Chaospy:

A modular implementation of Polynomial Chaos expansions and Monte Carlo methods

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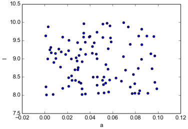
Chaospy is a Python toolbox for forward model UQ

Properties of Chaospy



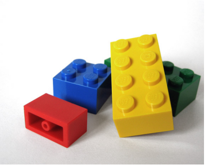
Monte Carlo methods

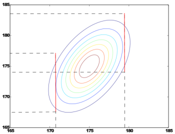
$$\sum_{n=0}^{N} c_n(x) P_n(q)$$

Polynomial Chaos

What is new in Chaospy

Chaospy is modular and therefore very flexible





Chaospy has support for dependent variables

Chaospy has a large collection of methods and distributions

It is easy to compare different methods on given a problem

Comparing Chaospy with Turns and Dakota

Feature	Dakota	Turns	Chaospy
Distributions	11	26	**64**
Copulas	1	7	**6**
Sampling schemes	4	7.5	**7**
Orthogonal polynomial schemes	4	3	**5**
Numerical integration strategies	7	0	**7**
Regression methods	5	4	**8**
Analytical metrics	6	6	**7**

Chaospy has support for many different methods

- Monte Carlo with variance reduction techniques
- Intrusive and non-intrusive polynomial chaos
  - Pseudo-spectral method
  - Point collocation/regression

All Chaospy needs is a Python wrapper around the forward model

```python
def solver(*node):
    # node: tuple of the uncertain stochastic parameters

    model.set_parameters(node)

    model.run()

    results = model.post_processing()

    return results
```

Chaospy is a completly generic software; for simplicity we use a very simple example problem

$$\frac{du(x)}{dx} = -au(x), \qquad u(0) = I.$$

u The quantity of interest.

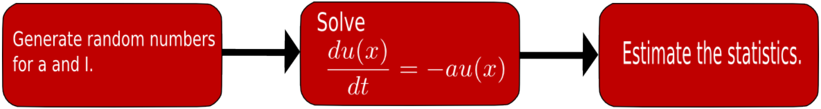
x Spatial location.

a, I Parameters containing uncertainties.

$$a \sim \text{Uniform(0, 0.1)} \qquad\qquad I \sim \text{Uniform(8, 10)}$$

We want to compute E(u) and Var(u).

Monte Carlo integration can be used for any model

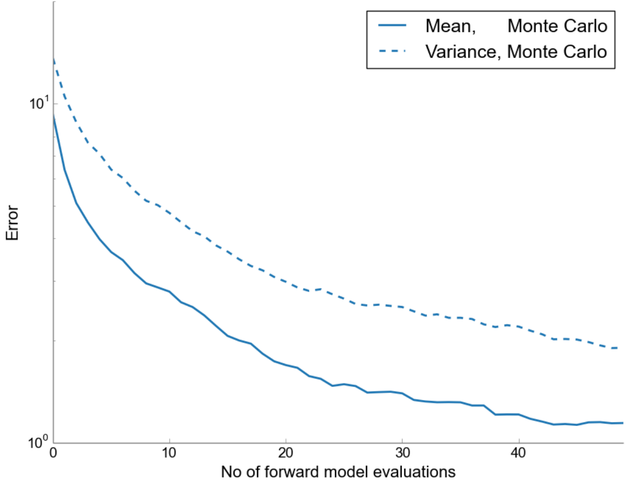


Monte Carlo with Chaospy

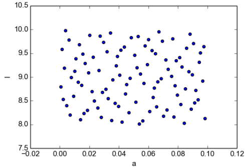
```
import chaospy as cp
import numpy as np

dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)

# Joint distribution
dist = cp.J(dist_a, dist_I)

samples = dist.sample(size=1000)

# solver returns u(x), where x is fixed
# samples_u: list of all u(x) for each set of a and I
samples_u = [solver(a, I) for a, I in samples]

E = np.mean(samples_u, 0)
Var = np.var(samples_u, 0)
```

Convergence of Monte Carlo is slow

$$\varepsilon_E = \int |\mathrm{E}(u) - \mathrm{E}(\hat{u})|\, dx \qquad \varepsilon_{Var} = \int |\mathrm{Var}(u) - \mathrm{Var}(\hat{u})|\, dx$$

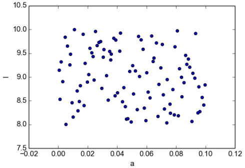


Chaospy has several variance reduction techniques for sampling a distribution



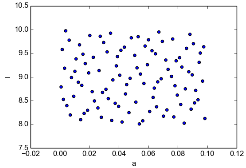
Hammersley sampling:

`nodes = dist.sample(100, "M")`



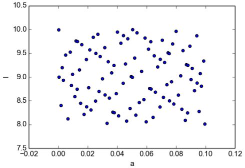
Latin Hypercube sampling:

`nodes = dist.sample(100, "L")`



Halton sampling

`nodes = dist.sample(100, "H")`



Sobol sampling

`nodes = dist.sample(100, "S")`

The different sampling schemes available in Chaospy compared to Turns and Dakota

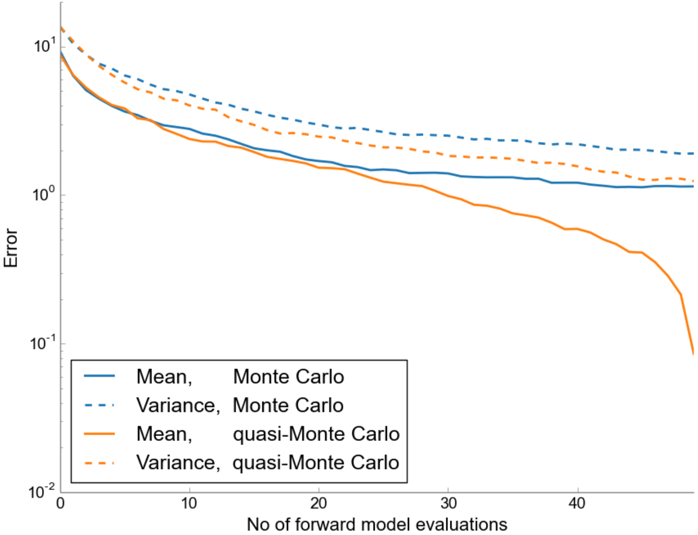
Quasi-Monte Carlo scheme	Dakota	Turns	Chaospy
Faure sequence	No	Yes	**No**
Halton sequence	Yes	Yes	**Yes**
Hammersley sequence	Yes	Yes	**Yes**
Haselgrove sequence	No	Yes	**No**
Korobov latice	No	No	**Yes**
Niederreiter sequence	No	Yes	**No**
Sobol sequence	No	Yes	**Yes**

Other methods			
Antithetic variables	No	No	**Yes**
Importance sampling	Yes	Yes	**Yes**
Latin Hypercube sampling	Yes	Limited	**Yes**

Quasi-Monte Carlo with Latin Hypercube sampling

```
import chaospy as cp
import numpy as np

dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a, dist_I)

samples = dist.sample(size=1000, rule="L")

samples_u = [solver(a, I) for a, I in samples]

E = np.mean(samples_u, 0)
Var = np.var(samples_u, 0)
```

Convergence of quasi-Monte Carlo is better than Monte Carlo, but still slow



Mapping in probability space; the idea behind Polynomial Chaos (PC) theory is to approximate our forward model with a polynomial

$$u(x;q) \quad \approx \quad \hat{u}_M(x;q) \quad = \quad \sum_{n=0}^{N} \quad \underbrace{c_n(x)}_{\text{Coefficient}} \quad \underbrace{P_n(q)}_{\text{Polynomial}}$$

$\hat{u}_M(x;q)$ is the mapping from the uncertain variables q to the response variable u, x is a fixed variable.

Mean and variance are calculated from $\hat{u}_M(x;q)$.

P_n are orthogonal polynomials and are generaly calculated through the three-term discretized Stiltjes recursion

```
dist = cp.Normal()

P = cp.orth_ttr(3, dist)

print P
[1.0, q0, q0^2-1.0, q0^3-3.0q0]
```

Methods for generating expansions of orthogonal polynomials

Orthogonalization Method	Dakota	Turns	Chaospy
Askey–Wilson scheme	Yes	Yes	**Yes**
Bertran recursion	No	No	**Yes**
Cholesky decomposition	No	No	**Yes**
Discretized Stieltjes	Yes	No	**Yes**
Modified Chebyshev	Yes	Yes	**No**
Modified Gram–Schmidt	Yes	Yes	**Yes**

The pseudo-spectral method, used to calculate c_n, needs numerical integration, which demands generating quadrature nodes and weights

```
dist = cp.Normal()

nodes, weights = cp.generate_quadrature(2, dist, rule="G")

print nodes
[[-1.73205081  0.          1.73205081]]
print weights
[ 0.16666667  0.66666667  0.16666667]
```

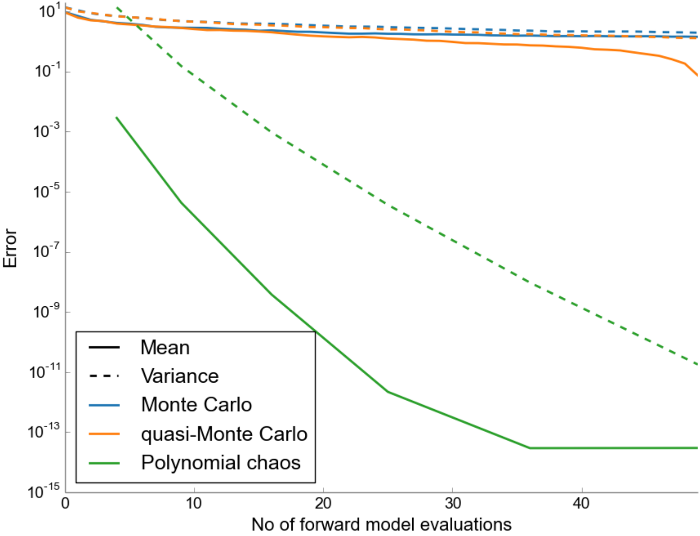
Numerical integration strategies implemented in the three software toolboxes

Node and weight generators	Dakota	Turns	Chaospy
Clenshaw-Curtis quadrature	Yes	No	**Yes**
Cubature rules	Yes	No	**No**
Gauss-Legendre quadrature	Yes	No	**Yes**
Gauss-Patterson quadrature	Yes	No	**Yes**
Genz-Keister quadrature	Yes	No	**Yes**
Leja quadrature	No	No	**Yes**
Monte Carlo integration	Yes	No	**Yes**
Optimal Gaussian quadrature	Yes	No	**Yes**

One slide is enough for the full implementation with the pseudo-spectral method in Chaospy

```
dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a,dist_I)

P = cp.orth_ttr(2, dist)

nodes, weights = cp.generate_quadrature(3, dist)

samples_u = [solver(*node) for node in nodes.T]

u_hat = cp.fit_quadrature(P, nodes, weights, samples_u
                          rule="Gaussian")

mean = cp.E(u_hat, dist)
var = cp.Var(u_hat, dist)
```

Convergence of polynomial chaos is much faster than the Monte Carlo methods



Chaospy is an ideal tool for research in UQ for the statistics expert

With a few lines of Python code it is easy to customize:

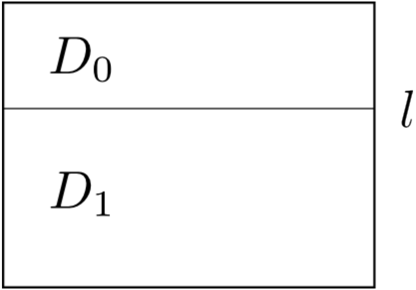
- distributions
- polynomials
- integration schemes
- sampling schemes
- statistical analysis of the result

Custom polynomials:

```
q0, q1 = cp.variable(2)

phi = cp.Poly([1, q0, q1, q0**2 - 1, q0*q1])

print phi
[1, q0, q1, q0^2-1, q0q1]
```

Chaospy handles Polynomial Chaos expansions with stochastically dependent variables

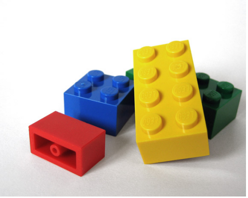
Diffusion in layered media with uncertain boundary, l, and uncertain diffusion constants, D_0, D_1.



Uncertain l slows down convergence, but introduction of auxiliary *dependent* variables restores convergence.

Summary: Chaospy is a Python toolbox for forward model UQ with advanced Monte Carlo methods and Polynomial Chaos expansions

Chaospy is modular, flexible, with syntax that resembles the mathematics



A vast collection of methods, ideal for method comparisons

Summary: Chaospy is a Python toolbox for forward model UQ with advanced Monte Carlo methods and Polynomial Chaos expansions

Installation instructions:

https://github.com/hplgit/chaospy

Reference:

Feinberg, J., & Langtangen, H. P. (2015). Chaospy: An open source tool for designing methods of uncertainty quantification. Journal Of Computational Science, 11, 46-57

http://hplgit.github.io/chaospy/doc/pub/chaospy-4screen.pdf

Questions?