

Sparse polynomial chaos expansions as a machine learning regression technique

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Sparse Polynomial Chaos Expansions as a Machine Learning Regression Technique

B. Sudret*, S. Marelli, C. Lataniotis



International Symposium on Big Data and Predictive Computational
Modeling

Introduction: supervised learning

- **Machine learning** aims at making **predictions** by building a model based on data
- **Unsupervised learning** aims at discovering a hidden structure within unlabelled data $\{\mathbf{x}^{(i)}, i = 1, \dots, n\}$
- **Supervised learning** considers a **training data set**:

$$\mathcal{X} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \dots, n\}$$

where:

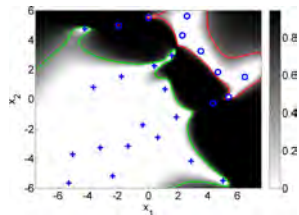
- $\mathbf{x}^{(i)}$'s are the **attributes** / features (input space)
- $y^{(i)}$'s are the **labels** (output space)

Classical problems and algorithms

Classification

- In **classification** problems, the labels are discrete, e.g. $y^{(i)} \in \{-1, 1\}$. The goal is to **predict the class** of a new point \boldsymbol{x}

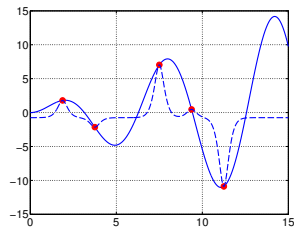
Logistic regression - Support vector machines



Regression

- In **regression** problems, the labels are continuous, say $y^{(i)} \in \mathcal{D}_Y \subset \mathbb{R}$. The goal is to **predict the value** $\hat{y} = \tilde{\mathcal{M}}(\boldsymbol{x})$ for a new point \boldsymbol{x}

Artificial neural networks - Gaussian process models - Support vector regression



Uncertainty quantification

- A **computational model** is defined as a map:

$$\mathbf{x} \in \mathcal{D}_X \mapsto y = \mathcal{M}(\mathbf{x})$$



- Uncertainties in the input are represented by a **probabilistic model**:

$$\mathbf{X} \sim f_X \quad (\text{joint PDF})$$

- **Uncertainty propagation** aims at estimating the statistics of $Y = \mathcal{M}(\mathbf{X})$
- **Sensitivity analysis** aims at finding the input parameters (or combination thereof) which drive the variability of Y

Uncertainty quantification

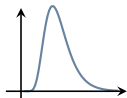
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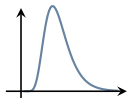
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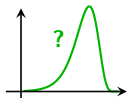


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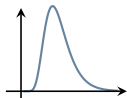
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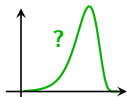


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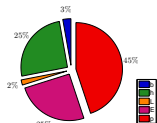
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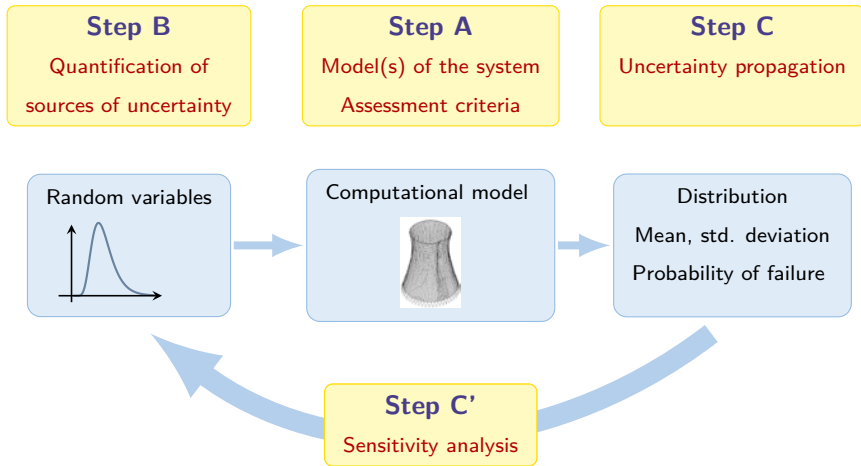
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Global framework for uncertainty quantification

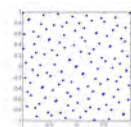


B.S., Uncertainty propagation and sensitivity analysis in mechanical models, Habilitation thesis, 2007.

Surrogate models for uncertainty quantification

A **surrogate model** $\tilde{\mathcal{M}}$ is an **approximation** of the original computational model:

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

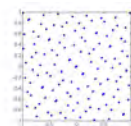


Name	Shape	Parameters
	$\tilde{\mathcal{M}}(x) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(x)$	y_{α}
Gaussian process modelling	$\tilde{\mathcal{M}}(x) = \beta^{\top} \cdot \mathbf{f}(x) + \sigma^2 Z(x, \omega)$	β, σ^2, θ
Support vector machines	$\tilde{\mathcal{M}}(x) = \sum_{i=1}^m y_i K(x_i, x) + b$	\mathbf{y}, b

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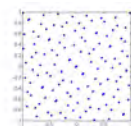


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Support vector machines	$\tilde{\mathcal{M}}(\mathbf{x}) = \sum_{i=1}^m y_i K(\mathbf{x}_i, \mathbf{x}) + b$	\mathbf{y}, b

Bridging supervised learning and PC expansions

Features	Machine learning	Unc. Quant. /PCE
Computational model \mathcal{M}	✗	✓
Probabilistic model of the input $\mathbf{X} \sim f_{\mathbf{X}}$	✗	✓
Training data: $\mathcal{X} = \{(\mathbf{x}_i, y_i), i = 1, \dots, n\}$	✓	✓
	Training data set	Experimental design
Prediction goal: for a new $\mathbf{x} \notin \mathcal{X}$, $y(\mathbf{x})$?	$\sum_{i=1}^m y_i K(\mathbf{x}_i, \mathbf{x}) + b$	$\sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{x})$
Validation (resp. cross-validation)	✓	✓
	Validation set	Leave-one-out CV

Outline

- 1 Introduction
- 2 Polynomial chaos expansions for supervised learning
 - PCE in a nutshell
 - Ad-hoc input probabilistic model
- 3 Applications
 - Combined cycle power plant
 - Boston Housing

Polynomial chaos expansions in a nutshell

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

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

where :

- y_{α} : **coefficients** to be computed (coordinates)
- $\Psi_{\alpha}(\mathbf{X})$: **basis** functions
- The PCE basis $\{\Psi_{\alpha}(\mathbf{X}), \alpha \in \mathbb{N}^M\}$ is made of **multivariate orthonormal polynomials**

$$\Psi_{\alpha}(\mathbf{x}) \stackrel{\text{def}}{=} \prod_{i=1}^M \Psi_{\alpha_i}^{(i)}(x_i) \quad \mathbb{E}[\Psi_{\alpha}(\mathbf{X})\Psi_{\beta}(\mathbf{X})] = \delta_{\alpha\beta}$$

Practical implementation

- The input random variables are first transformed into **reduced variables** (e.g. standard normal variables $\mathcal{N}(0, 1)$, uniform variables on $[-1, 1]$, etc.):

$$\mathbf{X} = \mathcal{T}(\boldsymbol{\xi}) \quad \dim \boldsymbol{\xi} = M \quad (\text{isoprobabilistic transform})$$

e.g. : $X_i = F_i^{-1} \circ \Phi(\xi_i)$, $\xi_i \sim \mathcal{N}(0, 1)$ in the independent case

- The model response is cast as a function of the reduced variables and expanded:

$$Y = \mathcal{M}(\mathbf{X}) = \mathcal{M} \circ \mathcal{T}(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

- A **truncation scheme** is selected and the associated **finite set** of multi-indices is generated, e.g. :

$$\mathcal{A}^{M,p} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : |\boldsymbol{\alpha}| \leq p\} \quad \text{card } \mathcal{A}^{M,p} \equiv P = \binom{M+p}{p}$$

Statistical approach: least-square minimization

Berveiller *et al.* (2006)

Principle

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

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) + \varepsilon_P(\mathbf{X}) \equiv \mathbf{Y}^{\top} \Psi(\mathbf{X}) + \varepsilon_P(\mathbf{X})$$

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

$$\Psi(\mathbf{x}) = \{\Psi_0(\mathbf{x}), \dots, \Psi_{P-1}(\mathbf{x})\}$$

Least-square minimization

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

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

Least-Square Minimization: discretized solution

Ordinary least-square (OLS)

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

$$\hat{\mathbf{Y}} = \arg \min_{\mathbf{Y} \in \mathbb{R}^P} \hat{\mathbb{E}} \left[\left(\mathbf{Y}^T \Psi(\mathbf{X}) - \mathcal{M}(\mathbf{X}) \right)^2 \right] = \arg \min_{\mathbf{Y} \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^n \left(\mathbf{Y}^T \Psi(\mathbf{x}^{(i)}) - \mathcal{M}(\mathbf{x}^{(i)}) \right)^2$$

Penalized least-squares

- ℓ_1 - penalty is introduced to induce **sparsity** in the solution

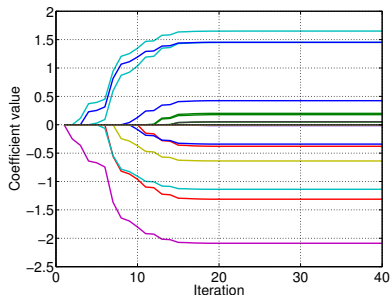
$$\mathbf{y}_\alpha = \arg \min \frac{1}{n} \sum_{i=1}^n \left(\mathbf{Y}^T \Psi(\mathbf{x}^{(i)}) - \mathcal{M}(\mathbf{x}^{(i)}) \right)^2 + \lambda \|\mathbf{Y}\|_1$$

- The **Least-angle regression** (LAR) algorithm is used

Efron *et al.*, *Ann. Stat.* (2004), Blatman and S., *J. Comp. Phys.* (2011)

Least angle regression

Path of solutions

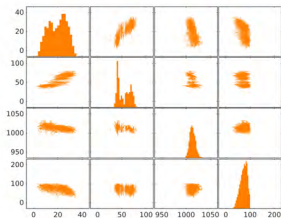


- A path of solutions is obtained containing $1, 2, \dots, \min(n, |\mathcal{A}|)$ terms.
- Leave-one-out error E_{LOO} is computed for each solution and the best model (smallest error) is selected

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

where h_i is the i -th diagonal term of matrix $\mathbf{A}(\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top$ and $\mathbf{A}_{ij} = \Psi_j(\mathbf{x}^{(i)})$

Back to supervised learning



- Assume all features are continuous variables
- Data: training set
 $\mathcal{X} = \{(\mathbf{x}_i, y_i), i = 1, \dots, n\}$
- A **probabilistic model** needs to be set up from this data

Statistical inference

Probabilistic modelling of (sufficiently) big data

Premise

- Machine learning is often used for **big data**, *i.e.* thousands to even millions of training points
- No need for parametric estimation of the input distribution
- **Full non-parametric** representation remains difficult in high dimensions

Proposed solution

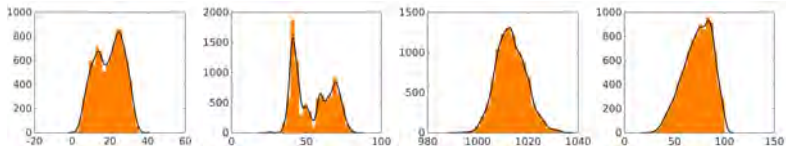
- Non parametric estimation of the marginals X_i , $i = 1, \dots, M$
- Parametric copula for the (possible) dependence

Modelling of the marginals

- For each univariate sample $\mathcal{X}_k \stackrel{\text{def}}{=} \{x_k^{(1)}, \dots, x_k^{(n)}\}$ a **kernel smoothing** technique is used:

$$\hat{f}_{X_k}(x) = \frac{1}{n h_k} \sum_{i=1}^n K\left(\frac{x - x_k^{(i)}}{h_k}\right)$$

- K : kernel function, e.g. the Gaussian kernel $\varphi(t) = e^{-t^2/2}/\sqrt{2\pi}$
- h_k : bandwidth to be adapted to the data (default value by Silverman's rule)



Dependence modelling: copula theory

Reminder (Sklar's theorem)

A continuous joint distribution $F_{\mathbf{X}}$ may be represented uniquely through the marginal distributions $\{F_{X_k}, k = 1, \dots, M\}$ and a copula function \mathcal{C} :

$$F_{\mathbf{X}}(\mathbf{x}) = \mathcal{C}(F_{X_1}(x_1), \dots, F_{X_M}(x_M))$$

Example

The **Gaussian copula** reads:

$$\mathcal{C}^{\mathcal{N}}(\mathbf{u}; \Theta) = \Phi_M(\Phi^{-1}(u_1), \dots, \Phi^{-1}(u_M); \Theta)$$

where:

- Φ_M is the multivariate Gaussian CDF (of dim. M)
- Θ is the **copula parameters matrix** ("correlation matrix")

Inference of the Gaussian copula

- The **Spearman rank correlation** matrix is computed from the training set:

$$\hat{\rho}_{kl}^S = \text{corr}(\mathcal{R}_k, \mathcal{R}_l)$$

where $\mathcal{R}_k, \mathcal{R}_l$ are the ranks of univariate samples $\mathcal{X}_k, \mathcal{X}_l$:

$$\hat{\rho}_{kl}^S = 1 - \frac{6}{n} \frac{\sum_{j=1}^n (\mathcal{R}_k^{(j)} - \mathcal{R}_l^{(j)})^2}{n^2 - 1}$$

- The copula correlation matrix reads:

$$\Theta_{kl} = 2 \sin\left(\frac{\pi}{6} \hat{\rho}_{kl}^S\right)$$

NB: The invertibility of this correlation matrix is not guaranteed



Charles Spearman
(1863-1945)

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Wrap-up: PCE-based supervised learning

- **Data:** $\mathcal{X} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \dots, n\}$
- Use **kernel smoothing** for setting marginals and e.g. the Gaussian copula, so as to get the joint distribution

$$F_{\mathbf{X}}(\mathbf{x}) = C^{\mathcal{N}}(\hat{F}_{X_1}^{-1}(x_1), \dots, \hat{F}_{X_M}^{-1}(x_M); \hat{\Theta})$$

- Transform data into a standardized space, e.g. $[-1, 1]^M$:

Remove marginals $z_k^{(i)} = \Phi^{-1}(\hat{F}_{X_k}(x_k^{(i)}))$

Decorrelate z 's $\tilde{z}^{(i)} = \mathbf{L}^{-1} \cdot \mathbf{z}^{(i)}$ where $\hat{\Theta} = \mathbf{L} \cdot \mathbf{L}^T$

Normalize over $[-1, 1]$ $u_k^{(i)} = 2\Phi(\tilde{z}_k^{(i)}) - 1$

Wrap-up: PCE-based supervised learning

- From the data set in the U -space $[-1, 1]^M$, compute the coefficient of the multivariate Legendre polynomials using least-square analysis:

$$Y \stackrel{\text{def}}{=} \mathcal{M}^{\text{PC}}(\mathbf{u}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} L_{\alpha_1}(u_1) \otimes \cdots \otimes L_{\alpha_M}(u_M)$$

New predictions for $\mathbf{x}^{(0)} \in \mathcal{D}_X$

- Transform input:

$$\mathbf{x}^{(0)} \longrightarrow \mathbf{z}^{(0)} \longrightarrow \tilde{\mathbf{z}}^{(0)} \longrightarrow \mathbf{u}^{(0)}$$

- Predict:

$$\hat{y}^{(0)} = \mathcal{M}^{\text{PC}}(\mathbf{u}^{(0)})$$

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Combined cycle power plant (CCPP)

Data set

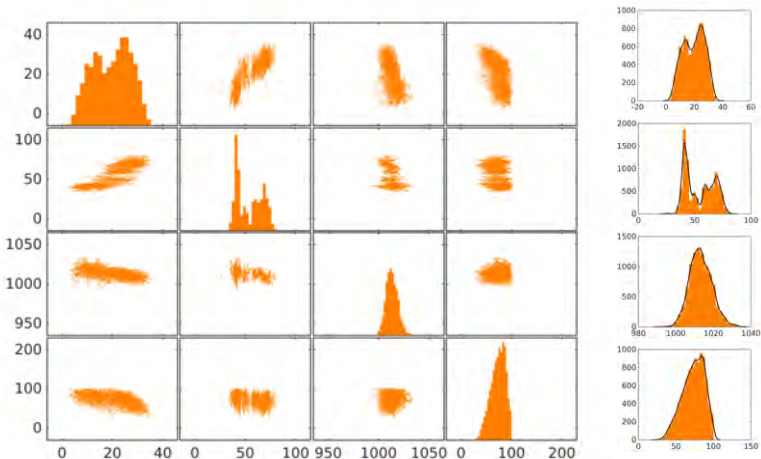
UC Irvine Machine Learning Repository

- 9568 data points
- 4 features:
 - Temperature $T \in [1.81, 37.11]$ °C
 - Ambient pressure $P \in [992.89, 1033.30]$ mB
 - Relative humidity $RH \in [25.56 - 100.16]\%$
 - Exhaust vacuum $V \in [25.36, 81.56]$ cm Hg
- 1 output: net hourly electrical energy output $EP \in [420.26, 495.76]$ MW

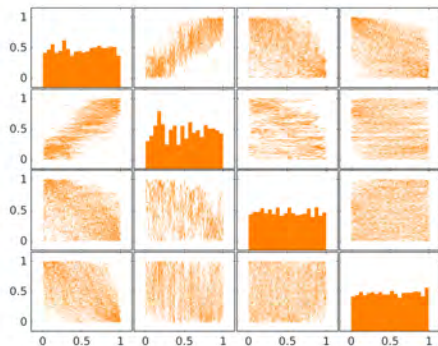
Strategy

- Non parametric kernel density smoothing of the distribution
- Fitting of a Gaussian copula

CCPP: Training data (X -space)



CCPP: Training data (U -space)

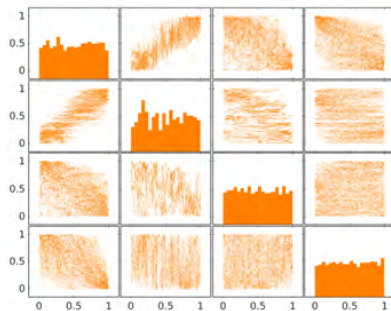


Samples of the data dependence structure

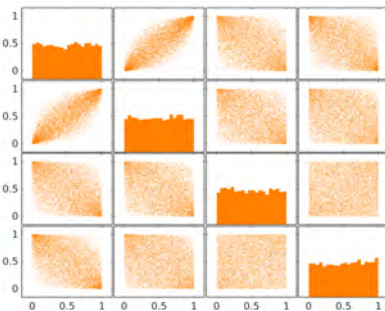
Correlation matrix:

$$\hat{\Theta} = \begin{pmatrix} 1.00 & 0.85 & -0.52 & -0.54 \\ 0.85 & 1.00 & -0.43 & -0.30 \\ -0.52 & -0.43 & 1.00 & 0.09 \\ -0.54 & -0.30 & 0.09 & 1.00 \end{pmatrix}$$

Validation of the probabilistic model

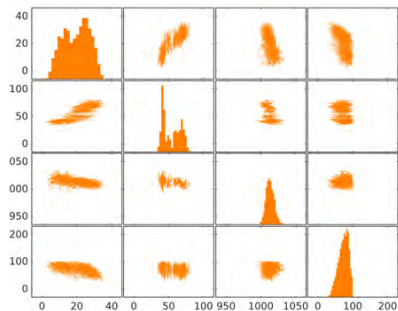


Training data – U -space

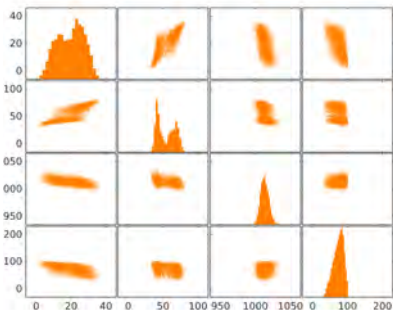


Probabilistic model – U -space

Validation of the probabilistic model



Training data – X -space



Probabilistic model – X -space

Error estimation

- The data set is divided into a training set and a validation set

$$\mathcal{X}_{val} = \left\{ \mathbf{x}_{val}^{(1)}, \dots, \mathbf{x}_{val}^{(n)} \right\}$$

- Given the validation set of data \mathcal{X}_{val} and the corresponding responses $\mathcal{V} = \left\{ v^{(1)}, \dots, v^{(n)} \right\}$, one can define two error estimates to assess the model performance:

- Mean absolute error

$$MAE = \frac{1}{n} \sum_{j=1}^n \left| v^{(j)} - \mathcal{M}^{PC}(\mathbf{x}_{val}^{(j)}) \right|$$

- Root-mean square error

$$RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^n \left(v^{(j)} - \mathcal{M}^{PC}(\mathbf{x}_{val}^{(j)}) \right)^2}$$

Leave-one-out cross-validation

- PCE also provides an **a posteriori** error estimate that is closely related to **RMSE** **without requiring a validation set**:

$$\varepsilon_{LOO} = \frac{1}{n_{ED} \text{Var}[\mathcal{Y}]} \sum_{j=1}^{n_{ED}} \left(y^{(j)} - \mathcal{M}^{PC \setminus k}(\mathbf{x}_{ED}^{(k)}) \right)^2$$

where $M^{PC \setminus k}$ refers to the metamodel built on the experimental design $\mathcal{X} \setminus \mathbf{x}_{ED}^{(k)}$

- The leave-one-out error ε_{LOO} can be used to compare with validation RMSE

$$RMSE \approx RMSE_{LOO} \stackrel{\text{def}}{=} \sqrt{E_{LOO} \cdot \text{Var}[\mathcal{Y}]}$$

Setup

- **10 data sets** are generated as follows
 - The dataset is randomly permuted 5 times
 - For each permutation, first half is used for training, second half for validation ($n_{train} = n_{val} = 4784$ points)
 - ... and the other way around (first half for validation, second half for training)

CCPP: Results

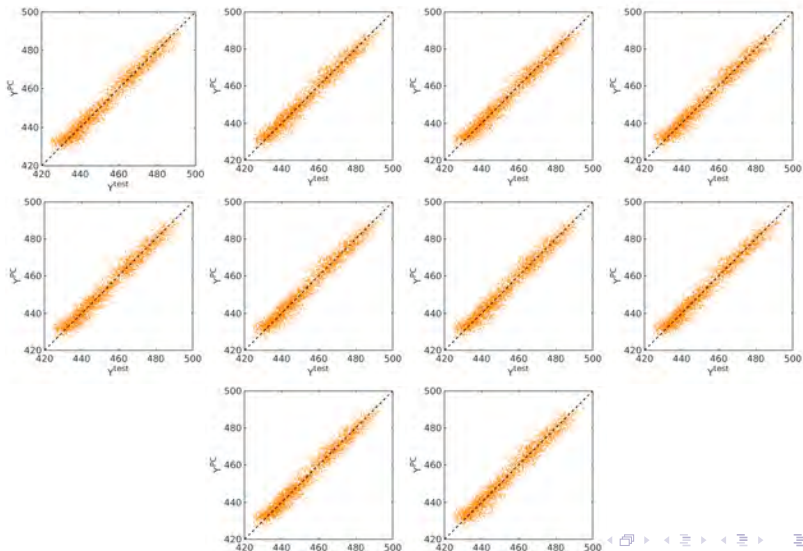
Method	$RMSE$ (best)	$RMSE$ (mean)	$RMSE_{LOO}$
LMS	4.572	4.888	-
SMOReg	4.563	4.887	-
K*	3.861	4.552	-
BREP	3.787	4.239	-
M5R	4.128	4.462	-
M5P	4.087	4.428	-
REP	4.211	4.518	-
PCE	3.6182	3.855	3.860

Reference results: Tüfecki, Electrical Power and Energy Systems (2014)

Polynomial chaos features

- Maximum PCE degree: 14 (full truncation: $P = \binom{14+4}{4} = 3,060$)
- Non-zero coefficients: $nnz = 117$
- Index of sparsity: $IS = nnz/P = 3.82\%$
- $\varepsilon_{LOO} = 5.4 \cdot 10^{-2}$

CCPP: Scatter plots (10 different data sets)



Outline

- 1 Introduction
- 2 Polynomial chaos expansions for supervised learning
- 3 Applications
 - Combined cycle power plant
 - **Boston Housing**

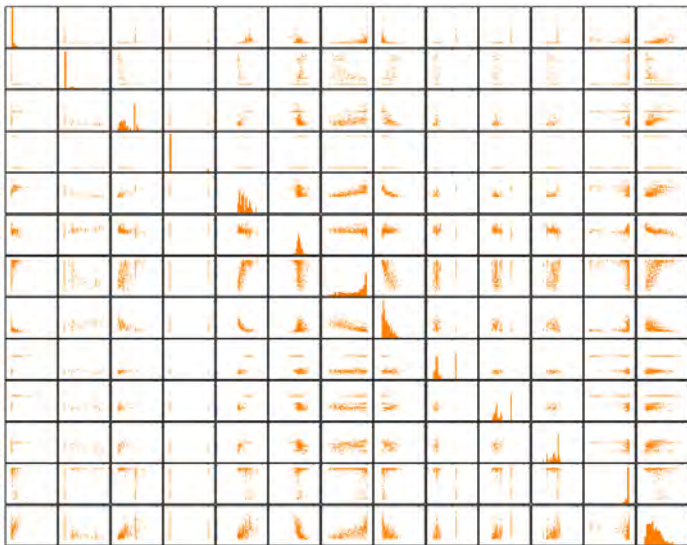
Boston Housing

Data set

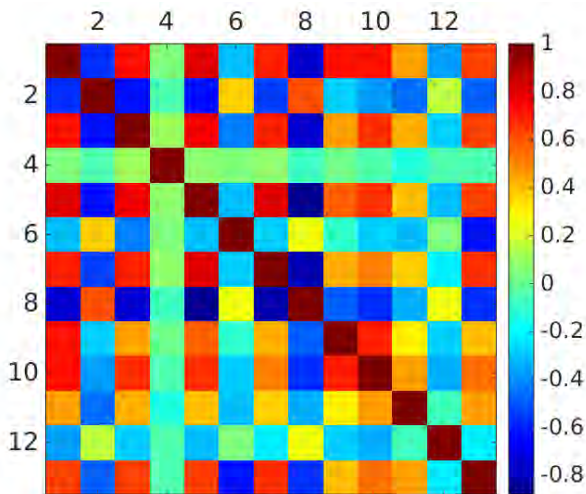
UC Irvine Machine Learning Repository

- 506 real data points
- 13 features:
 - CRIM: per capita crime rate by town
 - ZN: proportion of residential land zoned for lots over 25,000 sq.ft.
 - INDUS: proportion of non-retail business acres per town
 - CHAS: River (= 1 if near river; 0 otherwise)
 - NOX: nitric oxides concentration (parts per 10 million)
 - RM: average number of rooms per dwelling
 - AGE: proportion of owner-occupied units built prior to 1940
 - DIS: weighted distances to five Boston employment centres
 - RAD: index of accessibility to radial highways
 - TAX: full-value property-tax rate per \$10,000
 - PTRATIO: pupil-teacher ratio by town
 - B : $1000(Bk - 0.63)^2$ where Bk is the proportion of blacks by town
 - LSTAT: % lower status of the population
- 1 output: median value of owner-occupied homes (MEDV) in \$1000's

Boston housing: training data

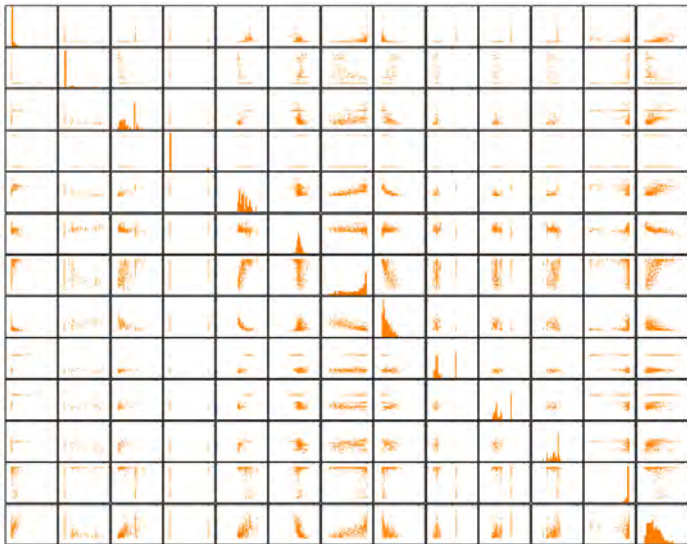


Boston housing: training data



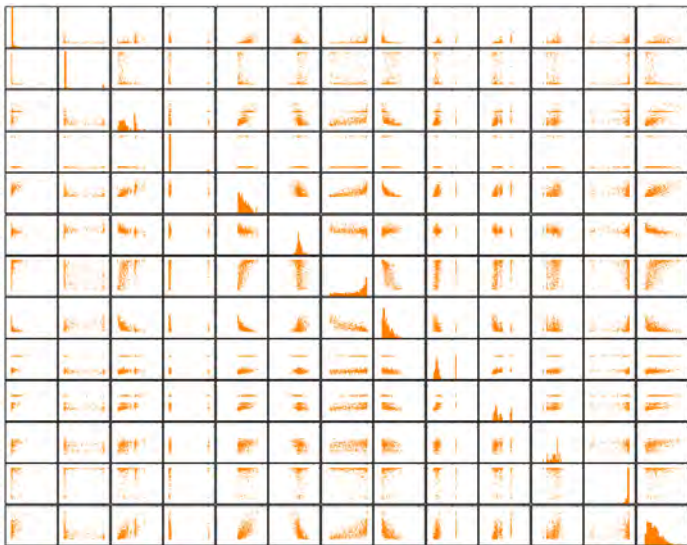
Data rank-correlation matrix

Boston housing: probabilistic model (X space)



Training data – X -space

Boston housing: probabilistic model (X space)



Probabilistic model – X -space

Validation strategy: leave- k -out cross validation

- $N_p = 200$ permutations of the full data set (506 points)
- For each permutation, last 25 points used for validation ($n_{train} = 481$)
- A PCE is generated using the training data set and the validation errors ($RMSE$) is computed using $n_{val} = 25$ points
- Comparison with in-house Gaussian process models (UQLab)

Polynomial chaos features

(one particular run)

- Maximum PCE degree: 6 (full truncation: $P = \binom{13+6}{6} = 27,132$)
- Non-zero coefficients: $nnz = 77$
- Index of sparsity: $IS = nnz/P = 77/27132 = 0.28\%$
- $\varepsilon_{LOO} = 0.2041$

Boston housing: results

Method	<i>RMSE</i> (best)	<i>RMSE</i> (mean)	<i>RMSE</i> (variance)
GP (Matérn 3/2)	1.7720	3.0747	0.8224
GP (Matérn 5/2)	1.8579	3.2882	0.7191
GP (Gaussian)	1.9663	3.3538	0.6346
PCE	2.0353	3.9009	1.1217

Comments

- Results not so good as in the CCPP case
- One categorical variable (just handled as the others here)
- Significant correlations between features
- ... Additional investigations required, e.g. using PC-Kriging

Conclusions and outlook

- Sparse polynomial chaos expansions are introduced as a tool for supervised learning
- Pre-processing of the data required to build a “reasonable” probabilistic model: **non parametric marginals** + **Gaussian copula**
- Current approach: **isoprobabilistic transform** into a space of independent uniform variables
- Excellent results in the CCPP case, yet to be improved in the Boston housing case
- **Many open questions**: best joint probabilistic model, suitable data-driven orthogonal polynomials, handling categorical variables
- Extension to **classification** problems?

Questions ?

Thank you very much for
your attention !



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