Bayesian inference through MCMC sampling with OpenTURNS

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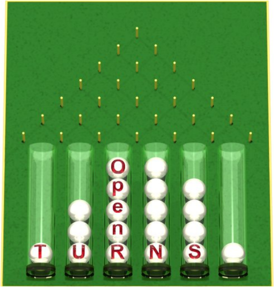
OpenTURNS: www.openturns.org



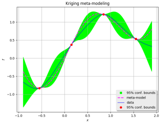
- Multivariate probabilistic modeling including dependence
- Numerical tools dedicated to the treatment of uncertainties
- Generic coupling to any type of physical model
- Open source, LGPL licensed, C++/Python library

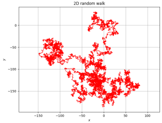
OpenTURNS: www.openturns.org

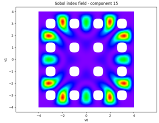
- Linux, Windows, macOS
- First release : 2007
- 5 full time developers
- Users ≈ 1000, mainly in France (785 000 Total Conda downloads)
- Project size : 800 classes, more than 6000 services

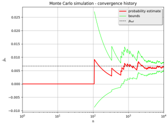
OpenTURNS: content

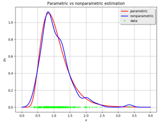
- Data analysis
  - Distribution fitting
  - Statistical tests
  - Estimate dependency and copulas
  - Estimate stochastic processes
- Probabilistic modeling
  - Dependence modeling
  - Univariate distributions
  - Multivariate distrbutions
  - Copulas
  - Processes
  - Covariance kernels
- Surrogate 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







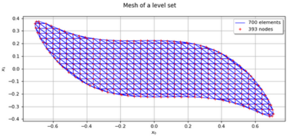




OpenTURNS: documentation

LevelSetMesher

(Source code, png, hires.png, pdf)



class **LevelSetMesher**(**args*)

Creation of mesh of box type.

Available constructor:

LevelSetMesher(*discretization*)

Parameters: **discretization** : sequence of int, of dimension ≤ 3.

Discretization of the levelset bounding box.

solver : `OptimizationAlgorithm`

Optimization solver used to project the vertices onto the level set. It must be able to solve nearest point problems. Default is `AbdoRackwitz`.

Notes

The meshing algorithm is based on the `IntervalMesher` 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 projected onto the levelset using a linear interpolation
- If the *project* flag is *True*, then the projection is refined using an optimization solver.

Examples

Create a mesh:

```
>>> import openturns as ot
>>> mesher = ot.LevelSetMesher([5, 10])
>>> level = 1.0
>>> function = ot.SymbolicFunction(['x0', 'x1'], ['x0^2+x1^2'])
>>> levelSet = ot.LevelSet(function, level)
>>> mesh = mesher.build(levelSet)
```

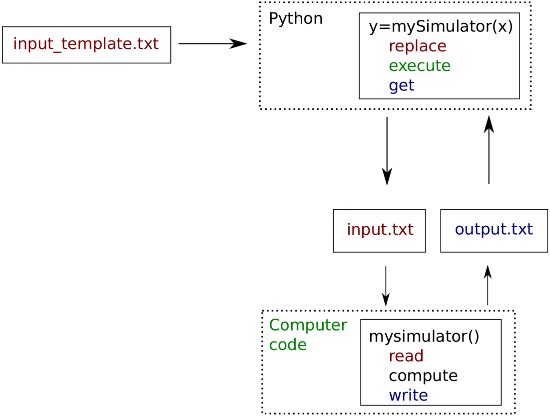
Methods

`build`(*args)	Build the mesh of levelset type.
`getClassName`()	Accessor to the object's name.
`getDiscretization`()	Accessor to the discretization.

- <u>Content</u>:
  - Programming interface (API)
  - Examples
  - Theory
- *All* classes and methods are documented, partly automatically.
- Examples are automatically tested at *each* update of the code and outputs are checked.

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
- otwrapy: interfacing tool to allow easy parallelization

Contents

OpenTURNS: Metropolis-Hastings

We want to sample from the distribution π of a random variables X. Here is one step of the algorithm, starting from the point x:

1. Simulate a candidate $x' \sim q(\cdot|x)$ for some conditional distribution q.
2. Compute $\alpha(x'|x, y, z) = \min\left\{ \frac{\pi(x')\, q(x|x')}{\pi(x) q(x'|x)}, 1 \right\}$.
3. Simulate $u \sim \mathcal{U}(0, 1)$. If $u \leqslant \alpha(x'|x)$, then the next state is x', otherwise it is x.

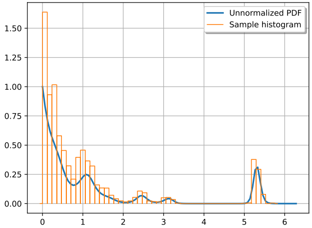
Throughout the presentation, our code is prefaced by:

```
import openturns as ot
import math as m
import numpy as np
```

Random walk Metropolis Hastings

When $q(\cdot|x) = x + \mu$, where μ is a distribution that does not depend on x, the algorithm is called "Random walk Metropolis-Hastings" and μ is called the "proposal distribution".

Sample from a nonstandard distribution[1]



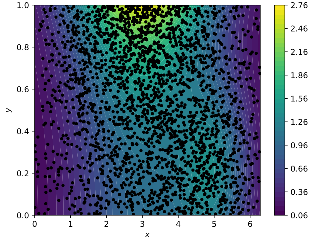
$$\pi(x) \propto \frac{1}{2}\left(2 + \sin(x)^2\right) \exp\left[-\left(2 + \cos(3x)^3 + \sin(2x)^3\right) x\right] \mathbf{1}_{[0,2\pi]}(x)$$

```
logdensity = ot.SymbolicFunction('x','log(2+sin(x)^2) - (2+cos(3*x)^3+sin(2*x)^3) * x')
support = ot.Interval([0.0], [2.0 * m.pi])
proposal = ot.Normal(0.0, 2.0) # mu
initialState = [3.0]
sampler = ot.RandomWalkMetropolisHastings(logdensity, support, initialState, proposal)
x = sampler.getSample(10000)
```

[1] Marin , J.M. and Robert, C.P. (2007). Bayesian Core: A Practical Approach to Computational Bayesian Statistics. *Springer-Verlag*, New York

2D Random walk Metropolis Hastings

Sample from a 2D nonstandard distribution

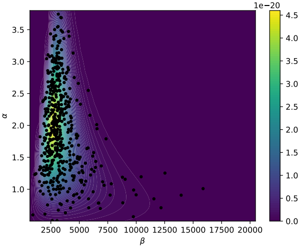


$$\pi(x) \propto \left(\exp\left[-\frac{1}{4}(x-3)^2 + y^2 \right] + \exp\left[-(x-5)^2 - 5\left(y - \frac{1}{5}\right)^2 \right] \right) \mathbf{1}_{[0,2\pi]}(x)\mathbf{1}_{[0,1]}(y)$$

```
logdensity = ot.SymbolicFunction(
    ["x", "y"], ["log(exp(-0.25 * (x-3)^2 + y^2) + exp(-(x-5)^2 - 5 * (y-0.2)^2))"]
)
support = ot.Interval([0.0, 0.0], [2.0 * m.pi, 1.0])
proposal = ot.Normal([0.0] * 2, [1.0, 0.2])
initialState = [3.0, 0.8]
sampler = ot.RandomWalkMetropolisHastings(logdensity, support, initialState, proposal)
x = sampler.getSample(50000)
```

2D Random walk Metropolis Hastings in a Bayesian setting

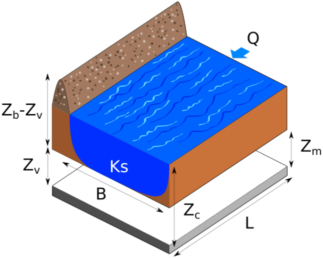
Posterior distribution of the parameters of a Weibull model



$$\beta \sim \Gamma(k = 2, \lambda = 2 \cdot 10^{-4})$$
$$\alpha \sim \mathcal{U}(0.5, 3.8)$$
$$T|\beta, \alpha \sim \mathcal{W}(\beta, \alpha, 0)$$
$$F_{\mathcal{W}}(t) = 1 - \exp\left[-\left(\frac{t-0}{\beta}\right)^{\alpha}\right]$$

```
alpha_min, alpha_max, a_beta, b_beta = 0.5, 3.8, 2.0, 2.0e-4
priorMarginals = [ot.Gamma(a_beta, b_beta), ot.Uniform(alpha_min, alpha_max)]
prior = ot.ComposedDistribution(priorMarginals)
proposal = ot.Normal([0.0]*2, [0.1*m.sqrt(a_beta/b_beta**2), 0.1*(alpha_max-alpha_min)])
initialState = [a_beta / b_beta, 0.5 * (alpha_max - alpha_min)]
sampler = ot.RandomWalkMetropolisHastings(prior, initialState, proposal)

conditional = ot.WeibullMin()
Tobs = [[4380], [1791], [1611], [1291]]

# WeibullMin expects beta, alpha, and localization, but the prior is only on beta, alpha
linkFunction = ot.SymbolicFunction(["beta", "alpha"], ["beta", "alpha", "0"])
sampler.setLikelihood(conditional, Tobs, linkFunction)
sample = sampler.getSample(100000)
```

A flood model



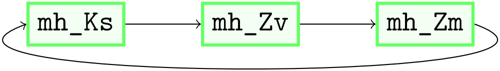
$$\forall 1 \leq i \leq 8, H^{(i)} \sim \mathcal{N}\left(G(Q^{(i)}, K_s, Z_v, Z_m), \frac{1}{2}\right)$$

$$K_s \sim \mathcal{N}(20, 5)$$
$$Z_v \sim \mathcal{N}(49, 1)$$
$$Z_m \sim \mathcal{N}(51, 1)$$

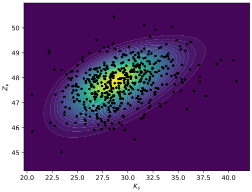
```
Qobs = [[2097], [1448], [1516], [2173], [387], [3016], [651], [541]]
Hobs = [[3.4], [2.5], [2.7], [3.5], [1.0], [4.2], [1.6], [1.6]]

def flooding(X):
    L = 5.0e3
    B = 300.0
    Q, K_s, Z_v, Z_m = X
    alpha = (Z_m - Z_v) / L
    if alpha < 0.0 or K_s <= 0.0:
        H = np.inf
    else:
        H = (Q / (K_s * B * np.sqrt(alpha))) ** (3.0 /
    5.0)
    return [H, 0.5]

functionG = ot.PythonFunction(4, 2, flooding)

# Q (input #0) is not calibrated
linkFunction = ot.ParametricFunction(functionG, [0], [100])
```

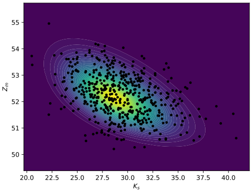
```
conditional = ot.Normal()

parameterPriorMean = [20.0, 49.0, 51.0]
parameterPriorSigma = [5.0, 1.0, 1.0]
prior = ot.Normal(parameterPriorMean, parameterPriorSigma)

initialState = parameterPriorMean
```

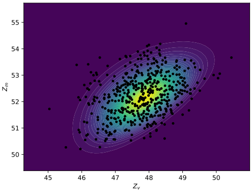
Single component Random Walk Metropolis-Hastings



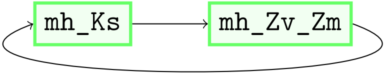

```
mh_coll = [
  ot.RandomWalkMetropolisHastings(prior, initialState, ot.Uniform(-5.0, 5.0), [0]),
  ot.RandomWalkMetropolisHastings(prior, initialState, ot.Uniform(-1.0, 1.0), [1]),
  ot.RandomWalkMetropolisHastings(prior, initialState, ot.Uniform(-1.0, 1.0), [2]),
]

for mh in mh_coll:
    mh.setLikelihood(conditional, Hobs, linkFunction, Qobs)

sampler = ot.Gibbs(mh_coll) # NB: the order can be made random: cf. setUpdatingMethod
sample = sampler.getSample(10000)
```



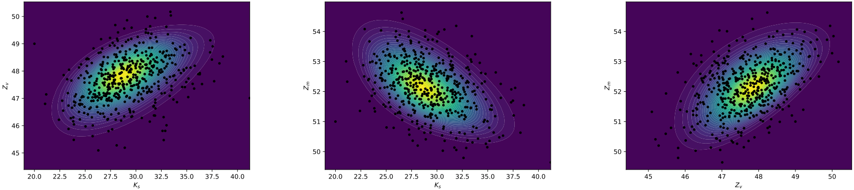




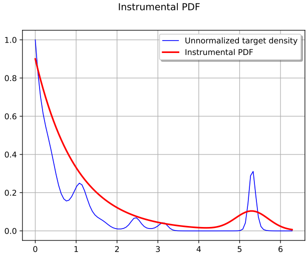
Blocks of components can be considered



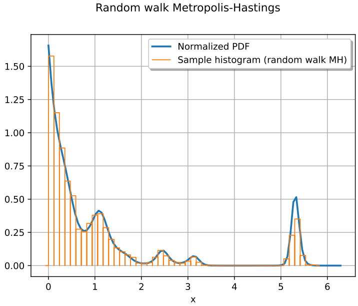

```python
mh_coll = [
  ot.RandomWalkMetropolisHastings(prior, initialState, ot.Uniform(-5.0, 5.0), [0]),
  ot.RandomWalkMetropolisHastings(prior,
                                  initialState,
                                  ot.ComposedDistribution([ot.Uniform(-1.0,1.0)]*2),
                                  [1, 2])
]
for mh in mh_coll:
    mh.setLikelihood(conditional, Hobs, linkFunction, Qobs)
sampler = ot.Gibbs(mh_coll) # NB: the order can be made random: cf. setUpdatingMethod
sample = sampler.getSample(10000)
```

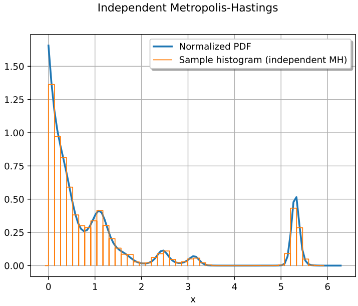


Independent Metropolis-Hastings: $q(\cdot|x) = \mu$



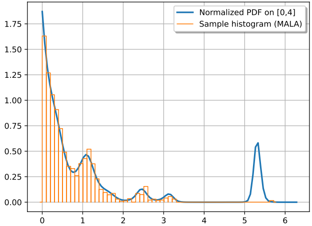

```
logdensity = ot.SymbolicFunction('x','...') # replace ...
support = ot.Interval([0.0], [2.0 * m.pi])
initialState = [3.0] # unimportant for independent MH

exp = ot.Exponential(1.0)
unif = ot.Normal(5.3, 0.4)
instrumental = ot.Mixture([exp, unif], [0.9, 0.1])

independentMH = ot.IndependentMetropolisHastings(
  logdensity, support, initialState, instrumental
)
x = independentMH.getSample(10000)
```





User-defined Metropolis-Hastings: $q(\cdot|x) = \mu(x)$

Metropolis adjusted Langevin algorithm[2] implementation



With $h > 0$ a fixed parameter:

$$q(\cdot|x) = \mathcal{N}\left(x + \frac{h}{2}\frac{d}{dx}[\log(\pi(x)], \sqrt{h}\right)$$

```
from openturns.experimental import UserDefinedMetropolisHastings
logdensity = ot.SymbolicFunction('x','log(2+sin(x)^2) - (2+cos(3*x)^3+sin(2*x)^3) * x')
support, proposal, initialState = ot.Interval([0.0], [2.0 * m.pi]), ot.Normal(), [2.5]
h = 0.5
std_deviation = m.sqrt(h)

def python_link(x):
    derivative_log_density = logdensity.getGradient().gradient(x)[0, 0]
    mean = x[0] + h / 2 * derivative_log_density
    return [mean, std_deviation]
link = ot.PythonFunction(1, 2, python_link)

mala = UserDefinedMetropolisHastings(logdensity, support, initialState, proposal, link)
z = mala.getSample(10000)
```

[2] Robert, C. P. *The Metropolis-Hastings algorithm*. arXiv preprint arXiv:1504.01896, 2015

Random vector "Metropolis Hastings"

$$\boldsymbol{Y}|\boldsymbol{\theta}, \tau \sim \mathcal{N}_n(\boldsymbol{X}\boldsymbol{\theta}, \tau^{-1}\boldsymbol{I}_n + \boldsymbol{Q}^{-1})$$

$$\boldsymbol{X} \in \mathbb{R}^{n\times p}, \boldsymbol{Q} \in \mathbb{R}^{n\times n}(\text{diagonal})$$

$$\boldsymbol{\theta}|\tau \sim 1, \tau \sim \tau^{-1}$$

```
n = 10; p = 2
X = ot.Sample([[1.0]] * n)
Xcol = [[9.6], [9.5], [-16.6], [3.9],
     [-10.9], [7.8], [10.9], [-6.5], [15.8],
      [6.1]]
X.stack(Xcol)
Q = np.array([[1.4], [1.1], [4.1], [1.0],
     [2.9], [3.3], [1.0], [2.1], [2.9],
     [1.6]]) # Diagonal of Q
Y = [4.9, 8.0, -16.8, 6.1, -7.1, 2.3, 10.9,
     -3.0, 20.2, 3.7]}

def py_link_y(x):
    theta = [x[i] for i in range(p)]
    tau = x[p]
    mean = np.dot(X, theta)
    std = np.sqrt(1.0 / tau + 1.0 / Q)
    params = np.zeros(2 * n)
    params[::2] = mean
    params[1::2] = std.ravel()
    return params
link_y = ot.PythonFunction(3,20,py_link_y)
```

$$\boldsymbol{\theta}|\boldsymbol{Y}, \tau \sim \mathcal{N}_p(\boldsymbol{\mu}_n, \boldsymbol{\Sigma}_n)$$

$$\boldsymbol{\mu}_n = (\boldsymbol{X}^T(\boldsymbol{I}_n + \tau\boldsymbol{Q}^{-1})^{-1}\boldsymbol{X})^{-1} (\boldsymbol{X}^T(\boldsymbol{I}_n + \tau\boldsymbol{Q}^{-1})^{-1}\boldsymbol{Y})$$

$$\boldsymbol{\Sigma}_n = \tau^{-1}(\boldsymbol{X}^T(\boldsymbol{I}_n + \tau\boldsymbol{Q})^{-1}\boldsymbol{X})^{-1}$$

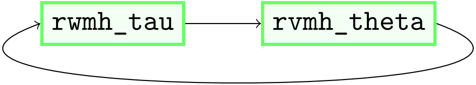
```
def py_link_theta(x):
    tau = x[p]
    Itilde_inv = 1.0 / (1.0 + tau / Q)
    Xtilde = Itilde_inv * X
    Sigma_n = np.linalg.inv(np.dot(Xtilde.T,
      X)) / tau
    mu_n = np.dot(Xtilde.T, Y)
    mu_n = tau * np.dot(Sigma_n, mu_n)
    dist = ot.Normal(mu_n,
           ot.CovarianceMatrix(Sigma_n)
    )
    return dist.getParameter()

link_theta = ot.PythonFunction(3, 5,
     py_link_theta)

RVtheta = ot.RandomVector(ot.Normal(p))
rvmh_theta = ot.RandomVectorMetropolisHastings(
    RVtheta, [1.0] * 3, [0,1], link_theta)
```

Random vector "Metropolis Hastings" – continued

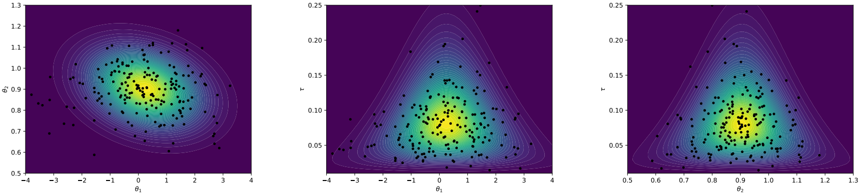
τ must be sampled the hard way, using Random walk Metropolis

```
proposal_tau = ot.Normal(0.0, 1e-1)
logprior = ot.SymbolicFunction(["theta1", "theta2", "tau"], ["-log(tau)"])
support = ot.Interval([-np.inf, -np.inf, 0.0], [np.inf] * 3)}
rwmh_tau = ot.RandomWalkMetropolisHastings(logprior, support, [1.0]*3, proposal_tau,[p])
rwmh_tau.setLikelihood(ot.ComposedDistribution([ot.Normal()]*len(Y)), [Y], link_y)
```

Samplers are combined in a Gibbs algorithm




```
gibbs = ot.Gibbs([rwmh_tau, rvmh_theta])
sample = gibbs.getSample(10000)
sample.setDescription([r"$\theta_1$", r"$\theta_2$", r"$\tau$"])
```



Conclusion

OpenTURNS provides an MCMC sampling framework through the following classes:

- MetropolisHastings variants:
  - RandomWalkMetropolisHastings
  - IndependentMetropolisHastings
  - UserDefinedMetropolisHastings
  - RandomVectorMetropolisHastings
- Gibbs

These classes can be freely combined to sample from nonstandard distributions in a “smart” manner.

In a Bayesian setting, this framework allows users to create and implement the MCMC algorithm most suited to a particular posterior distribution.