Technical University of Denmark

On Generalized Polynomial Chaos

Documentation of the Spectral Toolbox

Author:
Daniele Bigoni

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1 Introduction

Why this paper? Why Spectral Methods? Why a Spectral Toolbox? Why Python?

2 Orthogonal Polynomials

Orthogonal polynomials can be used in order to approximate functions in space. There exist infinite sets of orthogonal polynomials, however some of them have been studied extensively due to their simplicity and performances.

The Spectral Toolbox includes several polynomials for bounded as well as for unbounded domains. The available polynomials will be presented in the following. More information about orthogonal polynomials can be found in literature (e.g. [3]).

2.1 Jacobi Polynomials

2.1.1 Legendre Polynomials

2.1.2 Chebyshev Polynomials

2.2 Hermite Polynomials

Hermite polynomials span the interval $I := (-\infty, \infty)$.

2.2.1 Hermite Physicists' Polynomials

The Hermite Physicists Polynomials denoted by $H_n(x)$ are eigenfunctions of the Sturm-Liouville problem:

$$e^{x^2}\left(e^{-x^2} H_n'(x)\right)' + \lambda_n H_n(x) = 0, \qquad \forall x \in I := (-\infty, \infty) \tag{1}$$

- **Recurrence relation**

$$\begin{cases} H_0(x) = 1 \\ H_1(x) = 2x \\ H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \end{cases} \tag{2}$$

- **Derivatives**

$$\begin{cases} H_n^{(k)}(x) = 2nH_{n-1}^{(k-1)}(x) \\ H_n^{(0)}(x) = H_n(x) \\ H_0^{(k)}(x) = 0 \qquad \text{for } k > 0 \end{cases} \tag{3}$$

- **Orthogonality**

$$w(x) = e^{-x^2} \tag{4}$$

$$\gamma_n = \sqrt{\pi} 2^n n! \tag{5}$$

- **Gauss Quadrature points and weights**
  The Gauss points $\{x_j\}_{j=0}^N$ corresponding to $H_{N+1}(x)$ can be obtained using the Golub-Welsh algorithm [2] where:

$$a_j = 0 \qquad b_j = \frac{j}{2} \tag{6}$$

The Gauss weights are obtained by:

$$w_j = \frac{\lambda_N}{\lambda_{N-1}} \frac{(H_N(x), H_N(x))}{H_N(x_j)H'_{N+1}(x_j)} = \frac{\gamma_N}{(N+1)H_N^2(x_j)} \tag{7}$$

2.2.2 Hermite Functions

Hermite Functions are used because of their better behavior respect to Hermite Polynomials at infinity.

- **Recurrence relation**

$$\begin{cases} \tilde{H}_0(x) = e^{-x^2/2} \\ \tilde{H}_1(x) = \sqrt{2}xe^{-x^2/2} \\ \tilde{H}_{n+1}(x) = x\sqrt{\frac{2}{n+1}}\tilde{H}_n(x) - \sqrt{\frac{n}{n+1}}\tilde{H}_{n-1}(x), \qquad n \geq 1 \end{cases} \tag{8}$$

- **Derivatives**
The recursion relation for the k-th derivative of the function of order n is:

$$\tilde{H}_n^{(k)}(x) = \sqrt{\frac{n}{2}}\tilde{H}_{n-1}^{(k-1)}(x) - \sqrt{\frac{n+1}{2}}\tilde{H}_{n+1}^{(k-1)}(x) \tag{9}$$

Using this recursion formula we end up having an expression involving only Hermite Functions $\tilde{H}_n^{(0)}(x)$, that can be computed using the recurrence relation, and derivatives of the first Hermite Function $\tilde{H}_0^{(k)}$ that have the following form:

$$\tilde{H}_0^{(k)} = a_0e^{-x^2/2} + a_1xe^{-x^2/2} + a_2x^2e^{-x^2/2} + \ldots + a_kx^ke^{-x^2/2} \tag{10}$$

The values $\{a_i\}_{i=0}^k$ can be found using the following table:

k	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	$\ldots$
0	1									$\ldots$
1		-1								$\ldots$
2	-1		1							$\ldots$
3		3		-1						$\ldots$
4	3		-6		1					$\ldots$
5		-15		10		-1				$\ldots$
6	-15		45		-15		1			$\ldots$
7		105		-105		21		-1		$\ldots$
8	105		-420		210		-28		1	$\ldots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	

that can be generated iteratively using the following rules:

$$\begin{cases} A(0,0) = 1 & \\ A(i,j) = 0 & \text{if } i < j \\ A(i,j) = A(i,j) - A(i-1,j-1) & \text{if } j \neq 0 \\ A(i,j) = A(i,j) + A(i-1,j+1)(j+1) & \text{if } i > j \end{cases}$$

- **Orthogonality**

$$w(x) = 1 \tag{11}$$
$$\gamma_n = \sqrt{\pi} \tag{12}$$

- **Gauss Quadrature points and weights** The Gauss points $\{\tilde{x}_j\}_{j=0}^N$ corresponding to $\tilde{H}_{N+1}(x)$ can be obtained using the Golub-Welsh algorithm [2] where:

$$a_j = 0 \qquad b_j = \frac{j}{2} \tag{13}$$

These points are exactly the same of the Hermite Polynomials in (6).
The Gauss weights are obtained by:

$$\tilde{w}_j = \frac{\gamma_N}{(N+1)\tilde{H}_N^2(x_j)} \tag{14}$$

2.2.3 Hermite Probabilists' Polynomials

The Hermite Physicists Polynomials denoted by $H_n(x)$ are eigenfunctions of the Sturm-Liouville problem:

$$\left(e^{-x^2} He_n'(x)\right)' + \lambda_n e^{-x^2} He_n(x) = 0, \qquad \forall x \in I := (-\infty, \infty) \wedge \lambda \geq 0 \tag{15}$$

- **Recurrence relation**

$$\begin{cases} He_0(x) = 1 \\ He_1(x) = x \\ He_{n+1}(x) = xHe_n(x) - nHe_{n-1}(x) \end{cases} \tag{16}$$

- **Derivatives**

$$\begin{cases} He_n^{(k)}(x) = nHe_{n-1}^{(k-1)}(x) \\ He_n^{(0)}(x) = He_n(x) \\ He_0^{(k)}(x) = 0 \qquad \text{for } k > 0 \end{cases} \tag{17}$$

- **Orthogonality**

$$w(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \tag{18}$$
$$\gamma_n = n! \tag{19}$$

- **Gauss Quadrature points and weights**
The Gauss points $\{x_j\}_{j=0}^N$ corresponding to $He_{N+1}(x)$ can be obtained using the Golub-Welsh algorithm [2] where:

$$a_j = 0 \qquad b_j = j \tag{20}$$

The Gauss weights are obtained by:

$$w_j = \frac{\gamma_N}{(N+1)He_N^2(x_j)} \tag{21}$$

2.3 Laguerre Polynomials

3 Generalized Polynomial Chaos

Example 3.1 (Stochastic Test Equation)**.**
Consider the stochastic test equation

$$\frac{du(t,\xi)}{dt} = -k(\xi)u(t,\xi), \qquad u(0,\xi) = u_0 \tag{22}$$
$$\xi \sim \mathcal{U}(-1,1), \qquad \rho_\xi(\xi) = \frac{1}{2}, \qquad k(\xi) = \frac{1}{2}\xi + \frac{1}{2}$$

where the decay rate is uniformly distributed in $I \in [0,1]$*. Let's apply* ***non-normalized Legendre-chaos*** *on the random input as well as on the function* $u(t,\xi)$*, where* $\left\{J_i^{(0,0)}(\xi)\right\}_{i=0}^{N}$ *are the orthogonal Legendre basis functions.*

$$k(\xi) \approx k_N(\xi) = \sum_{i=0}^{N} \hat{k}_i J_i^{(0,0)} \tag{23}$$

$$\hat{k}_i = \frac{1}{\gamma_i}\int_{-1}^{1} k(\xi)J_i^{(0,0)}(\xi)w(\xi)d\xi \approx A^T k(\underline{\xi}) \tag{24}$$

$$u(t,\xi) \approx u_N(t,\xi) = \sum_{i=0}^{N} \hat{u}_i(t) J_i^{(0,0)} \tag{25}$$

$$\hat{u}_i(t) = \frac{1}{\gamma_i}\int_{-1}^{1} u(t,\xi)J_i^{(0,0)}(\xi)w(\xi)d\xi \approx A^T u(t,\underline{\xi}) \tag{26}$$

where $A_{j,i} = \frac{J_i^{(0,0)}(\xi_j)}{\gamma_i}w_j$ *and* $\{\xi_i, w_i\}_{i=0}^N$ *is a set of quadrature points. The* ***gPC-expansion*** *of* (22) *is given by:*

$$\mathbf{E}\left[\frac{du(t,\xi)}{dt}J_k^{(0,0)}(\xi)\right]_{\rho_\xi(\xi)} = \mathbf{E}\left[-k(\xi)u(t,\xi)J_k^{(0,0)}(\xi)\right]_{\rho_\xi(\xi)} \tag{27}$$

$$\int_{-1}^{1}\sum_{i=0}^{N}\frac{d\hat{u}_i(t,\xi)}{dt}J_i^{(0,0)}(\xi)J_k^{(0,0)}(\xi)\rho_\xi(\xi)d\xi = \tag{28}$$
$$-\int_{-1}^{1}\sum_{i,j=0}^{N}\hat{k}_i\hat{u}_j(t)J_i^{(0,0)}(\xi)J_j^{(0,0)}(\xi)J_k^{(0,0)}(\xi)\rho_\xi(\xi)d\xi$$

$$\frac{d\hat{u}_k(t)}{dt} = -\frac{1}{\gamma_k}\sum_{i,j=0}^{N}\hat{k}_i\hat{u}_j(t)\underbrace{\int_{-1}^{1}J_i^{(0,0)}(\xi)J_j^{(0,0)}(\xi)J_k^{(0,0)}(\xi)w(\xi)d\xi}_{\approx\sum_l^{2N}J_i^{(0,0)}(\xi_l)J_j^{(0,0)}(\xi_l)J_k^{(0,0)}(\xi_l)w_l=e_{ijk}} \tag{29}$$

The ***initial conditions*** *for the gPC-expansion are:*

$$\hat{u}_i(0) = \frac{1}{\gamma_i}\int_{-1}^{1}u(0,\xi)J_i^{(0,0)}(\xi)w(\xi)d\xi = \begin{cases} u_0 & i = 0 \\ 0 & i \geq 1 \end{cases} \tag{30}$$

*The **expectation** of the solution is given by*

$$\begin{aligned}\mathbf{E}\left[u(t,\xi)\right]_{\rho_\xi} &= \int_{-1}^{1} u(t,\xi)\rho_\xi(\xi)d\xi \approx \int_{-1}^{1}\sum_{i=0}^{N}\hat{u}_i(t)J_i^{(0,0)}(\xi)\rho_\xi(\xi)d\xi \\ &= \sum_{i=0}^{N}\hat{u}_i(t)\frac{1}{2}\int_{-1}^{1}J_i^{(0,0)}(\xi)w(\xi)d\xi = \hat{u}_0(t)\end{aligned} \tag{31}$$

*The **variance** of the solution is given by*

$$\begin{aligned}\mathbf{Var}[u(t,\xi)]_{\rho_\xi(\xi)} &= \mathbf{E}\left[\left(u(t,\xi)-\mu_u(t)\right)^2\right]_{\rho_\xi(\xi)} \\ &\approx \mathbf{E}[u_N^2(t,\xi)]_{\rho_\xi(\xi)} - 2\mu_u(t)\mathbf{E}[u_N(t,\xi)]_{\rho_\xi(\xi)} + \mu_u^2(t) \\ &= \int_{-1}^{1}\sum_{i,j=0}^{N}\hat{u}_i(t)\hat{u}_j(t)J_i^{(0,0)}(\xi)J_j^{(0,0)}(\xi)\rho_\xi(\xi)d\xi - \mu_u^2(t) \\ &= \frac{1}{2}\sum_{i=0}^{N}\hat{u}_i^2(t)\gamma_i - \hat{u}_0^2(t) = \frac{1}{2}\sum_{i=1}^{N}\hat{u}_i^2(t)\gamma_i\end{aligned} \tag{32}$$

*If **normalized Legendre-chaos** is employed, then some modifications to the equations have to be considered. The normalized basis are given by* $\tilde{J}_i^{(0,0)}(\xi) = \frac{J_i^{(0,0)}(\xi)}{\sqrt{\gamma_i}}$, *thus*

$$\hat{k}_i = \int_{-1}^{1} k(\xi)\tilde{J}_i^{(0,0)}(\xi)w(\xi)d\xi \approx A^T k(\underline{\xi}) \tag{33}$$

$$\hat{u}_i(t) = \int_{-1}^{1} u(t,\xi)\tilde{J}_i^{(0,0)}(\xi)w(\xi)d\xi \approx A^T u(t,\underline{\xi}) \tag{34}$$

where $A_{j,i} = \tilde{J}_i^{(0,0)}(\xi_j)w_j$ *and* $\{\xi_i, w_i\}_{i=0}^N$ *is a set of quadrature points. The **gPC-expansion** is then written as*

$$\frac{d\hat{u}_k(t)}{dt} = -\sum_{i,j=0}^{N}\hat{k}_i\hat{u}_j(t)\underbrace{\int_{-1}^{1}\tilde{J}_i^{(0,0)}(\xi)\tilde{J}_j^{(0,0)}(\xi)\tilde{J}_k^{(0,0)}(\xi)w(\xi)d\xi}_{\approx\sum_l^{2N}\tilde{J}_i^{(0,0)}(\xi_l)\tilde{J}_j^{(0,0)}(\xi_l)\tilde{J}_k^{(0,0)}(\xi_l)w_l=e_{ijk}} \tag{35}$$

*The **initial conditions** are given by*

$$\hat{u}_i(0) = \int_{-1}^{1} u(0,\xi)\tilde{J}_i^{(0,0)}(\xi)w(\xi)d\xi = \begin{cases}2\frac{u_0}{\sqrt{\gamma_0}} & i=0\\ 0 & i\geq 1\end{cases} \tag{36}$$

*The **expectation** and the **variance** of the solution for the normalized gPC are given by*

$$\begin{aligned}
\mathbf{E}\left[u(t,\xi)\right]_{\rho_\xi} &= \int_{-1}^{1} u(t,\xi)\rho_\xi(\xi)d\xi \approx \int_{-1}^{1}\sum_{i=0}^{N}\hat{u}_i(t)\tilde{J}_i^{(0,0)}(\xi)\rho_\xi(\xi)d\xi && (37)\\
&= \sum_{i=0}^{N}\frac{\hat{u}_i(t)}{\sqrt{\gamma_i}}\frac{1}{2}\int_{-1}^{1}J_i^{(0,0)}(\xi)w(\xi)d\xi = \frac{\hat{u}_0(t)}{\sqrt{\gamma_0}}\\
\mathbf{Var}[u(t,\xi)]_{\rho_\xi(\xi)} &= \mathbf{E}\left[(u(t,\xi)-\mu_u(t))^2\right]_{\rho_\xi(\xi)} && (38)\\
&\approx \mathbf{E}[u_N^2(t,\xi)]_{\rho_\xi(\xi)} - 2\mu_u(t)\mathbf{E}[u_N(t,\xi)]_{\rho_\xi(\xi)} + \mu_u^2(t)\\
&= \int_{-1}^{1}\sum_{i,j=0}^{N}\hat{u}_i(t)\hat{u}_j(t)\tilde{J}_i^{(0,0)}(\xi)\tilde{J}_j^{(0,0)}(\xi)\rho_\xi(\xi)d\xi - \mu_u^2(t)\\
&= \frac{1}{2}\sum_{i=0}^{N}\hat{u}_i^2(t) - \hat{u}_0^2(t) = \frac{1}{2}\sum_{i=1}^{N}\hat{u}_i^2(t)
\end{aligned}$$

An advantage of using orthonormal polynomials is that we don't need to compute $\{\gamma_i\}_{i=1}^N$ values that involve factorials and can become hard to compute accurately for big N values.

3.1 Time Dependent generalized Polynomial Chaos

In order to improve the performances on time dependent ODEs, one can employ Time Dependent generalized Polynomial Chaos (TDgPC) first introduced in [1].

Stop criteria

$$\max\left(|_j\hat{u}_2(t)|,\dots,|_j\hat{u}_N(t)|\right) \geq \frac{|_j\hat{u}_1(t)|}{\theta} \tag{39}$$

Integral relation

$$\int_{I_{\psi_j}} g(\psi_j)f_{\psi_j}(\psi_j)d\psi_j = \int_{I_\xi} g(\mathbf{T}(\xi))f_\xi(\xi)d\xi \tag{40}$$

where $\mathbf{T}_j(\xi)$ is the composition $T_1\circ\cdots\circ T_j$ of transformations from the variable ξ to the variables $\psi_1,\dots,\psi_j$.

Example 3.2 (Stochastic Test Equation - continuing example 3.1)**.**
*Consider the solution $u(t_j,\psi_{j-1})$ at time t_j that satisfy the stopping criteria (39). Let's define a **new random variable** ψ_j corresponding to such solution:*

$$\begin{aligned}
\psi_j = \mathbf{T}_j(\xi) = u(t_j,\psi_{j-1}) &\approx \sum_{i=0}^{N}[_{j-1}\hat{u}_i(t)][_{j-1}\phi_i(\psi_{j-1})] && (41)\\
&= \sum_{i=0}^{N}[_{j-1}\hat{u}_i(t)][_{j-1}\phi_i(\mathbf{T}_{j-1}(\xi))]
\end{aligned}$$

We now seek for the best set of orthonormal polynomials in order to describe the distribution of this random variable. We use a generalized version of ***Gram-Schmidt orthogonalization*** *algorithm [4] for weighted normed spaces. The orthogonalization is started with the Vandermonde matrix of ψ. We finally obtain a set $\left\{{}_j\phi_i(\psi_j)\right\}_{i=0}^N$ of basis functions s.t.*

$$\int_I [{}_j\phi_i(\psi_j)][{}_j\phi_k(\psi_j)]f_{\psi_j}(\psi_j)d\psi = \delta_{ik}, \qquad \text{for } i,k = 0,\dots,N \tag{42}$$

We now need to rewrite the system of ODE with respect to this basis functions. First we rewrite the ***initial conditions****, that are given by:*

$$u(t,\psi_j) \approx \sum_{i=0}^N [{}_j\hat{u}_i(t)][{}_j\phi_i(\psi_j)] \tag{43}$$

$$\begin{aligned} {}_j\hat{u}_i(t_j) &= \frac{1}{\|{}_j\phi_i\|_{f_{\psi_j}}} \int_{I_{\psi_j}} u(t_j,\psi_j)[{}_j\phi_i(\psi_j)]f_{\psi_j}(\psi_j)d\psi_j \\ &= \frac{1}{\|{}_j\phi_i\|_{f_{\psi_j}}} \underbrace{\int_{I_\xi} u(t_j,\mathbf{T}(\xi))[{}_j\phi_i(\mathbf{T}(\xi))]f_\xi(\xi)d\xi}_{\approx\sum_{l=0}^{QN} u(t_j,\mathbf{T}(\xi_l))[{}_j\phi_i(\mathbf{T}(\xi_l))]w_l} \end{aligned} \tag{44}$$

where Q determines the precision of the quadrature rule, that is used for estimating an integral that can possibly not be a polynomial. We now ***rewrite the ODE*** *in terms of the new polynomials. For the parameter $k(\xi)$ the expansion (33) can still be used, while the new expansion (43) will be used for $u(t,\psi_j)$. We plug these expansion in the weak formulation of gPC, obtaining*

$$\mathbf{E}\left[\frac{du(t,\psi_j)}{dt}{}_j\phi_i(\psi_j)\right]_{f_{\psi_j}} = \mathbf{E}\left[-k(\xi)u(t,\psi_j)[{}_j\phi_i(\psi_j)]\right]_{f_{\psi_j}} \tag{45}$$

$$\frac{d[{}_j\hat{u}_i(t)]}{dt} = -\frac{1}{\|{}_j\phi_i\|_{f_{\psi_j}}} \sum_{l,i=0}^N \hat{k}_l[{}_j\hat{u}_i(t)] \underbrace{\int_{-1}^1 \tilde{J}_l^{(0,0)}(\xi)[{}_j\phi_i(\mathbf{T}(\xi))][{}_j\phi_k(\mathbf{T}(\xi))]f_\xi(\xi)d\xi}_{\approx\sum_{n=0}^{QN}\tilde{J}_l^{(0,0)}(\xi_n)[{}_j\phi_i(\mathbf{T}(\xi_n))][{}_j\phi_k(\mathbf{T}(\xi_n))]w_n=e_{lik}} \tag{46}$$

The ***mean*** *and the* ***variance*** *can now be computed using*

$$\mathbf{E}\left[u(t,\psi_j)\right]_{f_{\psi_j}} = \sum_{i=0}^N {}_j\hat{u}_i(t) \underbrace{\int_{-1}^1 [{}_j\phi_i(\mathbf{T}(\xi))]f_\xi(\xi)d\xi}_{\approx\sum_{n=0}^{QN}[{}_j\phi_i(\mathbf{T}(\xi_n))]w_n} \tag{47}$$

$$\mathbf{Var}\left[u(t,\psi_j)\right]_{f_{\psi_j}} = \left[\sum_{i=0}^N {}_j\hat{u}_i(t) \underbrace{\int_{-1}^1 [{}_j\phi_i(\mathbf{T}(\xi))][{}_j\phi_i(\mathbf{T}(\xi))]f_\xi(\xi)d\xi}_{\approx\sum_{n=0}^{QN}[{}_j\phi_i(\mathbf{T}(\xi_n))][{}_j\phi_i(\mathbf{T}(\xi_n))]w_n}\right] - \mu_u^2(t) \tag{48}$$

4 Probabilistic Collocation Method

Probabilitsic collocation is a non-intrusive approach used to solve stochastic problems.
Let

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