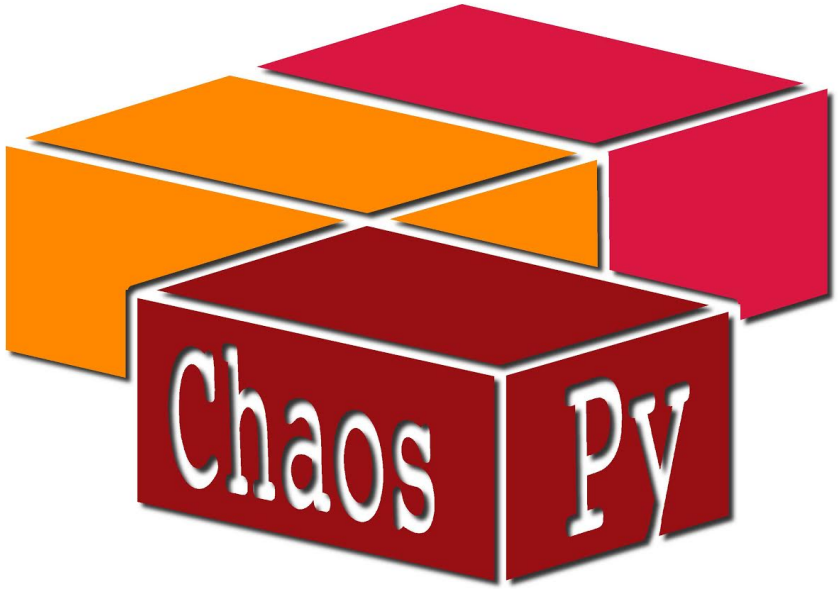
# Polynomial chaos expansions part I: Method Introduction

Jonathan Feinberg and Simen Tennøe

Kalkulo AS

January 27, 2015

# Lectures will include many examples using the Chaospy software

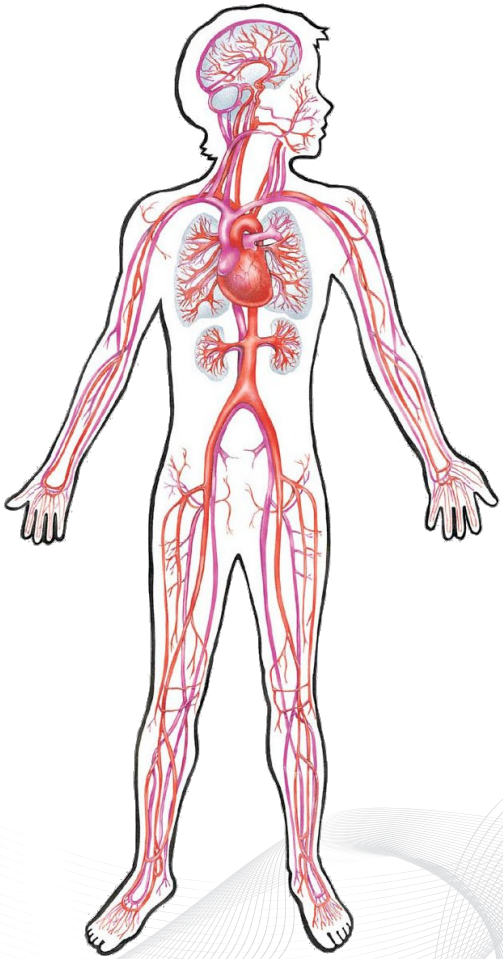



A very basic introduction to scientific Python programming:
http://hplgit.github.io/bumpy/doc/pub/sphinx-basics/index.html

Installation instructions:
https://github.com/hplgit/chaospy

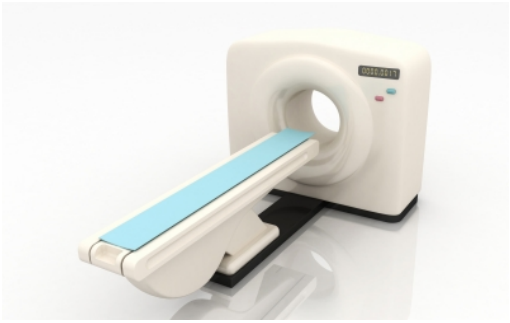
Interactive session:
http://10.50.3.247:8888/

# Example: 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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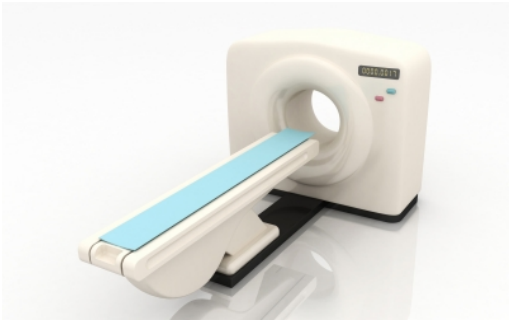

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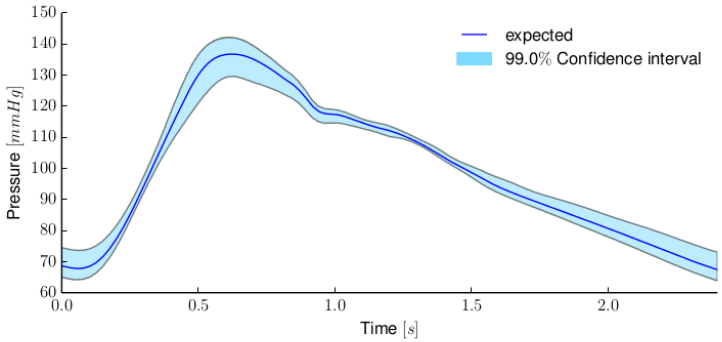


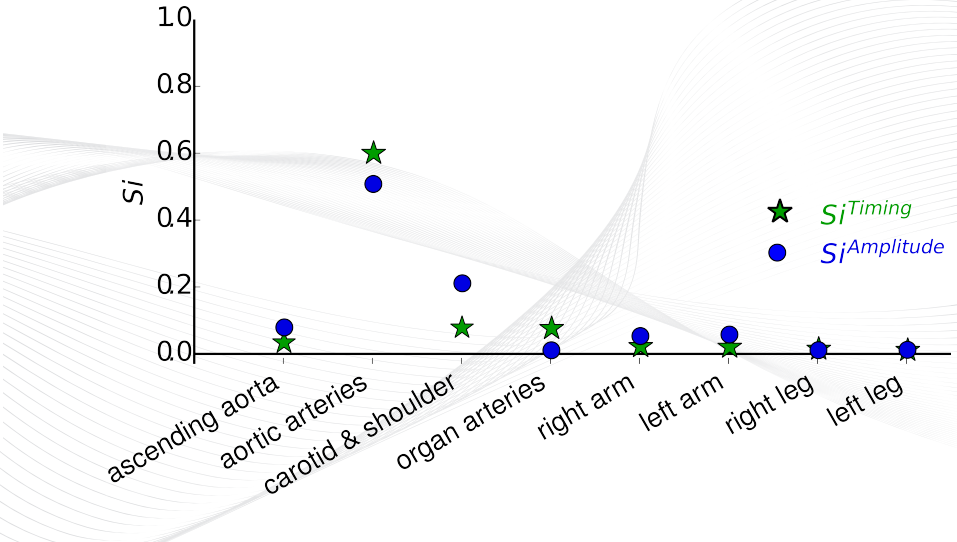

# Introducing a testcase as a working example

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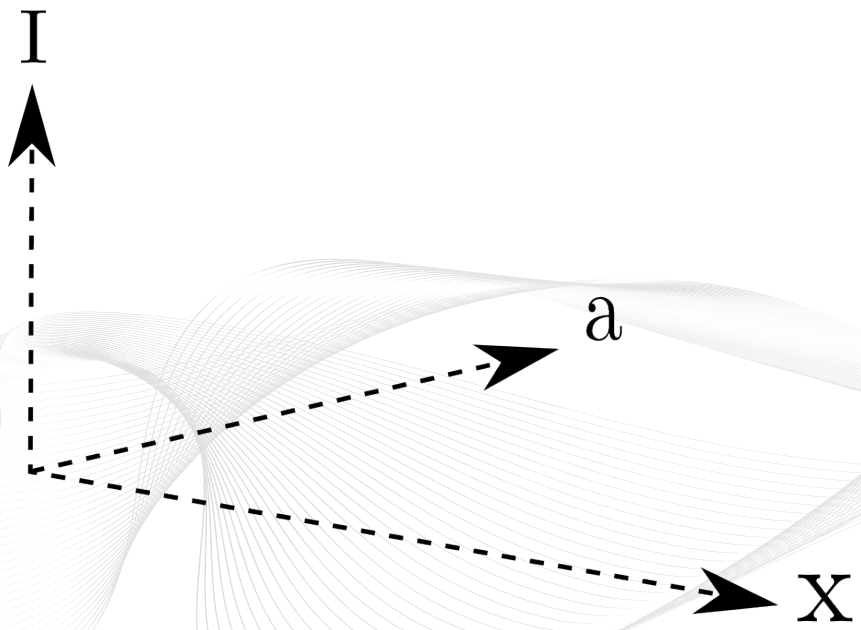

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$$\mathrm{E}(u) = \int_{-\infty}^{\infty} u(x; a) f_a(a) da = \int_0^{0.1} e^{-ax} \frac{1}{10} da = \frac{1 - e^{-0.1x}}{10x}$$

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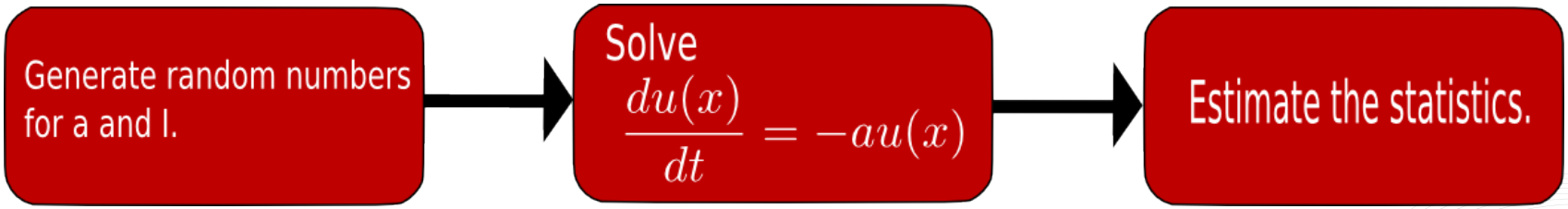
$$\mathrm{Var}(u) = \int_{-\infty}^{\infty} (u(x; a) - \mathrm{E}(u))^2 f_a(a) da = \frac{1 - e^{-0.2ax}}{20x} - \left(\frac{1 - e^{-0.1x}}{10x}\right)^2$$

# In general, models can be analysed using Monte Carlo integration



# Monte Carlo with Chaospy

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import chaospy as cp
import numpy as np

def u(x, a):
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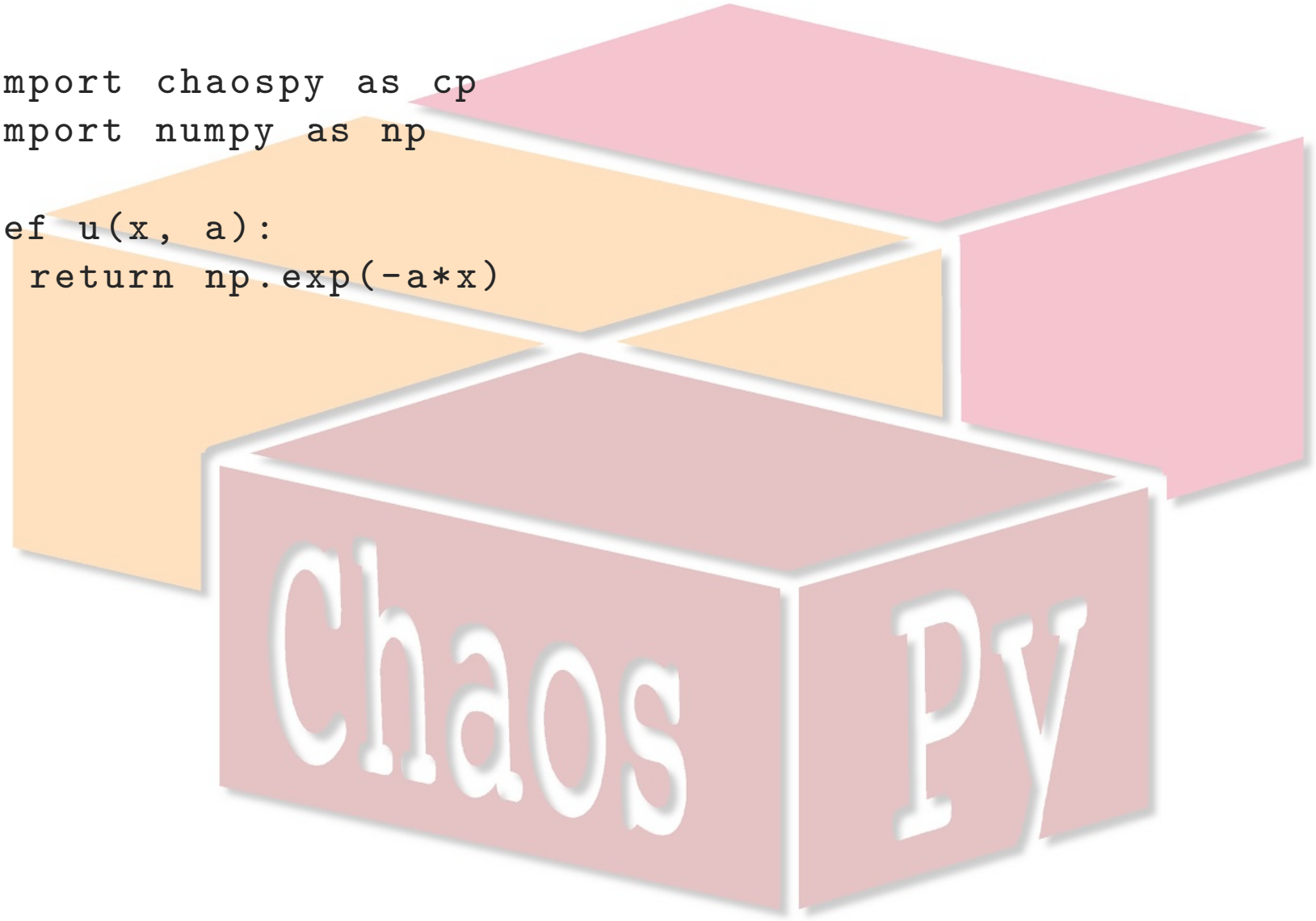

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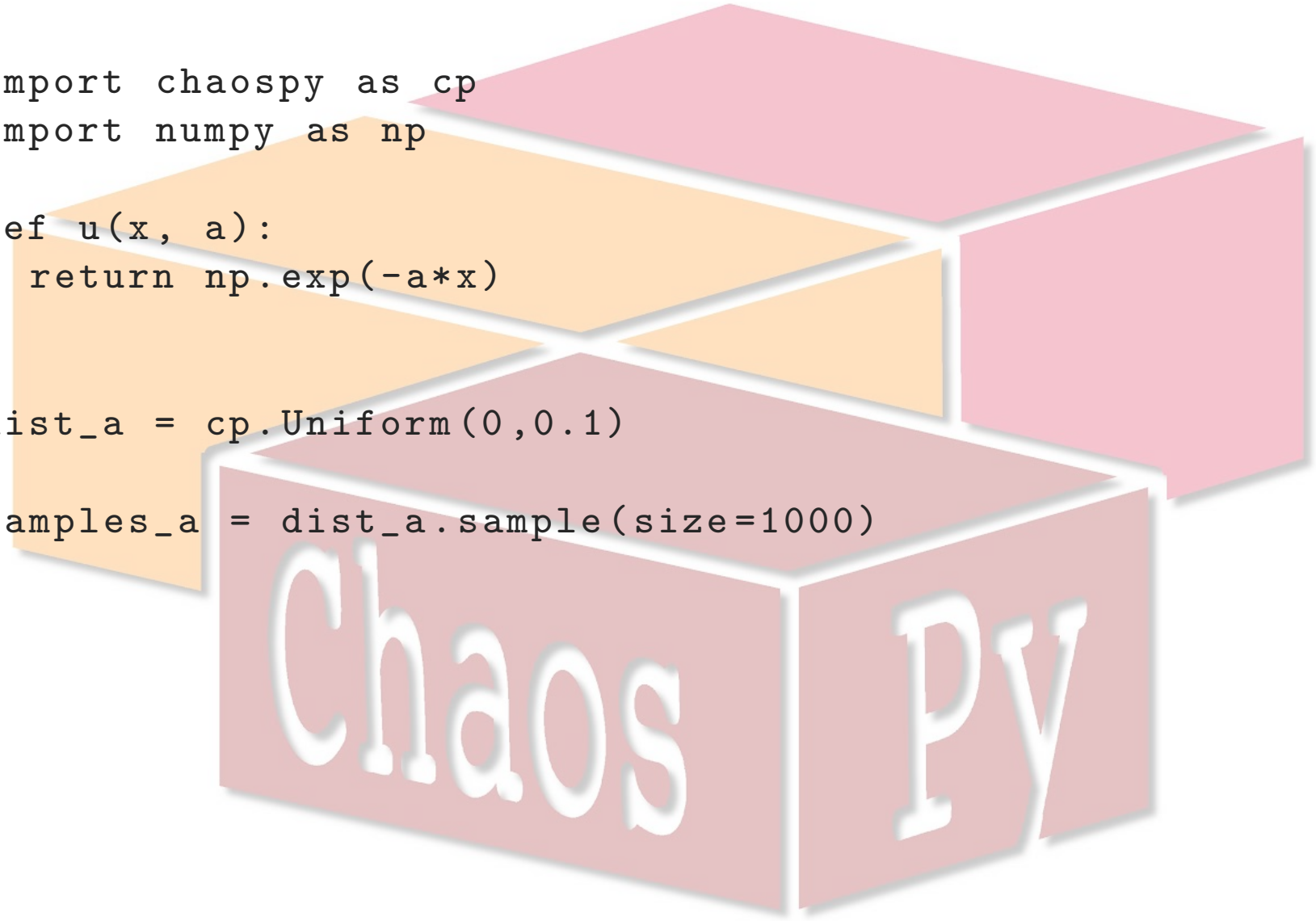

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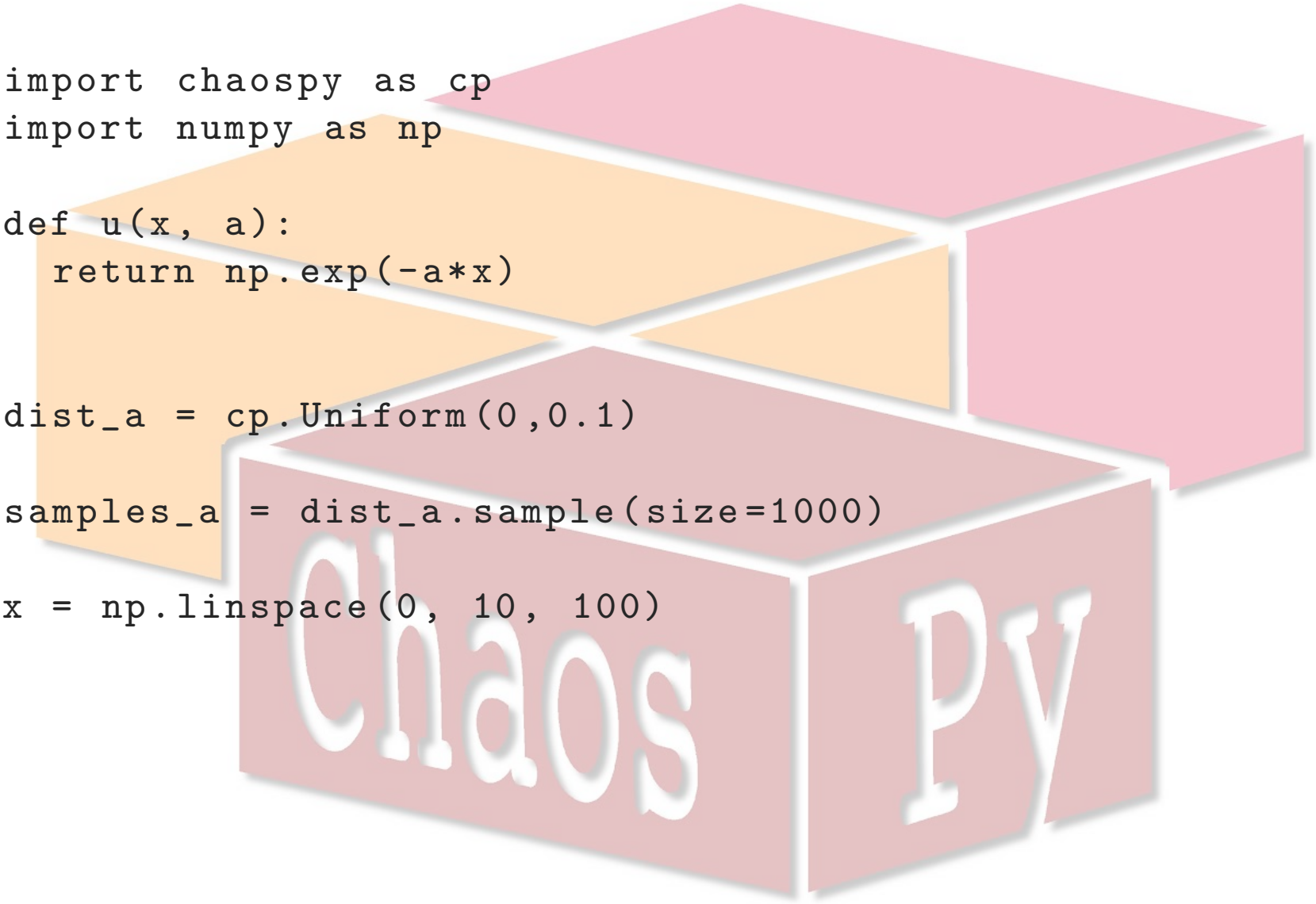

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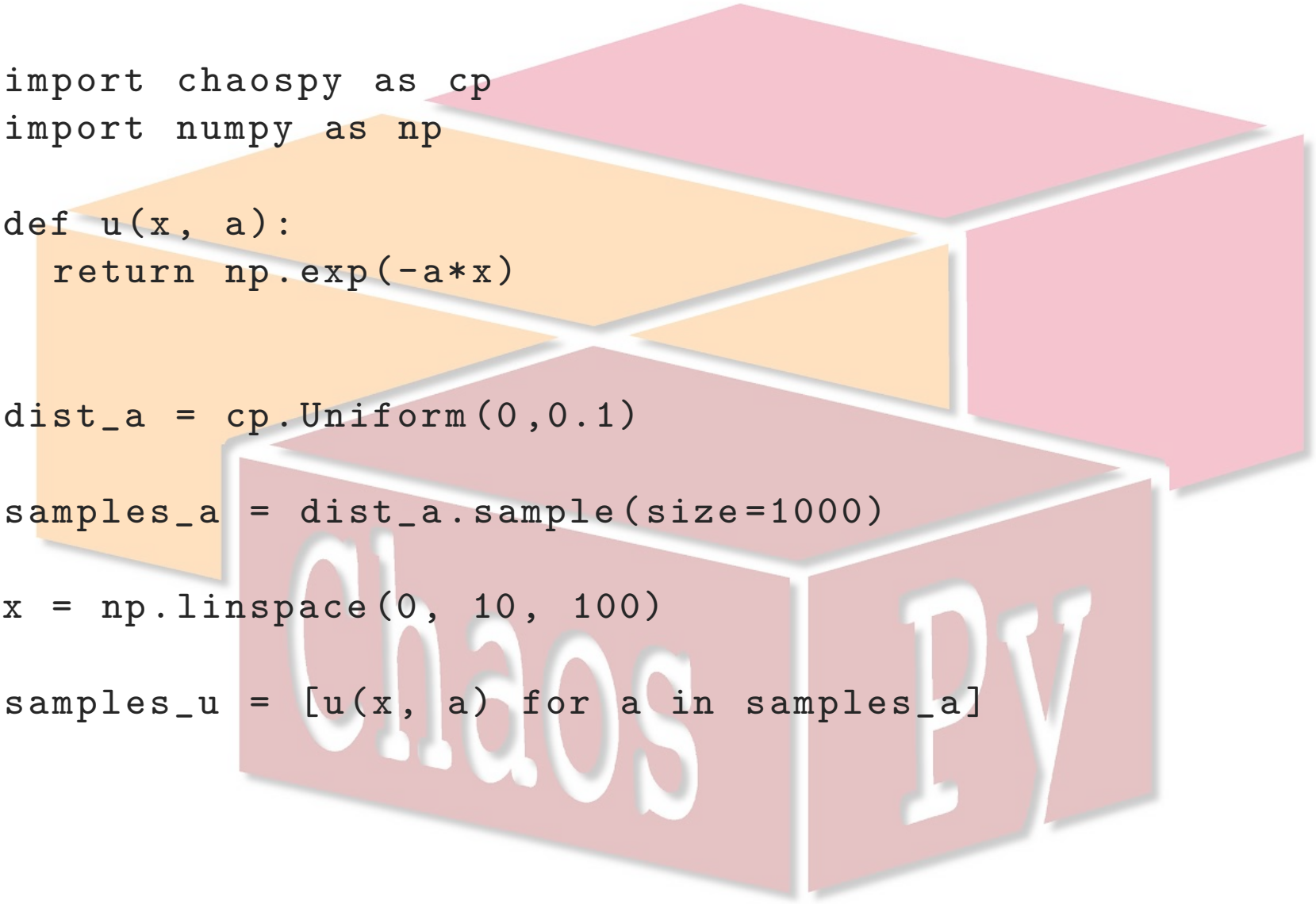

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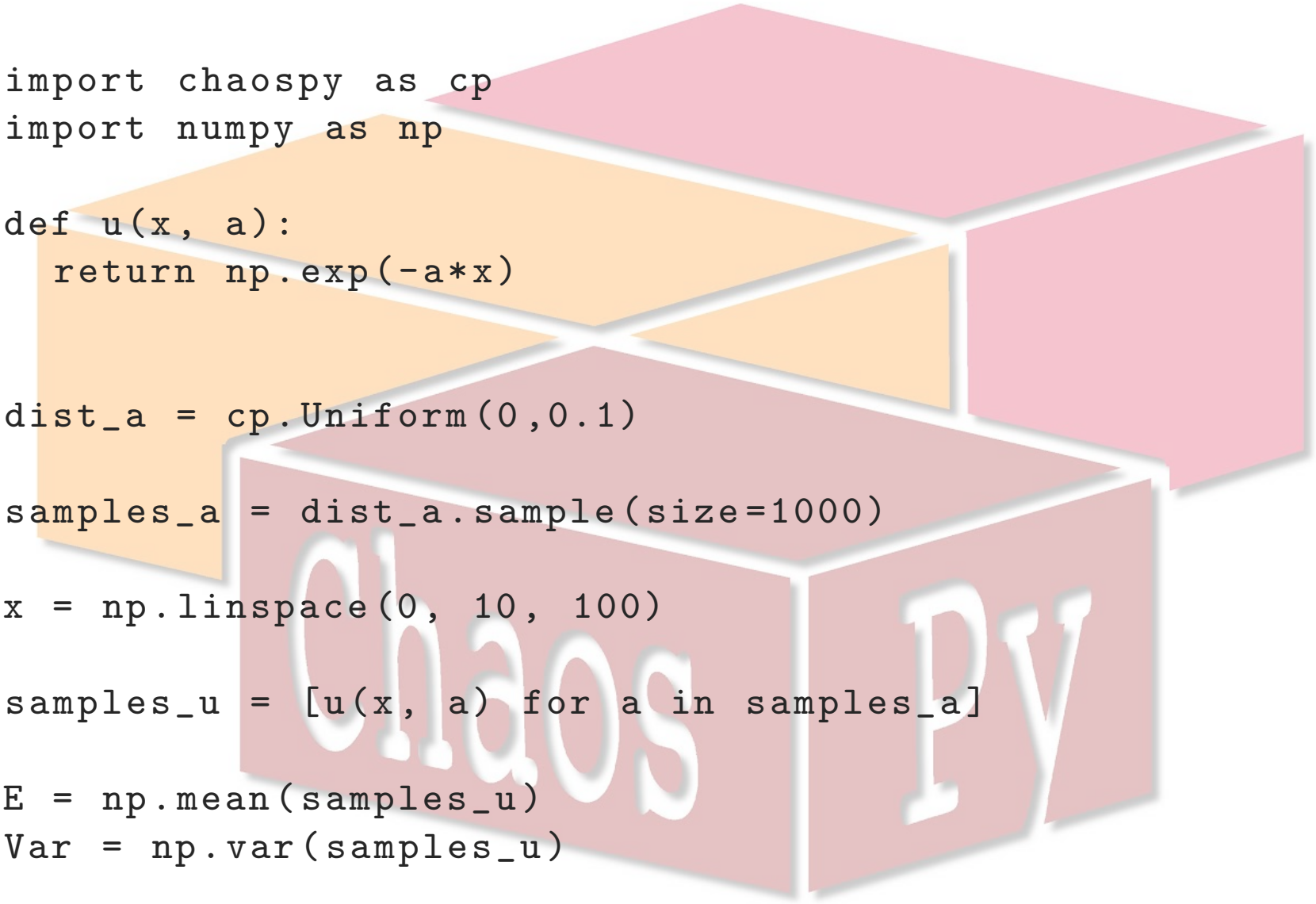
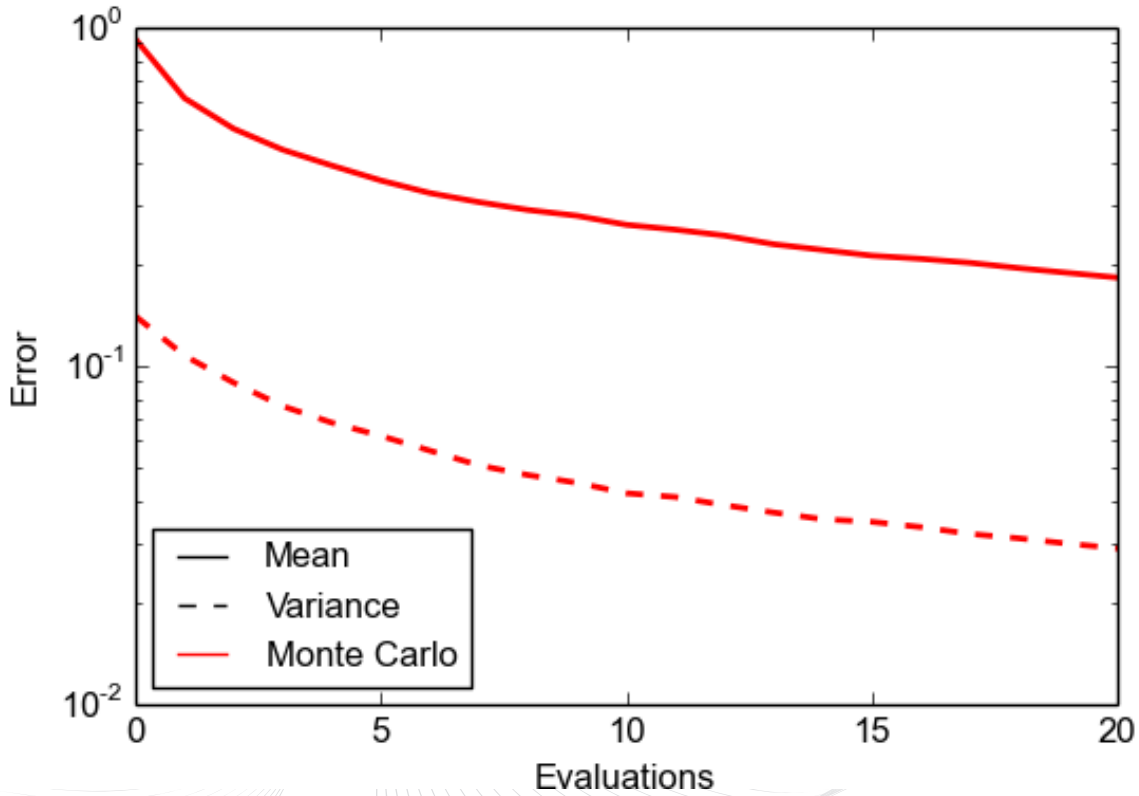
samples_u = [u(x, a) for a in samples_a]

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

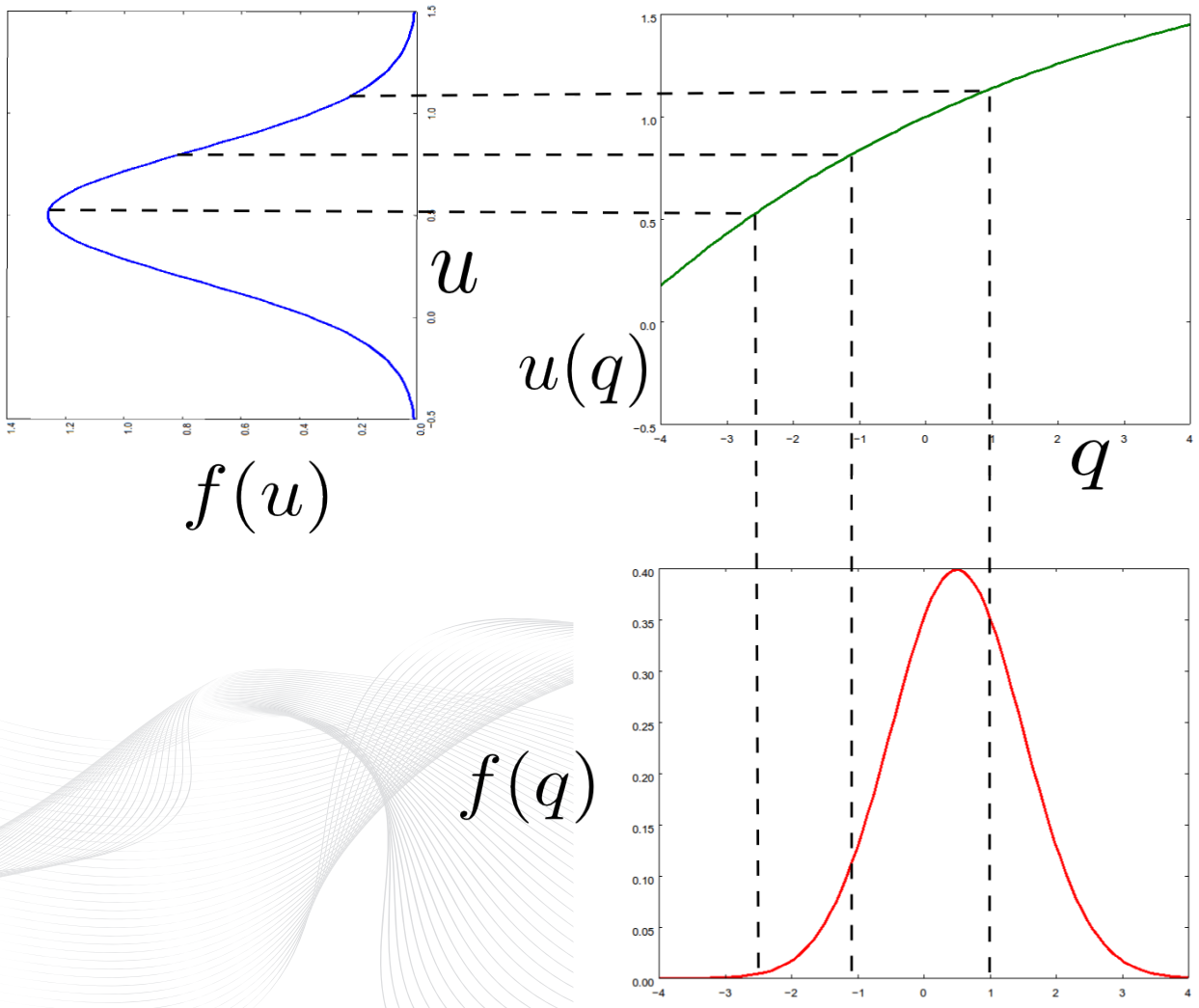


# Convergence of Monte Carlo is slow

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



# Assumption: mapping from input $q$ to output $u$ is smooth



# Using Lagrange polynomials to approximate $u(q)$ ($N$-th degree polynomial interpolation)

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

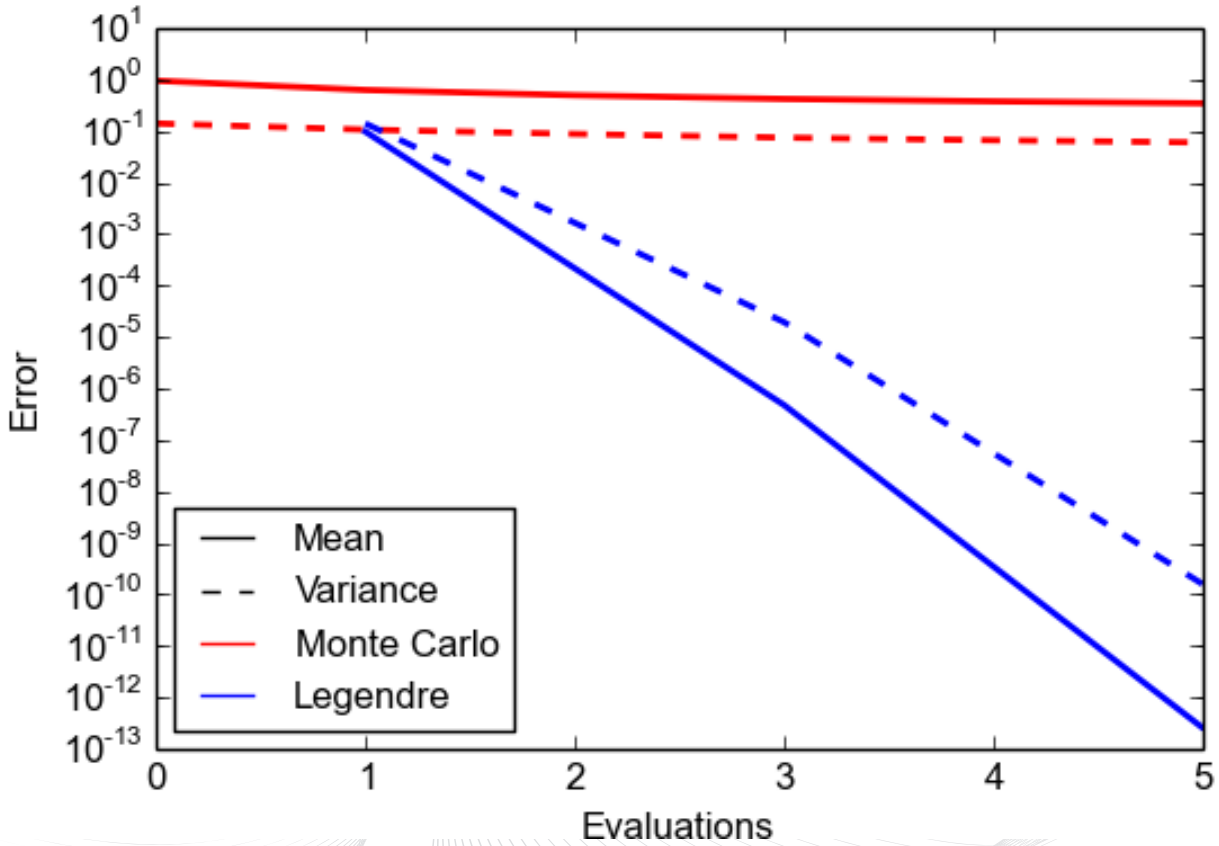
where

- $c_n$ are model evaluations $u(x, a_n)$
- $P_n$ are Lagrange polynomials:

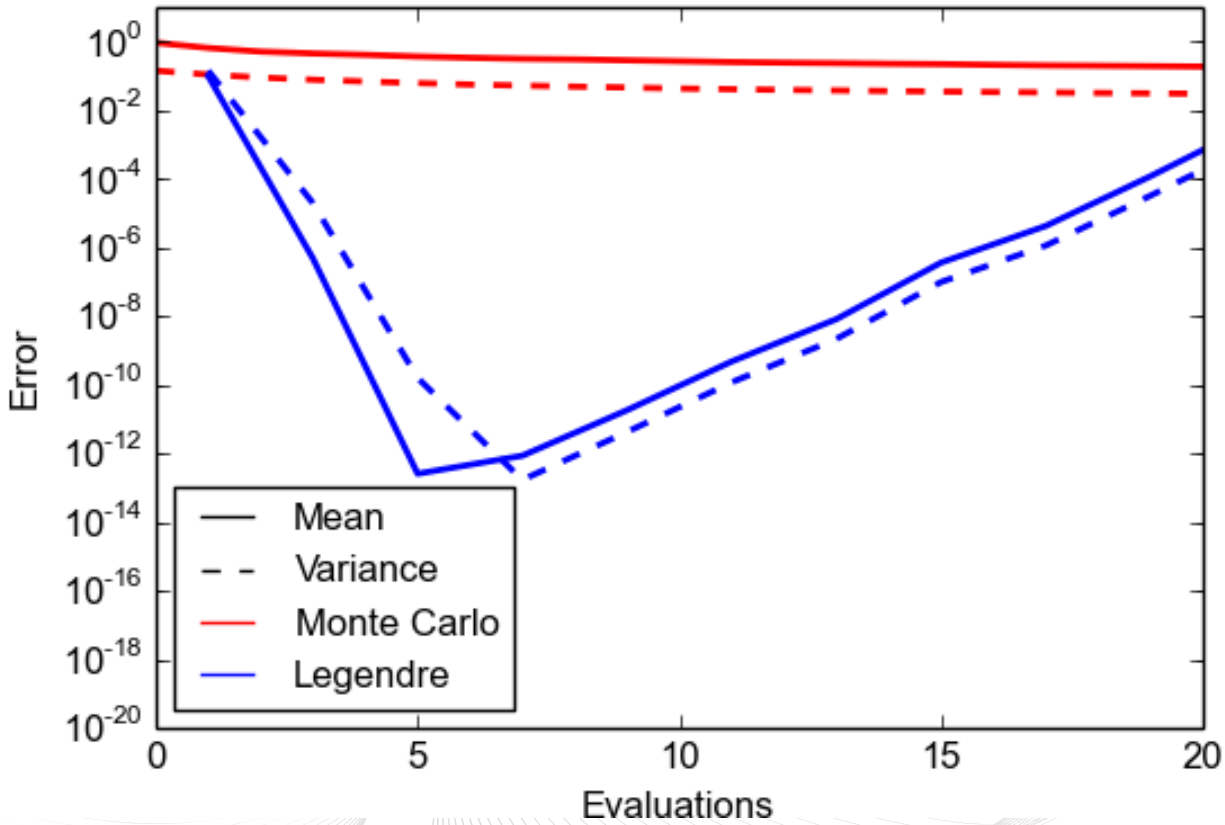
$$P_n(a) = \prod_{\substack{m=0 \\ m \neq n}}^{N} \frac{a - a_n}{a_m - a_n}$$

- $a_n$ are collocation nodes

# The interpolation has much better convergence properties than Monte Carlo!



# Oscillations in Lagrange polynomials (for large $N$) destroy the convergence



# Let us introduce a better polynomial approximation: Polynomial Chaos (PC) theory

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

# PC employs inner product spaces weighted with the probability distribution

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

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

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Orthogonality:

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

# Coefficients are determined by least squares minimization

$$\min_{c_0,\ldots,c_N} ||u - \hat{u}_M||_Q^2$$

$$\vdots$$

$$\left\langle \sum_{n=0}^{N} c_n P_n, P_k \right\rangle_Q$$

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$$c_k = \frac{\langle u, P_k \rangle_Q}{\|P_k\|_Q^2}$$

Fourier coefficients

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

# Construct an orthogonal polynomial expansion using Gram-Schmidt orthogonalization

$$v_0, v_1, ..., v_N = 1, q, ..., q^N$$

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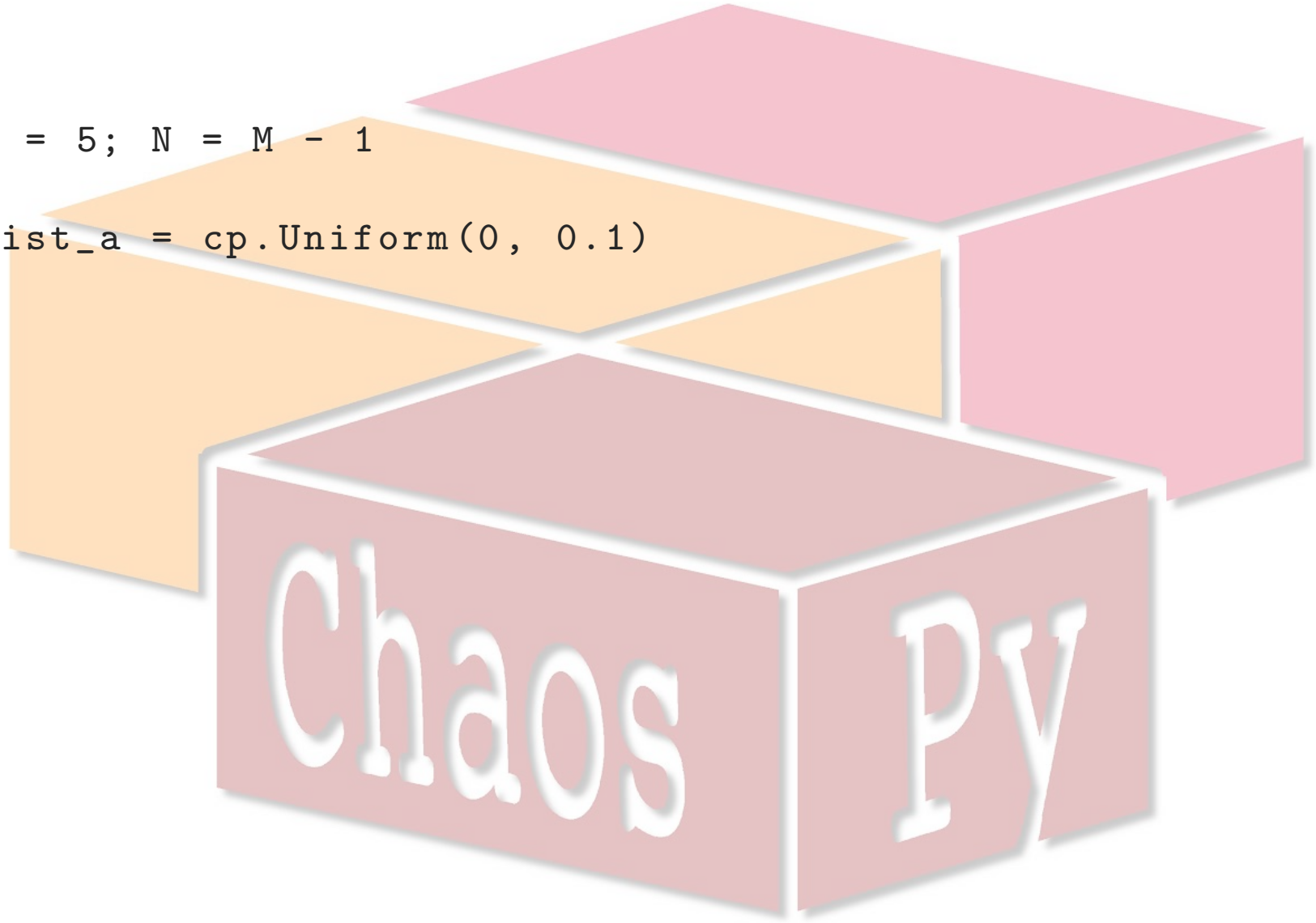
The Gram Schmidt method is

$$\begin{aligned} P_0 &= v_0 \\ P_n &= v_n - \sum_{m=0}^{n-1} \frac{\langle v_n, P_m \rangle_Q}{\|P_m\|_Q^2} \\ &= v_n - \sum_{m=0}^{n-1} \frac{\mathrm{E}(v_n P_m)}{\mathrm{E}(P_m^2)} \end{aligned}$$

# Gram-Schmidt with chaospy

```
M = 5; N = M - 1

dist_a = cp.Uniform(0, 0.1)
```



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dist_a = cp.Uniform(0, 0.1)

v = cp.basis(0, M, 1)
P = [v[0]]
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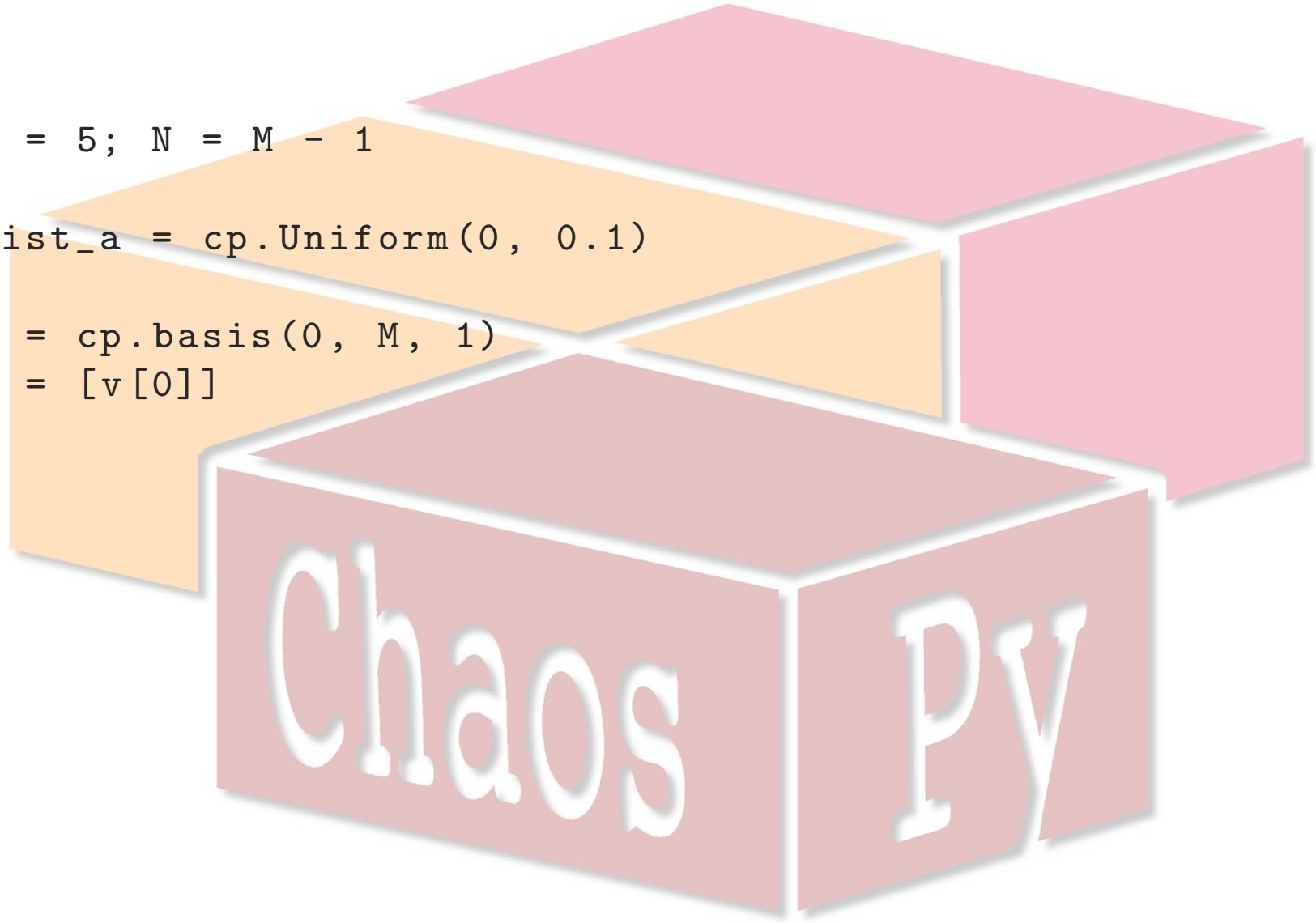

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v = cp.basis(0, M, 1)
P = [v[0]]

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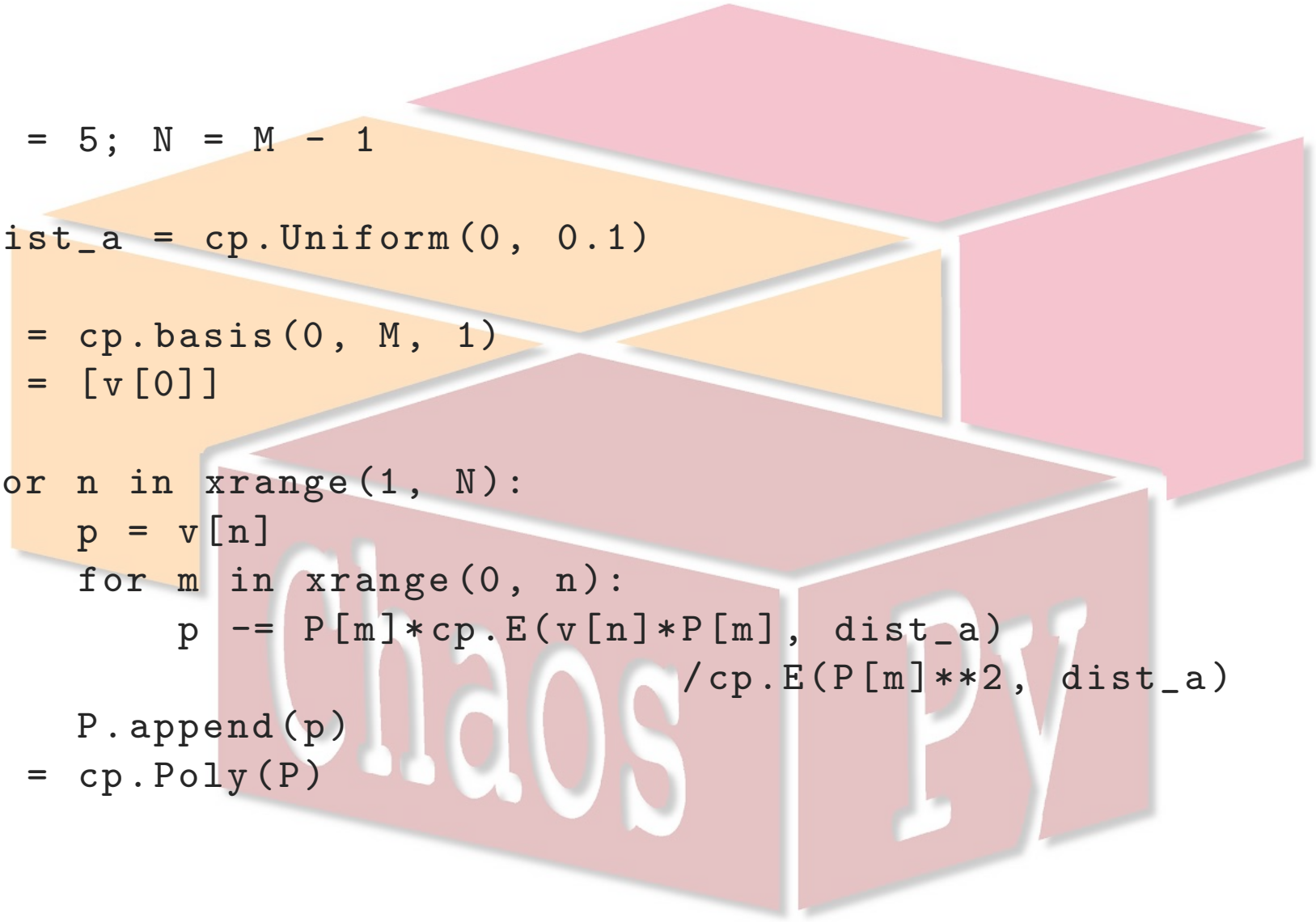
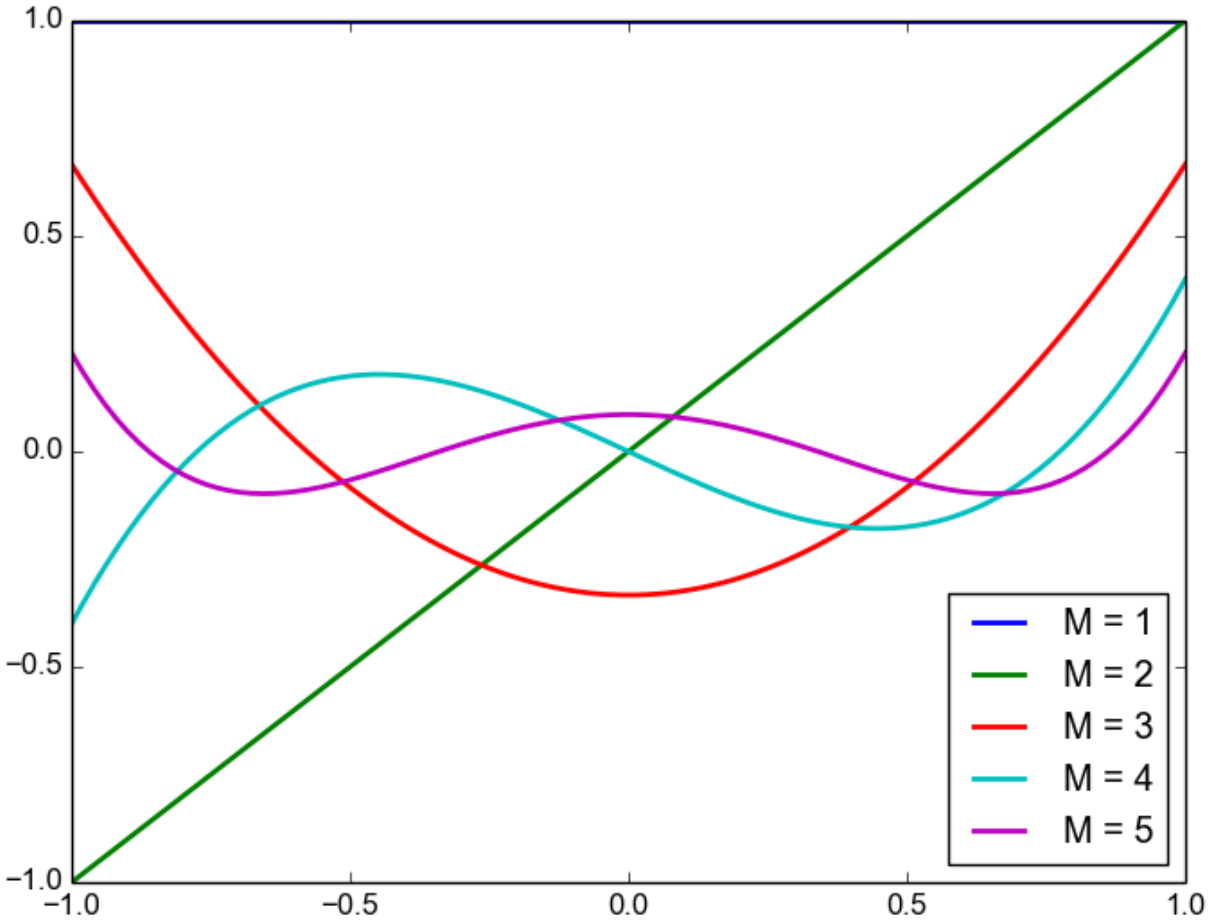
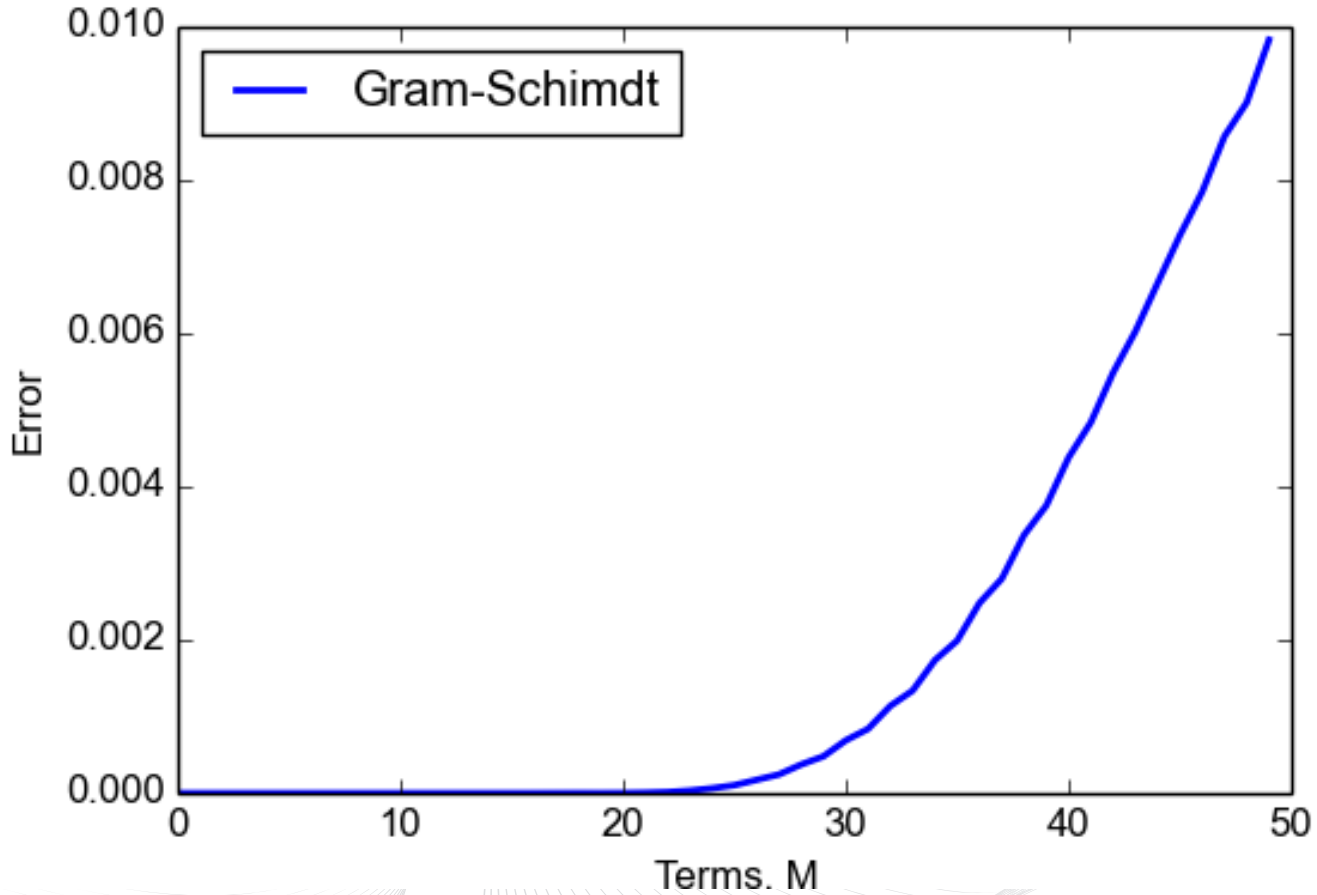



# Plot of all generated polynomials



# Most constructors of orthogonal polynomials are ill-conditioned



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Three terms recursion relation:

$$P_{n+1} = (x - A_n)P_n - B_n P_{n-1} \qquad P_{-1} = 0 \qquad P_0 = 1,$$

# The only numerically stable method for calculating orthogonal polynomials is through the three-term discretized Stiltjes recursion

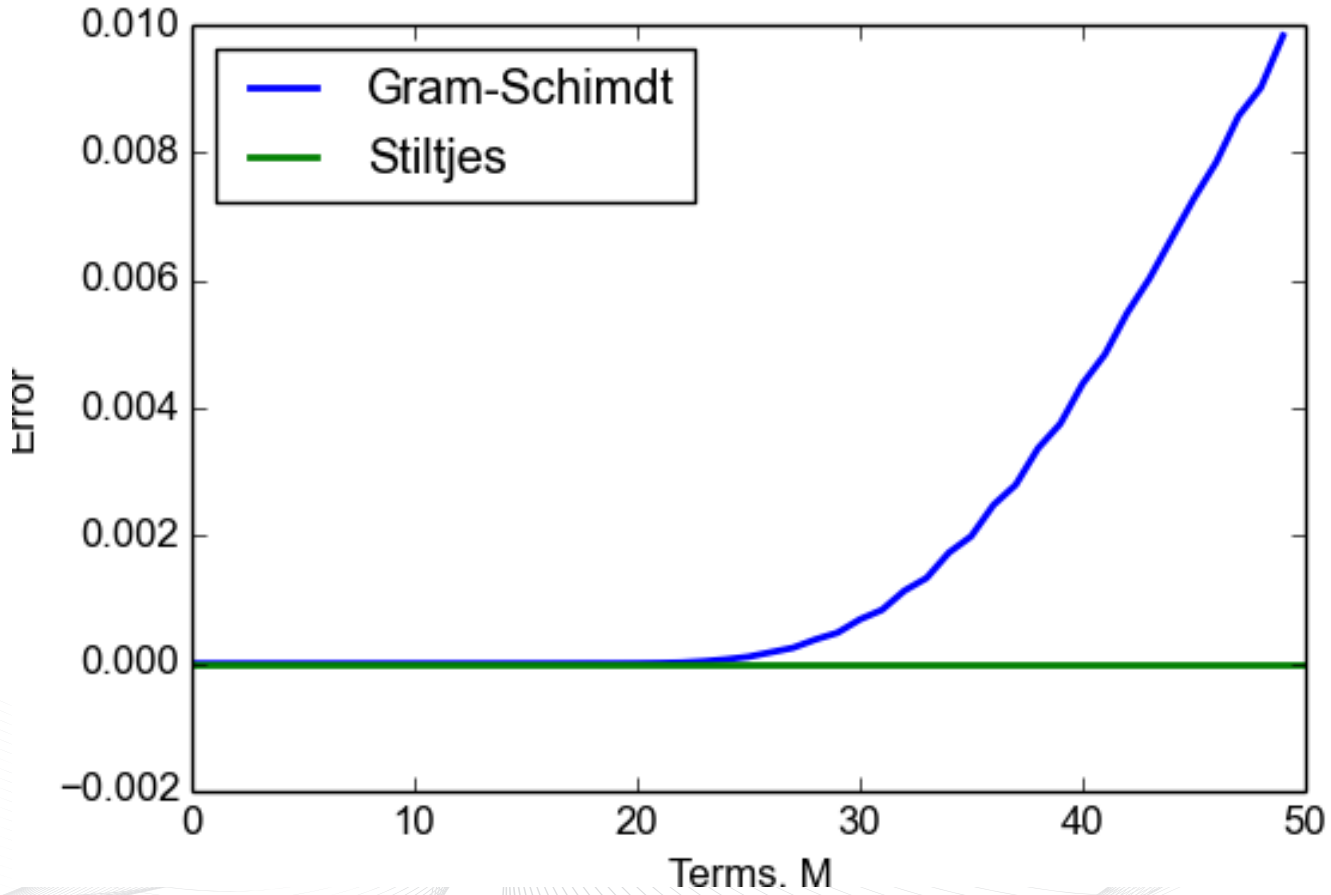
Three terms recursion relation:

$$P_{n+1} = (x - A_n)P_n - B_n P_{n-1} \qquad P_{-1} = 0 \qquad P_0 = 1,$$

where

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

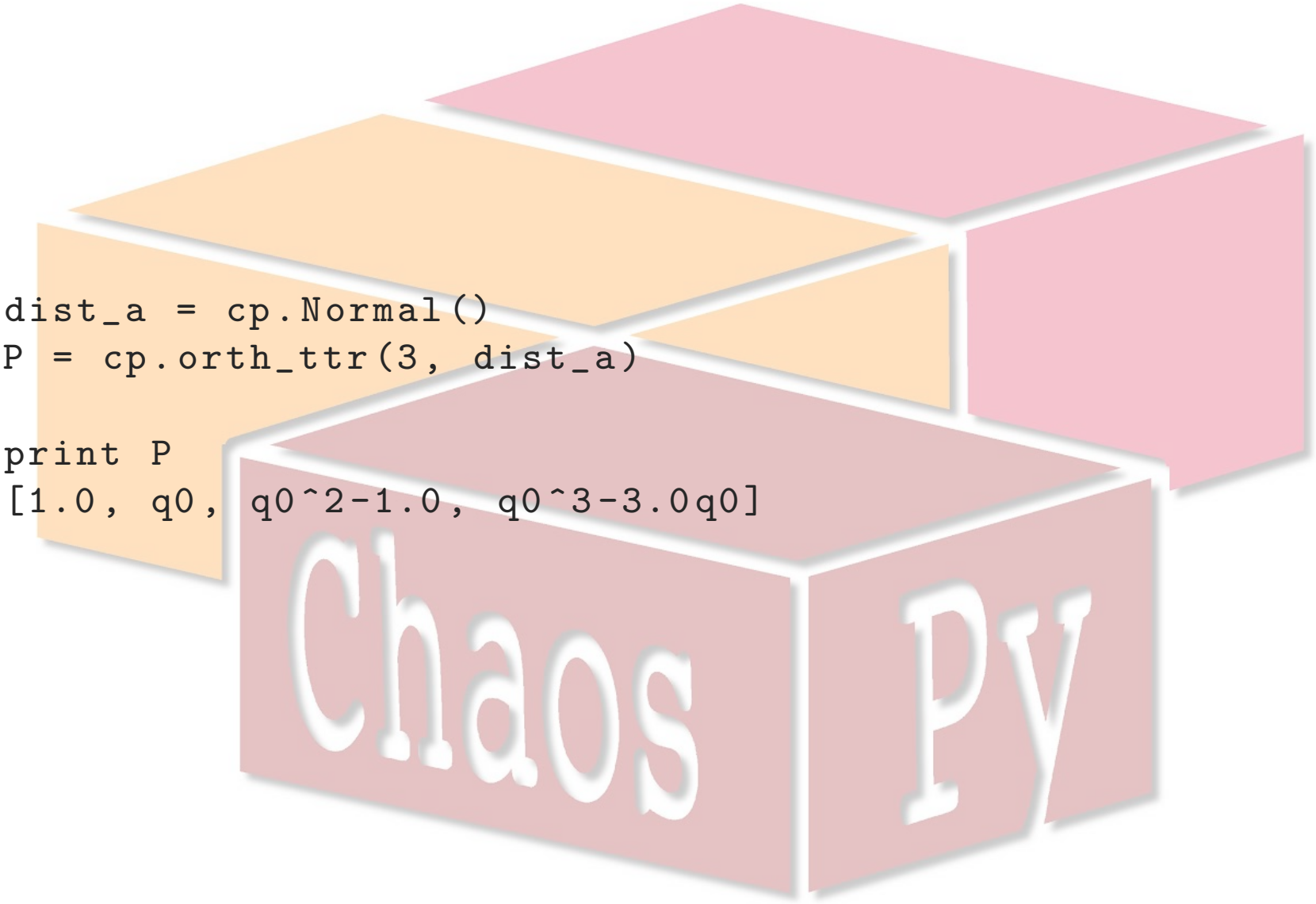
# Discretized Stiltjes method is numerically stable



# People have found analytical orthogonal polynomials for many common probability distributions

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

# Three terms recursion in Chaospy




```
dist_a = cp.Normal()
P = cp.orth_ttr(3, dist_a)

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

# Repetition of the problem

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

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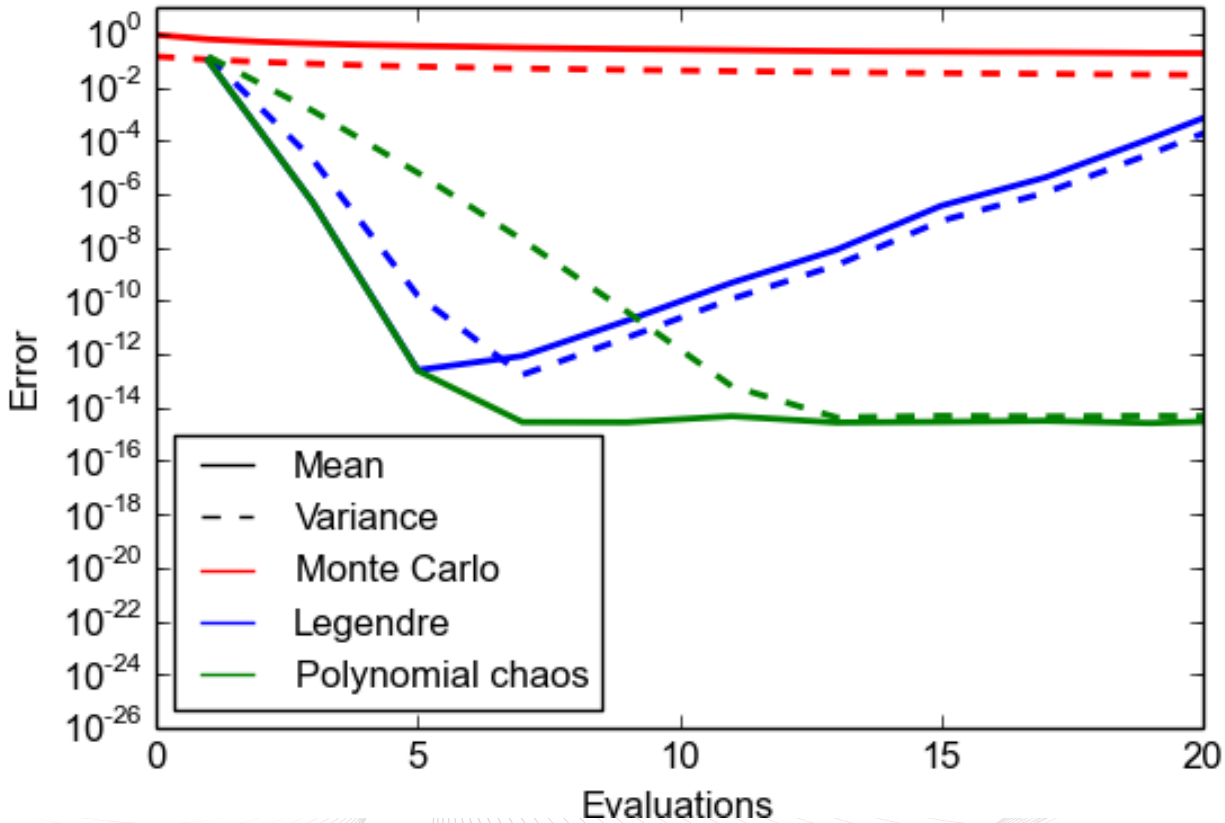
$$\varepsilon_E = \int_0^{10} |E(u) - E(\hat{u})|\, dx \quad \varepsilon_{Var} = \int_0^{10} |Var(u) - Var(\hat{u})|\, dx$$

# Convergence of orthogonal polynomial approximation



# Next step: Extend the theory to multiple dimensions

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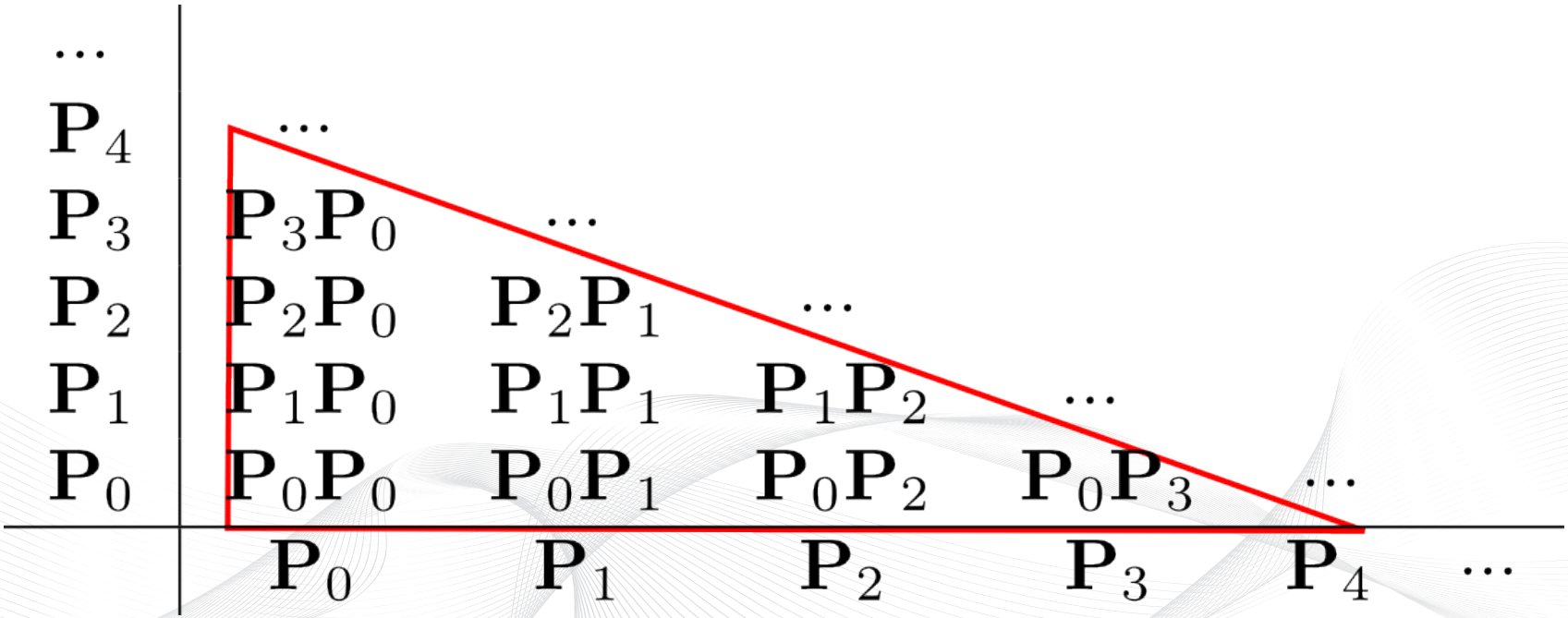

# We need a mapping from multiple indices to single index

Multi-index

$$
\begin{array}{ccccc}
 & & \mathbf{P}_{00} & & \\
 & \mathbf{P}_{10} & & \mathbf{P}_{01} & \\
\mathbf{P}_{20} & & \mathbf{P}_{11} & & \mathbf{P}_{02} \\
\mathbf{P}_{30} & \mathbf{P}_{21} & & \mathbf{P}_{12} & \cdots
\end{array}
$$

Single-index

$$
\begin{array}{ccccc}
 & & \mathbf{P}_{0} & & \\
 & \mathbf{P}_{1} & & \mathbf{P}_{2} & \\
\mathbf{P}_{3} & & \mathbf{P}_{4} & & \mathbf{P}_{5} \\
\mathbf{P}_{6} & \mathbf{P}_{7} & & \mathbf{P}_{8} & \cdots
\end{array}
$$

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$$\mathbf{P}_{30} \quad \mathbf{P}_{21} \quad \mathbf{P}_{12} \quad \dots$$

Single-index

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

$$N = \binom{M+D}{M}$$

# Orthogonality for multivariate polynomials

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

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$$= \left\| P_{n_1}^{(1)} \right\|_Q \delta_{n_1 m_1} \cdots \left\| P_{n_D}^{(D)} \right\|_Q \delta_{n_D m_D}$$

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

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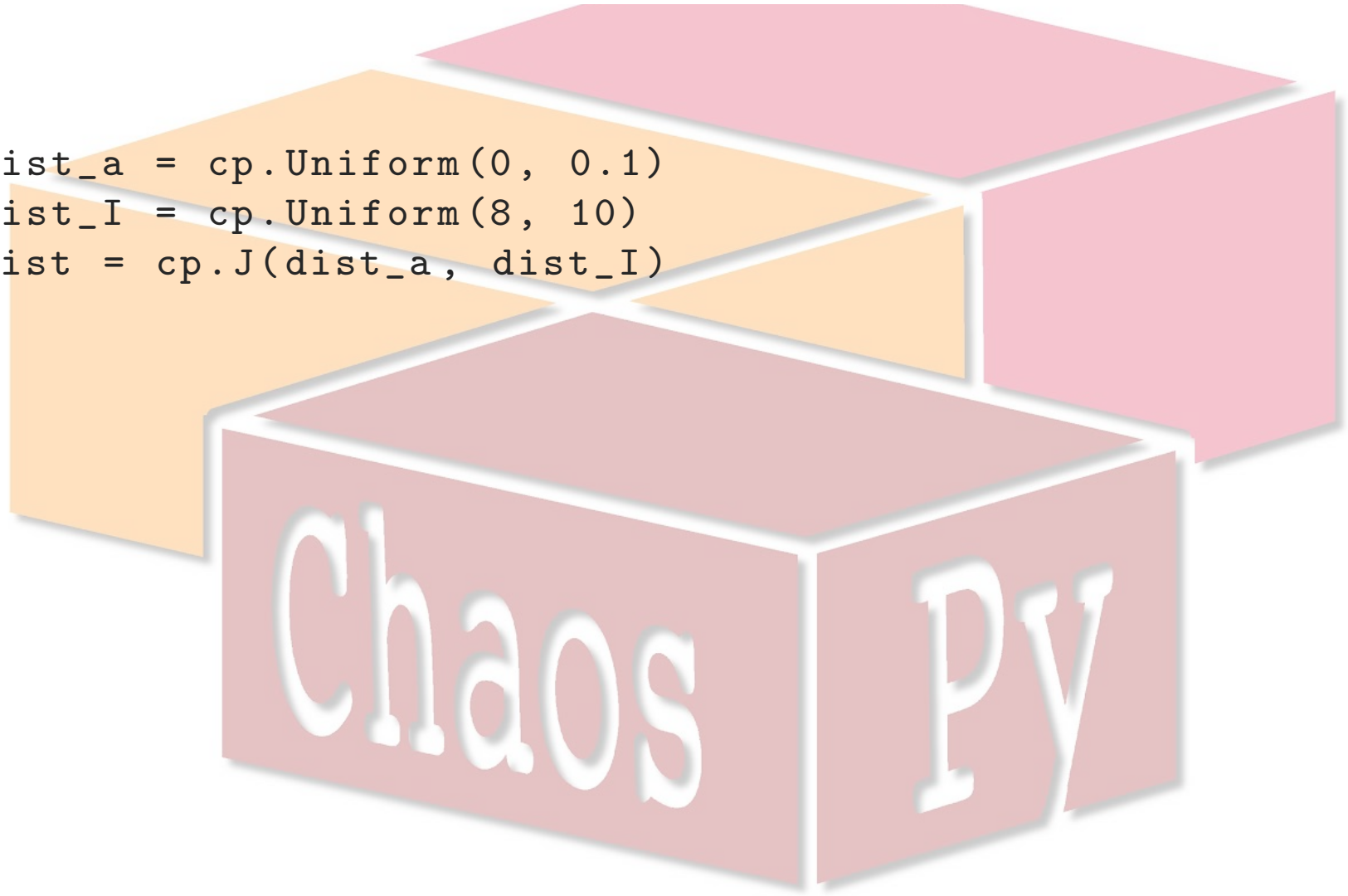
$$= \left\| P_{n_1}^{(1)} \right\|_Q \delta_{n_1 m_1} \cdots \left\| P_{n_D}^{(D)} \right\|_Q \delta_{n_D m_D}$$

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

# Creating multivariate orthogonal polynomials in Chaospy

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



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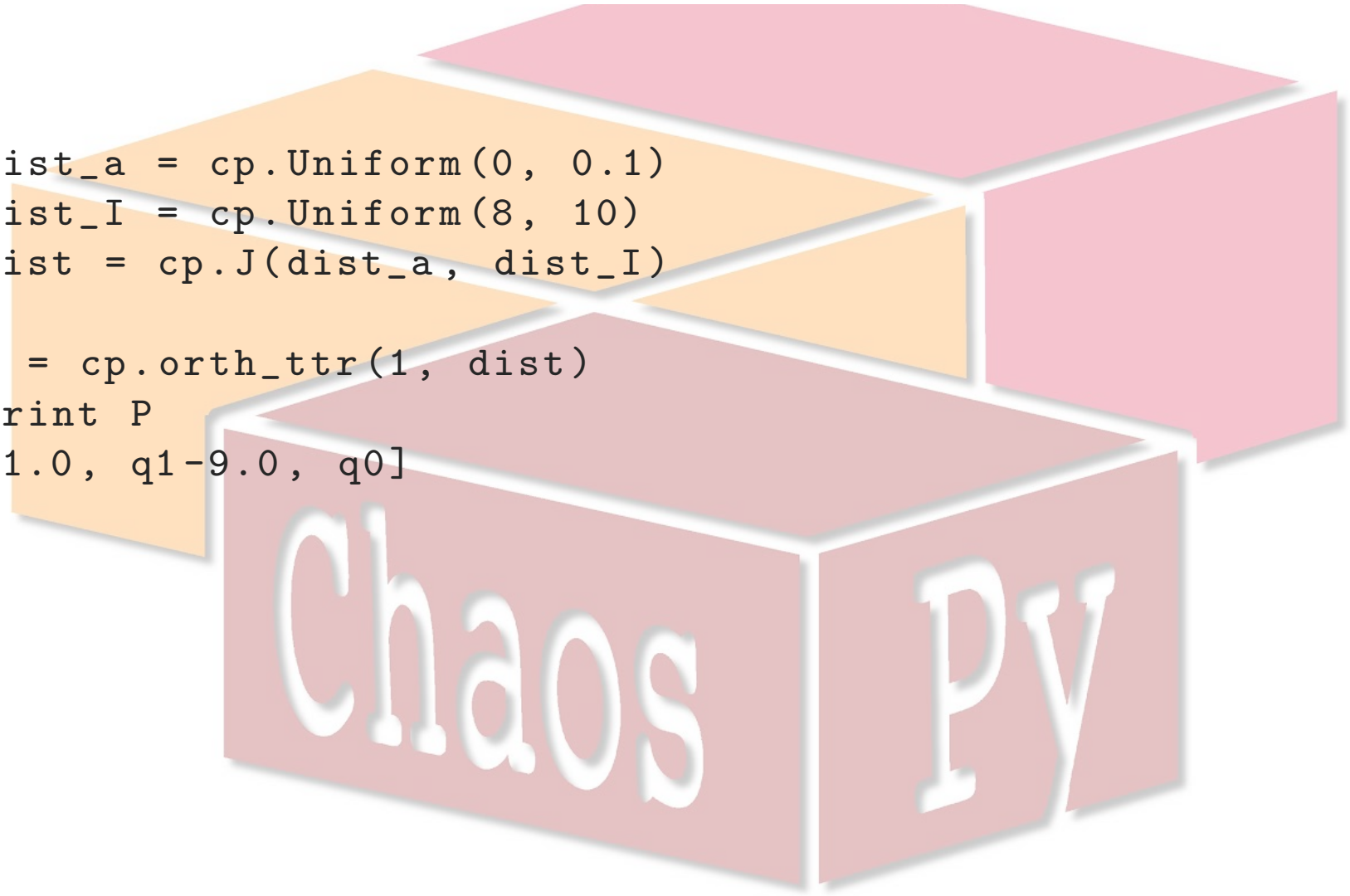
```
dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a, dist_I)

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



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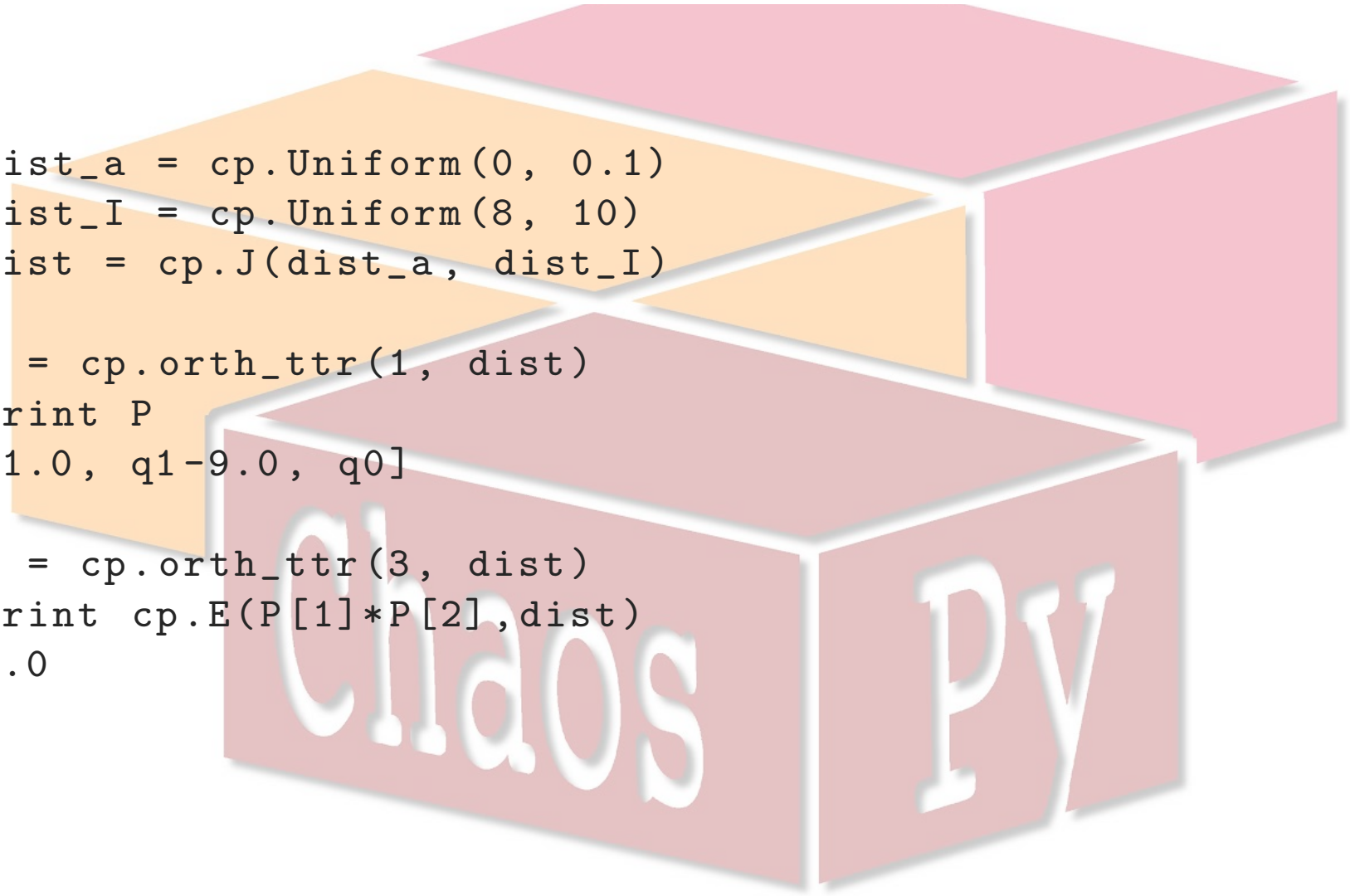


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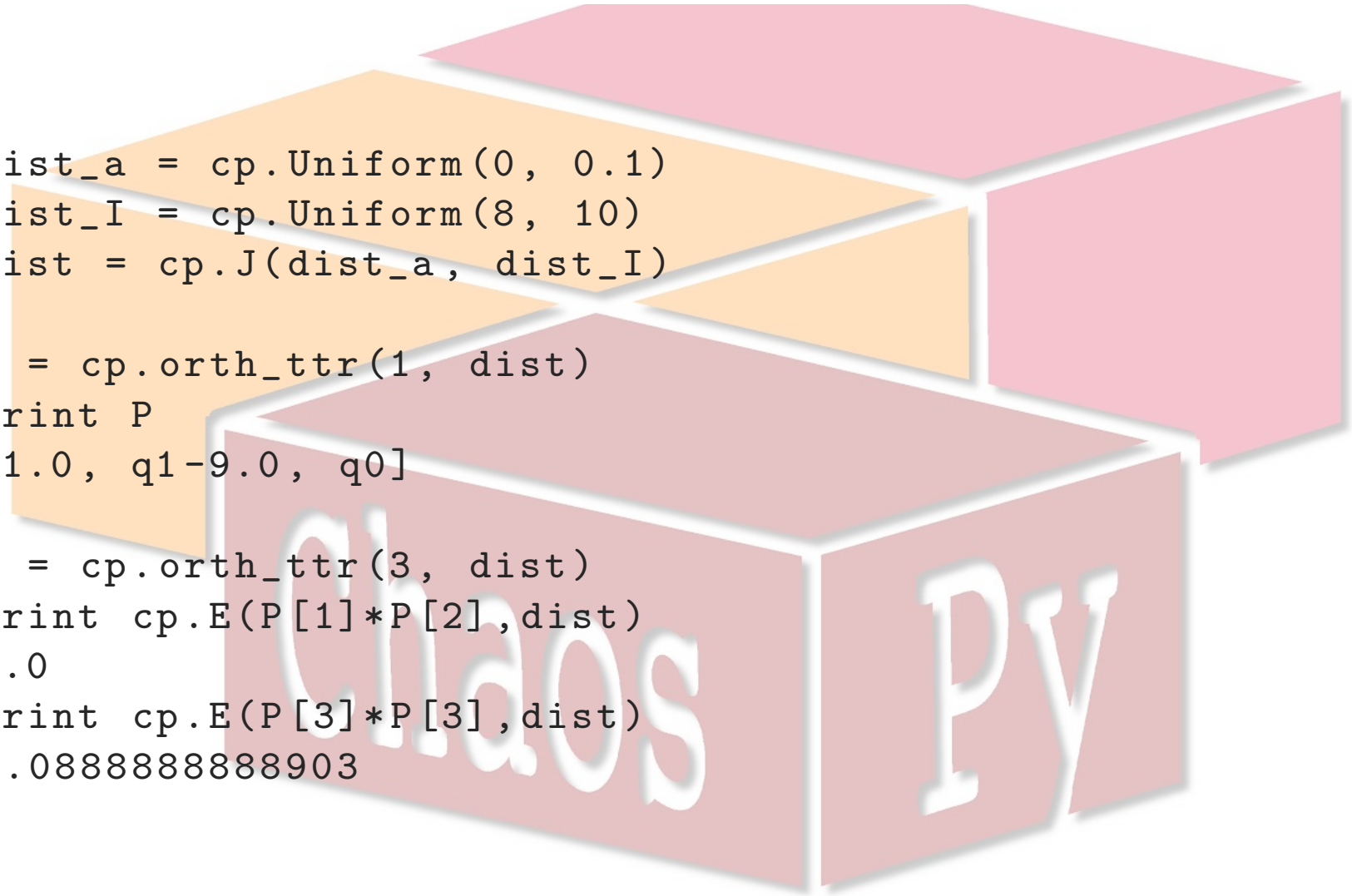
P = cp.orth_ttr(3, dist)
print cp.E(P[1]*P[2],dist)
0.0
```

# Creating multivariate orthogonal polynomials in Chaospy

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P = cp.orth_ttr(1, dist)
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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
```

# A two-dimensional problem

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

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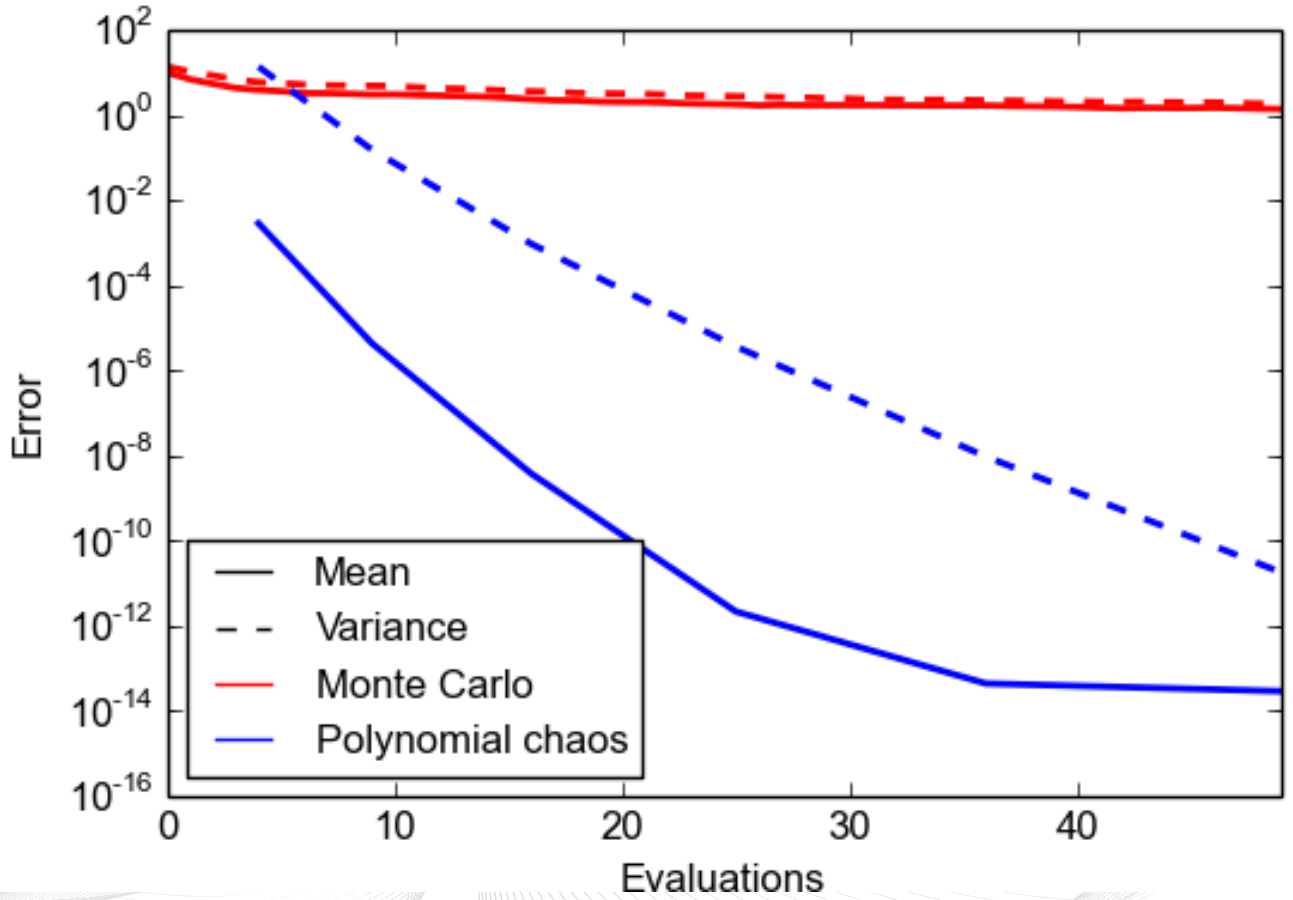
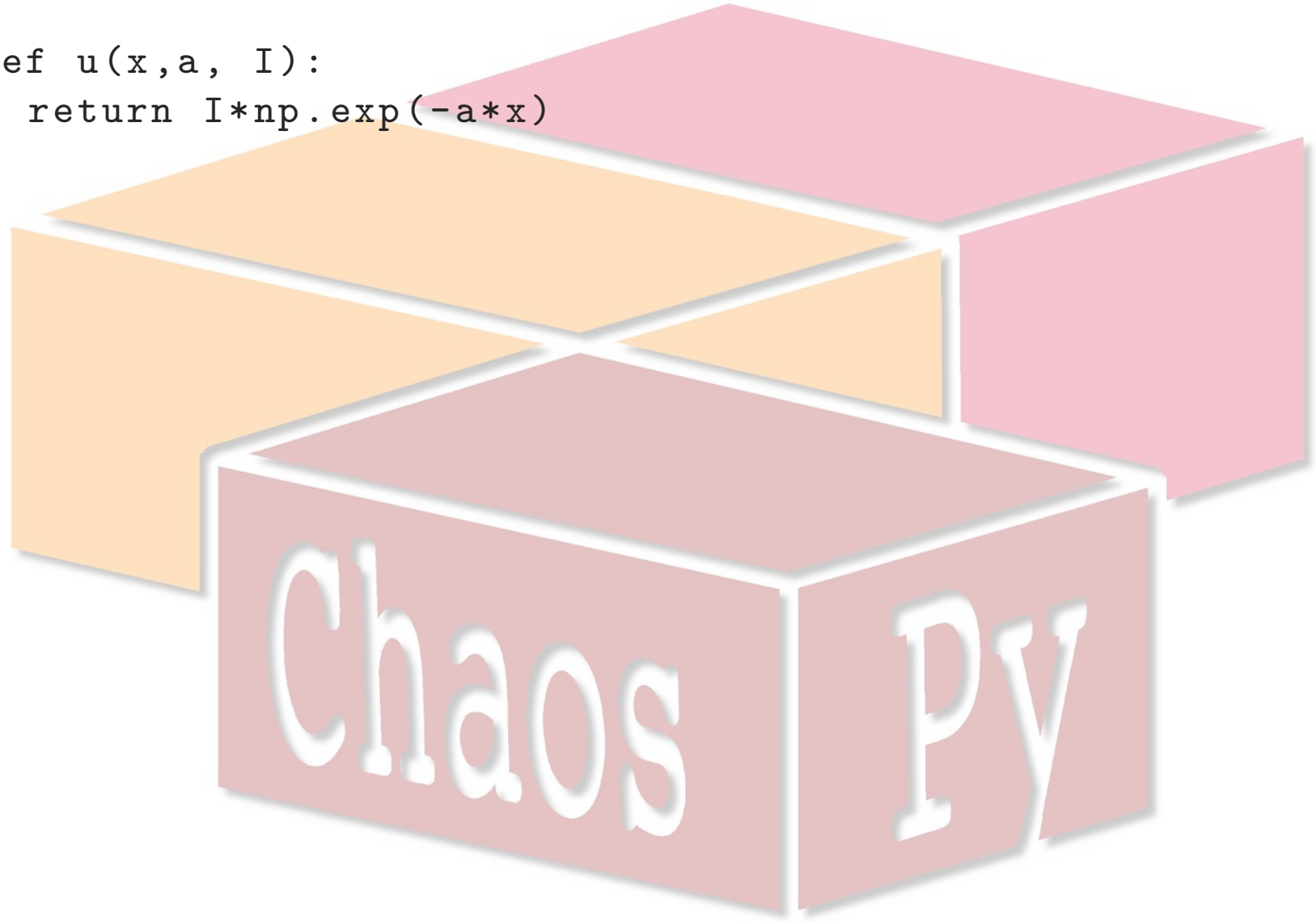
# Convergence of the two-dimensional $(a, l)$ problem



# Teaser of the full implementation

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



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```
def u(x,a, I):
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dist_a = cp.Uniform(0, 0.1)
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```

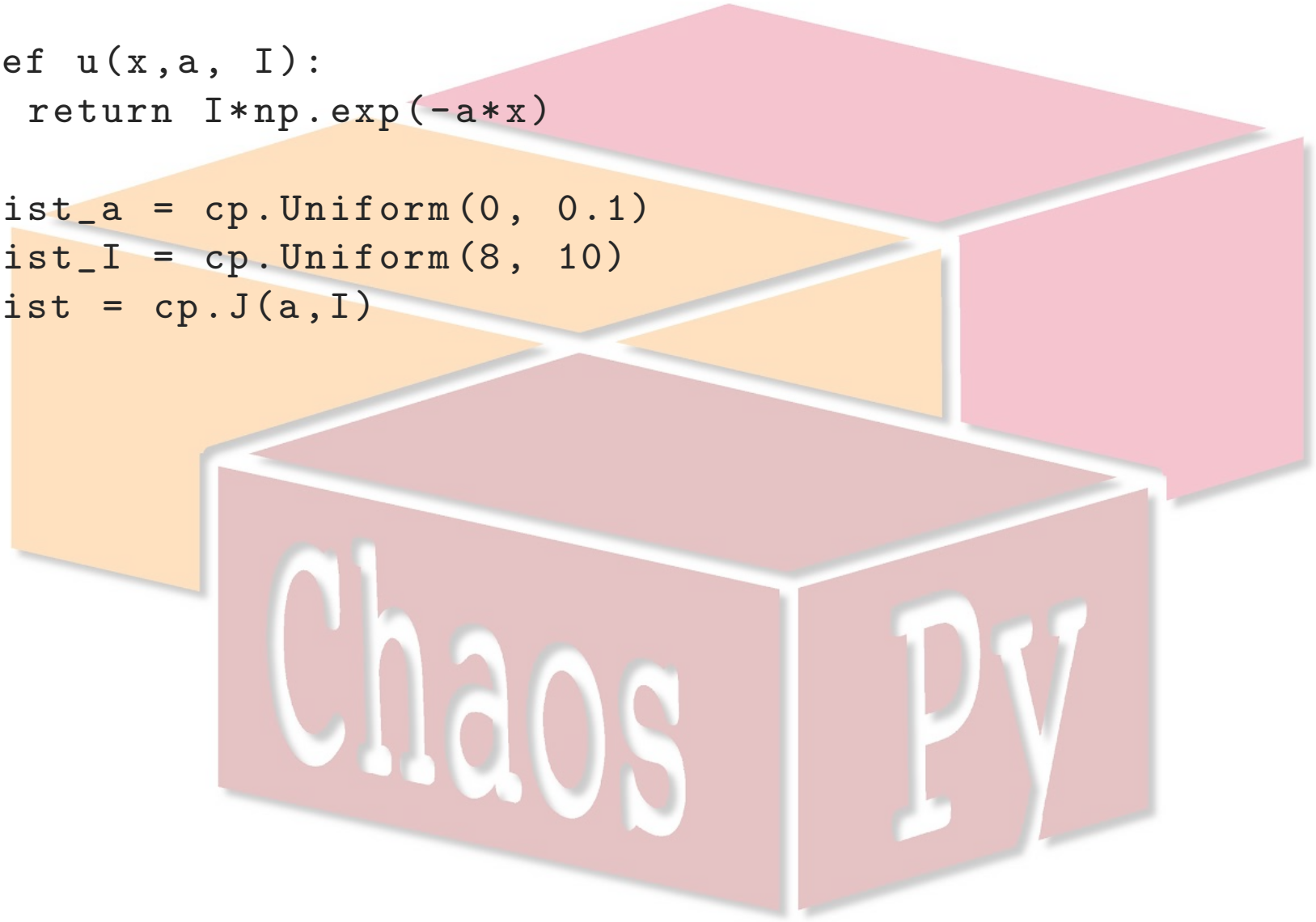

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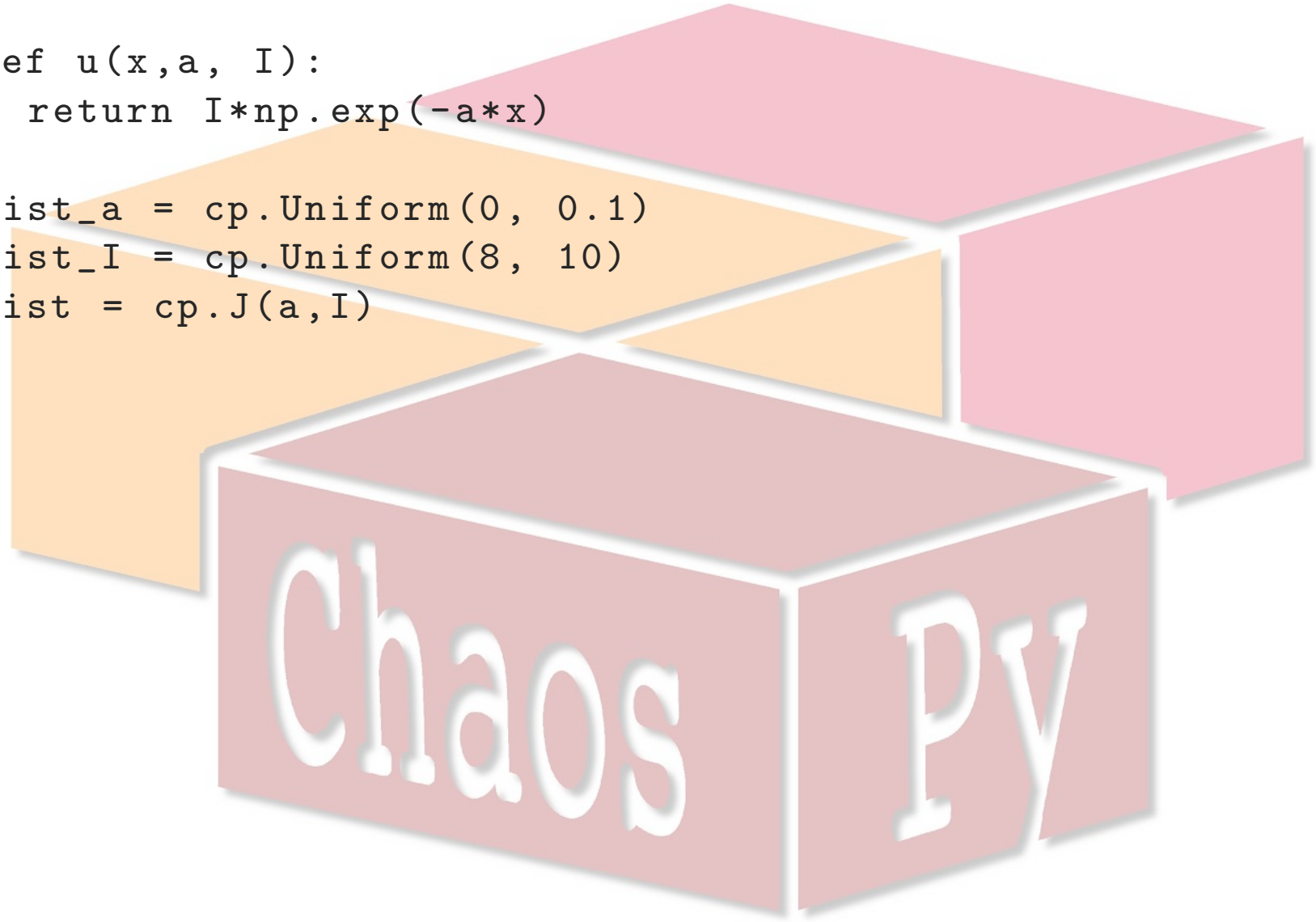

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dist_a = cp.Uniform(0, 0.1)
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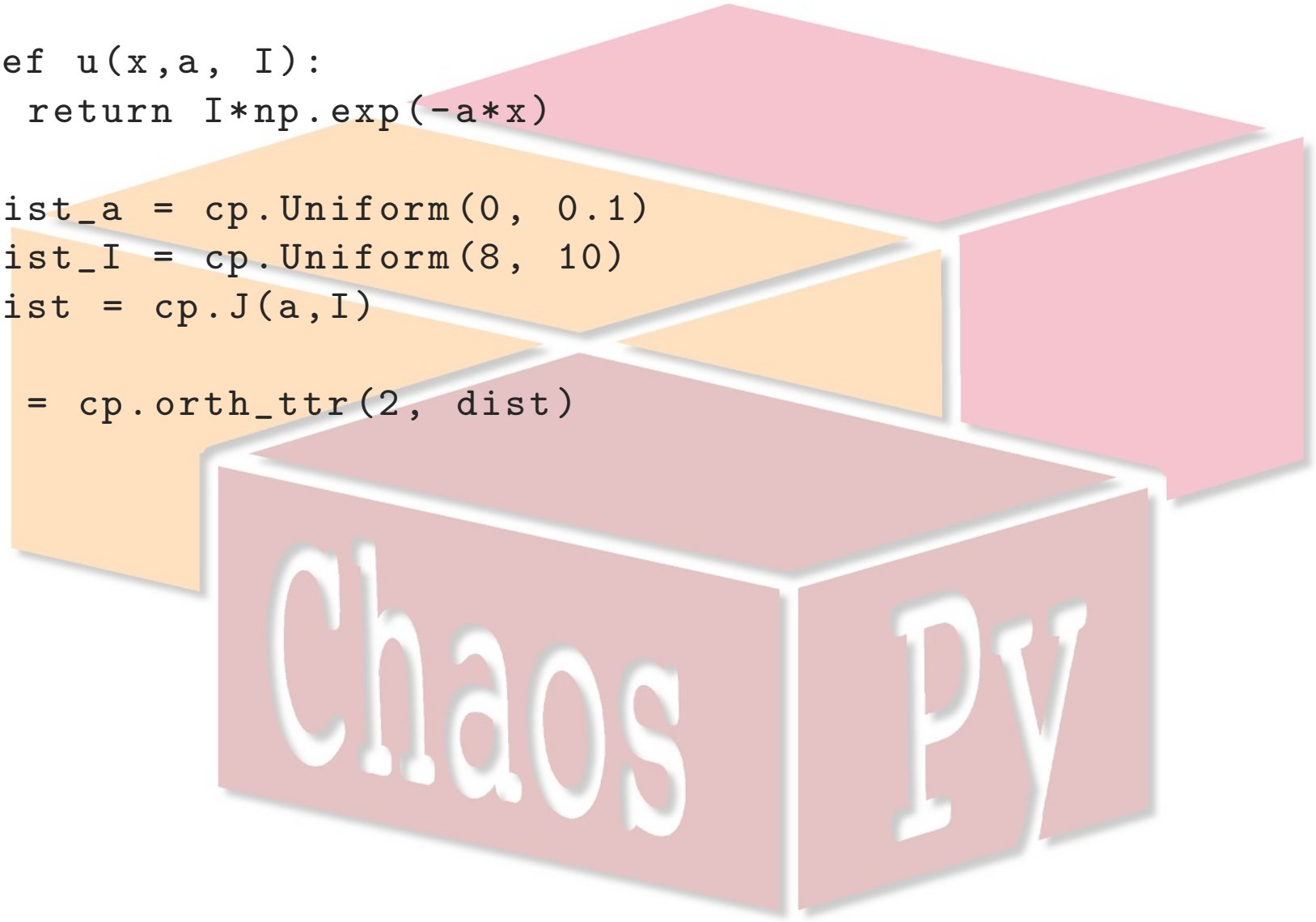
dist = cp.J(a,I)

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



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dist_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)
samples_u = [u(x, *node) for node in nodes.T]

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

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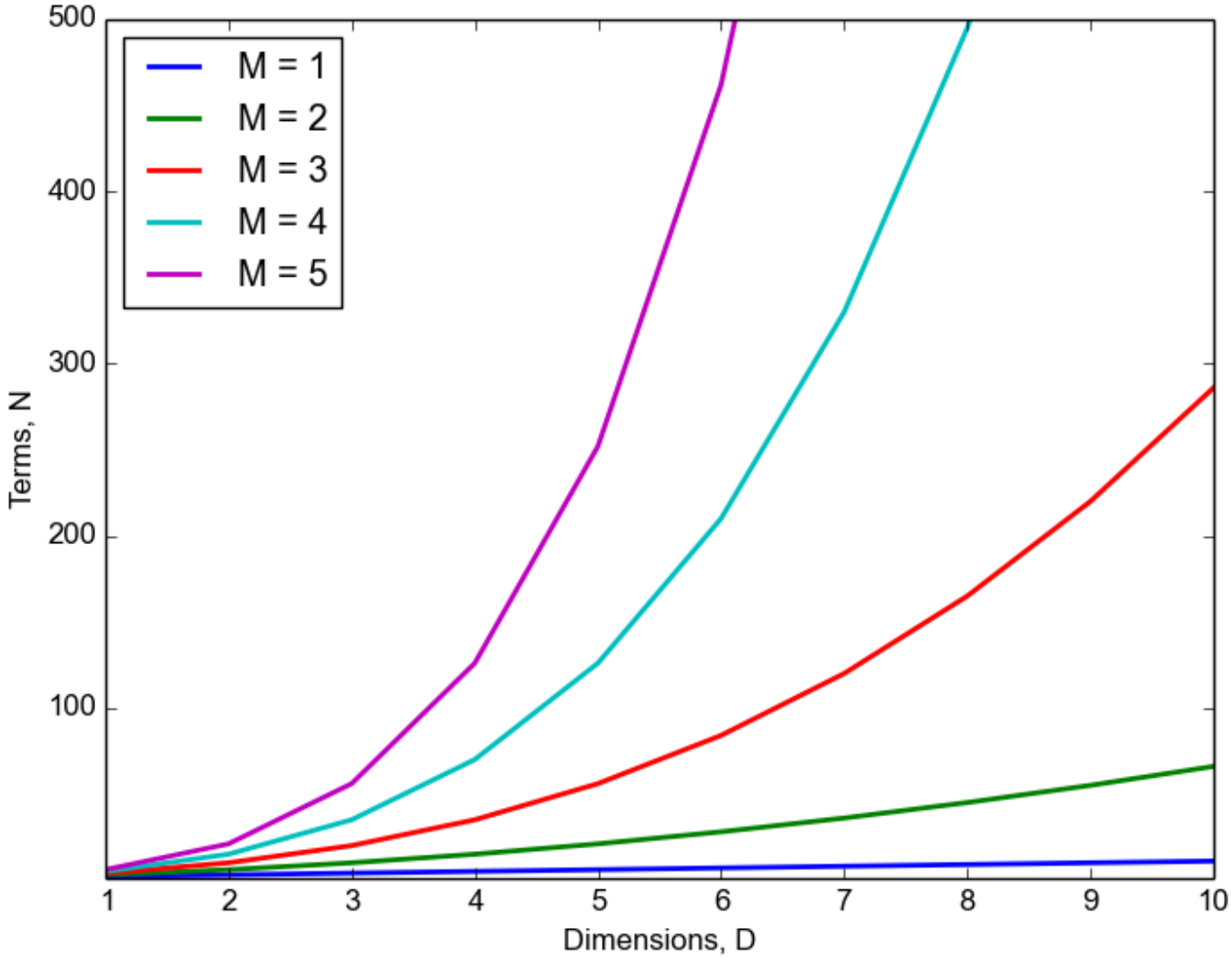
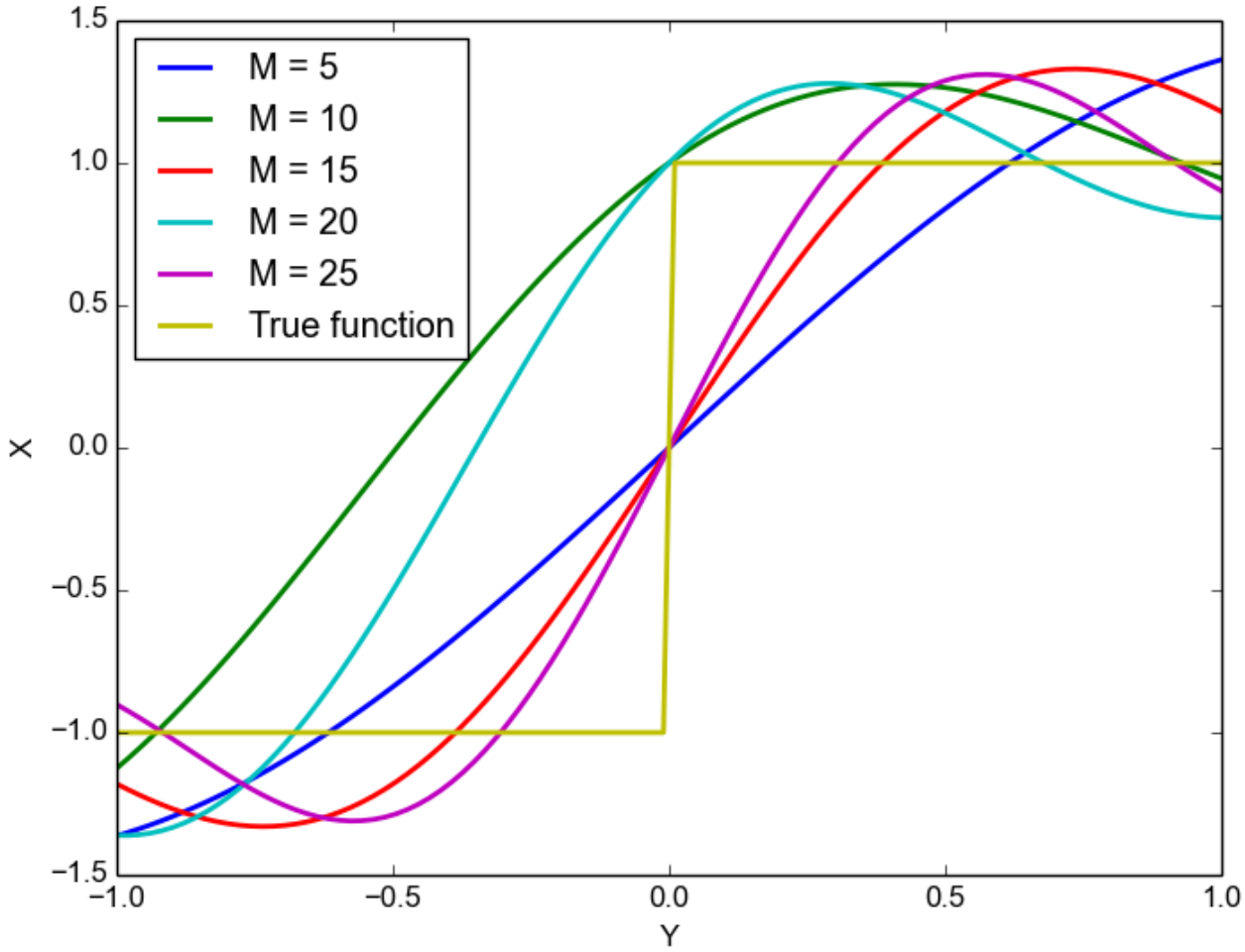
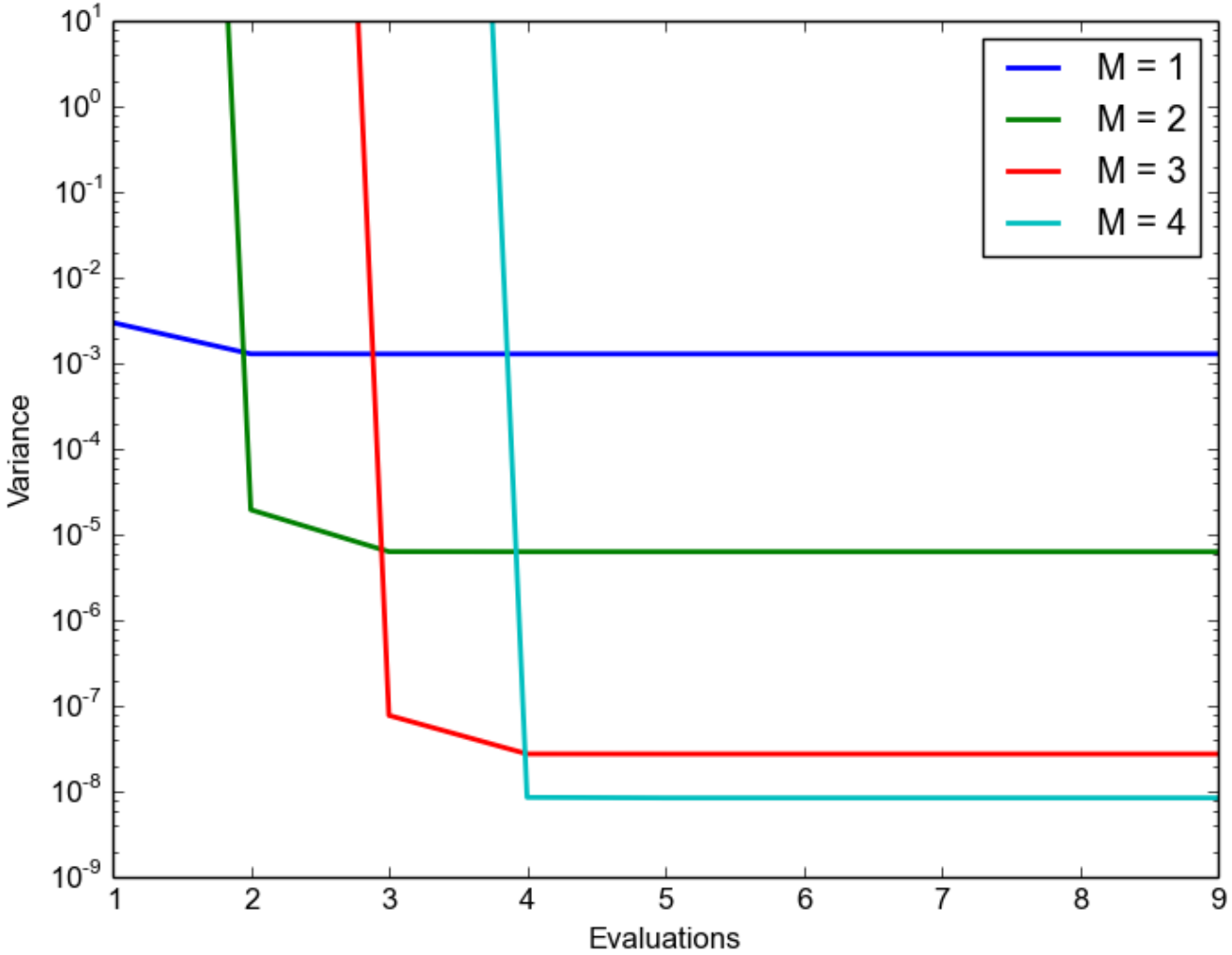

# The curse of dimensionality



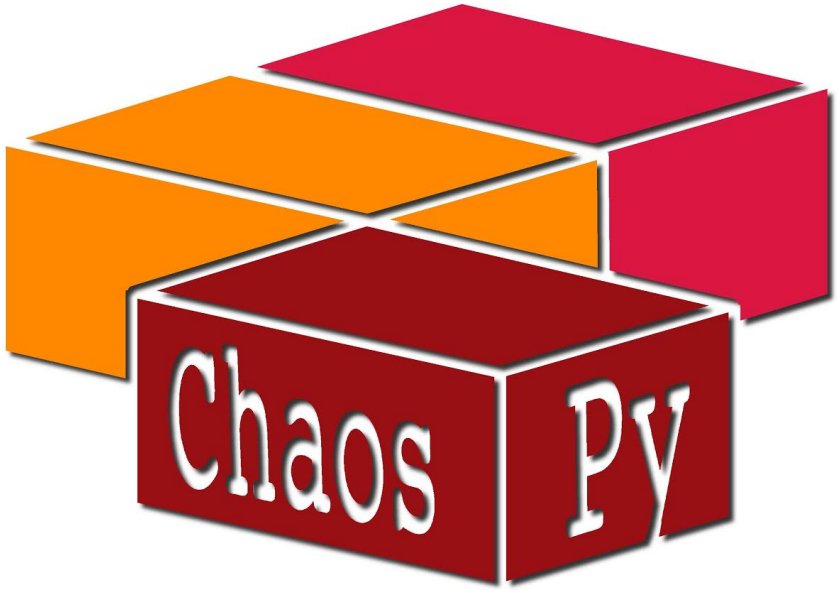
# Gibb's Phenomena: discontinuities give oscillations



# Higher number of samples justifies higher number of collocation nodes



# Thank you




A very basic introduction to scientific Python programming:
http://hplgit.github.io/bumpy/doc/pub/sphinx-basics/index.html

Installation instructions:
https://github.com/hplgit/chaospy

Interactive session:
http://10.50.3.247:8888/