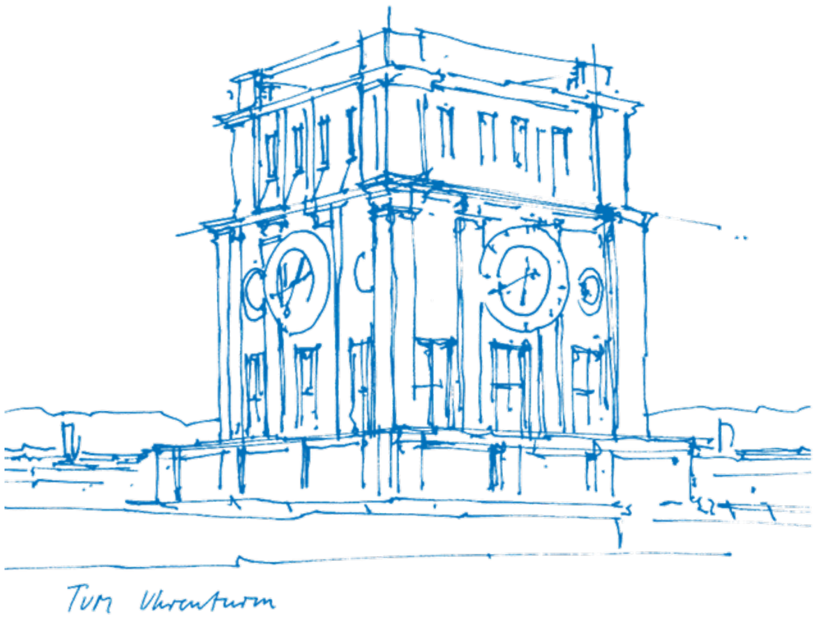
Algorithms for Uncertainty Quantification

Tobias Neckel

Lehrstuhl Informatik V

Summer Semester 2017



Lecture 9:

Sensitivity analysis

Repetition from previous lecture

Sparse grids in Uncertainty Quantification

Repetition from previous lecture

Sparse grids in Uncertainty Quantification

- concept of sparse grids (SG)
  - basic idea: "truncate on diagonal"
  - SG save many grid points but often provide similar accuracy compared to full tensor grids
  - rule of thumb: SG useful for $4 \leq d \leq 20$
- specific SG versions: depend on
  - 1D grid point sequence (w/o nesting, point positions/stretching, boundary points)
  - 1D discrete operator
- focus in this lecture: SG for quadrature in UQ
- adaptivity possible
- example: damped linear oscillator

Today's lecture

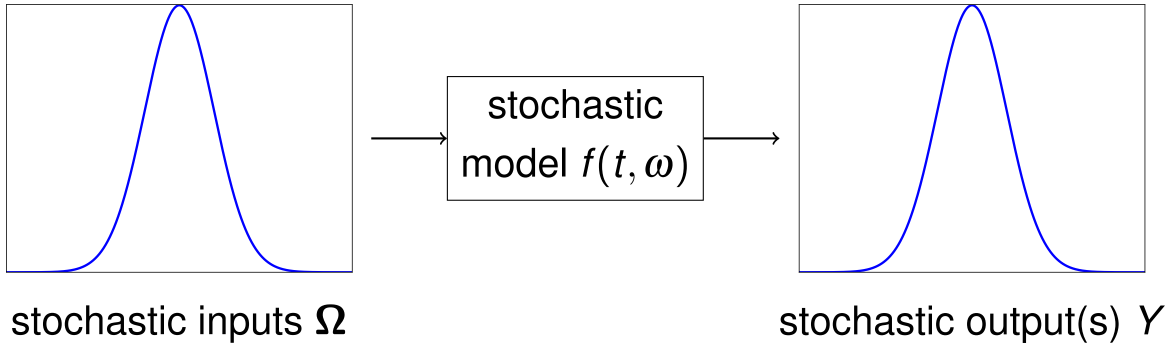
Topic

Global sensitivity analysis (SA) in UQ

Content

- motivation of SA
- categorisation: local vs. global SA
- variance-based global SA
- Sobol' indices and gPC approximation
- example: damped linear oscillator

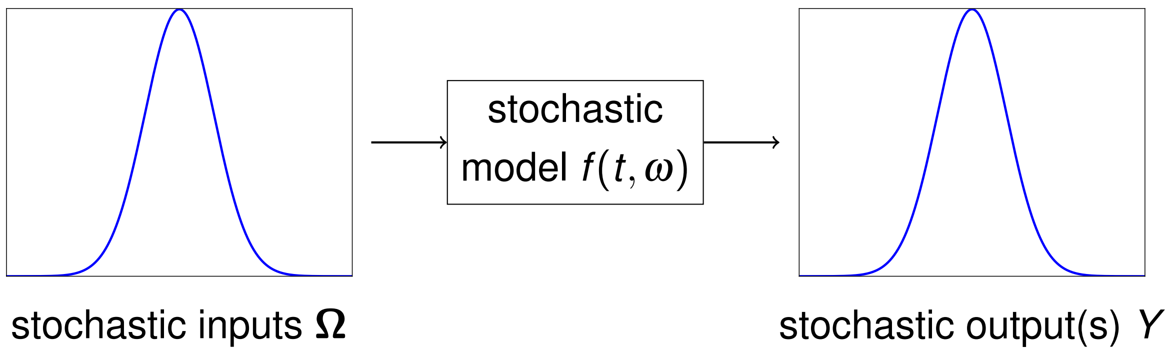
Multi-dimensional forward propagation of uncertainty



Problem

- how sensitive is Y to changes in $\omega \in \boldsymbol{\Omega}$?
- what is the relative contribution of $\omega_i, i = 1,\dots,d$ to the output uncertainty?

Multi-dimensional forward propagation of uncertainty



Problem

- how sensitive is Y to changes in $\omega \in \boldsymbol{\Omega}$?
- what is the relative contribution of $\omega_i, i = 1,\dots,d$ to the output uncertainty?

What we want

- compute “sensitivities” at a very low computational cost: Which uncertain parameters contribute most to the stochasic output Y?
- a reasonable “measure” of the output uncertainty

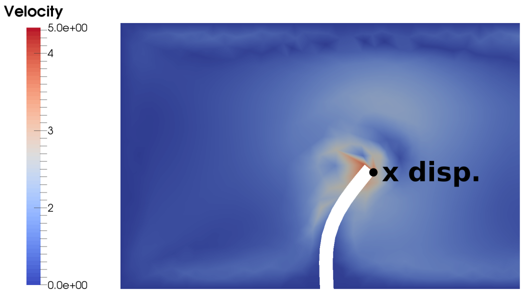
Motivation: Reasons for sensitivity analysis

- ascertain robustness of underlying model w.r.t. to various parameters
  example: safe flight mode for airplanes
- stochastic dimensionality reduction $\Rightarrow$ Can model be simplified by fixing insensitive parameters to deterministic value?
- specify regimes in parameters space that optimally impact responses or their uncertainties
- guide experimental design to determine measurement regimes that have greatest impact on parameter or response sensitivity

Motivation: Example of SA usage/results

Fluid-structure interaction scenario

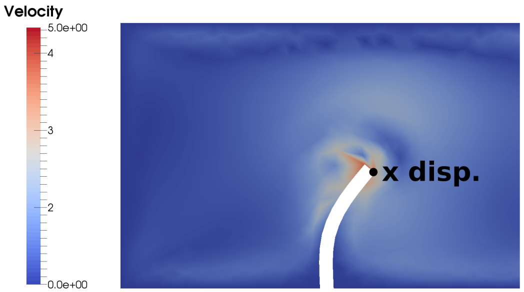
- scenario: bending beam in channel flow
- 5 stochastic parameters:
  fluid density and viscosity (ρ_f and μ), structural density (ρ_s), elastic module (E), Poisson ratio (ν)
- Q.o.I.: displacement of beam tip (at different times)
- total Sobol' indices (at different times t)

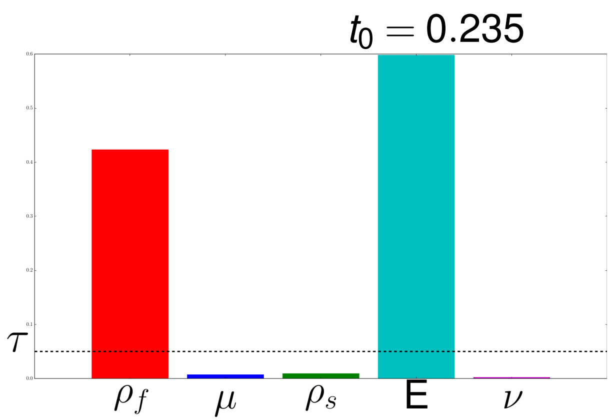


Motivation: Example of SA usage/results

Fluid-structure interaction scenario

- scenario: bending beam in channel flow
- 5 stochastic parameters:
  fluid density and viscosity (ρ_f and μ), structural density (ρ_s), elastic module (E), Poisson ratio (ν)
- Q.o.I.: displacement of beam tip (at different times)
- total Sobol' indices (at different times t)



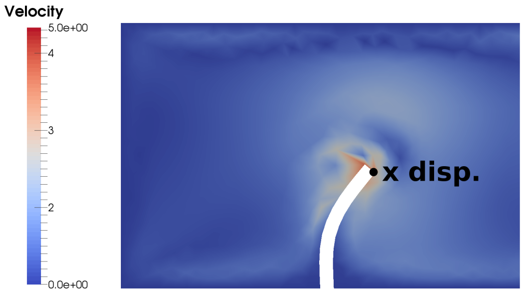


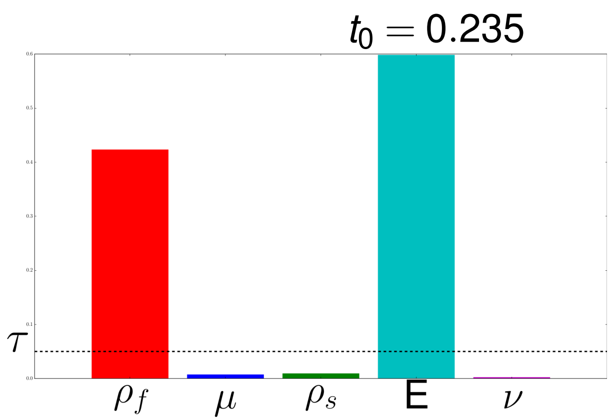
- threshold $\tau \Rightarrow$ dim. reduction $5 \rightarrow 2$
- > 50 h compute time saved

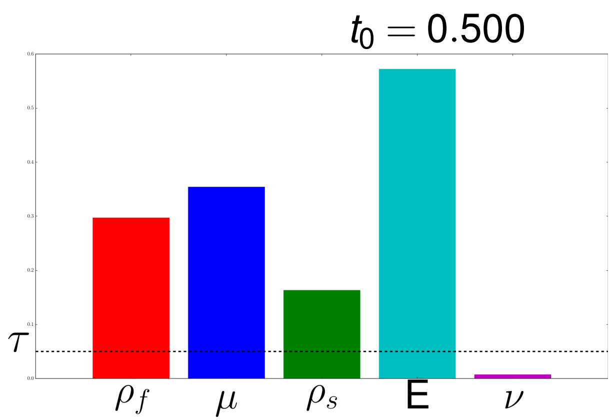
Motivation: Example of SA usage/results

Fluid-structure interaction scenario

- scenario: bending beam in channel flow
- 5 stochastic parameters:
  fluid density and viscosity (ρ_f and μ), structural density (ρ_s), elastic module (E), Poisson ratio (ν)
- Q.o.I.: displacement of beam tip (at different times)
- total Sobol' indices (at different times t)







- threshold $\tau \Rightarrow$ dim. reduction $5 \to 2$
- $>$ 50 h compute time saved

- dim. reduction $5 \to 4$
- $>$ 20 h compute time saved

Remember: multivariate polynomial chaos expansion

- random vector $\boldsymbol{\Omega}$ consisting of independent random variables Ω_i, $i = 1, \ldots, d$
- multiindices $\boldsymbol{n} = (n_1, \ldots, n_d), \boldsymbol{k} = (k_1, \ldots, k_d) \in \mathbb{N}_0^d$
- multivariate polynomials: product of univariate polynomials

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

Remember: multivariate polynomial chaos expansion

- random vector $\boldsymbol{\Omega}$ consisting of independent random variables Ω_i, $i = 1, \ldots, d$
- multiindices $\boldsymbol{n} = (n_1, \ldots, n_d), \boldsymbol{k} = (k_1, \ldots, k_d) \in \mathbb{N}_0^d$
- multivariate polynomials: product of univariate polynomials

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

- multivariate polynomial chaos expansion

$$f(t, \omega) \approx \sum_{|\boldsymbol{n}|_1 = 0}^{N-1} \hat{f}_{\boldsymbol{n}}(t) \phi_{\boldsymbol{n}}(\omega),$$

where $|\boldsymbol{n}|_1 = n_1 + \ldots + n_d$

Remember: multivariate polynomial chaos expansion

- random vector $\boldsymbol{\Omega}$ consisting of independent random variables Ω_i, $i = 1, \ldots, d$
- multiindices $\boldsymbol{n} = (n_1, \ldots, n_d), \boldsymbol{k} = (k_1, \ldots, k_d) \in \mathbb{N}_0^d$
- multivariate polynomials: product of univariate polynomials

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

- multivariate polynomial chaos expansion

$$f(t,\omega) \approx \sum_{|\boldsymbol{n}|_1=0}^{N-1} \hat{f}_{\boldsymbol{n}}(t) \phi_{\boldsymbol{n}}(\omega),$$

where $|\boldsymbol{n}|_1 = n_1 + \ldots + n_d$

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

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

where $|\boldsymbol{k}|_\infty = \max_i |k_i|$

Multivariate polynomial chaos expansion

- multivariate polynomial chaos expansion

$$f(t,\omega) \approx \sum_{|\boldsymbol{n}|_1=0}^{N-1} \hat{f}_{\boldsymbol{n}}(t)\phi_{\boldsymbol{n}}(\omega)$$

- $\boldsymbol{n}$ typically chosen such as $n_1 + \ldots n_d \leq N$ for a given N
- with this setup: $P = \binom{d+N}{d}$ is the number of serialised summation terms
- multivariate pseudo-spectral approach

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

- standard approach: $M = K^d$ where K is number of quadrature points in one direction
- *sparse grid quadrature*: reduce number of quadrature nodes

Local vs. global sensitivity analysis

Local and global sensitivity analysis

Local sensitivity analysis

- aim: asses the “sensitivity” of output w.r.t. inputs perturbed about a nominal value
- generally: using gradients of output w.r.t. inputs
- can be used to “screen” out the “insensitive” uncertain inputs $\Rightarrow$ one input at a time
- tool for stochastic dimensionality reduction before doing the actual forward uncertainty propagation
- however: may be computationally expensive

Local and global sensitivity analysis

Local sensitivity analysis

- aim: asses the "sensitivity" of output w.r.t. inputs perturbed about a nominal value
- generally: using gradients of output w.r.t. inputs
- can be used to "screen" out the "insensitive" uncertain inputs $\Rightarrow$ one input at a time
- tool for stochastic dimensionality reduction before doing the actual forward uncertainty propagation
- however: may be computationally expensive

Global sensitivity analysis

- based on analyzing a suitable "measure" of uncertainty, e.g. the variance
- quantifies the contribution of each input to the output uncertainty
- relies solely on properties of the model and not on experimental data
- in this lecture $\rightarrow$ variance-based global sensitivity analysis

Time for Evaluation!

Variance-based global sensitivity analysis

Variance-based global sensitivity analysis

ANOVA decomposition

- output uncertainty “measure” = output variance
- assume, for simplicity that $\omega \in \boldsymbol{\Omega}$ are i.i.d.
- starting point: ANOVA decomposition

$$f(t,\omega) = f_0(t) + \sum_{i=1}^{d} f_i(t,\omega_i) + \sum_{1\leq i<j\leq d} f_{ij}(t,\omega_i,\omega_j) + \ldots + f_{12..d}(t,\omega),$$

where $f_0(t)$ is the *mean*, $f_i(t,\omega_i)$ are *univariate functions*, $f_{ij}(t,\omega_i,\omega_j)$ are *bivariate functions*, etc.

Variance-based global sensitivity analysis

ANOVA decomposition

- output uncertainty “measure” = output variance
- assume, for simplicity that $\omega \in \mathbf{\Omega}$ are i.i.d.
- starting point: ANOVA decomposition

$$f(t,\omega) = f_0(t) + \sum_{i=1}^{d} f_i(t,\omega_i) + \sum_{1\leq i<j\leq d} f_{ij}(t,\omega_i,\omega_j) + \ldots + f_{12..d}(t,\omega),$$

  where $f_0(t)$ is the *mean*, $f_i(t,\omega_i)$ are *univariate functions*, $f_{ij}(t,\omega_i,\omega_j)$ are *bivariate functions*, etc.
- let $\Gamma^d = \text{supp}(\mathbf{\Omega})$
- make the above expansion unique by imposing orthogonality, i.e.

$$\forall \{i_1,\ldots,i_n\} \neq \{i_1,\ldots,i_m\} \Rightarrow \int_{\Gamma^d} f_{i_1\ldots i_n}(t,\omega_{i_1},\ldots,\omega_{i_n}) f_{i_1\ldots i_m}(t,\omega_{i_1},\ldots,\omega_{i_m}) d\omega = 0$$

Variance-based global sensitivity analysis

ANOVA terms computation

- let $\Gamma^d = \text{supp}(\boldsymbol{\Omega})$

$$
\begin{aligned}
f_i(t, \omega_i) &= \int_{\Gamma^{d-1}} f(t, \omega) d\omega_{\sim i} - f_0(t), \\
f_{ij}(t, \omega_i, \omega_j) &= \int_{\Gamma^{d-2}} f(t, \omega) d\omega_{\sim ij} - f_i(t, \omega_i) - f_j(t, \omega_j) - f_0(t), \\
& \ldots,
\end{aligned}
$$

  where $\int_{\Gamma^{d-1}} (\cdot) d\omega_{\sim i}$ means that the integration is performed over all variables, except the i^{th}
- standard approach to evaluate the above quantities $\Rightarrow$ Monte Carlo sampling

Variance-based global sensitivity analysis

ANOVA terms computation

- let $\Gamma^d = \text{supp}(\mathbf{\Omega})$

$$f_i(t, \omega_i) = \int_{\Gamma^{d-1}} f(t, \omega) d\omega_{\sim i} - f_0(t),$$
$$f_{ij}(t, \omega_i, \omega_j) = \int_{\Gamma^{d-2}} f(t, \omega) d\omega_{\sim ij} - f_i(t, \omega_i) - f_j(t, \omega_j) - f_0(t),$$
$$\ldots,$$

where $\int_{\Gamma^{d-1}} (\cdot) d\omega_{\sim i}$ means that the integration is performed over all variables, except the i^{th}

- standard approach to evaluate the above quantities $\Rightarrow$ Monte Carlo sampling

Total Variance

- denoting $D_{i_1 \ldots i_s}(t) = \int_{\Gamma^s} f^2_{i_1 \ldots i_s}(f, \omega_{i_1} \ldots \omega_{i_s}) d\omega_{i_1} \ldots d\omega_{i_s}$, we have

$$\text{Var}[f(t, \omega)] = \sum_{i=1}^{d} D_i(t) + \sum_{1 \leq i < j \leq d} D_{ij}(t) + \ldots + D_{12..d}(t)$$

Variance-based global sensitivity analysis

Sobol' indices

- remember

$$\mathrm{Var}[f(t,\omega)] = \sum_{i=1}^{d} D_i(t) + \sum_{1\le i<j\le d} D_{ij}(t) + \ldots + D_{12..d}(t)$$

- use the above equation to asses the contribution of each term to $\mathrm{Var}[f(t,\omega)] \Rightarrow$ Sobol' indices
- local/partial Sobol' indices: measure individual contributions OR "interactions" between inputs

$$S_{i_1\ldots i_s}(t) = \frac{D_{i_1\ldots i_s}}{\mathrm{Var}[f(t,\omega)]}$$

- total Sobol' indices: measure individual contributions AND "interactions" between inputs

$$S_i^T(t) = \sum_{i\in\{i_1,\ldots,i_s\}} S_{i_1,\ldots,i_s}(t)$$

Sobol' indices and the polynomial chaos approximation

Computation of Sobol' indices

Standard approach

- remember
- remember ANOVA decomposition ⇒ partial variances ⇒ Sobol' indices
- terms in ANOVA decomposition ⇒ integrals

$$f_{i_1,\ldots i_s}(t,\omega_i,\ldots,\omega_s) = \int_{\Gamma^{d-s}} f(t,\omega)d\omega_{\sim i_1\ldots i_s} - f_{i_1}(t,\omega_{i_1}) - \ldots f_{i_s}(t,\omega_{i_s}) - f_0(t)$$

- therefore, standard approach ⇒ Monte Carlo sampling ⇒ computationally expensive

Computation of Sobol' indices

Standard approach

- remember
- remember ANOVA decomposition $\Rightarrow$ partial variances $\Rightarrow$ Sobol' indices
- terms in ANOVA decomposition $\Rightarrow$ integrals

$$f_{i_1,\ldots i_s}(t,\omega_i,\ldots,\omega_s) = \int_{\Gamma^{d-s}} f(t,\omega)d\omega_{\sim i_1\ldots i_s} - f_{i_1}(t,\omega_{i_1}) - \ldots f_{i_s}(t,\omega_{i_s}) - f_0(t)$$

- therefore, standard approach $\Rightarrow$ Monte Carlo sampling $\Rightarrow$ computationally expensive

Using polynomial chaos expansion

- ANOVA decomposition and the polynomial chaos expansion $\Rightarrow$ orthogonal series/sums
- orthogonality $\Rightarrow$ uniqueness $\Rightarrow$ ANOVA $\Leftrightarrow$ polynomial chaos expansion
- idea: derive Sobol' indices directly from polynomial chaos expansion coefficients

Computation of Sobol' indices (2)

Using polynomial chaos expansion

- remember: multivariate polynomial chaos expansion

$$f(t,\omega) \approx \sum_{|\boldsymbol{n}|_1=0}^{N-1} \hat{f}_{\boldsymbol{n}}(t)\phi_{\boldsymbol{n}}(\omega),$$

  where $|\boldsymbol{n}|_1 = n_1 + \ldots + n_d$

- Sobol' indices for global sensitivity analysis

$$S_i(t) = \frac{D_i(t)}{\mathrm{Var}[f(t,\omega)]}, \quad D_i(t) = \sum_{\boldsymbol{n}\in A_i} \hat{f}^2_{\boldsymbol{n}}(t) \qquad (1)$$

Computation of Sobol' indices (2)

Using polynomial chaos expansion

- remember: multivariate polynomial chaos expansion

$$f(t,\omega) \approx \sum_{|\boldsymbol{n}|_1=0}^{N-1} \hat{f}_{\boldsymbol{n}}(t)\phi_{\boldsymbol{n}}(\omega),$$

  where $|\boldsymbol{n}|_1 = n_1 + \ldots + n_d$
- Sobol' indices for global sensitivity analysis

$$S_i(t) = \frac{D_i(t)}{\mathrm{Var}[f(t,\omega)]}, \quad D_i(t) = \sum_{\boldsymbol{n}\in A_i} \hat{f}^2_{\boldsymbol{n}}(t) \tag{1}$$

- for first order indices

$$A_i = \{\boldsymbol{n} \in \mathbb{N}^d : \forall j \neq i, \boldsymbol{n}_j = 0\}$$

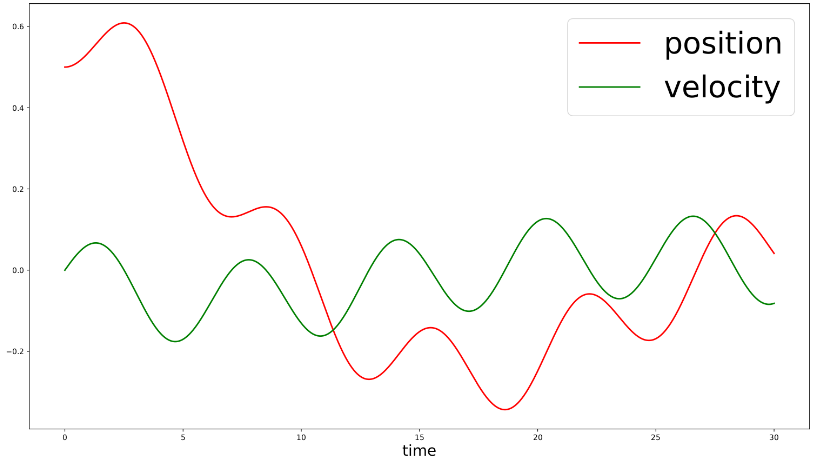
- for higher order contributions

$$A_i = \{\boldsymbol{n} \in \mathbb{N}^d : \boldsymbol{n}_i > 0\}$$

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: sensitivity analysis

Stochastic setup

- $t \in [0, 30]$
- $T = 15$
- assume
  - $c = 0.10$
  - $k \sim \mathcal{U}(0.03, 0.04)$
  - $f \sim \mathcal{U}(0.08, 0.12)$
  - $\omega_O \sim \mathcal{U}(0.8, 1.2)$
  - $y_0 \sim \mathcal{U}(0.45, 0.55)$
  - $y_1 \sim \mathcal{U}(-0.05, 0.05)$

Damped linear oscillator: sensitivity analysis

Stochastic setup

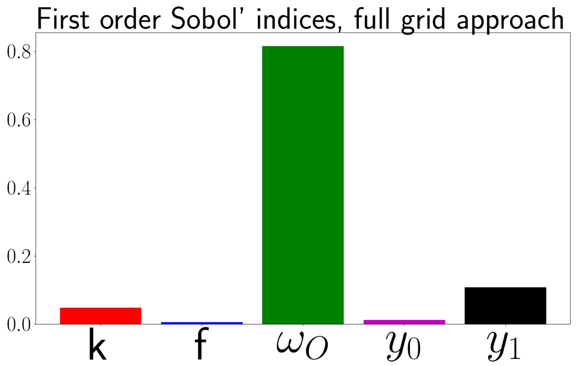
- $t \in [0,30]$
- $T = 15$
- assume
  - $c = 0.10$
  - $k \sim \mathscr{U}(0.03, 0.04)$
  - $f \sim \mathscr{U}(0.08, 0.12)$
  - $\omega_O \sim \mathscr{U}(0.8, 1.2)$
  - $y_0 \sim \mathscr{U}(0.45, 0.55)$
  - $y_1 \sim \mathscr{U}(-0.05, 0.05)$

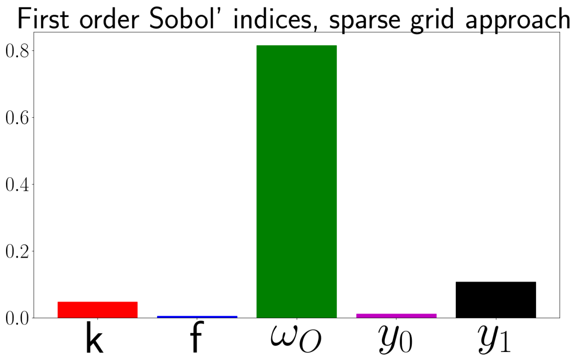
Uncertainty propagation setup

- polynomial chaos expansion + the pseudo-spectral approach
- full Gaussian grid (7776 nodes) vs. sparse Gaussian grid (2203 nodes)

Damped linear oscillator: sensitivity analysis

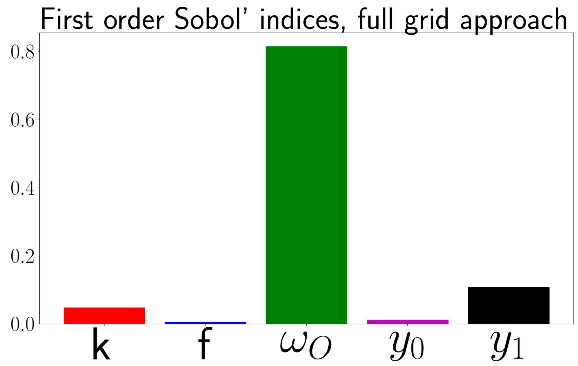
First order indices: full vs. sparse grid

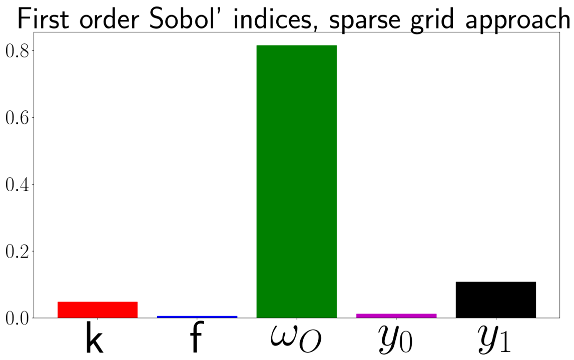




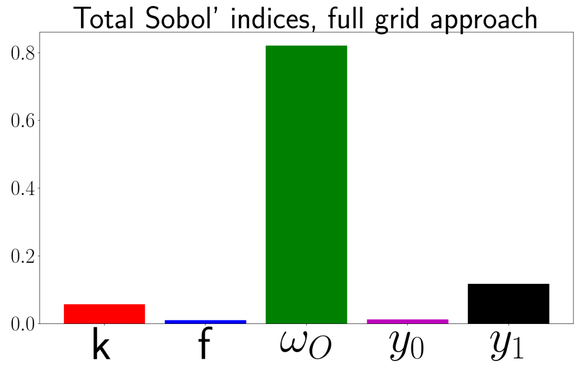
Damped linear oscillator: sensitivity analysis

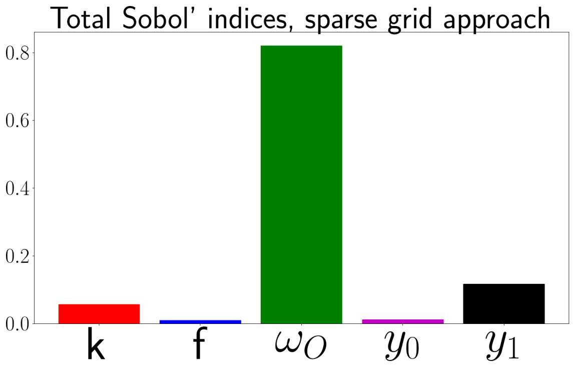
First order indices: full vs. sparse grid





Total indices: full vs. sparse grid





Literature

- Local sensitivity analysis: Chapter 14 in *R. C. Smith, Uncertainty Quantification – Theory, Implementation, and Applications, SIAM, 2014*
- Global sensitivity analysis: Chapter 15 in *R. C. Smith, Uncertainty Quantification – Theory, Implementation, and Applications, SIAM, 2014*

Summary

Sensitivity analysis

- categorisation: local vs. global SA
- global SA can provide useful insight
- variance-based global SA & Sobol' indices (for gPC)
- example: damped linear oscillator