Stochastic polynomial chaos expansions for emulating stochastic simulators

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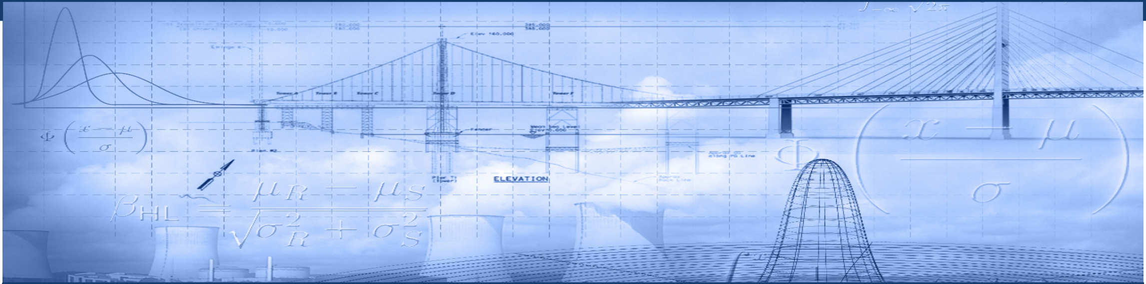

Stochastic polynomial chaos expansions for emulating stochastic simulators

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Outline

Stochastic simulators

Stochastic polynomial chaos expansions
- Motivations
- Formulation
- Stochastic surrogate

Examples
- Bimodal toy example
- Geometric Brownian motion

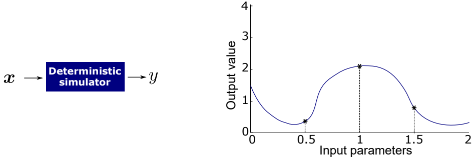
Conclusions & outlook

Deterministic vs. stochastic simulators

Deterministic simulators

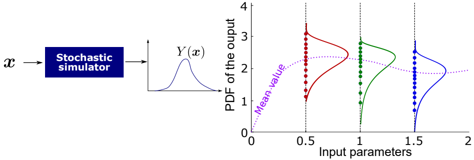
- Each set of input variables has a unique corresponding output

$$\mathcal{M}_d : \mathcal{D}_{\boldsymbol{X}} \subset \mathbb{R}^M \rightarrow \mathbb{R}$$



Stochastic simulators

- A given set of input parameters can lead to different values for the output
- $\mathcal{M}_s(\boldsymbol{x})$ is a random variable
- Source of randomness: $Y(\boldsymbol{x}) = \mathcal{M}_d(\boldsymbol{x}, \boldsymbol{Z})$, $\boldsymbol{Z}$ are latent variables



Stochastic emulators

Questions

- What are the mean/variance/quantiles or the probability density function (PDF) of the output for a given set of input parameters?
- What range (or distribution) of outputs can I expect? $\rightarrow$ uncertainty propagation
- What is the probability that the model response exceeds a threshold? $\rightarrow$ reliability analysis
- Which input variable is most important, which ones hardly affect the output? $\rightarrow$ sensitivity analysis
- ...

Stochastic emulators

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Large number of model runs

Stochastic emulators

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Large number of model runs

Need for surrogate models

- Easy to evaluate
- Accurate for estimating the response distribution
- Non-intrusive: treat the simulator as a black box

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Motivations

Model description

- A random variable Y can be represented by

$$Y = \mathcal{M}_d(\boldsymbol{Z}) \overset{\mathrm{d}}{=} g(\tilde{Z}) = \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{Z})$$

- $\tilde{Z}$ is a latent random variable with the cumulative distribution function $F_{\tilde{Z}}$
- Ψ_α's are the associated polynomial chaos basis functions, i.e., $\mathbb{E}\left[\Psi_{\alpha_1}(\tilde{Z})\,\Psi_{\alpha_2}(\tilde{Z})\right] = \delta_{\alpha_1 \alpha_2}$
- Weak approximation[1]

Mathematical foundation

- Iso-probabilistic transform $Y \overset{\mathrm{d}}{=} F_Y^{-1}(F_{\tilde{Z}}(\tilde{Z}))$
- Cameron-Martin theorem $Y \overset{\mathrm{d}}{=} F_Y^{-1}(F_{\tilde{Z}}(\tilde{Z})) = \sum_{\alpha=0}^{+\infty} c_\alpha \Psi_\alpha(\tilde{Z})$
- Convergence in L^2 implies convergence in distribution

[1] Xiu (2010). *Numerical methods for stochastic computations: a spectral method approach.* Princeton University Press

However...

Estimation method

- Maximum likelihood estimation (MLE) [2]: $f_Y(y) = \sum_j \frac{f_{\tilde{Z}}(\tilde{z}_j)}{|g'(\tilde{z}_j)|}$ with $\tilde{z}_j$ being the j-th root of the equation $y = g(\tilde{z}) = \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{z})$
- The likelihood can reach infinity
- Remedy: forcing $g(\cdot)$ to be strictly monotone, but nontrivial

[2] Desceliers et al. (2006). *Maximum likelihood estimation of stochastic chaos representations from experimental data*, Int. J. Numer. Meth. Engng. (66): 978–1001

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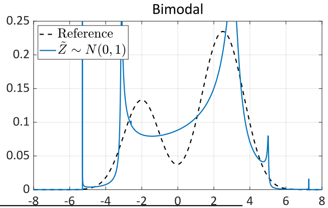
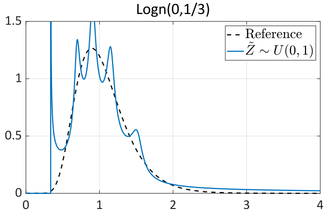
Oracle

- The best fit would be to build a surrogate directly from $Y = F_Y^{-1}(F_{\tilde{Z}}(\tilde{Z}))$





[2] Desceliers et al. (2006). *Maximum likelihood estimation of stochastic chaos representations from experimental data*, Int. J. Numer. Meth. Engng. (66): 978–1001

Stochastic polynomial chaos expansions

$$Y \stackrel{\mathrm{d}}{=} g(\tilde{Z}) + \epsilon = \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{Z}) + \epsilon$$

- Additional noise variable $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- ϵ is a smoother:

$$f_Y(y) = \int_{-\infty}^{+\infty} f_{Y \mid \tilde{Z}}(y \mid \tilde{z}) \, f_{\tilde{Z}}(\tilde{z}) \mathrm{d}\tilde{z} = \int_{-\infty}^{+\infty} f_\epsilon(y - g(\tilde{z}); \sigma) \, f_{\tilde{Z}}(\tilde{z}) \, \mathrm{d}\tilde{z}$$
$$= \int_{-\infty}^{+\infty} f_\epsilon(y - t; \sigma) \sum_j \frac{f_{\tilde{Z}}(\tilde{z}_j)}{|g'(\tilde{z}_j)|} \, \mathrm{d}t = (f_T * f_\epsilon)(y)$$

  where $T = g(\tilde{Z})$, and $\tilde{z}_j$ is the j-th root of the equation $t = g(\tilde{z})$
- c_α's and σ should be estimated from data

Estimation method

Maximum likelihood estimation

- The likelihood for $Y = y$ can be written as:

$$l(\boldsymbol{c}, \sigma; y) = \int_{\mathcal{D}_{\tilde{Z}}} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y - \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{z})\right)^2}{2\sigma^2} \right) f_{\tilde{Z}}(\tilde{z}) \mathrm{d}\tilde{z}$$

- The integral is calculated by quadrature:

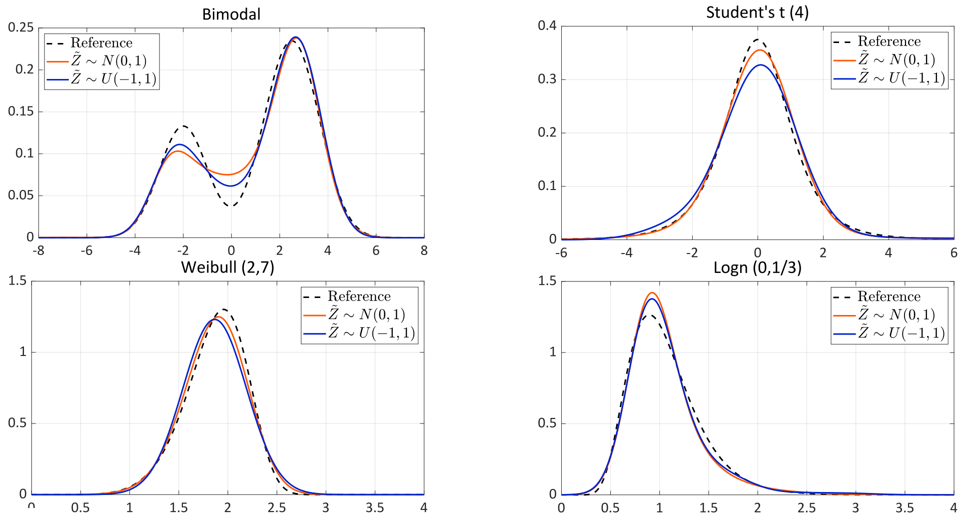
$$l(\boldsymbol{c}, \sigma; y) \approx \tilde{l}(\boldsymbol{c}, \sigma; y) = \sum_{j=1}^{N_Q} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y - \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{z}_j)\right)^2}{2\sigma^2} \right) w_j$$

- For a given σ, the maximum likelihood estimation is used for estimating the coefficients from data $\mathcal{Y} = \left\{ y^{(1)}, \ldots, y^{(N)} \right\}$: $\hat{\boldsymbol{c}} = \arg\max_{\boldsymbol{c}} \sum_{i=1}^{N} \log\left(\tilde{l}\left(\boldsymbol{c}, \sigma; y^{(i)} \right) \right)$

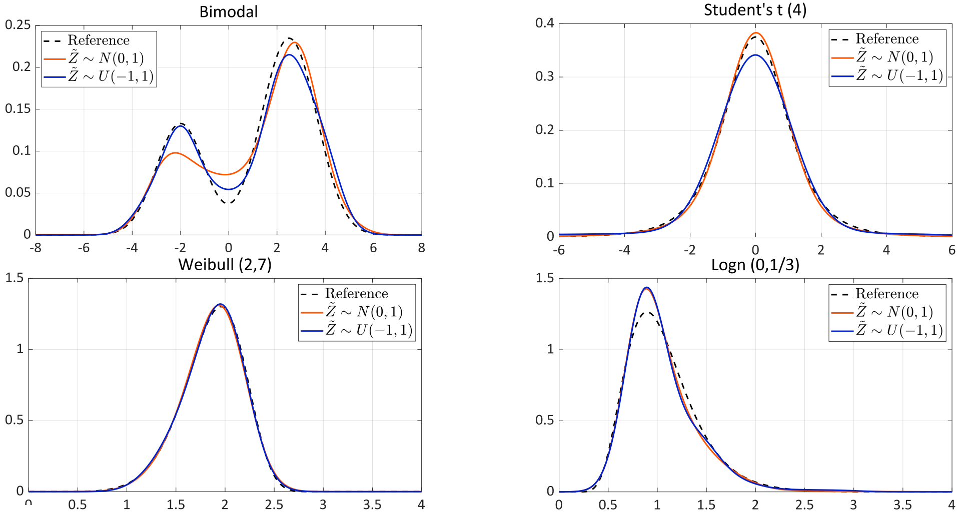
Cross-validation

- For fixed basis functions, cross-validation is applied for σ selection

Preliminary results (500 training points)



Preliminary results (1000 training points)



Remarks

Properties

- The stochastic PCE is a latent variable model, and also a generative model
- The additional noise variable ϵ is used to prevent overfitting
- The equality in $Y \overset{\mathrm{d}}{=} g(\tilde{Z}) = \sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\tilde{Z}) + \epsilon$ is in distribution, i.e., the latent variable $\tilde{Z}$ does not have real physical meanings

Links with machine learning

- Variational autoencoder[3]: variational Bayesian, Evidence Lower BOund (ELBO)
- Normalizing flow[4]: special bijective and easy-to-inverse functions $\boldsymbol{Y} \overset{\mathrm{d}}{=} \boldsymbol{g}(\tilde{\boldsymbol{Z}})$
- GAN[5]: adversarial loss (minimax)

[3] Kingma and Welling (2014). *Auto-encoding variational Bayes.*, Proc. of the 2nd International Conference on Learning Representations (ICLR)

[4] Dinh et. al. (2016). *Density estimation using real NVP.* arXiv:1605.08803

[5] Goodfellow et. al. (2014). *Generative Adversarial Networks.* Proc. of the International Conference on Neural Information Processing Systems (NeurIPS): 2672–2680

Stochastic PCE as a stochastic surrogate

Formulation

$$Y(\boldsymbol{x}) \stackrel{\mathrm{d}}{=} \sum_{\boldsymbol{\alpha}\in\mathcal{A}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}, \tilde{Z}) + \epsilon$$

- For a given x, $Y(\boldsymbol{x})$ is a function of the latent variable $\tilde{Z}$ perturbed by a Gaussian additive noise ϵ

Estimation

- The conditional likelihood for a data point $(\boldsymbol{x}, y)$ is

$$l(\boldsymbol{c}, \sigma; \boldsymbol{x}, y) = \int_{\mathcal{D}_{\tilde{Z}}} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y - \sum_{\boldsymbol{\alpha}\in\mathcal{A}} c_{\boldsymbol{\alpha}} \Psi(\boldsymbol{x}, \tilde{z})\right)^2}{2\sigma^2}\right) f_{\tilde{Z}}(\tilde{z}) \mathrm{d}\tilde{z}$$

- Numerical integration by quadrature $l(\boldsymbol{c}, \sigma; \boldsymbol{x}, y) \approx \tilde{l}(\boldsymbol{c}, \sigma; \boldsymbol{x}, y)$
- Maximum likelihood to estimate the PC coefficients $\hat{\boldsymbol{c}} = \arg\max_{\boldsymbol{c}} \sum_{i=1}^{N} \log\left(\tilde{l}\left(\boldsymbol{c}, \sigma; \boldsymbol{x}^{(i)}, y^{(i)}\right)\right)$
- Cross-validation for σ selection

Cross-validation

- The data set is divided into N_{cv} equal sized groups $\{V_k : k = 1, \dots, N_{\mathrm{cv}}\}$
- For $k \in \{1, \dots, N_{\mathrm{cv}}\}$, we pick the $k-$th group V_k as the validation set and the other $N_{\mathrm{cv}} - 1$ folds $V_{\sim k}$ as training set to build a stochastic PCE,

$$\hat{\boldsymbol{c}}_k(\sigma) = \arg\max_{\boldsymbol{c}} \sum_{i \in V_{\sim k}} \log\left(\tilde{l}\left(\boldsymbol{c}, \sigma; \boldsymbol{x}^{(i)}, y^{(i)}\right)\right)$$

- We evaluate the likelihood on the validation set, which gives the out-of-sample performance

$$\mathbf{l}_k(\sigma) = \sum_{i \in V_k} \log\left(\tilde{l}\left(\hat{\boldsymbol{c}}_k(\sigma), \sigma; \boldsymbol{x}^{(i)}, y^{(i)}\right)\right)$$

- We repeat the procedure for all $k \in \{1, \dots, N_{\mathrm{cv}}\}$, and the optimal σ^* is selected as

$$\sigma^* = \arg\max_{\sigma} \sum_{k=1}^{N_{\mathrm{cv}}} \mathbf{l}_k(\sigma)$$

Model selection

Adaptivity

- Truncation scheme $\mathcal{A}^{p,q,M} = \left\{ \boldsymbol{\alpha} \in \mathbb{N}^M : \|\boldsymbol{\alpha}\|_q \overset{\text{def}}{=} \left(\sum_{i=1}^{M} \alpha_i^q\right)^{\frac{1}{q}} \leq p \right\}$
  - Choose the appropriate degree (p-adaptivity)
  - Choose the appropriate q-norm (q-norm-adaptivity)
- Choose the appropriate latent variable: normal or uniform

Selection criteria

- Information criterion, e.g., Akaike information criterion (AIC), Bayesian information criterion (BIC)
- Cross-validation, e.g., the same quantity as for σ-selection

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Error metric

Wasserstein distance (of order 2)

- For continuous random variables, it is the L^2 distance between the quantile functions:

$$d_{\mathrm{WS}}^2(Y, \hat{Y}) = \|Q_Y - Q_{\hat{Y}}\|_{L^2}^2$$

Normalized Wasserstein distance

$$\varepsilon = \frac{\mathbb{E}_{\boldsymbol{X}}\left[d_{\mathrm{WS}}^2\left(Y(\boldsymbol{X}), \hat{Y}(\boldsymbol{X})\right)\right]}{\mathrm{Var}\left[Y\right]}$$

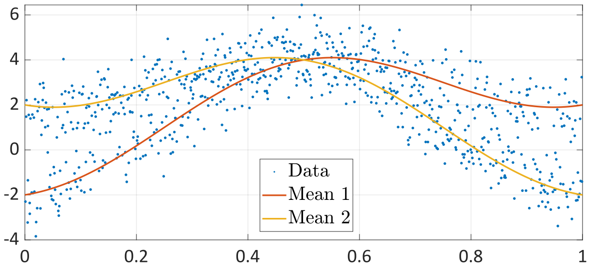
- Shift and scale invariant

Bimodal toy example

Description of the simulator

$$f_{Y|X}(y \mid X = x) = 0.6\, f_n(4\sin^2(\pi \cdot x) + 4x - 2) + 0.4\, f_n(4\sin^2(\pi \cdot x) - 4x + 2)$$

- f_n is the PDF of a normal distribution with mean 0 and standard deviation 0.8.
- The response distribution is a mixture of Gaussian PDFs
- $X \sim \mathcal{U}(0, 1)$



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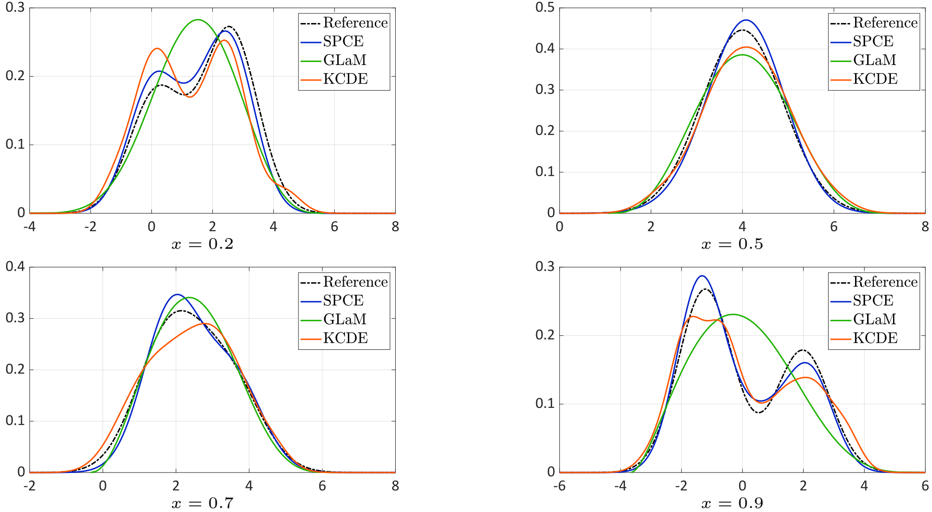
Surrogate setting

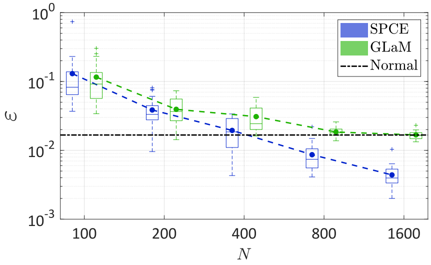
- Experimental design (ED): $\boldsymbol{\mathcal{X}}$ are generated using the Latin hypercube sampling
- Degree and q-norm adaptivity: $p \in \{1, 2, \ldots, 5\}$ and $q \in \{0.5, 0.75, 1\}$
- Latent variable selection: $\tilde{Z} \sim \mathcal{N}(0, 1)$ and $\tilde{Z} \sim \mathcal{U}(-1, 1)$

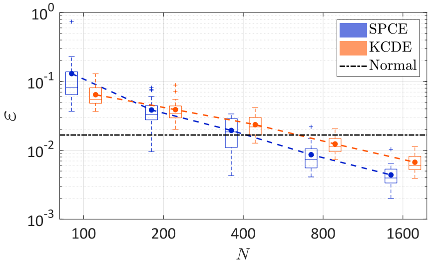
PDF predictions (ED with $N = 800$)



Convergence study

- Experimental design of size 100, 200, 400, 800, 1600
- 20 independent runs for each scenario
- Normalized Wasserstein distance as a performance indicator





Geometric Brownian motion

$$\mathrm{d}S_t = x_1\, S_t\, \mathrm{d}t + x_2\, S_t\, \mathrm{d}W_t$$

- S_t: price process, W_t: Wiener process, x_1: drift, x_2: volatility
- $X_1 \sim \mathcal{U}(0, 0.1)$, $X_2 \sim \mathcal{U}(0.1, 0.4)$, and $Y(\boldsymbol{x}) = S_1(\boldsymbol{x})$
- The analytical distribution of S_t exists (Itô's calculus)

$$S_1(\boldsymbol{x})/S_0 \sim \mathcal{LN}\left(x_1 - \frac{x_2^2}{2}, x_2\right)$$

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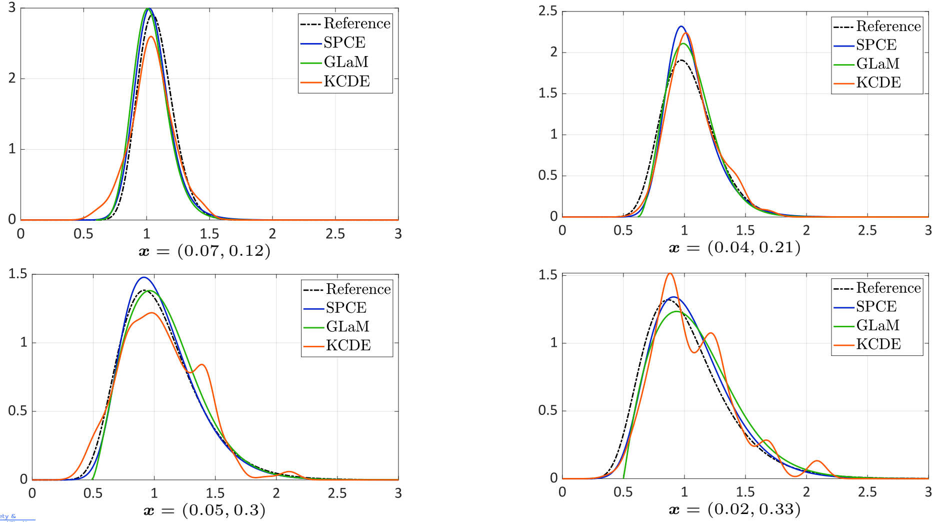
PDF predictions (ED with $N = 400$)



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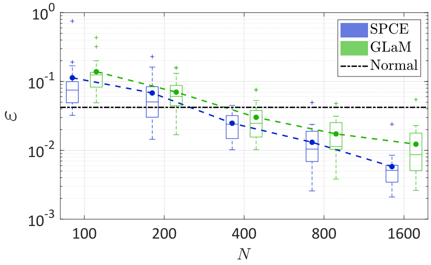

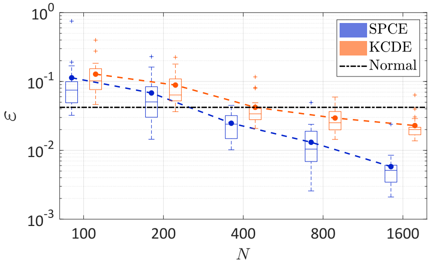

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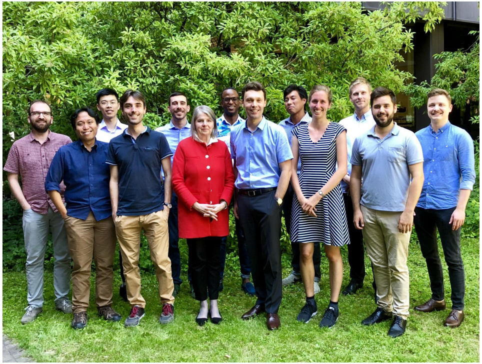
Conclusions

- Stochastic PCE is developed for general statistical inference of distributions
- On top of the input variables, a latent variable and a noise variable are introduced to represent the intrinsic randomness of a stochastic simulator
- The PC coefficients are calibrated by the maximum likelihood estimation
- The noise variable is a smoother, and its standard deviation σ is a hyperparameter
- The proposed algorithm does not require replications

Outlook

- Theoretical properties of the surrogate model (consistency, asymptotic properties)
- More applications
- Sparse stochastic PCE
- Conditional Wasserstein GAN [6]

[6] Ariovsky et al. (2017). *Wasserstein Generative Adversarial Networks*, Proc. of the 34th International Conference on Machine Learning (70): 214–223



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Thank you very much for your attention !

Statistical models

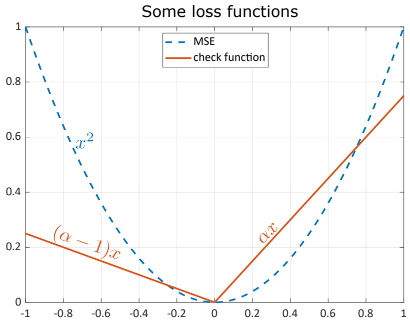
Statistical assumptions

- Data generation process, e.g., linear models

$$Y = a\,X + b + \epsilon$$

Estimation method

- A framework to infer the model
- Loss function, e.g. mean estimation: mean-squared error, quantile estimation: check function loss



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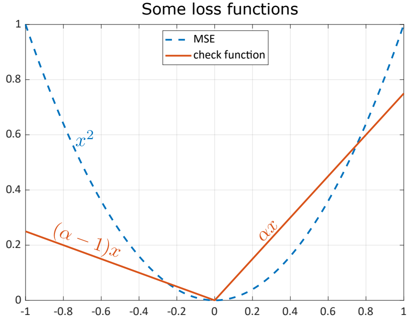

Distribution estimation

- Parametric family (e.g. exponential family): maximum likelihood estimation
- Kernel estimation: $f(y \mid \boldsymbol{x}) = f(\boldsymbol{x}, y)/f(\boldsymbol{x})$
- Latent variable models: variational auto-encoder, GAN