

Surrogate models for uncertain dynamical systems: applications to earthquake engineering

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Chair of Risk, Safety and Uncertainty Quantification

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Research topics

- **•** Uncertainty modelling for engineering systems
- Structural reliability analysis
- Surrogate models (polynomial chaos expansions, Kriging, support vector machines)
- Bayesian model calibration and stochastic inverse problems
- Global sensitivity analysis
-

• Reliability-based design optimization **<http://www.rsuq.ethz.ch>**

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Global framework for uncertainty quantification

B. Sudret, Uncertainty propagation and sensitivity analysis in mechanical models – contributions to structural reliability and stochastic spectral

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Surrogate models for uncertainty quantification

A surrogate model \tilde{M} is an approximation of the original computational model M with the following features:

- It is built from a limited set of runs of the original model M called the experimental design $\mathcal{X} = \left\{ x^{(i)}, \, i = 1, \, \ldots \, , n \right\}$
- It assumes some regularity of the model M and some general functional shape

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Ingredients for building a surrogate model

- Select an experimental design X that covers at best the domain of input parameters: Latin hypercube sampling (LHS), low-discrepancy sequences
- Run the computational model M onto $\mathcal X$ exactly as in Monte Carlo simulation

• Smartly post-process the data $\{X, M(X)\}\$ through a learning algorithm

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Advantages of surrogate models

Usage

$$
\mathcal{M}(x) \approx \tilde{\mathcal{M}}(x)
$$

hours per run seconds for 10⁶ runs

Advantages

- Non-intrusive methods: based on runs of the computational model, exactly as in Monte Carlo simulation
- Construction suited to high performance computing: "embarrassingly parallel"

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- Need for rigorous validation
- Communication: advanced mathematical background

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Efficiency: 2-3 orders of magnitude less runs compared to Monte Carlo

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Polynomial chaos expansions in a nutshell

Ghanem & Spanos (1991); Xiu & Karniadakis (2002); Soize & Ghanem (2004); Lemaˆıtre & Knio (2010)

- Consider the input random vector X (dim $X = M$) with given probability density function (PDF) $f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^M f_{X_i}(x_i)$
- Assuming that the random output $Y = \mathcal{M}(X)$ has finite variance, it can be cast as the following polynomial chaos expansion:

$$
Y = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})
$$

where :

- \mathbb{F} $\Psi_{\alpha}(X)$: basis functions
- \bullet *y*_{α} : coefficients to be computed (coordinates)
- **•** The PCE basis $\left\{\Psi_{\alpha}(X), \alpha \in \mathbb{N}^{M}\right\}$ is made of multivariate orthonormal polynomials

Computing the coefficients by least-square minimization

Isukapalli (1999); Berveiller, Sudret & Lemaire (2006)

Principle

The exact (infinite) series expansion is considered as the sum of a truncated series and a residual:

$$
Y = \mathcal{M}(\boldsymbol{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\boldsymbol{X}) + \varepsilon_{P} \equiv \mathbf{Y}^{\mathsf{T}} \Psi(\boldsymbol{X}) + \varepsilon_{P}(\boldsymbol{X})
$$

where : $\mathbf{Y} = \{y_{\alpha}, \alpha \in \mathcal{A}\} \equiv \{y_0, \ldots, y_{P-1}\}$ (*P* unknown coef.)

$$
\boldsymbol{\Psi}(\boldsymbol{x}) = \left\{\Psi_0(\boldsymbol{x}),\,\ldots\,,\Psi_{P-1}(\boldsymbol{x})\right\}
$$

The unknown coefficients are estimated by minimizing the mean square

$$
\hat{\mathbf{Y}} = \arg\min \mathbb{E}\left[\left(\mathbf{Y}^{\mathsf{T}}\mathbf{\Psi}(\boldsymbol{X}) - \mathcal{M}(\boldsymbol{X})\right)^2\right]
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Least-square minimization

The unknown coefficients are estimated by minimizing the mean square residual error:

$$
\left[\hat{\mathbf{Y}} = \arg\min \mathbb{E}\left[\left(\mathbf{Y}^{\mathsf{T}}\mathbf{\Psi}(\boldsymbol{X}) - \mathcal{M}(\boldsymbol{X})\right)^2\right]\right]
$$

An estimate of the mean square error (sample average) is minimized:

$$
\hat{\mathbf{Y}} = \arg \min_{\mathbf{Y} \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^n (\mathbf{Y}^{\mathsf{T}} \boldsymbol{\Psi}(\boldsymbol{x}^{(i)}) - \mathcal{M}(\boldsymbol{x}^{(i)}))^{2}
$$

Procedure

- **•** Select a truncation scheme, e.g. $\mathcal{A}^{M,p} = \{ \alpha \in \mathbb{N}^M : |\alpha|_1 \leq p \}$
- Select an experimental design and evaluate the model response

$$
\mathsf{M} = \left\{\mathcal{M}(\boldsymbol{x}^{(1)}), \, \ldots \, , \mathcal{M}(\boldsymbol{x}^{(n)})\right\}^{\mathsf{T}}
$$

• Compute the experimental matrix

$$
\mathbf{A}_{ij} = \Psi_j\left(x^{(i)}\right) \quad i = 1, \ldots, n \; ; \; j = 0, \ldots, P - 1
$$

• Solve the resulting linear system

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\hat{\mathbf{Y}} = (\mathbf{A}^{\mathsf{T}} \mathbf{A})^{-1} \mathbf{A}^{\mathsf{T}} \mathbf{M}
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Simple is beautiful !

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Error estimators

• In least-squares analysis, the generalization error is defined as:

$$
E_{gen} = \mathbb{E}\left[\left(\mathcal{M}(X) - \mathcal{M}^{PC}(X)\right)^2\right] \qquad \mathcal{M}^{PC}(X) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(X)
$$

• The empirical error based on the experimental design $\mathcal X$ is a poor estimator in case of overfitting

$$
E_{emp} = \frac{1}{n} \sum_{i=1}^{n} (\mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{PC}(\boldsymbol{x}^{(i)}))^{2}
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$$

Leave-one-out cross validation

• From statistical learning theory, model validation shall be carried out using independent data

$$
E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{\mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{PC}(\boldsymbol{x}^{(i)})}{1 - h_i} \right)^2
$$

where h_i is the i -th diagonal term of matrix $\mathbf{A} (\mathbf{A} ^\mathsf{T} \mathbf{A})^{-1} \mathbf{A} ^\mathsf{T}$

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Why brute-force PCE fails in dynamics?

Non-linear SDOF Duffing oscillator

$$
\ddot{x}(t) + 2\omega\zeta\,\dot{x}(t) + \omega^2\,\left(x(t) + \varepsilon\,x^3(t)\right) = 0
$$

Initial conditions: $x(0) = 1$, $\dot{x}(0) = 0$

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Time-frozen PCE

Why time-frozen PCE does not work?

- The map $\xi \mapsto \mathcal{M}(\xi, t)$ becomes increasingly non linear with time
- The time-frozen distribution of the output at time t_0 becomes more complex (*e.g.*) multimodal)
- Expansions of higher degree would be required to keep sufficient accuracy with time
- For a fixed experimental design, the LOO error blows up

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Some literature

- Multi-elements PCEs: decomposition of the random space into non-overlapping sub-elements Wan & Karniadakis, 2005
- Constant phase interpolation: responses interpolated in the phase space

Witteveen & Bijl, 2008

- Asynchronous time integration: intrusive transformed time variable introduced to reduce variability and the Maître et al., 2010
- Time-dependent PCEs: new random variables added on-the-fly G Gerritsma et al., 2010
- PC flow map composition: long-term response obtained by composing intermediate PCE-based flow maps **Luchtenburg** et al., 2014
- PC-NARX: future state determined by current and past states

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Nonlinear AutoRegressive with eXogenous input model

NARX model **Billings, 2013**

Based on a time-dependent input excitation $x(t)$ and corresponding system response $y(t)$, the dynamics is captured through:

$$
y(t) = \mathcal{F}(x(t), \ldots, x(t - n_x), y(t - 1), \ldots, y(t - n_y)) + \varepsilon_t
$$

where:

- $\mathbf{z}(t) = (x(t), \ldots, x(t n_x), y(t 1), \ldots, y(t n_y))^{\mathsf{T}}$ is the vector of current and past values
- *n^x* and *n^y* denote the maximum input and output time lags
- $\varepsilon_t \sim \mathcal{N}(0, \sigma_{\varepsilon}^2(t))$ is the residual error
- $\mathcal{F}(\cdot)$ is a functional of NARX terms, usually linear-in-parameters:

$$
y(t) = \sum_{i=1}^{n_g} \vartheta_i g_i(\boldsymbol{z}(t)) + \varepsilon_t
$$

 $PC\text{-}NARX \text{ model}$ spiridonakos et al. , 2015a,2015b

Computational model with uncertainties

$$
y(t,\boldsymbol{\xi}_x,\boldsymbol{\xi}_s) \stackrel{\text{def}}{=} \mathcal{M}(x(t,\boldsymbol{\xi}_x),\boldsymbol{\xi}_s)
$$

- \bullet *ξ_x* : uncertainty in the input excitation
- *ξ^s* : uncertainty in the system

$$
y(t,\xi) = \sum_{i=1}^{n_g} \vartheta_i(\xi) g_i(z(t)) + \varepsilon_g(t,\xi) \qquad \xi = (\xi_x, \xi_s)
$$

The NARX stochastic coefficients $\vartheta_i(\xi)$ are represented by PCEs:

$$
\vartheta_i(\xi) = \sum_{\alpha \in \mathcal{A}_i} \vartheta_{i,\alpha} \psi_{\alpha}(\xi)
$$

PC-NARX model Spiridonakos et al. , 2015a,2015b

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PC-NARX expansion

$$
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PC-NARX model

$$
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$$

Interpretation

- PC-NARX is a NARX model in which each (random) coefficient is expanded as a PCE
- Compared to time-frozen PCE, a specific dynamics of the random coefficients is imposed
- Similar to flow map composition since the response at current instant is used to predict the response at future instants

Experimental design

Data

- *N* realizations of the input excitation, cast as $(x_k[1], \ldots, x_k[T])^{\mathsf{T}}$, $k = 1, \ldots, N$ (*T* time instants)
- The corresponding system response computed by a simulator, cast as $(y_k[1], \ldots, y_k[T])$

Example: quarter car model

Deterministic NARX calibration

For a particular realization *ξ^k*

• Select NARX model (candidate terms):

$$
\mathbf{z}(t) = (x(t), \dots, x(t - n_x), y(t - 1), \dots, y(t - n_y))^\mathsf{T}
$$

$$
\phi(t) = \{g_i(\mathbf{z}(t)), i = 1, \dots, n_y\}^\mathsf{T}
$$

- Use least angle regression (LARS) to select the best explanatory subset of terms Efron et al., 2004
- Compute the coefficients ϑ_k by ordinary least-squares

Prediction error (of model #*k* on trajectory *l*)

$$
\varepsilon_l^{\#k} = \frac{\sum\limits_{t=1}^T (y(t,\xi_l) - \hat{y}^{\#k}(t,\xi_l))^2}{\sum\limits_{t=1}^T (y(t,\xi_l) - \bar{y}(t,\xi_l))^2}
$$

Common NARX basis

Premise

To expand the NARX coefficients onto a PC basis, it is necessary to have a common NARX model for all trajectories

Procedure

- Select *K* ≤ *N* trajectories ("NARX learning set"), e.g. with the strongest non linear behaviour (peak displacement, velocities, etc.)
- Determine the sparse deterministic NARX models for realizations $k = 1, \ldots, K$, which leads to $P \leq K$ different possible models called $#1, \ldots,#P$
- Compute the NARX coefficients of the N trajectories, for each model $\#p$, and evaluate an average error:

$$
\varepsilon_p = \frac{1}{N} \sum_{k=1}^{N} \varepsilon_k^{\# p}
$$

• Select the final best NARX model that minimizes ε_p

PCE of the NARX coefficients

PCE calibration

• Once a common NARX basis has been found, *N* realizations of the NARX coefficients are available:

$$
\mathcal{ED} = \{ \vartheta_{i,k}, i = 1, \ldots, n_g; k = 1, \ldots, N \}
$$

 n_q different sparse PC expansions are built from this experimental design, using least-angle regression (LAR) Blatman & Sudret, 2011

$$
\vartheta_i(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_i} \vartheta_{i,\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})
$$

PC-NARX prediction

- For a new realization of the input parameters ξ_0 , the NARX coefficients are first evaluated from PCFs
- Then they are plugged into the NARX model

Bouc-Wen model

Governing equations **Kafali & Grigoriu (2007)**, Spiridonakos & Chatzi (2015)

$$
\ddot{y}(t) + 2\zeta \omega \dot{y}(t) + \omega^2 (\rho y(t) + (1 - \rho) z(t)) = -x(t),
$$

\n
$$
\dot{z}(t) = \gamma \dot{y}(t) - \alpha |\dot{y}(t)| |z(t)|^{n-1} z(t) - \beta \dot{y}(t) |z(t)|^n,
$$

Excitation

 $x(t)$ is generated by a probabilistic ground motion model Rezaeian & Der Kiureghian (2010) $x(t) = q(t, \alpha) \sum s_i(t, \lambda(t_i)) U_i$

Bouc-Wen model: prediction

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Introduction to fragility curves

- Earthquake engineering aims at assessing the performance of structures and infrastructures w.r.t recorded or potential quakes
- Due to uncertainties in the localization, magnitude, structural behaviour and resistance, etc. probabilistic approaches are commonly used

Fragility curves

For a given performance criterion $q \leq q_{adm}$, the fragility curve represents the conditional probability of failure given an intensity measure *IM*:

$$
Frag(IM; g_{adm}) = \mathbb{P}\left(g \geq g_{adm} \,|\, IM\right)
$$

Example

- $g = \max_{k} \max_{t_i \in [0,T]} |\delta_{t_i}^k|$ (*k*-th interstorey drift)
- *IM*: peak ground acceleration (PGA), pseudo-spectral acceleration (PSa), cumulative absolute velocity (CAV), etc.

Fragility curves

Classical approach

- Select a set of ground motions (recorded / synthetic)
- Compute the transient structural response (finite element analysis)
- Assume a parametric shape for the fragility curve, e.g. a lognormal shape:

$$
\mathsf{Frag}(IM; \delta_o) = \mathbb{P}\left(\Delta \ge \delta_o \,|\, IM\right) = \Phi\left(\frac{\log IM - \alpha}{\beta}\right)
$$

• Fit the parameters (α, β) form data

Limitations

- Predefined shape of the curve
- Subject to epistemic uncertainties when the number of ground motions is small

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$$

• Fit the parameters (α, β) form data

New proposal

- Use non parametric statistics for the fragility curves
- Use surrogate models of the transient analysis based on polynomial chaos expansions

Parametric methods

Linear regression (LR) Ellingwood (2001)

• Probabilistic demand model:

$$
\log \Delta = A \, \log IM + B + \zeta \, Z \qquad Z \sim \mathcal{N}(0,1)
$$

- *A* and *B* determined by ordinary least squares estimation in a log-log scale
- Results in a lognormal-like fragility curve:

$$
\begin{aligned} \widehat{\text{Frag}}(IM; \, \delta_o) &= \mathbb{P} \left[\log \Delta \ge \log \delta_o \right] = 1 - \mathbb{P} \left[\log \Delta \le \log \delta_o \right] \\ &= \Phi \left(\frac{\log IM - \left(\log \delta_o - B \right) / A}{\zeta / A} \right). \end{aligned}
$$

• Lognormal shape:

$$
\widehat{\text{Frag}}(IM; \delta_o) = \Phi\left(\frac{\log IM - \log \alpha}{\beta}\right)
$$

• Estimation of *α* and *β* by maximum likelihood for each *δo*:

$$
\mathcal{L}\left(\alpha, \beta, \{IM_i\}_{i=1}^N\right) = \prod_{IM_i: \Delta_i \ge \delta_o} \left[\widehat{\text{Frag}}(IM_i; \delta_o)\right] \prod_{IM_i: \Delta_i < \delta_o} \left[1 - \widehat{\text{Frag}}(IM_i; \delta_o)\right]
$$

B. Sudret (Chair of Risk, Safety & UQ) [Surrogates for dynamical systems](#page-0-0) BRGM – January 16th, 2018 28 /

Parametric methods

Linear regression (LR) Ellingwood (2001)

• Probabilistic demand model:

$$
\log \Delta = A \, \log IM + B + \zeta \, Z \qquad Z \sim \mathcal{N}(0,1)
$$

- *A* and *B* determined by ordinary least squares estimation in a log-log scale
- Results in a lognormal-like fragility curve:

$$
\begin{aligned} \widehat{\text{Frag}}(IM; \, \delta_o) &= \mathbb{P} \left[\log \Delta \ge \log \delta_o \right] = 1 - \mathbb{P} \left[\log \Delta \le \log \delta_o \right] \\ &= \Phi \left(\frac{\log IM - \left(\log \delta_o - B \right) / A}{\zeta / A} \right). \end{aligned}
$$

Maximum likelihood estimation (ML) Shinozuka et al. (2000)

• Lognormal shape:

$$
\widehat{\mathsf{Frag}}(IM;\,\delta_o) = \Phi\left(\frac{\log IM - \log \alpha}{\beta}\right)
$$

• Estimation of *α* and *β* by maximum likelihood for each *δo*:

$$
\mathcal{L}\left(\alpha,\,\beta,\,\left\{IM_i\right\}_{i=1}^N\right)=\prod_{\substack{IM_i:\,\Delta_i\geq\delta_o\\ \text{Surrogates for dynamical systems}}} \left[\widehat{\text{Frag}}(IM_i;\,\delta_o)\right]\prod_{\substack{IM_i:\,\Delta_i<\delta_o\\ \text{BRGM - January 16th, 2018}}} \left[1-\widehat{\text{Frag}}(IM_i;\,\delta_o)\right]
$$

Non parametric methods

Binned Monte Carlo estimate Mai, Konakli & Sudret, Frontiers Struct. Civ. Eng., (2017)

■ Suppose N_s analyses are available for $IM = IM_o$, with N_f such that $\Delta > \delta_o$. The fragility curve in this point could be estimated by Monte Carlo simulation:

$$
\widehat{\text{Frag}}(IM_o) = \frac{N_f(IM_o)}{N_s(IM_o)}
$$

• From the data cloud, a bin centered on IM_o is considered, and points within the beam are "projected" onto the vertical line $IM = IM_o$ by linearization $\widetilde{\Delta_{j}}(IM_{o}) = \Delta_{j}\frac{IM_{o}}{IM_{j}}$ $\frac{1+10}{IM_j}$.

Kernel density estimation

Fragility curves as a conditional CCDF Mai et al., Frontiers Struct. Civ. Eng., (2017)

$$
\text{Frag}(a; \delta_o) = \mathbb{P}\left(\Delta \ge \delta_o | IM = a\right) = \int_{\delta_o}^{+\infty} f_{\Delta}(\delta | IM = a) d\delta
$$

where:

$$
f_{\Delta}(\delta | IM = a) = \frac{f_{\Delta,IM}(\delta, a)}{f_{IM}(a)}
$$

• The joint- and the marginal PDFs are estimated by:

$$
\hat{f}_X(x) = \frac{1}{Nh} \sum_{i=1}^N K\left(\frac{x - x_i}{h}\right) \qquad \hat{f}_X(x) = \frac{1}{N |H|^{1/2}} \sum_{i=1}^N K\left(H^{-1/2}(x - x_i)\right)
$$

NB: Use of a constant bandwidth in the logarithmic scale

Kernel density estimation

Fragility curves as a conditional CCDF Mai et al., Frontiers Struct. Civ. Eng., (2017)

$$
\text{Frag}(a; \delta_o) = \mathbb{P}\left(\Delta \ge \delta_o | IM = a\right) = \int_{\delta_o}^{+\infty} f_{\Delta}(\delta | IM = a) d\delta
$$

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Kernel density estimation

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NB: Use of a constant bandwidth in the logarithmic scale

Mai, C., Polynomial chaos expansions for uncertain dynamical systems – Applications in earthquake engineering, PhD Thesis, ETH

Zurich, 2016

Outline

1 [Introduction](#page-4-0)

2 [Polynomial chaos expansions](#page-17-0)

3 [PC-NARX expansions](#page-31-0)

4 [Fragility curves](#page-45-0) [Theory](#page-46-0) [Application: steel frame](#page-54-0)

Application : steel frame

- 2D steel frame submitted to synthetic ground motions
- Synthetic earthquakes generated in time domain

Stochastic ground motion

Stochastic excitation

• Obtained by a modulated filtered white noise process Rezaeian & Der Kiureghian (2010)

$$
x(t) = q(t, \alpha) \sum_{i=1}^{n} s_i(t, \lambda(t_i)) \cdot \xi_i \qquad \xi_i \sim \mathcal{N}(0, 1)
$$

- Parameters of the filter $\boldsymbol\lambda = \left(\omega_{mid}, \omega', \zeta_f\right)^\mathsf{T}$ are calibrated on recorded signals
- Global parameters (Arias intensity *I*^a, duration *D*_{5−95}, strong phase peak *tmid*) are transformed into the parameters α of the modulation function $q(t, \alpha)$ (e.g. gamma distribution)

Stochastic ground motion

Parameters of the excitation

Training and validation data

- Reference solution: Monte Carlo sampling of 10,000 non linear transient analyses
- PC-NARX: 300 samples

300 simulations (training PC-NARX) 10,000 simulations

Two trajectories (first floor displacement)

- Reference solution: Monte Carlo sampling of 10,000 non linear transient analyses
- PC-NARX: 300 samples

Statistics of the first floor drift

Fragility curve – maximal drift

- Reference solution: Monte Carlo sampling of 10,000 non linear transient analyses
- PC-NARX: 300 samples

Fragility curves

Kernel density estimation

Fragility curve – maximal drift

- Reference solution: Monte Carlo sampling of 10,000 non linear transient analyses
- PC-NARX: 300 samples

Fragility curves

Conclusions

- Polynomial chaos expansions are facing challenging issues when modelling time-dependent systems such as arising in structural dynamics
- A non-intrusive approach based on NARX models (from structural identification) and sparse PCE is proposed
- The accuracy is remarkable on the statistical moments (mean/std. deviation), PDF of the maximum output, but also on particular trajectories
- The method was successfully used for computing fragility curves in earthquake engineering applications

[Conclusions](#page-64-0)

Questions ?

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<www.uqlab.com>

Thank you very much for your attention !

[Conclusions](#page-65-0)

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