Overview of OpenTURNS, its new features and its graphical user interface

The OpenTURNS Dev Team

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OpenTURNS: www.openturns.org

OpenTURNS

An Open source initiative for the Treatment of Uncertainties, Risks'N Statistics

- Multivariate probabilistic modeling including dependence
- Numerical tools dedicated to the treatment of uncertainties
- · Generic coupling to any type of physical model
- Open source, LGPL licensed, C++/Python library
- Multivariate probabilistic modeling including complex dependencies
- Numerical tools dedicated to the treatment of uncertainties
- Generic coupling to any type of physical model
- ▶ Open source, LGPL licensed, C++ library with a Python interface

OpenTURNS: www.openturns.org









- Linux, Windows, macOS, Android
- First release: 2007
- ▶ 5 full time developers
- ho pprox 1~000~000 Total Conda downloads since 2016, pprox 5000 monthly pipy downloads
- Project size: 800 classes, more than 6000 services
- Available in Debian Bookworm, Ubuntu, ...

OpenTURNS: content

- Data analysis
 - Parametric Distribution fitting
 - Non-parametric Distribution fitting
 - Statistical tests
 - Estimate dependency and copulas
 - Estimate stochastic processes

- Probabilistic modeling
 - Dependence modeling
 Univariate distributions
 - Multivariate distributions
 - Copulas
 - Processes
 - Covariance kernels

Surrogate models

- Linear regression
 - Polynomial chaos expansion
- Gaussian process regression
- Spectral methods
- Low rank tensors
- Fields metamodel

Reliability, sensitivity

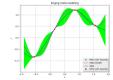
- Sampling methods
- Approximation methods
- Sensitivity analysis
- Design of experiments

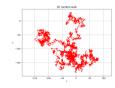
Calibration

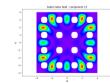
- Least squares calibration
- Gaussian calibration
 - Bayesian calibration

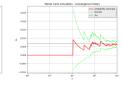
Numerical methods

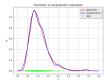
- Optimization
- Integration
- Least squares
- Meshing
- Coupling with external codes







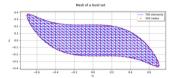




OpenTURNS: documentation

LevelSetMesher





classLevelSetHesher(*args)

Creation of mesh of box type. Available constructor

LevelSetMesher(discretization)

Parameters: discretization : sequence of int. of dimemion < 3.

Discretization of the level set bounding how

solver: On timization& loss ithm

Optimization solver used to project the vertices onto the level set. It must be able to solve nearest point problems. Default is & bdoRackwi, tz

The meshing alterithm is based on the Interval Nesher class. First the bounding box of the level set (provided by the user or automatically computed) is meshed. Then, all the simplices with all vertices outside of the level set are rejected, while the simplices with all vertices inside of the level set are kept. The remaining simplices are adapted the following way:

- . The mean point of the vertices inside of the level set is computed. Each vertex outside of the level set is remierted onto the level set using all near interpolation.
- If the project flaz is True, then the projection is refined using an optimization solver.

Examples

Create a mesh:

```
yes import apportures as at
>>> mesher = ot LevelSetMesher([5, 10])
son level - 1.0
```

>>> function = of SymbolicFunction(['x0', 'x1'], ['x0'2+x1'2'])
>>> levelSet = of LevelSet(function, level)

>>> mesh = mesher.build(levelSet)

build(*args)	Build the mesh of level set type.
getClassName()	Accessor to the object's name.
getDiscretization()	Accessor to the discretization.
getId()	Accessor to the object's id.
getName()	Accessor to the object's name.
getOptimizationAlgorithm()	Accessor to the optimization solver.
get ShadowedId()	Accessor to the object's shadowed id.
getVisibility()	Accessor to the object's visibility state.
hasNane()	Test if the object is named.
hasVisibleName()	Test if the object has a distinguishable name.
setDiscretization(discretization)	Accessor to the discretization.
setNane(name)	Accessor to the object's name.
setOptimirationAlgorithm(SONOT)	Accessor to the optimization solver.
setShadowedId(id)	Accessor to the object's shadowed id.
setVisibility/visible)	Accessor to the object's visibility state.

init(*ares) but1d(*ones)

Build the mesh of level set type

Parameters: Javelflet : Louis Lat. The level set to be meshed, of dimension equal to the dimension of associative tipe tion

> boundingBox : Interval The bounding box used to mesh the level set.

Flag to tell if the vertices outside of the level set of a simpley partially included into the level set have to be projected onto the level set. Default is True

mean to make The mesh built

Content:

- Programming interface (API)
- Examples
- Theory
- All classes and methods are documented, partly automatically.
- Examples and unit tests are automatically run at each code update

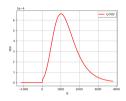
OpenTURNS: practical use

- Compatibility with several popular python packages
 - Numpy
 - Scipy
 - Matplotlib
 - Scikit-learn
 - Pandas
- Parallel computational with shared memory (TBB)
- Optimized linear algebra with LAPACK and BLAS
- Possibility to interface with a computation cluster
- ► Focused towards handling numerical data
- ▶ Installation through conda, pip, packages for various Linux distros and source code

Probabilistic modeling

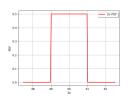
Random variables distributions:

Q: Gumbel(scale=558, mode=1013)>0



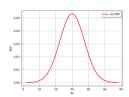
```
Dist = ot.Gumbel(558,1013)
Q = ot.TruncatedDistribution(Dist, 0.,
ot.TruncatedDistribution.LOWER)
```

Zv: Uniform(min=49, max=51)

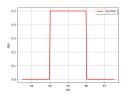


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Ks: Normal(mean=30, std=7.5)>0



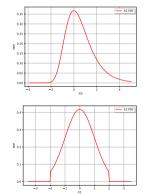
Zm: Uniform(min=54, max=56)



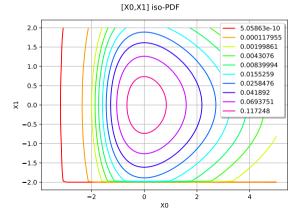
Design of experiments

- ▶ Different Design of experiment types are available
- We consider a 2-dimensional distribution with the following marginals:
 - ▶ Gumbel(min = -1, max = 1)
 - Truncated normal (mean = 0, std = 1, min = -2, max = 2)

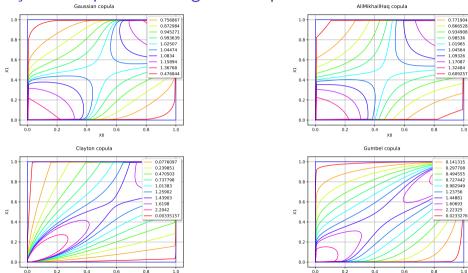
Marginals



Joint distributions

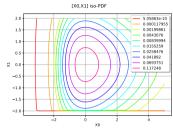


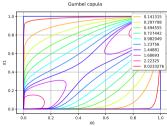
Beyond independent marginals: Copulas



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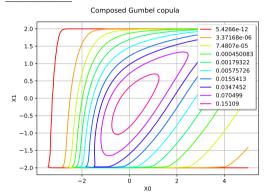
Composing marginal distributions and copulas





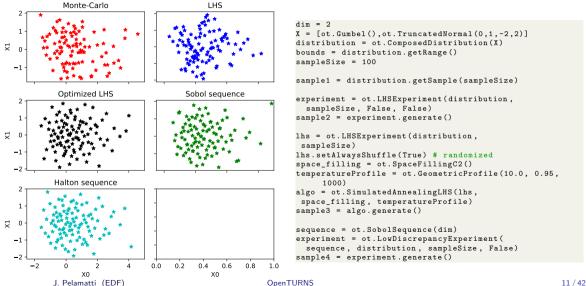
J. Pelamatti (EDF)

We obtain:



```
distribution =
  [ot.Uniform(),ot.TruncatedNormal(0,1,-2,2)]
composed = ot.ComposedDistribution(X,copula)
graph = composed.drawPDF()
graph.setTitle('Composed Gumbel copula')
viewer.View(graph)
```

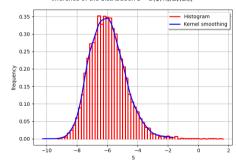
Design of experiments



Monte-Carlo sampling

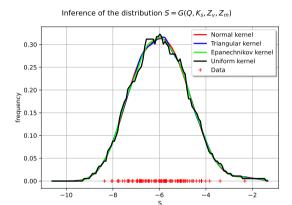
- ► The input distribution and relative output value are evaluated 10000 times
- The output distribution can be infered as a parametric function or through histogram or kernel smoothing methods

Inference of the distribution $S = G(O, K_s, Z_v, Z_m)$



```
Distribution = ot.ComposedDistribution([Q.Ks.Zv.Zm])
#Python model
def floodFunction(X):
    Q . Ks . Zv . Zm = X
    alpha = (Zm - Zv)/5.0e3
    H = (Q/(300.0*Ks*np.sqrt(alpha)))**0.6
    S = [H + Zv - 58.5]
    return S
fun = ot.PvthonFunction(4.1.floodFunction)
#We define the output as a random vector
inputVector = ot.RandomVector(Distribution)
outputVector = ot.CompositeRandomVector(fun.
 inputVector)
#We sample and infere the output distribution
size = 10000
sampleY = outputVector.getSample(size)
graph = ot.HistogramFactory().build(sampleY).drawPDF()
loiKS = ot.KernelSmoothing().build(sampleY)
graph2 = loiKS.drawPDF()
```

Distribution and dependence inference

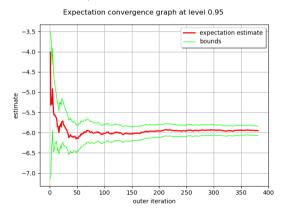


```
size = 100
sampleY = outputVector.getSample(size)
graph = ot.KernelSmoothing(ot.Normal()).build
    (sampleY).drawPDF()
loiKS = ot.KernelSmoothing(ot.Triangular()).
    build(sampleY)
graph2 = loiKS.drawPDF()
graph.add(graph2)
loiKS = ot.KernelSmoothing(ot.Epanechnikov())
    .build(sampleY)
graph2 = loiKS.drawPDF()
graph.add(graph2)
loiKS = ot.KernelSmoothing(ot.Uniform()).
    build(sampleY)
graph2 = loiKS.drawPDF()
```

- ► Parametric (1*d* − *Nd*) distribution inference
- Non-parametric (1d Nd) distribution inference
- Parametric copula inference
- Non-parametric copula inference (Bernstein copula)
- Resampling w.r.t. inferred distributions

Iterative Monte-Carlo: Central tendency anaysis

- The expected value and associated standard deviation are computed iteratively
- Different stopping criteria can be used
- Batch computation can be used



$$\widehat{\sigma}_{y} = \frac{1}{N} \sum_{1}^{N} G(\mathbf{X}_{i})$$

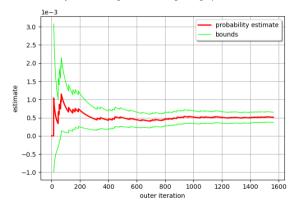
$$\widehat{\sigma}_{y} = \sqrt{\frac{1}{N} \sum_{1}^{N} (G(\mathbf{X}_{i}) - \widehat{m}_{y})}$$

```
algo = ot.ExpectationSimulationAlgorithm(
  outputVector)
algo.setMaximumOuterSampling(100000)
algo.setBlockSize(1)
algo.setCoefficientOfVariationCriterionType(
    'MAX')
algo.setMaximumCoefficientOfVariation(0.01)
algo.run()
graph = algo.drawExpectationConvergence()
view = View(graph)
```

Iterative Monte-Carlo: Reliability analysis

- We now consider the probability of flooding: (P(S > 0.))
- ▶ Same as before, but the function $\mathbb{I}_{G(\mathbf{X}_i)>0}$ is considered

ProbabilitySimulationAlgorithm convergence graph at level 0.95



$$\widehat{\rho}_{y} = \frac{1}{N} \sum_{1}^{N} \mathbb{I}_{G(\mathbf{X}_{i}) > 0}$$

$$\widehat{\sigma} = \sqrt{\frac{1}{N} \sum_{1}^{N} (\mathbb{I}_{G(\mathbf{X}_{i}) > 0} - \hat{\rho}_{y})^{2}}$$

$$\widehat{\sigma}_{\rho_{y}} = \widehat{\sigma} / \sqrt{N}$$

FORM/SORM reliability analysis

- We estimate the probability of flooding through FORM/SORM procedures
- ▶ MC estimation requires ≈ 1500 function evaluations
- ightharpoonup FORM and SORM only use $\simeq 150$
- Estimated probability:
 - MC: 5.099999999998 1e-4
 - FORM: 5.340929030055227 1e-4

```
SORM: 6.793780433482759 1e-4
```

Also:

- Directional sampling
- Importance sampling (FORM-IS, NAIS, Adaptive IS-Cross-entropy)
- Subset sampling

```
#FORM
OptAlgo = ot.Cobyla()
startingPoint = Distribution.getMean()
algoFORM = ot.FORM(OptAlgo, eventF,
startingPoint)
algoFORM.run()

#SORM
OptAlgo = ot.Cobyla()
startingPoint = Distribution.getMean()
algoSORM = ot.SORM(OptAlgo, eventF,
startingPoint)
algoSORM.run()
```

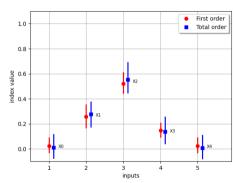
Different types and parameterizations of finite difference gradient computation are available

Sensitivity analysis

Various sensitivity analysis methods are available

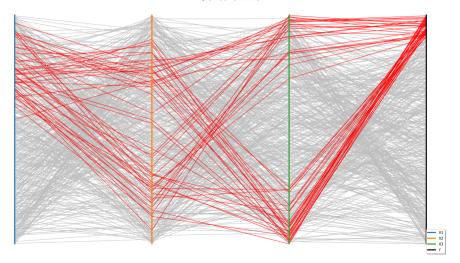
- Graphical analysis
 - Pair plots
 - Parallel coordinates plots
 - Cross-cuts
- Quantitative indices
 - ► SRC, SRRC, PRC, PRCC
 - Sobol' indices (multiple estimators)
 - ► FAST indices
 - ANCOVA indices
 - ► HSIC indices
 - ► Shapley Indices (available as a module)

Aggregated Sobol' indices - SaltelliSensitivityAlgorithm

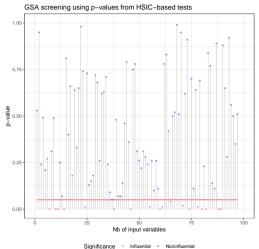


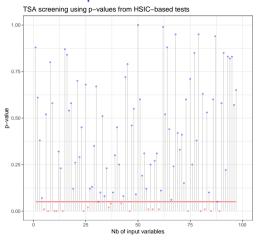
Sensitivity analysis: Parallel coordinates plot

Cobweb graph - [Y] vs [X1.X2.X3]



Sensitivity analysis: HSIC indices and associated p-values





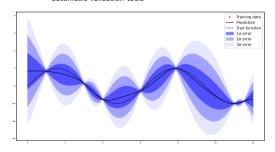
GSA-oriented screening.

TSA-oriented screening.

Influential
 Noninfluential

Surrogate modeling: Gaussian process regression

- Different surrogate modeling methods are available
 - Kriging
 - Polynomial chaos expansion
 - Linear regression & step-wise basis selection
 - Low rank tensors
 - automatic validation tools



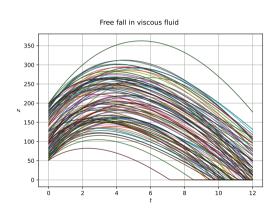
Gaussian process regression

- Different types of covariance functions and function basis can be used
- User-defined options are also available
- MLE optimization can be parameterized
- Large number of optimization algorithms available

Optimization

- OpenTURNS provides an interface with several optimization libraries
 - Bonmin
 - NLopt
 - dlib
 - pagmo
- Ad-hoc implementation of the COBYLA algorithm
- Constrained and unconstrained optimization
- Gradient-based and derivative-free optimizaiton
- Bound and unbound optimization
- Single and multi-objective optimization
- Multi-start wrapper

Field function modeling

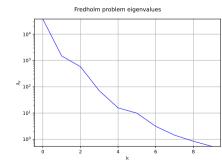


```
def FreeFall(X):
    g = 9.81
    z0.v0.m.c = X
    tau=m/c
    vinf = -m * g/c
    t = np.arrav(mesh.getVertices().asPoint())
    z=z0+vinf*t+tau*(v0-vinf)*(1-np.exp(-t/tau))
    z=np.maximum(z,0.0)
    return of Field (mesh. [[zeta] for zeta in z])
tmin=0.
tmax = 12.
gridsize=100
mesh = ot.IntervalMesher([gridsize-1]).build(
ot.Interval(tmin, tmax))
alti = ot.PvthonPointToFieldFunction(4, mesh, 1, AltiFunc)
distZ0 = ot.Uniform(50.0.200.0)
distV0 = ot.Normal(55.0.10.0)
distM = ot.Normal(80.0, 8.0)
distC = ot.Uniform(0.0, 30.0)
distX = ot.ComposedDistribution([distZ0, distV0.
 distM, distC])
size = 100
inputSample = distX.getSample(size)
outputField = alti(inputSample)
```

Dimension reduction: Karhunen-Loeve decomposition

- ▶ We wish to reduce the dimension of the problem from a infinite dimensional output to a finite dimensional one
- ▶ We can perform a Karhunen-Loeve decomposition with a finite truncature
- This requires to solve a Fredholm's problem in order to identify the eigenfunctions and associated eigenvalues of the considered process

$$Y(\omega,\underline{t}) = \sum_{k=1}^{\infty} \sqrt{\lambda_k} \xi_k(\omega) \underline{\varphi}_k(\underline{t}) \to \tilde{Y}(\omega,\underline{t}) = \sum_{k=1}^{p} \sqrt{\lambda_k} \xi_k(\omega) \underline{\varphi}_k(\underline{t})$$



```
meanFunction = ot.PiLagrangeEvaluation(
    meanField)
trend = ot.TrendTransform(meanFunction, myMesh)
invTrend = trend.getInverse()
outputFieldCentered = invTrend(outputField)

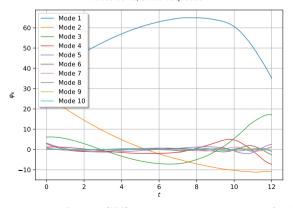
truncThreshold = 1.0e-5
algo = ot.KarhunenLoeveSVDAlgorithm(
    outputFieldCentered, truncThreshold)
algo.run()
KLResult = algo.getResult()
eigenValues = KLResult.getEigenValues()
```

Dimension reduction: Karhunen-Loeve decomposition

$$\tilde{Y}(\omega,\underline{t}) = \sum_{k=1}^{p} \sqrt{\lambda_k} \xi_k(\omega) \underline{\varphi}_k(\underline{t})$$

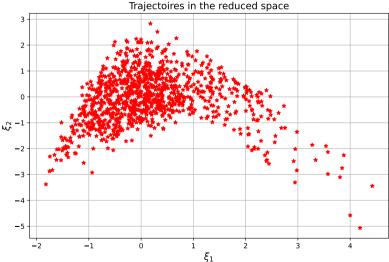
Main modes:

Modes de KL. chute visqueuse



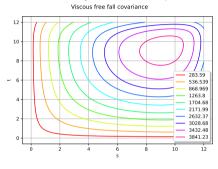
Dimension reduction: Karhunen-Loeve decomposition

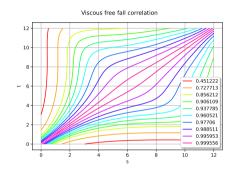
We only consider the first 2 terms of the decomposition:



Field function analysis

We center the trajectories with respect to the mean field:





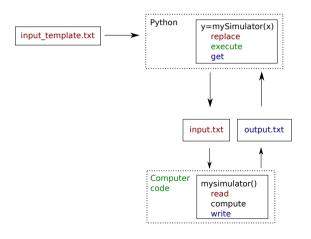
```
cov = KLResult.getCovarianceModel()

# As a covariance function
isStationary = False
asCorrelation = False
graph = cov.draw(0, 0, tmin, tmax, 128, isStationary, asCorrelation)

# As a correlation function
asCorrelation = True
graph = cov.draw(0, 0, tmin, tmax, 128, isStationary, asCorrelation)
```

Coupling OpenTURNS with computer codes

OpenTURNS provides a text file exchange based interface in order to perform analyses on complex computer codes



- Replaces the need for input/output text parsers
- Wraps a simulation code under the form of a standard python function
- Allows to interface OpenTURNS with a cluster

Support, discussion and contribution

- github repository: github.com/openturns/openturns
 - Bug report
 - Enhancement suggestions
 - Contribute
 - Review contributions
- Discourse forum: https://openturns.discourse.group/
 - Practical questions
 - Theoretical questions
 - ► Feature request
 - Forum layout
- Gitter chat: https://gitter.im/openturns
 - Practical questions
 - ► Theoretical questions
 - ► Feature request
 - Chat lavout

A few recent highlights

- Introduction of the **experimental** sub-module
- New services
 - Introduction of generalized extreme value distributions
 - ► Cross-entropy importance sampling & Non-parametric adaptive importance sampling
 - Uniform sampling on a mesh
 - ► Field to vector surrogate modeling & sensitivity
 - ► Iterative statistics (Mean, variance, Sobol')
 - ► HSIC indices
 - New examples and use-cases
 - **.** . .
- Performance enhancement
 - ▶ Parallelization and optimized computation of HSIC indices & p-values
 - Improved interface and flexibility of the Metropolis-Hastings sampling classes
 - Improved polynomial chaos expansion API
 - Coupling with the Pagmo optimization library
 - **•** ...

Reliability analysis: cross-entropy importance sampling

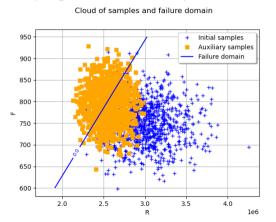
We wish to evaluate the probability of a given event through importance sampling:

$$\hat{P}_{\mathsf{IS}} = \frac{1}{N} \sum_{i=1}^{N} 1_{g(\mathbf{x}_i) < T} \frac{f_{\mathbf{X}}(\mathbf{x}_i)}{h(\mathbf{x}_i)}$$

- ► f_X input distribution
- h parametric auxiliary distribution
- \triangleright \mathbf{x}_i generated according to h
- ▶ h is updated during the sampling process so as to tend towards its optimal value
- ▶ We can work in both the **physical** and the **standard** spaces

Reliability analysis: cross-entropy importance sampling

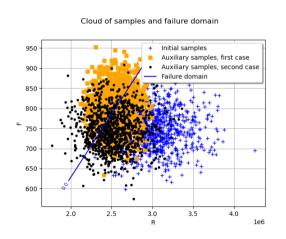
Sampling in the standard space



- Probability of failure: 0.029465848610494363
- Coefficient of variation: 0.045029988245260714

Reliability analysis: cross-entropy importance sampling

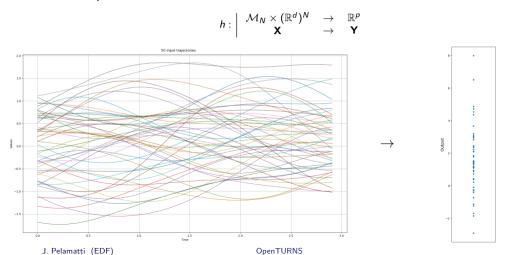
Sampling in the physical space



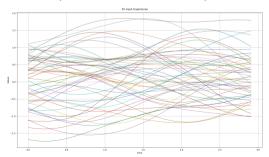
```
marginR = ot.LogNormalMuSigma().getDistribution()
marginF = ot.Normal()
auxiliaryDistribution = ot.ComposedDistribution([marginR
     . marginFl)
# Case 1: optimize al parameters
physicalSpaceIS1 = otexp.
     PhysicalSpaceCrossEntropyImportanceSampling(
    event, auxiliaryDistribution, activeParameters,
     initialParameters, bounds
physicalSpaceIS1.run()
# Case 2: only distribution means are optimized
activeParameters = ot. Indices([0. 3])
physicalSpaceIS2 = otexp.
     PhysicalSpaceCrossEntropyImportanceSampling(
    event, auxiliaryDistribution, activeParameters,
     initialParameters, bounds
physicalSpaceIS2.run()
```

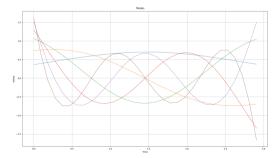
- Probability of failure: 0.029702353119720654
- ► Coefficient of variation: 0.04321365594527282

► We consider here an application which takes a random field as input, and provides a vectorial output:



- \blacktriangleright We want to create a surrogate model, \tilde{h} , of the function at hand
- ► The class **FieldToPointFunctionalChaosAlgorithm** allows to do so by combining the following functionalities:
 - ► Karhunen-Loeve decomposition of the functional input over a discrete mesh
 - Creation of a polynomial chaos expansion surrogate model between the resulting reduced space and the vectorial outputs

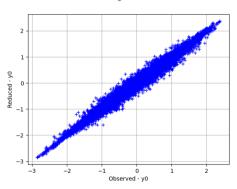




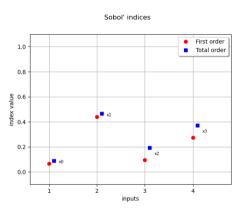
```
algo = otexp.FieldToPointFunctionalChaosAlgorithm(x, y)
# 1. KL parameters
algo.setThreshold(4e-2)  # we expect to explain 96% of
    variance
algo.setNbModes(10)  # max KL modes (default=unlimited)
algo.run()
result = algo.getResult()
kl_results = result.getInputKLResultCollection()

for i in range(x.getDimension()):
    validation = ot.KarhunenLoeveValidation(x.
        getMarginal(i), kl_results[i])
    graph = validation.drawValidation().getGraph(0, 0)
```

KL validation - marginal #1 ratio=98.52 %



```
sensitivity = otexp.FieldFunctionalChaosSobolIndices(
    result)
graph = sensitivity.draw()
```

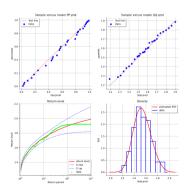


Modeling generalized extreme value (GEV) distributions

Estimation techniques

- Likelihood maximization
- Profile likelihood maximization

Estimation of a return level (sea level data)

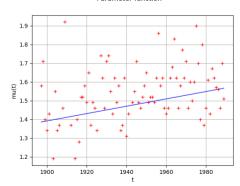


Stationary and non-stationary data

The GEV parameters can be made to vary as a function of time:

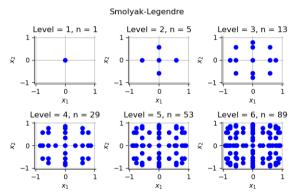
$$\mathsf{GEV}(\mu(t), \sigma(t), \xi(t))$$





Efficient numerical quadrature: Smolyak-Legendre quadrature

► Combines multi-dimensional Gauss-Legendre quadrature with an efficient selection of the polynomial multi-indices.



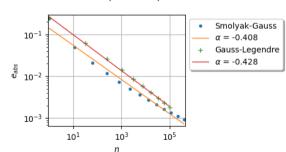
Efficient numerical quadrature: Smolyak-Legendre quadrature

Example on the integration of:

$$g(\mathbf{x}) = (1 + 1/d)^d \prod_{i=1}^d x_i^{1/d}$$

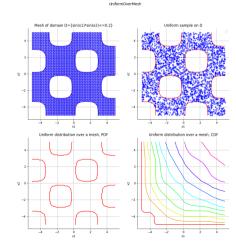
uniform = ot.GaussProductExperiment(ot.Uniform(0.0, 1.0)) collection = [uniform] * dimension level = 5 print("level = ", level) experiment = otexp.SmolyakExperiment(collection, level) nodes, weights = experiment.generateWithWeights() g_values = g_function(nodes) g_values_point = g_values.asPoint() approximate_integral = g_values_point.dot(weights) lre10 = -np.log10(abs(approximate_integral - integral) / abs(integral)

Exponential problem



Sampling on a mesh

We wish to sample over a mesh, proportionally to the size of each cell, and uniformly in a given cell



PERSALYS, the graphical user interface of OpenTURNS

- Provides a graphical interface of OpenTURNS in and out of the SALOME integration platform
- ▶ Features: probabilistic model, distribution fitting, central tendency, sensitivity analysis, probability estimate, surrogate modeling (polynomial chaos, kriging, linear regression), screening (Morris), optimization, design of experiments
- ► GUI language: English, French
- Partners: EDF, Phiméca
- Licence: LGPL
- ► OS: Windows and Linux
- ➤ Schedule: Since summer 2016, two releases per year, currently V13

https://persalys.fr/



The end

Thanks!

Questions?



