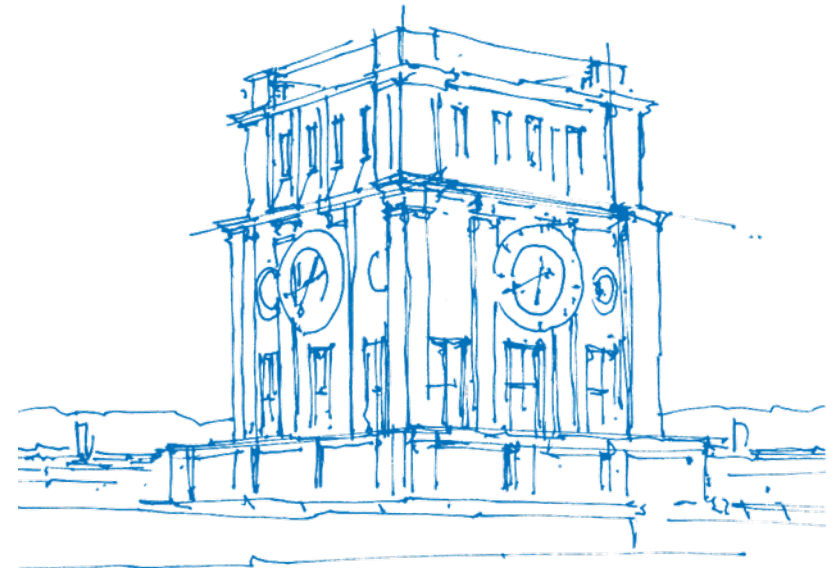


# Algorithms for Uncertainty Quantification

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## Lecture 6:

# Polynomial chaos approximation 1: the pseudo-spectral approach

# Repetition from previous lecture

- Interpolation concepts
  - every continuous function can be interpolated uniquely
  - interpolation with Lagrange cardinal polynomials
  - uniform grid not always a good choice

# Repetition from previous lecture

- Interpolation concepts
  - every continuous function can be interpolated uniquely
  - interpolation with Lagrange cardinal polynomials
  - 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

# Today's lecture

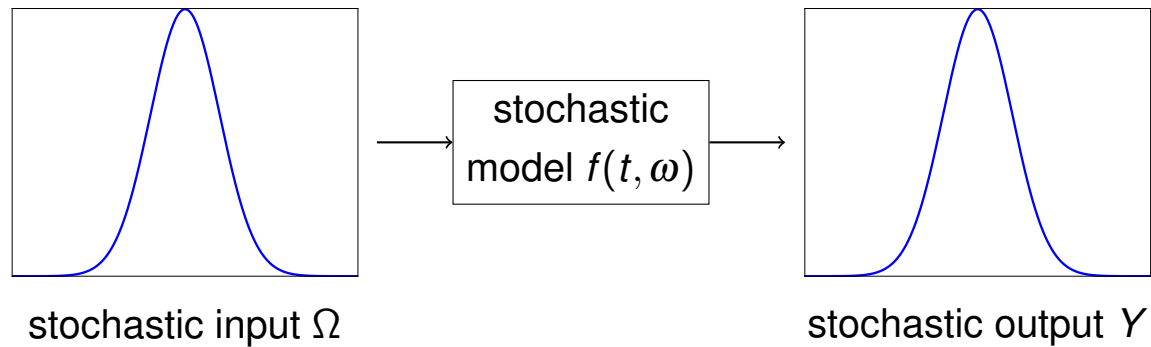
## Topic

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

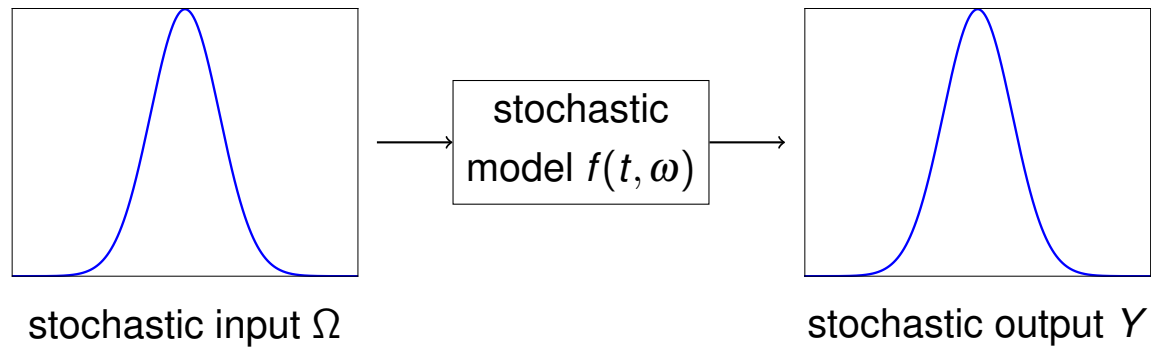
# Forward propagation of uncertainty



## Problem

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

# Forward propagation of uncertainty



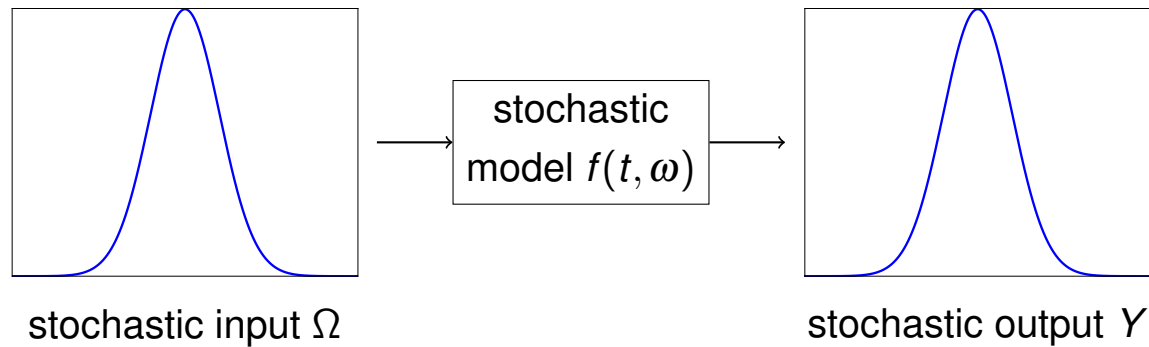
## Problem

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

## What we want

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

# Forward propagation of uncertainty



## 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  $s(t)$

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

# Polynomial chaos methods

## Analogy: Fourier series

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

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

## 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

## Polynomial chaos expansion

- truncate series after  $N$  terms

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

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

# Polynomial chaos methods

## 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

# Polynomial chaos methods

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# Inner product of functions

## Remember: Scalar product of vectors

- vectors in Euclidean space:  $\mathbf{a}$ ,  $\mathbf{b}$

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

## (Weighted) inner product of functions

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

$$\langle p(\omega), q(\omega) \rangle_{\rho} = \int_{\text{supp}(\rho)} p(\omega) q(\omega) \rho(\omega) d\omega$$

# Orthogonality

## Remember: Orthogonal vectors

- scalar product is zero

$$\langle \mathbf{a}, \mathbf{b} \rangle = 0 \iff \mathbf{a} \perp \mathbf{b}$$

## Orthogonal functions

- inner product is zero

$$\langle p(\omega), q(\omega) \rangle_{\rho} = \int_{\text{supp}(\rho)} p(\omega) q(\omega) \rho(\omega) d\omega = 0 \iff p(\omega) \perp q(\omega)$$

# Univariate Orthogonal Polynomials

## Orthogonal basis

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

$$\langle \phi_i(\omega), \phi_j(\omega) \rangle_\rho = \int \phi_i(\omega) \phi_j(\omega) \rho(\omega) d\omega = \gamma_i \delta_{ij}$$

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



# Univariate Orthogonal Polynomials

## Orthogonal basis

$$\langle \phi_i(\omega), \phi_j(\omega) \rangle_\rho = \int \phi_i(\omega) \phi_j(\omega) \rho(\omega) d\omega = \gamma_i \delta_{ij}$$

## 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

$$\langle \phi_i(\omega), \phi_j(\omega) \rangle_\rho = \delta_{ij}$$

# 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?

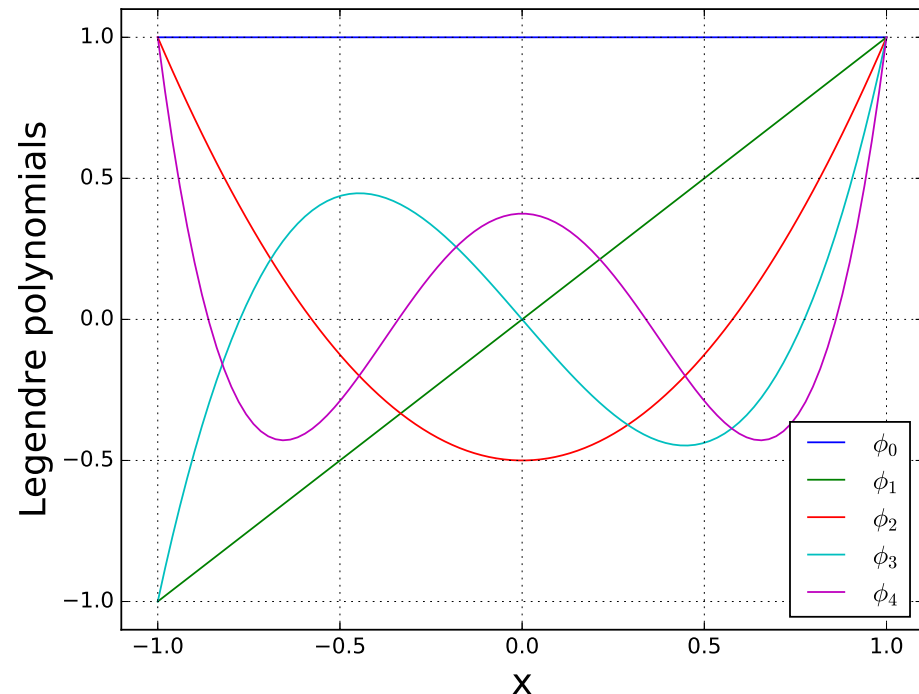
- chosen w.r.t. probability distribution  $\rho(\omega)$
- examples:
  - $\Omega \sim \mathcal{U}(-1, 1) \rightarrow$  Legendre polynomials
  - $\Omega \sim \mathcal{N}(0, 1) \rightarrow$  Hermite polynomials
- the idea can be generalized to all probability distributions

# Legendre Polynomials

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

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

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

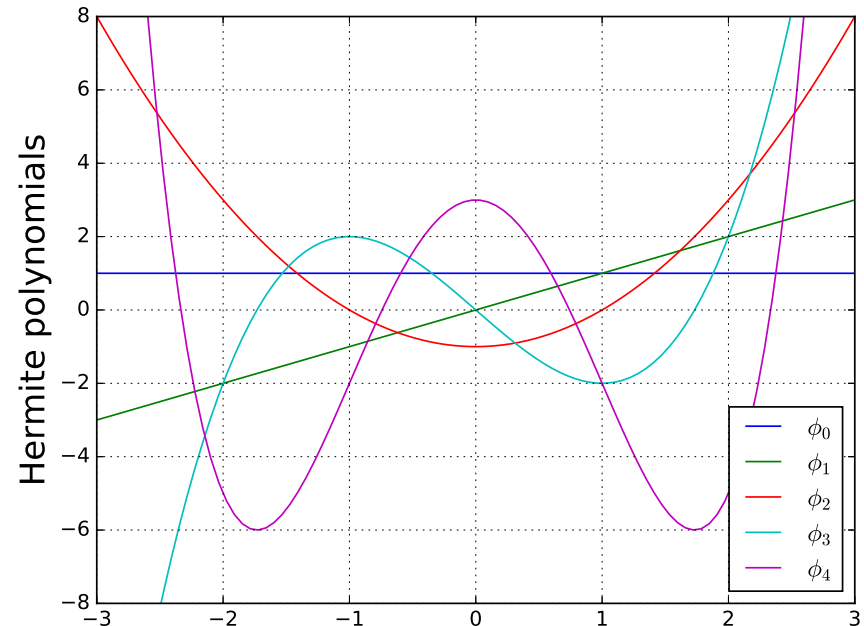


# Hermite Polynomials

- orthogonal w.r.t. integral from  $-\infty$  to  $\infty$
- 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 terms recursion

## Computation of polynomials

- Stieltjes' three-terms recursion relation

$$\phi_{-1}(\omega) \equiv 0$$

$$\phi_0(\omega) \equiv 1$$

$$\phi_{n+1}(\omega) = (A_n\omega + B_n)\phi_n(\omega) - C_n\phi_{n-1}(\omega) \quad n \geq 0$$

- $A_n, B_n, C_n$  constants (computed by recursion, depending on weight  $\rho$  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

## 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

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

$$\left\langle \sum_{n=0}^{N-1} \hat{f}_n(t) \phi_n(\omega), \phi_m(\omega) \right\rangle_{\rho} = \left\langle f(t, \omega), \phi_m(\omega) \right\rangle_{\rho}$$

$$\sum_{n=0}^{N-1} \hat{f}_n(t) \underbrace{\left\langle \phi_n(\omega), \phi_m(\omega) \right\rangle_{\rho}}_{\delta_{nm}} = \left\langle f(t, \omega), \phi_m(\omega) \right\rangle_{\rho}$$

$$\hat{f}_n(t) = \left\langle f(t, \omega), \phi_n(\omega) \right\rangle_{\rho}$$

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

# The pseudo spectral approach

## Computation of coefficients

$$\hat{f}_n(t) = \langle f(t, \omega), \phi_n(\omega) \rangle_\rho = \int_{\Omega} f(t, \omega) \phi_n(\omega) \rho(\omega) d\omega$$

- 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

## Nodes and weights

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

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**Algorithm 1:** compute coefficients

---

**Require:**  $N, K, \rho$

generate polynomials  $\phi_i$

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

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# Polynomial chaos approximation

## 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

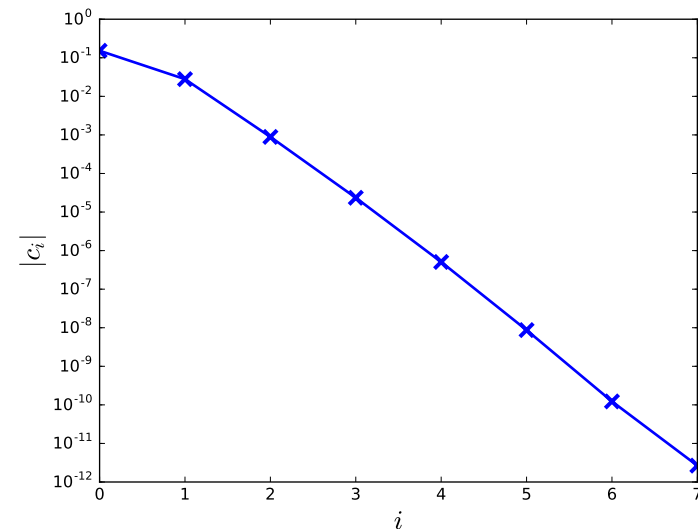
# Number of terms and nodes

## 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

## Polynomial chaos expansion and pseudo spectral approach

$$f(t, \omega) \approx \sum_{n=0}^{N-1} \hat{f}_n(t) \phi_n(\omega)$$
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### 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:  $\phi_0(\omega) \equiv 1$
- $E[\phi_0(\omega) \phi_n(\omega)] = \langle \phi_0(\omega), \phi_n(\omega) \rangle_\rho$

# Expectation and Variance

## Expectation

- remember:  $\phi_0(\omega) \equiv 1$
- $E[\phi_0(\omega) \phi_n(\omega)] = \langle \phi_0(\omega), \phi_n(\omega) \rangle_\rho$

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

# Expectation and Variance

## Expectation

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 &= \sum_{n=0}^{N-1} \hat{f}_n(t) \underbrace{E[\phi_0(\omega) \phi_n(\omega)]}_{=\delta_{0n}} = \hat{f}_0(t)
 \end{aligned}$$

# Expectation and Variance

## Variance

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

- squared sum  $\rightarrow$  sum of squares
- mixed terms are 0 because of the orthogonality  $E[\phi_n(\omega) \phi_m(\omega)] = \delta_{nm}$



# Expectation and Variance

## Variance

$$\begin{aligned}
 \text{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(x) \phi_n(\omega) \right)^2 \right] \\
 &= \sum_{n=1}^{N-1} \hat{f}_n^2(t) \underbrace{E[\phi_n(t)^2]}_{=1} = \sum_{n=1}^{N-1} \hat{f}_n^2(t)
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- squared sum  $\rightarrow$  sum of squares
- mixed terms are 0 because of the orthogonality  $E[\phi_n(\omega) \phi_m(\omega)] = \delta_{nm}$

# Polynomial chaos methods

## 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

$$\begin{cases} \frac{d^2 y}{dt^2}(t) + c \frac{dy}{dt}(t) + ky(t) = f \cos(\omega_0 t) \\ y(0) = y_0 \\ \frac{dy}{dt}(0) = y_1 \end{cases}$$

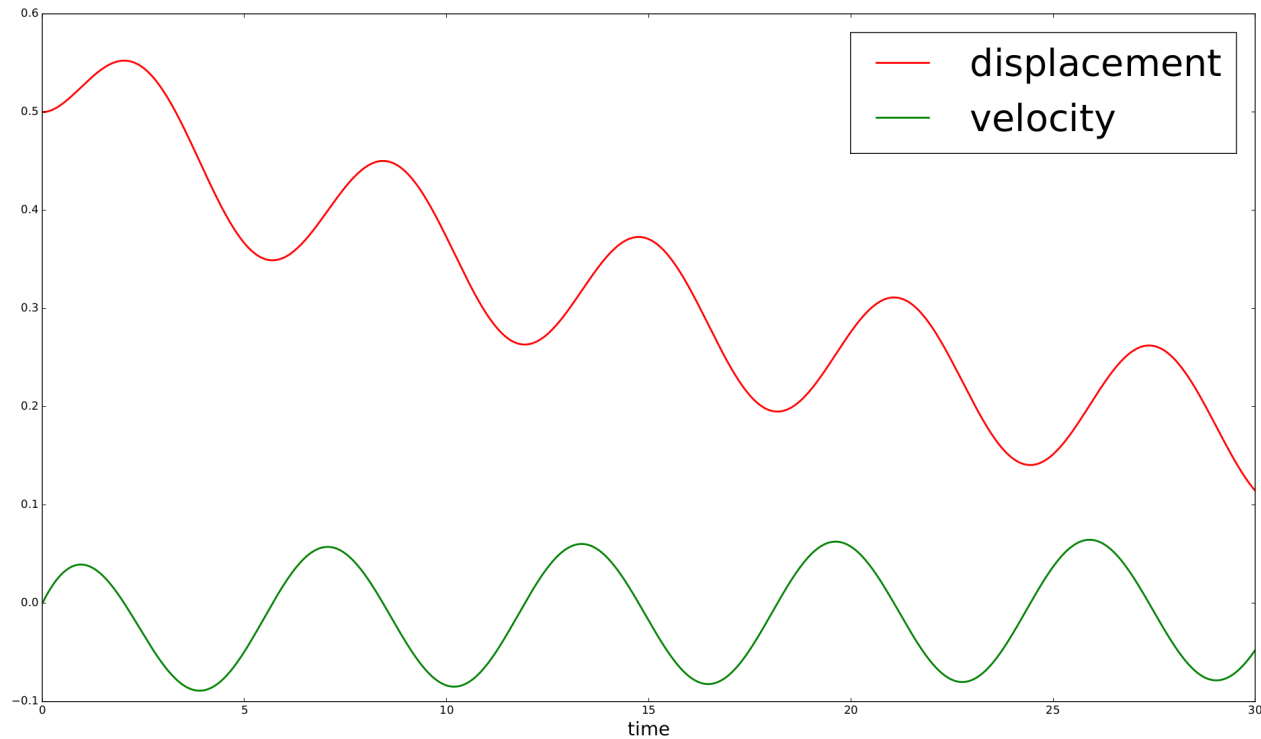
# Model problem – damped linear oscillator

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

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

# Damped linear oscillator

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



# 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

- $T = 15$

## Deterministic result

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

## Stochastic results – Monte Carlo sampling

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

## Stochastic results – the pseudo-spectral approach

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

# The pseudo-spectral approach – example

## Convergence

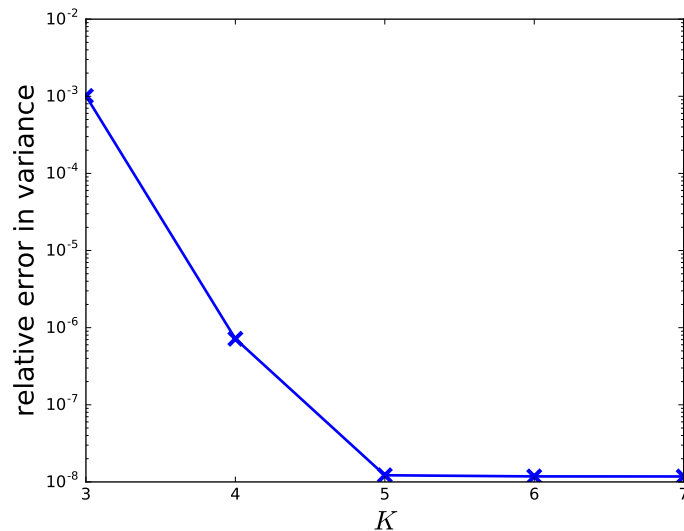
- sufficient to use small  $K$  and  $N = \frac{1}{2}K$
- oscillator example: stoch. Galerkin with 10 terms as reference



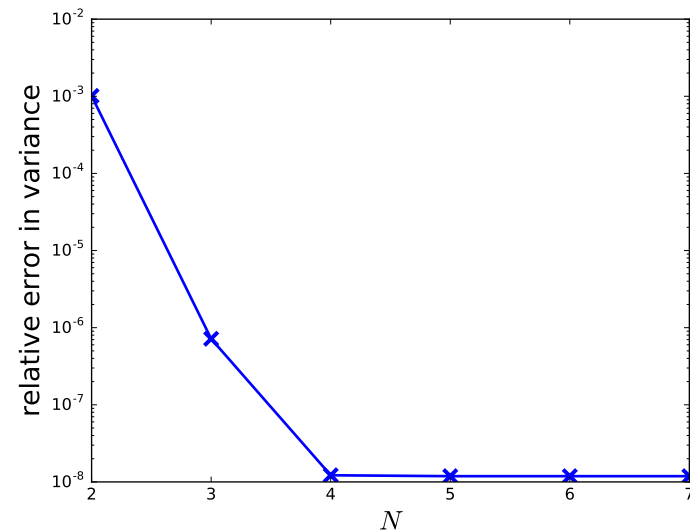
# The pseudo-spectral approach – example

## 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  $\Omega_i, i = 1, \dots, d$
- multi-index  $\mathbf{n} = (n_1, \dots, n_d) \in \mathbb{N}_0^d$
- multivariate polynomials: product of univariate polynomials

$$\begin{aligned}\phi_{\mathbf{n}}(\boldsymbol{\omega}) &= \phi_{n_1}(\omega_1) \cdots \phi_{n_d}(\omega_d), \\ \langle \phi_{\mathbf{n}}(\boldsymbol{\omega}), \phi_{\mathbf{m}}(\boldsymbol{\omega}) \rangle_w &= \delta_{\mathbf{n}\mathbf{m}}, \quad \delta_{\mathbf{n}\mathbf{m}} = \delta_{n_1 m_1} \cdots \delta_{n_d m_d}\end{aligned}$$

- multivariate polynomial chaos expansion

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

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

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

# Multivariate polynomial chaos expansion

- multivariate polynomial chaos expansion

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

- $\mathbf{n}$  typically chosen such as  $n_1 + \dots + n_d \leq N$  for a given  $N$
- in this situation, the number of elements of  $\{\mathbf{n} \in \mathbb{N}_0^d : n_1 + \dots + n_d \leq N\} = \binom{d+N}{d} := P$
- 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  $d = 5, N = 4 \rightarrow P = 126$
  - ...

# Multivariate polynomial chaos expansion

- multivariate polynomial chaos expansion

$$f(t, \omega) \approx \sum_n \hat{f}_n(t) \phi_n(\omega)$$

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  - 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
  - $\langle \phi_i(\omega), \phi_j(\omega) \rangle_\rho = \delta_{ij}$
  - choose polynomial type according to input distribution
- the pseudo-spectral approach
  - use quadrature rule to compute coefficients
  - $\hat{f}_n = \sum_{k=0}^{K-1} f(t, x_k) \phi_n(x_k) w_k$
- model problem: damped linear oscillator
- multivariate polynomial chaos expansion