueCopula` (see `lib/src/Uncertainty/Distribution`). This copula is defined by its Pickand function:

$$\forall t \in [0, 1], A(t) = 1 - \left[\{\psi_1(1 - t)\}^{-1/\theta} + \{\psi_2 t\}^{-1/\theta} \right]^{-\theta} \quad (13)$$

where $\theta > 0$ and $0 \leq \psi_1, \psi_2 \leq 1$.

- ❷ (**) **ArchiMaxCopula** as a specialization of `CopulaImplementation` (see `lib/src/Uncertainty/Distribution`). Given an Archimedean copula with generator ψ and an extreme value copula with Pickand function A , an archimax copula C is defined by:

$$\forall (u, v) \in [0, 1]^2, C(u, v) = \psi^{-1} \left(\min \left(\psi(0), [\psi(u) + \psi(v)] A \left(\frac{\psi(u)}{\psi(u) + \psi(v)} \right) \right) \right) \quad (14)$$

It becomes (***) if one wants to implement an efficient sampling algorithm.

Library development 8/9

Projects

- 13 (*) **SquaredNormal** as a specialization of `ContinuousDistribution` (see `lib/src/Uncertainty/Distribution`). If X is distributed according to the $\mathcal{N}(\mu, \sigma)$ distribution, $Y = X^2$ is distributed according to the squared normal distribution with parameters μ and $\sigma > 0$. This distribution has already been implemented in Python, see `SquaredNormal.py`.
- 14 (**) **ConditionalEventDistribution** as a specialization of `ContinuousDistribution` (see `lib/src/Uncertainty/Distribution`). Given the joint distribution of an $(m + n)$ dimensional random vector (X, Y) and an m dimensional interval I such that $\mathbb{P}(X \in I) > 0$, it is the distribution of Y knowing that $X \in I$. This distribution has already been implemented in Python, see `ConditionalEventDistribution.py`. It becomes (***) if one wants to implement an efficient simplification mechanism.
- 15 (***) Extend archimedian copulas from 2-d to n -d. Given a 2-d Archimedean copula with generator ψ , implement its n -d counterpart using:

$$\forall (u_1, \dots, u_n) \in [0, 1]^n, C(u_1, \dots, u_n) = \psi^{-1}(\psi(u_1) + \dots + \psi(u_n)) \quad (15)$$

The main difficulties are the architecture of this extension and the implementation of an efficient sampling algorithm.

Library development 9/9

Projects

- 16 (**) **BlockComposedDistribution** as a specialization of **DistributionImplementation** (see `lib/src/Uncertainty/Distribution`). Given a collection of distributions D_1, \dots, D_n of dimensions d_1, \dots, d_n , it is the distribution of the random vector (X_1, \dots, X_n) of dimension $d_1 + \dots + d_n$ where X_i is distributed as D_i and X_1, \dots, X_n are independent. It becomes (****) if one wants to propagate this new distribution in every places it could go within the library.
- 17 (*) Extend **SolverImplementation** and **Solver** to the resolution of systems of nonlinear equations and provide a generic implementation using the **LeastSquaresProblem** class. The solutions x^* of a nonlinear system of equations $f_1(x) = 0, \dots, f_n(x) = 0$ where $x = (x_1, \dots, x_n)$, if they exist, have to be found in the set of solutions of the following least-squares problem:

$$x^* = \arg \min \sum_{j=1}^n f_j^2(x) \quad (16)$$

for which many solvers are available in OpenTURNS.

Module development 1/2

Projects

- 18 (*) or (**) **CloudMesher**: mesh generation over a cloud of points using kernel mixture, pca, rotation, then levelset mesher on an interval
- 19 (*) **UniformSphereRandomVector** as a specialization of `RandomVectorImplementation` (see `lib/src/Uncertainty/Model`). This random vector is distributed uniformly on the sphere of center $c \in \mathbb{R}^n$ and radius $r > 0$. The sampling is done using the fact that $Y/\|Y\|$ is uniformly distributed over S_{n-1} , the unit sphere in \mathbb{R}^n , if Y is an n dimensional random vector with independent $\mathcal{N}(0, 1)$ components.
- 20 (*) **UniformBallRandomVector** as a specialization of `RandomVectorImplementation` (see `lib/src/Uncertainty/Model`). This random vector is distributed uniformly on the ball of center $c \in \mathbb{R}^n$ and radius $r > 0$. The sampling is done using the fact that $Y/\sqrt{\|Y\|^2 + Z}$ is uniformly distributed over B_{n-1} , the unit ball in \mathbb{R}^n , if Y is an n dimensional random vector with independent $\mathcal{N}(0, 1)$ components, and Z is $\mathcal{E}(1)$ independent from Y .
- 21 (*) **UniformSimplexRandomVector** as a specialization of `RandomVectorImplementation` (see `lib/src/Uncertainty/Model`). This random vector is distributed uniformly in the simplex given by $n + 1$ points in \mathbb{R}^n . The sampling is done using the fact that Y is uniformly distributed over the standard simplex in \mathbb{R}^n if it follows the Dirichlet distribution with parameter $(\theta_1 = 1, \dots, \theta_n = 1)$.

Module development 2/2

Projects

- 22 (**) **SmoliakExperiment** as a specialization of `WeightedExperiment` (see `lib/src/Uncertainty/Algorithm/WeightedExperiment`). This design of experiment is obtained by interfacing the `smolpack` C library. A possible name for the module is **OTSmolpack**.
- 23 (**) **CubaIntegration** as a specialization of `IntegrationAlgorithmImplementation` (see `lib/src/Base/algo`). This algorithm is obtained by interfacing the `cuba` C library. A possible name for the module is **OTCuba**.
- 24 (**) **HIntLibIntegration** as a specialization of `IntegrationAlgorithmImplementation` (see `lib/src/Base/algo`). This algorithm is obtained by interfacing the `HIntLib` C++ library, see <https://github.com/JohannesBuchner/HIntLib>. A possible name for the module is **OTHIntLib**.