Polynomial chaos expansions part I: Method Introduction

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Kalkulo AS

January 15, 2015

Lecture will include many examples using the Chaospy software

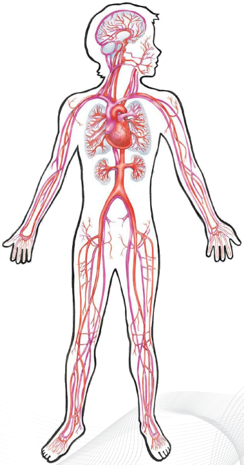
Installation instructions:

`http://github.com/hplgit/chaospy/`

Interactive sessions:

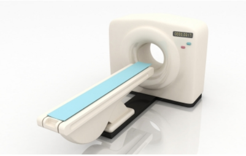
`path/to/ipython/notebook/sessions`

Practicle application involving bloodflow simulations



In colaboration with V. Eck and L. Hellevik

Modelling require uncertainty quantification



STARFiSh
STochastic ARterial Flow Simulations

Chaos Py

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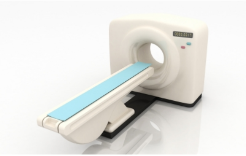

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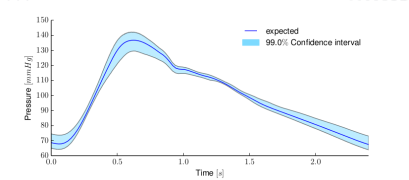

ntnu/results/sensitivity-point

Introducing a naive testcase as a working example

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

- u The quantity of interest
- x Spatio-temperal locations
- a, I Parameters containting uncertainties

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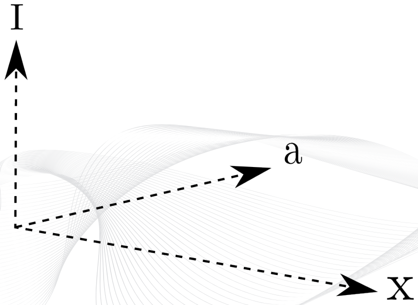

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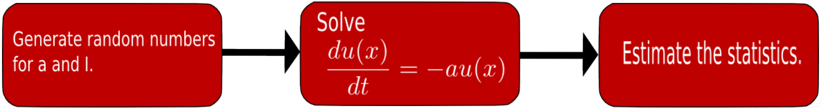
$$Var(u) = \int_0^{0.1} \left(e^{-ax}\right)^2\frac{1}{10}da - E(u)^2 = \frac{1 - e^{-0.2ax}}{20x} - \left(\frac{1 - e^{-0.1x}}{10x}\right)^2$$

Non-trivial models can be analysed using Monte Carlo integration



Monte Carlo with chaospy

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import chaospy as cp
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def u(x, a):
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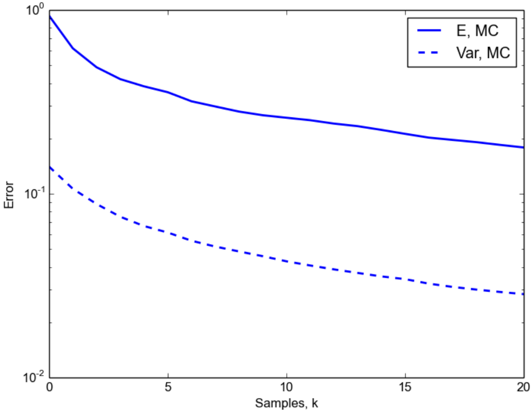
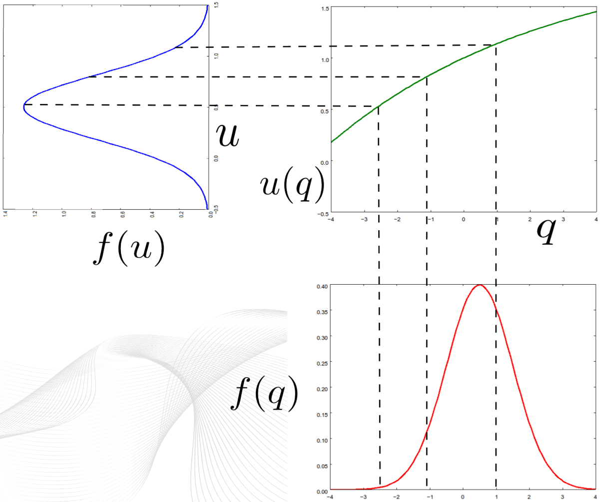
E = np.mean(U)
Var = np.var(U)
```

Convergence of Monte Carlo is slow

$$\varepsilon_E = \int_0^{10} |E(u) - E(\hat{u})| \, dx \quad \varepsilon_{Var} = \int_0^{10} |Var(u) - Var(\hat{u})| \, dx$$



Monte Carlo is based on the idea of indirect sampling



Using Lagrange polynomials to approximate the model

$$u(x;a) \approx \hat{u}_M(x;a) = \sum_{n=0}^{N} c_n(x) P_n(a) \qquad N = M + 1,$$

where

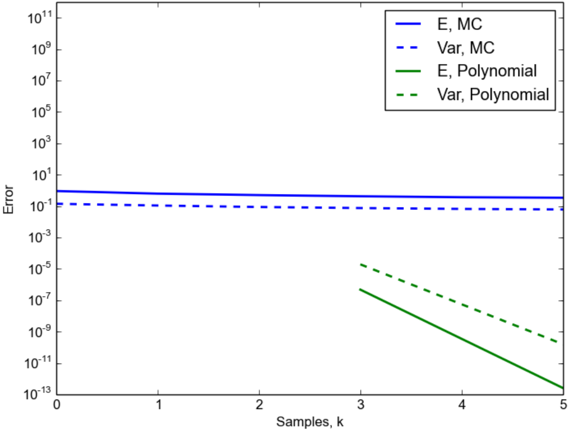
c_n are model evaluations $u(x, a_n)$

P_n are Lagrange polynomials:

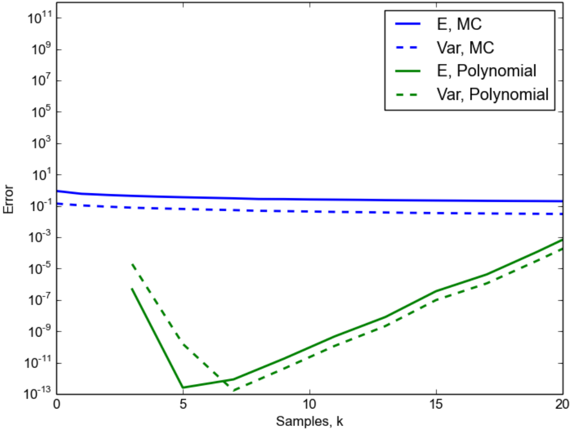
$$P_n(a) = \prod_{\substack{m=0 \\ m \neq n}}^{N} \frac{a - a_n}{a_m - a_n}$$

a_n are collocation nodes

Much better convergence properties than Monte Carlo



Stochastic analysis of model approximations can be dangerous



Combining polynomial approximation with uncertainty quantification well requires a better underlying theory

$$\langle u, v \rangle_Q = E(u \cdot v) \qquad \|u\|_Q = \sqrt{\langle u, u \rangle_Q}$$

where Q is a random vector, i.e. (a, I).

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Orthogonality:

$$\langle P_n, P_m \rangle = \begin{cases} \|P_n\|_Q^2 & n = m \\ 0 & n \neq m \end{cases}$$

Coefficients are Fourier when polynomials are orthogonal

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$$c_k = \frac{\langle u, P_k \rangle_Q}{\| P_k \|_Q^2} \qquad k = 0, \ldots, N$$

Optimality linked to statistical property

$$(c_0, \ldots, c_N) = \underset{c_0,\ldots,c_N}{\operatorname{argmin}} \|u - \hat{u}_M\|_Q$$

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$$\mathrm{E}(\hat{u}_M) = c_0 \qquad \mathrm{Var}(\hat{u}_M) = \sum_{n=1}^{N} c_n^2 \|P_n\|_Q$$

Construct an orthogonal polynomial expansion using Gram-Schmidt orthogonalization

$$v_0, v_1, \ldots, v_N = 1, q, \ldots, q^N$$

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M = 5; D = 1; N = M - 1

a = cp.Uniform(0,0.1)
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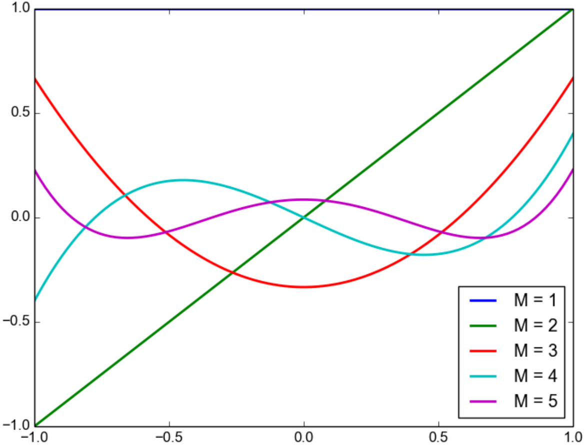
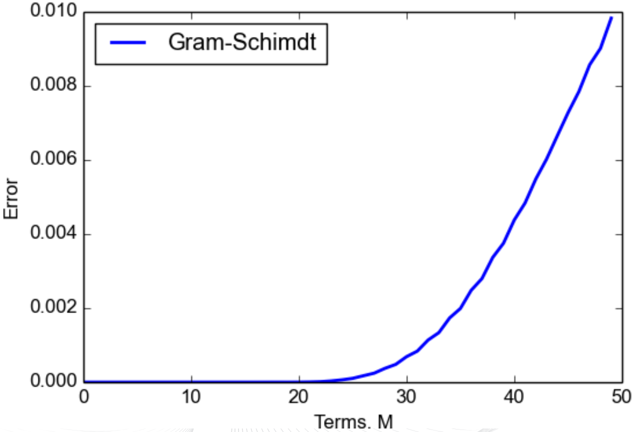
for n in xrange(1,N):
    p = v[n]
    for m in xrange(0,n):
        p -= P[m]*cp.E(v[n]*P[m],a)
                            /cp.E(P[m]**2,a)
    P.append(p)
P = cp.Poly(P)
```

Plot of all generated polynomials



Most constructors of orthogonal polynomials are illposed



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where

$$A_n = \frac{\langle qP_n, P_n \rangle_Q}{\|P_n\|_Q^2} \qquad\qquad B_n = \begin{cases} \frac{\|P_n\|_Q^2}{\|P_{n-1}\|_Q^2} & n > 0 \\ \|P_n\|_Q^2 & n = 0 \end{cases}$$

Askey scheme, organization of orthogonal polynomials

The askey scheme gives a relation between a probability distribution and the corresponding orhogonal polynomial.

Distribution	Polynomial	Support
Gaussian	Hermite	$(-\infty, \infty)$
Gamma	Laguerre	$[0, \infty]$
Beta	Jacobi	$[a, b]$
Uniform	Legendre	$[a, b]$

Three terms recursion in Chaospy

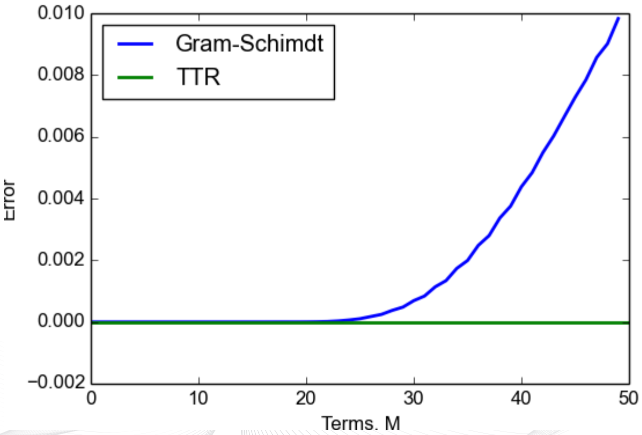
```
import chaospy as cp

M = 3
a = cp.Normal()
P = cp.orth_ttr(M, a)

print P

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

Discretized Stiltjes method is numerically stable



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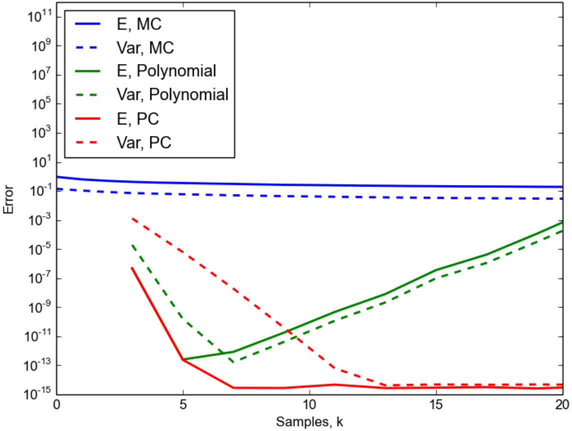
Convergence of orthogonal polynomial approximation



Extending the theory to multiple dimensions

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$\cdots$						
$\mathbf{P}_4$	$\cdots$					
$\mathbf{P}_3$	$\mathbf{P}_3\mathbf{P}_0$	$\cdots$				
$\mathbf{P}_2$	$\mathbf{P}_2\mathbf{P}_0$	$\mathbf{P}_2\mathbf{P}_1$	$\cdots$			
$\mathbf{P}_1$	$\mathbf{P}_1\mathbf{P}_0$	$\mathbf{P}_1\mathbf{P}_1$	$\mathbf{P}_1\mathbf{P}_2$	$\cdots$		
$\mathbf{P}_0$	$\mathbf{P}_0\mathbf{P}_0$	$\mathbf{P}_0\mathbf{P}_1$	$\mathbf{P}_0\mathbf{P}_2$	$\mathbf{P}_0\mathbf{P}_3$	$\cdots$	
	$\mathbf{P}_0$	$\mathbf{P}_1$	$\mathbf{P}_2$	$\mathbf{P}_3$	$\mathbf{P}_4$	$\cdots$

Construct polynomial approximation

Multi-index

$$\mathbf{P}_{00}$$
$$\mathbf{P}_{10} \quad \mathbf{P}_{01}$$
$$\mathbf{P}_{20} \quad \mathbf{P}_{11} \quad \mathbf{P}_{02}$$
$$\mathbf{P}_{30} \quad \mathbf{P}_{21} \quad \mathbf{P}_{12} \quad \dots$$

Single-index

$$\mathbf{P}_{0}$$
$$\mathbf{P}_{1} \quad \mathbf{P}_{2}$$
$$\mathbf{P}_{3} \quad \mathbf{P}_{4} \quad \mathbf{P}_{5}$$
$$\mathbf{P}_{6} \quad \mathbf{P}_{7} \quad \mathbf{P}_{8} \quad \dots$$

Orthogonality for multivariate polynomials

$$\langle \mathbf{P}_n, \mathbf{P}_m \rangle_Q = \mathrm{E}\Big(P_{n_1}^{(1)} \cdots P_{n_D}^{(D)} \cdot P_{m_1}^{(1)} \cdots P_{m_D}^{(D)} \Big)$$

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$$= \left\langle P_{n_1}^{(1)} \cdot P_{m_1}^{(1)} \right\rangle_Q \cdots \left\langle P_{n_D}^{(D)} \cdot P_{m_D}^{(D)} \right\rangle_Q$$

Orthogonality for multivariate polynomials

$$\begin{aligned}
\langle \mathbf{P}_n, \mathbf{P}_m \rangle_Q &= \mathrm{E}\left(P^{(1)}_{n_1} \cdots P^{(D)}_{n_D} \cdot P^{(1)}_{m_1} \cdots P^{(D)}_{m_D} \right) \\
&= \mathrm{E}\left(P^{(1)}_{n_1} \cdot P^{(1)}_{m_1} \right) \cdots \mathrm{E}\left(P^{(D)}_{n_D} \cdot P^{(D)}_{m_D} \right) \\
&= \left\langle P^{(1)}_{n_1} \cdot P^{(1)}_{m_1} \right\rangle_Q \cdots \left\langle P^{(D)}_{n_D} \cdot P^{(D)}_{m_D} \right\rangle_Q \\
&= \left\| P^{(1)}_{n_1} \right\|_Q \delta_{n_1 m_1} \cdots \left\| P^{(D)}_{n_D} \right\|_Q \delta_{n_D m_D}
\end{aligned}$$

Orthogonality for multivariate polynomials

$$
\begin{aligned}
\langle \mathbf{P}_n, \mathbf{P}_m \rangle_Q &= \mathrm{E}\left(P_{n_1}^{(1)} \cdots P_{n_D}^{(D)} \cdot P_{m_1}^{(1)} \cdots P_{m_D}^{(D)} \right) \\
&= \mathrm{E}\left(P_{n_1}^{(1)} \cdot P_{m_1}^{(1)} \right) \cdots \mathrm{E}\left(P_{n_D}^{(D)} \cdot P_{m_D}^{(D)} \right) \\
&= \left\langle P_{n_1}^{(1)} \cdot P_{m_1}^{(1)} \right\rangle_Q \cdots \left\langle P_{n_D}^{(D)} \cdot P_{m_D}^{(D)} \right\rangle_Q \\
&= \left\| P_{n_1}^{(1)} \right\|_Q \delta_{n_1 m_1} \cdots \left\| P_{n_D}^{(D)} \right\|_Q \delta_{n_D m_D}
\end{aligned}
$$

$$
\langle \mathbf{P}_n, \mathbf{P}_m \rangle_Q = \| \mathbf{P}_n \|_Q \, \delta_{nm}
$$

Creating multivariate orthogonal polynomials in Chaospy

```
a = cp.Uniform(0, 0.1)
I = cp.Uniform(8, 10)
dist = cp.J(a,I)
```

Creating multivariate orthogonal polynomials in Chaospy

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a = cp.Uniform(0, 0.1)
I = cp.Uniform(8, 10)
dist = cp.J(a,I)

P = cp.orth_ttr(1, dist)
print P
[1.0, q1-9.0, q0]
```

Creating multivariate orthogonal polynomials in Chaospy

```
a = cp.Uniform(0, 0.1)
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P = cp.orth_ttr(3, dist)
print cp.E(P[1]*P[2],dist)
0.0
```

Creating multivariate orthogonal polynomials in Chaospy

```
a = cp.Uniform(0, 0.1)
l = cp.Uniform(8, 10)
dist = cp.J(a,l)

P = cp.orth_ttr(1, dist)
print P
[1.0, q1-9.0, q0]

P = cp.orth_ttr(3, dist)
print cp.E(P[1]*P[2],dist)
0.0
print cp.E(P[3]*P[3],dist)
0.0888888888903
```

The multidimensional problrm

$$u(x; a, I) = Ie^{-ax}$$

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Initially assume model parameters:

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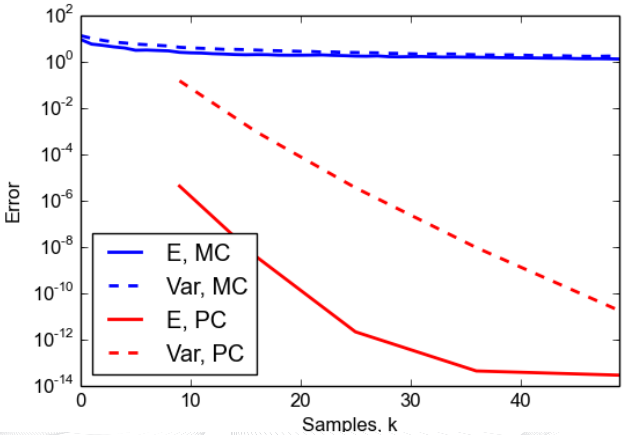
$$\varepsilon_E = \int_0^{10} |E(u) - E(\hat{u})|\, dx \quad \varepsilon_{Var} = \int_0^{10} |Var(u) - Var(\hat{u})|\, dx$$

Convergence of a multidimensional problem



Teaser of the full implementation

```
def u(x,a, I):
    return I*np.exp(-a*x)
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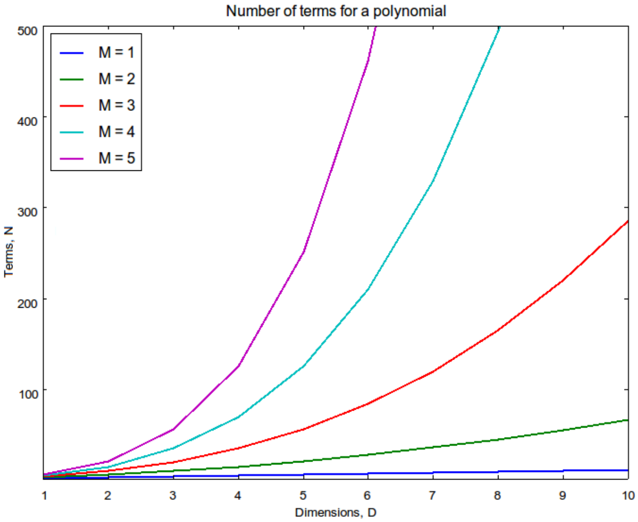
I = cp.Uniform(8, 10)
dist = cp.J(a,I)

P = cp.orth_ttr(2, dist)
```

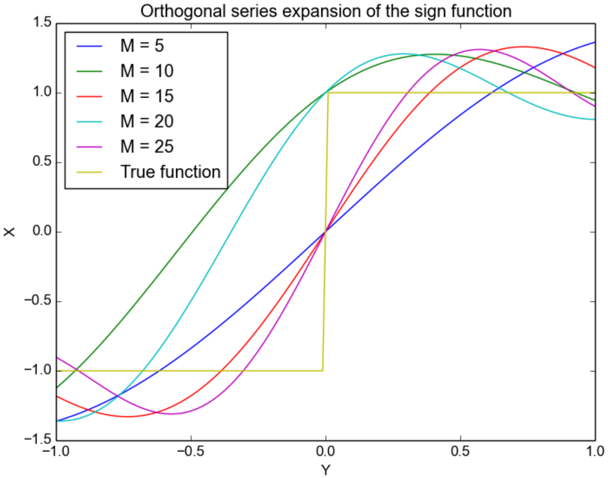
Teaser of the full implementation

```python
def u(x,a, I):
  return I*np.exp(-a*x)

a = cp.Uniform(0, 0.1)
I = cp.Uniform(8, 10)
dist = cp.J(a,I)

P = cp.orth_ttr(2, dist)

nodes, weights = \
    cp.generate_quadrature(3, dist, rule="G")

x = np.linspace(0, 10, 100)
solves = [u(x, *node) for node in nodes.T]

u_hat = cp.fit_quadrature(P, nodes, weights, solves)

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

The curse of dimensionality



Gibb's Phenomena, discontinues methods are troublesome



Higher number of samples justifies higher number of collocation nodes