Polynomial chaos expansions part 4: Generalized polynomial chaos

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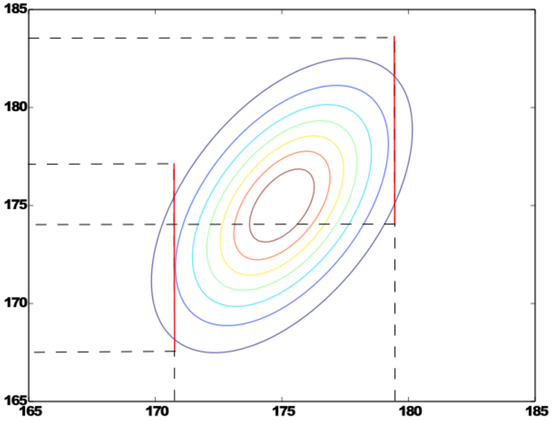
Relevant links

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

Some random variables are dependent



"Tall people have tall children"

Repetition of our model problem with two independent variables I and a

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

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, 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)
```

Dependent variables break the orthogonality property of polynomials!

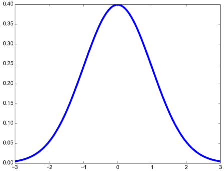
$$P_{\mathrm{i}} = P^{(1)}_{i_1} P^{(2)}_{i_2} \cdots P^{(D)}_{i_D} \qquad \mathrm{i} = (i_1, i_2, ..., i_D)$$

$$\begin{aligned}
\langle P_{\mathrm{i}}, P_{\mathrm{j}} \rangle_Q &= E(P_{\mathrm{i}}, P_{\mathrm{j}}) \\
&= \mathrm{E}\left(P^{(1)}_{i_1} \cdots P^{(D)}_{i_D} P^{(1)}_{j_1} \cdots P^{(D)}_{j_D} \right) \\
&= \mathrm{E}\left(P^{(1)}_{i_1} P^{(1)}_{j_1} \right) \cdots \mathrm{E}\left(P^{(D)}_{i_D} P^{(D)}_{j_D} \right) \\
&= \dots \\
&= \left\| P^{(1)}_{\mathrm{i}} \right\|_Q \delta_{\mathrm{ij}}
\end{aligned}$$

But the problem is:

$$\mathrm{E}(uv) \neq \mathrm{E}(u)\,\mathrm{E}(v) \qquad \text{when } u \text{ and } v \text{ are stochastically dependent}$$

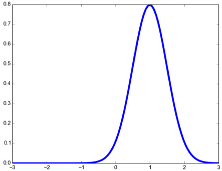
Transformations manipulates probability distributions



$R \sim N(0,1)$

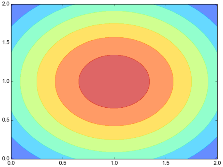
$R = \frac{Q-\mu}{\sigma}$

$Q = R\sigma + \mu$



$Q \sim N(\mu, \sigma^2)$

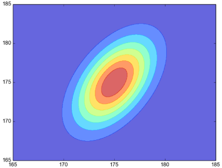
Transformation for multivariate distributions



$R \sim MvN(\mathbf{0}, I)$

$$R = L^{-1}(Q - \mu)$$

$$Q = LR + \mu$$



$Q \sim MvN(\boldsymbol{\mu}, \Sigma_Q)$

$$\Sigma_Q = L^T L$$

$$\boldsymbol{\mu}_Q = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \Sigma_Q = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \qquad \boldsymbol{\mu}_R = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \Sigma_R = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$Q_1(R_1, R_2) = R_1 \qquad Q_2(R_1, R_2) = \rho R_2 + \sqrt{1 - \rho^2} R_1$$

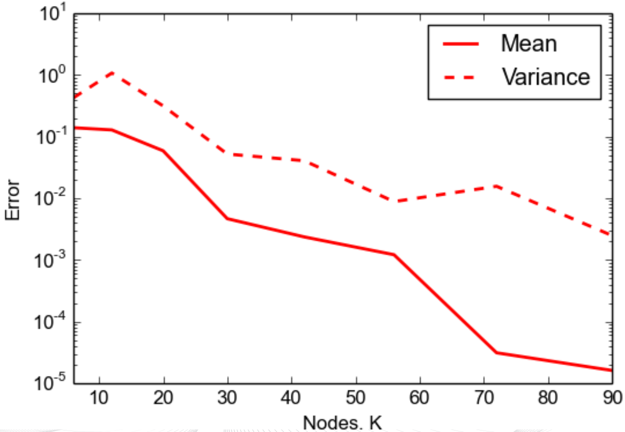
Transformations can be used to model dependent variables effectively as a parameterization of independent variables

$$\hat{u}_M(x; q) = \hat{u}_M(x; T(r)) = \sum_{n=0}^{N} c_n(x) P_n(r)$$

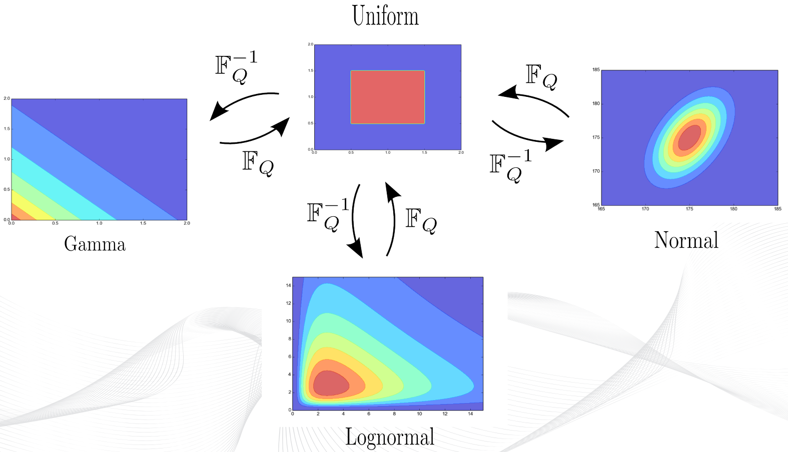
Code for dependent normal variables

```
x = np.linspace(0, 1, 100)
def u(x, a, I):
  return I*np.exp(-a*x)

C = [[2,1],[1,2]]
mu = [0.5,0.5]

dist_R = cp.J(cp.Normal(), cp.Normal())
P = cp.orth_ttr(M, dist_R)
L =  np.linalg.cholesky(C)        # C = np.dot(L.T, L)
def T(r):
    return np.dot(L,r) + mu

nodes_R = dist_R.sample(2*len(P), "M")
nodes_Q = T(nodes_R)

samples_u = [u(x, *node) for node in nodes_Q.T]
u_hat = cp.fit_quadrature(\
    P, nodes_R, weights, samples_u)
```

Convergence plot



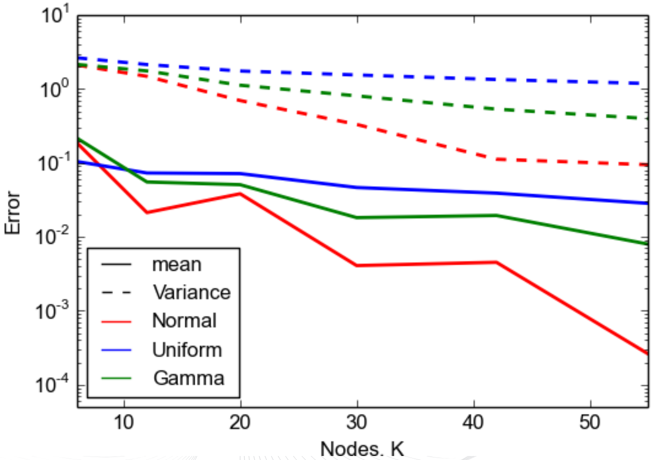
All random variables can with aid of the Rosenblatt transformations be transformed to/from the uniform distribution



Point collocation with Rosenblatt transformation

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

dist_R = cp.J(cp.Normal(), cp.Normal())
C = [[1, 0.5], [0.5, 1]]
mu = [0, 0]
dist_Q = cp.MvNormal(mu, C)

P = cp.orth_ttr(M, dist_R)
nodes_R = dist_R.sample(2*len(P), "M")
nodes_Q = dist_Q.inv(dist_R.fwd(nodes_R))

x = np.linspace(0, 1, 100)
samples_u = [u(x, *node) for node in nodes_Q.T]
u_hat = cp.fit_regression(P, nodes_R, samples_u)
```

Convergence of point collocation with Rosenblatt transformations



Rosenblatt transformations is essentially variable substitution

$$\mathrm{E}(u) = \int u(x;q) f_Q(q)\, dq \qquad = \int u\left(x;q\right) f_Q(q) \frac{f_R(r)}{f_Q(q)}\, dr$$

$$F_Q(q) = F_R(r) \qquad q = F_Q^{-1}\left(F_R(r)\right)$$

$$f_Q(q)\, dq = f_R(r)\, dr \qquad dq = \frac{f_R(r)}{f_Q(q)}\, dr$$

Pseudo-spectral with Rosenblatt transformation

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

C = [[1,0.5],[0.5,1]]
mu = np.array([0, 0])
dist_R = cp.J(cp.Normal(), cp.Normal())
dist_Q = cp.MvNormal(mu, C)

P = cp.orth_ttr(M, dist_R)
nodes_R, weights_R = cp.generate_quadrature(M+1, dist_R)
nodes_Q = dist_Q.inv(dist_R.fwd(nodes_R))
weights_Q = weights_R*\
    dist_Q.pdf(nodes_Q)/dist_R.pdf(nodes_R)

x = np.linspace(0, 1, 100)
samples_u = [u(x, *node) for node in nodes_Q.T]
u_hat = cp.fit_quadrature(P, nodes_R, weights_Q, samples_u)
```

Convergence of pseudo-spectral projection with Rosenblatt transformations