Algorithms for Uncertainty Quantification

Lecture 6: Polynomial Chaos Approximation 1: The Pseudo-spectral Approach

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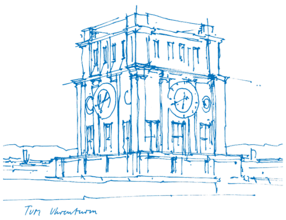
Scientific Computing in Computer Science
TUM



Repetition of Previous Lecture

- Interpolation concepts
  - every continuous function can be interpolated uniquely
  - interpolation with Lagrange cardinal polynomials
  - interpolation error $\Leftrightarrow$ Lebesgue constant
  - uniform grid not always a good choice
- Quadrature concepts
  - weighted inner product spaces
  - orthogonal polynomials
  - examples: Lagrange (uniform weight), Hermite (Gaussian weight) polynomials
  - Gaussian quadrature
    - nodes: zeros of the underlying orthogonal polynomial
    - weights: integral of the Lagrange cardinal polynomial evaluated at the nodes

Concept of Building Block:

- Time: $\approx$ 90 minutes
- Content
  - Polynomial Chaos: Basic concept & pseudo-spectral approach
  - Example: Damped linear oscillator
- Expected Learning Outcomes
  - The participants can describe the basic idea of generalized polynomial chaos (gPC) methods and underlying reasons.
  - They are able to list several ways to compute the gPC coefficients and to describe and relate the pseudo-spectral approach in this context.
  - They can give rough estimates for the dependency of the approximation orders N and K.
  - The participants are able to derive the formulas relating expectation and variance to the coefficients of the gPC approach.
  - They can indicate the relevant changes in the concept if several instead of one parameters are uncertain, i.e. in the multivariate context.

Agenda

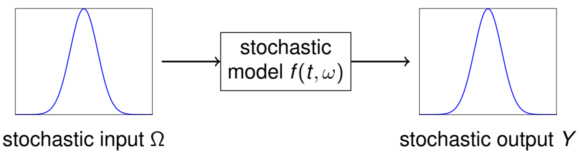
Topic

Methods based on polynomial chaos approximation

Content

- polynomial chaos expansion
- orthogonal polynomials
- the pseudo-spectral approach
- example: damped linear oscillator
- extension to multivariate polynomials
- summary

Forward Propagation of Uncertainty



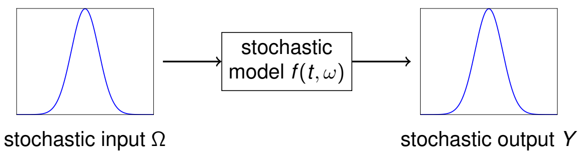
Problem

- assumption: f computationally expensive or available as a black-box
- deterministic independent variable: t (placeholder for $t, x, \ldots$)

What we want

- a good approximation of f (or statistical moments of its output Y) that is cheap to evaluate

Forward Propagation of Uncertainty (2)



Which method to use?

- remember: standard or improved Monte Carlo sampling
  1. sample from the input distribution
  2. solve system for each sample
  3. compute statistical output properties
- slow convergence in general
- computationally expensive (many samples)

Polynomial Chaos Methods

Analogy: Fourier series

- series of trigonometric functions for periodic functions $s(t)$

$$s(t) = \sum_{n=0}^{\infty} \hat{s}_n \, sin(\ldots)$$

Polynomial chaos expansion

- idea: approximate $f(t,\omega)$ by series of polynomials

$$f(t,\omega) = \sum_{n=0}^{\infty} \hat{f}_n(t)\, \phi_n(\omega)$$

- $\phi_n(\omega)$ polynomials of degree n, $\hat{f}_n(t)$ coefficients

Polynomial Chaos Methods (2)

Polynomial chaos expansion

- truncate series after N terms

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\, \phi_n(\omega)$$

- $\phi_n(\omega)$ orthogonal
- type of polynomials chosen w.r.t. input distribution $\rho(\omega)$

Polynomial Chaos Methods – Checklist

Polynomial chaos expansion

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\, \phi_n(\omega)$$

What we need to do

- **specify type of polynomials** $\phi_n(\omega)$
- compute coefficients $\hat{f}_n(t)$
- choose maximum order N
- compute statistical properties of $f(t,\omega)$ based on this approximation

Inner Product of Functions

Remember: Scalar product of vectors

- vectors in Euclidean space: **a**, **b**

$$< \mathbf{a}, \mathbf{b} > = \mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{N} a_i\, b_i$$

(Weighted) inner product of functions

- Euclidean space $\rightarrow$ Hilbert space
- vectors $\rightarrow$ functions: $p(\omega)$, $q(\omega)$
- sum $\rightarrow$ integral with weight function $\rho(\omega)$

$$< p(\omega), q(\omega) >_\rho = \int_{supp(\rho)} p(\omega)\, q(\omega)\, \rho(\omega)\, d\omega$$

Orthogonality

Remember: Orthogonal vectors

- scalar product is zero

$$< \mathbf{a}, \mathbf{b} > = 0 \iff \mathbf{a} \perp \mathbf{b}$$

Orthogonal functions

- inner product is zero

$$< p(\omega), q(\omega) >_\rho = \int_{supp(\rho)} p(\omega)\, q(\omega)\, \rho(\omega)\, d\omega = 0 \iff p(\omega) \perp q(\omega)$$

Univariate Orthogonal Polynomials

Orthogonal basis

- degree 0 to $N-1$: $\phi_0, \phi_1, \ldots, \phi_{N-1}$
- orthogonal w.r.t. weight $\rho(\omega)$

$$< \phi_i(\omega), \phi_j(\omega) >_\rho = \int \phi_i(\omega)\, \phi_j(\omega)\, \rho(\omega)\, d\omega = \gamma_i\, \delta_{ij}$$

- Kronecker delta $\delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$
- normalization constants $\gamma_i =< \phi_i(\omega), \phi_i(\omega) >_\rho$

Univariate Orthogonal Polynomials (2)

Orthogonal basis

$$< \phi_i(\omega), \phi_j(\omega) >_\rho = \int \phi_i(\omega)\, \phi_j(\omega)\, \rho(\omega)\, d\omega = \gamma_i\, \delta_{ij}$$

Orthonormal basis

- Normalization constants are 1

$$\tilde{\phi}_i = \frac{1}{\sqrt{\gamma_i}} \phi_i$$

- from now on: assume $\phi_i(\omega)$ are normalized

$$< \phi_i(\omega), \phi_j(\omega) >_\rho = \delta_{ij}$$

Type of Polynomials

Polynomial chaos expansion

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\, \phi_n(\omega)$$

What type of polynomials to use?

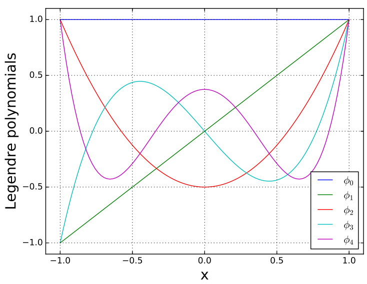
- chosen w.r.t. probability distribution $\rho(\omega)$
- examples:
  - $\Omega \sim \mathcal{U}(-1,1) \rightarrow$ Legendre polynomials
  - $\Omega \sim \mathcal{N}(0,1)$: $\rightarrow$ Hermite polynomials
- the idea can be generalized to all probability distributions

Legendre Polynomials

- orthogonal w.r.t. integral from -1 to 1 with weight function $\rho(\omega) = \frac{1}{2}$

$$\int_{-1}^{1} \phi_i(\omega)\, \phi_j(\omega)\, \rho(\omega)\, d\omega = \frac{2}{2i+1}\, \delta_{ij}$$

- $\phi_0 = 1$
- $\phi_1 = \omega$
- $\phi_2 = \frac{1}{2}\,(3\omega^2 - 1)$
- $\phi_3 = \frac{1}{2}\,(5\omega^3 - 3\omega)$
- $\phi_4 = \frac{1}{8}\,(35\omega^4 - 30\omega^2 + 3)$
- ...

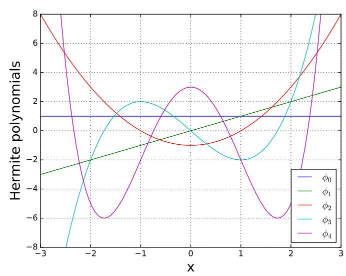


Hermite Polynomials

- orthogonal w.r.t. integral from $-\infty$ to ∞
- weight function $\rho(\omega) = \frac{1}{\sqrt{2\pi}} exp(-\frac{\omega^2}{2})$

$$\int_{-\infty}^{\infty} \phi_i(\omega)\, \phi_j(\omega)\, \rho(\omega)\, dx = i!\, \delta_{ij}$$

- $\phi_0 = 1$
- $\phi_1 = \omega$
- $\phi_2 = \omega^2 - 1$
- $\phi_3 = \omega^3 - 3\omega$
- $\phi_4 = \omega^4 - 6\omega^2 + 3$
- ...



Three-Term Recursion

Computation of polynomials

- Stieltjes' three-term recursion relation

$$\begin{aligned} \phi_{-1}(\omega) &\equiv 0 \\ \phi_0(\omega) &\equiv 1 \\ \phi_{n+1}(\omega) &= (A_n\omega + B_n)\,\phi_n(\omega) \;-\; C_n\,\phi_{n-1}(\omega) \qquad n \geq 0 \end{aligned}$$

- A_n, B_n, C_n constants (computed by recursion, depending on weight ρ via inner product)
- satisfied by all orthogonal polynomials
- numerically stable method for computation of polynomials
- other schemes possible, e.g. Gram-Schmidt algorithm

Polynomial Chaos Methods – Checklist

Polynomial chaos expansion

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)$$

What we need to do

- specify type of polynomials $\phi_n(\omega)$ ✓
- **compute coefficients $\hat{f}_n(t)$**
- choose maximum order N
- compute statistical properties of $f(t,\omega)$ based on this approximation

Computation of Coefficients

The pseudo-spectral approach

- exploit orthonormality of underlying basis

$$\sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega) = f(t,\omega)$$

$$< \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega), \phi_m(\omega) >_\rho \; = < f(t,\omega), \phi_m(\omega) >_\rho$$

$$\sum_{n=0}^{N-1} \hat{f}_n(t) \underbrace{< \phi_n(\omega), \phi_m(\omega) >_\rho}_{\delta_{nm}} \; = < f(t,\omega), \phi_m(\omega) >_\rho$$

$$\hat{f}_n(t) = < f(t,\omega), \phi_n(\omega) >_\rho$$

- other approaches: least squares, stochastic Galerkin (next lecture) ...

The Pseudo-spectral Approach

Computation of coefficients

$$\hat{f}_n(t) = < f(t,\omega), \phi_n(\omega) >_\rho = \int_\Omega f(t,\omega)\,\phi_n(\omega)\,\rho(\omega)\,d\omega$$

- possible difficulties:
  - $f(t,\omega)$ computationally expensive
  - $f(t,\omega)$ available only as a black box
- solution: use quadrature
- Gaussian quadrature optimal in one dimensional settings

$$\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$$

The Pseudo-spectral Approach (2)

Nodes and weights

- quadrature rule → nodes, weights $\{x_k, w_k\}_{k=0}^{K-1}$
- chosen w.r.t. the input probability distribution ρ
- the underlying model $f(t,\omega)$ needs be evaluated only once at x_k

Algorithm 1: compute coefficients

Require: N, K, ρ
  generate polynomials ϕ_i
  for $k = 0$ to $K-1$ **do**
    generate x_k, w_k
    evaluate $f(t, x_k)$
  for $n = 0$ to $N-1$ **do**
    compute $\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$

Polynomial Chaos Methods – Checklist

Polynomial chaos expansion and the pseudo-spectral approach

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)$$

$$\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$$

What we need to do

- specify type of polynomials $\phi_n(\omega)$ ✓
- compute coefficients $\hat{f}_n(t)$ ✓
- **choose maximum order** N and number of number of quadrature terms K
- compute statistical properties of $f(t,\omega)$ based on this approximation

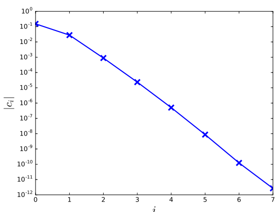
Number of Terms and Nodes

Number of quadrature nodes K

- expensive: evaluate $f(t, x_k)$
- K determines computational effort

Number of expansion terms N

- $\hat{f}_n(t)$ decay exponentially
- few coefficients sufficient
- low computational effort once $f(t, x_k)$ known
- rule of thumb: use $N \approx \frac{1}{2}K$



coefficients of oscillator example

Polynomial Chaos Methods – Checklist

Polynomial chaos expansion and pseudo spectral approach

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)$$

$$\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$$

What we need to do

- specify type of polynomials $\phi_n(\omega)$ ✓
- compute coefficients $\hat{f}_n(t)$ ✓
- choose maximum order N and number of quadrature terms K ✓
- **compute statistical properties of $f(t,\omega)$ based on this approximation**

Expectation and Variance

Expectation

- remember: $\phi_0(\omega) \equiv 1$
- $E[\phi_0(\omega)\,\phi_n(\omega)] = <\phi_0(\omega), \phi_n(\omega)>_\rho$

$$E[f(t,\omega)] \approx E\left[\sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)\right] = \sum_{n=0}^{N-1} \hat{f}_n(t)\,E[1\cdot\phi_n(\omega)] = \sum_{n=0}^{N-1} \hat{f}_n(t)\,\underbrace{E[\phi_0(\omega)\,\phi_n(\omega)]}_{=\delta_{0n}} = \hat{f}_0(t)$$

Expectation and Variance

Variance

$$Var[f(t,\omega)] = E\left[(f(t,\omega) - E[f(t,\omega)])^2\right] \approx E\left[\left(\sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega) - \hat{f}_0(x)\right)^2\right] = E\left[\left(\sum_{n=1}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)\right)^2\right] = \sum_{n=1}^{N-1} \hat{f}_n^2(t)\,\underbrace{E\left[\phi_n(\omega)^2\right]}_{=1} = \sum_{n=1}^{N-1} \hat{f}_n^2(t)$$

- squared sum $\rightarrow$ sum of squares
- mixed terms $= 0$ due to orthogonality: $E[\phi_n(\omega)\,\phi_m(\omega)] = \delta_{nm}$

Polynomial Chaos Methods – Checklist

Polynomial approximation and the pseudo-spectral approach

$$f(t,\omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)$$

$$\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$$

What we need to do

- specify type of polynomials $\phi_n(\omega)$ ✓
- compute coefficients $\hat{f}_n(t)$ ✓
- choose maximum order N and number of quadrature terms K ✓
- compute statistical properties of $f(t,\omega)$ based on this approximation ✓

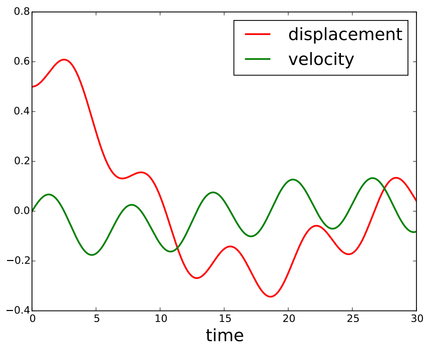
Model Problem – Damped Linear Oscillator

$$\begin{cases} \frac{d^2y}{dt^2}(t) + c\frac{dy}{dt}(t) + ky(t) = f\cos(\omega_O t) \\ y(0) = y_0 \\ \frac{dy}{dt}(0) = y_1 \end{cases}$$

- c – damping coefficient
- k – spring constant
- f – forcing amplitude
- ω_O – frequency
- y_0 – initial position
- y_1 – initial velocity

Damped Linear Oscillator (2)

- $c = 0.100$, $k = 0.035$, $f = 0.100$, $\omega_O = 1.000$, $y_0 = 0.500$, $y_1 = 0.000$
- $t \in [0, 30]$



The Pseudo-spectral Approach – Example

- assume $c \sim \mathcal{U}(0.08, 0.12)$

$$y(T,\omega) \approx \sum_{n=0}^{N-1} \hat{y}_n(T)\phi_n(\omega)$$

$$\hat{y}_n(T) = \sum_{k=0}^{K-1} y(T, x_k)\,\phi_n(x_k)\,w_k$$

- $\hat{y}_n(T)$ – coefficients
- $\phi_n(\omega)$ – Legendre polynomials
- x_k, w_k – Gauss-Legendre quadrature nodes and weights

The Pseudo-spectral Approach – Example (2)

- $T = 15$

Deterministic result

- $y(T) = -1.51e-01$

Stochastic results – Monte Carlo sampling

- 100000 samples $\rightarrow$ $E[y(T,\omega)] \approx -1.53e-01$, $\mathrm{Var}[y(T,\omega)] \approx 7.83e-04$

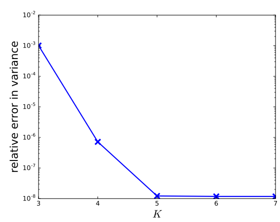
Stochastic results – the pseudo-spectral approach

- 5 nodes $\rightarrow$ $E[y(T,\omega)] \approx -1.52e-01$, $\mathrm{Var}[y(T,\omega)] \approx 7.80e-04$

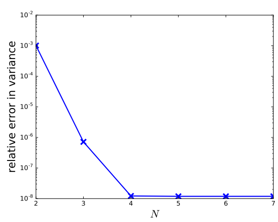
The Pseudo-spectral Approach – Example (3)

Convergence

- sufficient to use small K and $N = \frac{1}{2}K$
- oscillator example: stoch. Galerkin with 10 terms as reference



number of quadrature nodes



number of expansion terms (K=10)

Multivariate Polynomial Chaos Expansion

- random vector $\boldsymbol{\Omega}$ consisting of independent random variables Ω_i, $i = 1, \ldots, d$
- multi-index $\boldsymbol{n} = (n_1, \ldots, n_d) \in \mathbb{N}_0^d$
- multivariate polynomials: product of univariate polynomials

$$\phi_{\boldsymbol{n}}(\boldsymbol{\omega}) = \phi_{n_1}(\omega_1)\cdots\phi_{n_d}(\omega_d),$$
$$< \phi_{\boldsymbol{n}}(\omega), \phi_{\boldsymbol{m}}(\omega) >_w = \delta_{\boldsymbol{nm}}, \quad \delta_{\boldsymbol{nm}} = \delta_{n_1 m_1}\cdots\delta_{n_d m_d}$$

- multivariate polynomial chaos expansion:

$$f(t, \omega) \approx \sum_{\boldsymbol{n}} \hat{f}_{\boldsymbol{n}}(t)\phi_{\boldsymbol{n}}(\boldsymbol{\omega})$$

- use multivariate pseudo-spectral approach to obtain $\hat{f}_{\boldsymbol{n}}$:

$$\hat{f}_{\boldsymbol{n}}(t) = \sum_{k=0}^{K-1} f(t, \boldsymbol{x}_k)\,\phi_{\boldsymbol{n}}(\boldsymbol{x}_k)\,w_k$$

Multivariate Polynomial Chaos Expansion (2)

- multivariate polynomial chaos expansion

$$f(t, \boldsymbol{\omega}) \approx \sum_{\boldsymbol{n}} \hat{f}_{\boldsymbol{n}}(t)\phi_{\boldsymbol{n}}(\boldsymbol{\omega})$$

- $\boldsymbol{n}$ typically chosen such as $n_1 + \ldots n_d \leq N$ for a given N
- in this situation, the number of elements of $\{\boldsymbol{n} \in \mathbb{N}_0^d : n_1 + \ldots n_d \leq N\} = \binom{d+N}{d} := P$
- example
  - if $d = 2, N = 4 \rightarrow P = 15$
  - if $d = 3, N = 4 \rightarrow P = 35$
  - if $d = 4, N = 4 \rightarrow P = 70$
  - if $d = 5, N = 4 \rightarrow P = 126$
  - ...
- computational cost: K, only indirectly related to P

Literature

- Chapter 10 in *R. C. Smith, Uncertainty Quantification – Theory, Implementation, and Applications, SIAM, 2014*
- *D. Xiu, Numerical Methods for Stochastic Computations – A Spectral Method Approach, Princeton Univ. Press, 2010*

Summary

Polynomial chaos methods

- polynomial chaos expansion
  - approximate quantity of interest by polynomial series
  - $f(t, \omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\omega)$
- orthogonal polynomials and polynomial chaos
  - inner product 0 for orthogonal polynomials
  - $< \phi_i(\omega), \phi_j(\omega) >_\rho = \delta_{ij}$
  - choose polynomial type according to input distribution
- the pseudo-spectral approach
  - use quadrature rule to compute coefficients
  - $\hat{f}_n \approx \sum_{k=0}^{K-1} f(t, x_k)\,\phi_n(x_k)\,w_k$
- model problem: damped linear oscillator
- multivariate polynomial chaos expansion