Polynomial-Chaos-Kriging

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Problem Statement & Context

A **computational model** maps the input vector $\boldsymbol{x} \in \mathbb{D}_X \subset \mathbb{R}^N$ to $y \in \mathbb{R}$ and is represented by $y = \mathcal{M}(\boldsymbol{x})$. The input space is modelled by a random vector $\boldsymbol{X}$ (set of input variables) through probability distributions. The input variables are assumed statistically independent.

The goal is to approximate the computationally expensive-to-evaluate computational model by a cheap-to-evaluate function, *i.e.* a **meta-model**.
Further, the computational model is interpreted as a black-box model, *i.e.* only input/output data is available.

Polynomial Chaos Expansions

Polynomial-Chaos-Expansions (PCE) surrogate the computational model $\mathcal{M}(\boldsymbol{X})$ by a sum of orthonormal polynomials (Ghanem and Spanos, 2003):

$$\mathcal{M}^{(PCE)}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} \boldsymbol{a}_{\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

- $\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$: multivariate, orthonormal polynomials in coherency with the input distributions $\boldsymbol{X}$, indexed by multi-index $\boldsymbol{\alpha}$. An orthonormal basis is defined as $\langle \phi_i, \phi_j \rangle_k = \int_{\mathcal{D}_k} \phi_i(x)\, \phi_j(x)\, f_{X_k}(x) dx = \delta_{ij}$ where ϕ are univariate polynomials, $f_{X_k}(x)$ is the marginal PDF in dimension k and δ is the Kronecker symbol. The multivariate polynomials are $\psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \prod_{i=1}^{M} \phi_{\alpha_i}^{(i)}(X_i)$ where M is the number of dimensions.
- $\boldsymbol{a}_{\boldsymbol{\alpha}}$: coefficients of the polynomials, indexed by $\boldsymbol{\alpha}$.
- $\mathcal{A}$: index set of the orthonormal polynomials.

The set of candidate polynomials is defined by a maximal polynomial degree and a truncation scheme, such as *hyperbolic index sets*. The PCE meta-model is then calibrated through least-angle regression (LARS) (Blatman and Sudret, 2011).

Kriging

Kriging (a.k.a. Gaussian process modelling) is a stochastic meta-modelling technique assuming that the computational model $\mathcal{M}(\boldsymbol{x})$ is the realization of a Gaussian random field (Santner et al., 2003):

$$\mathcal{M}^{(\mathsf{K})}(\boldsymbol{x}) = \boldsymbol{\beta}^{\mathsf{T}} \cdot \boldsymbol{f}(\boldsymbol{x}) + \sigma^2 \, Z(\boldsymbol{x}, \omega)$$

- $\boldsymbol{\beta}^{\mathsf{T}} \cdot \boldsymbol{f}(\boldsymbol{x})$: mean value of the Gaussian process (a.k.a. trend).
- $Z(\boldsymbol{x}, \omega)$: zero mean, unit variance Gaussian process with autocorrelation function $R(|\boldsymbol{x}' - \boldsymbol{x}|; \boldsymbol{\theta})$ and its hyper-parameters $\boldsymbol{\theta}$.
- σ^2: Kriging variance.

Calibration of the model:

- Compute the hyper-parameters $\boldsymbol{\theta}$ via cross-validation (CV) or maximum likelihood estimate (MLE) (Bachoc, 2013).
- Compute the Kriging parameters $\{\boldsymbol{\beta}, \sigma^2\}$ via generalized least-squares solution.
- Predict new samples and obtain the prediction mean $\mu_{\widehat{Y}}(x)$ and variance $\sigma_{\widehat{Y}}(x)$.

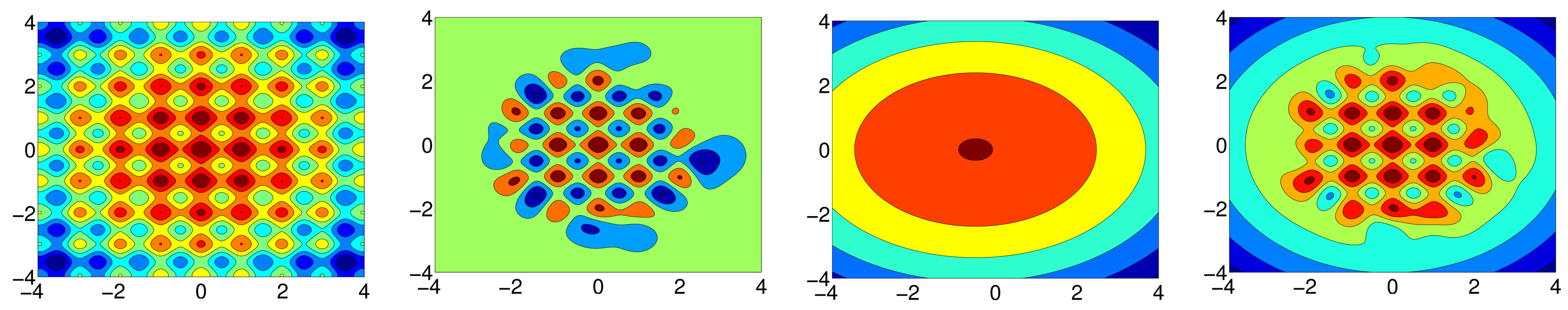
PC-Kriging

Polynomial-Chaos-Kriging (PC-Kriging) is a non-intrusive meta-modelling technique which combines the traditional methods PCE and Kriging in a universal Kriging model (Schöbi and Sudret, 2014).

$$\mathcal{M}(\boldsymbol{x}) \approx \mathcal{M}^{(\mathsf{PCK})}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) + \sigma^2 \, Z(\boldsymbol{x}, \omega)$$

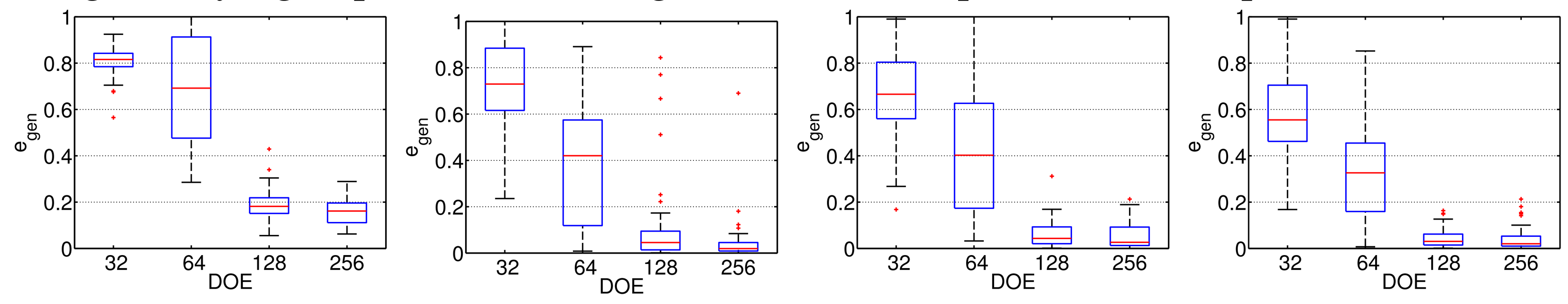
- $\sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ is the sum of a sparse set of multivariate **orthonormal polynomials**, representing the trend.
- Sequential PC-Kriging (**SPC-Kriging**): Determine a set of polynomials $\mathcal{A}$ by LARS and use $\mathcal{A}$ as trend of the PC-Kriging model.
- Optimal PC-Kriging (**OPC-Kriging**): Take $\mathcal{A}$ from SPC-Kriging, iteratively add one-by-one $\boldsymbol{\alpha} \in \mathcal{A}$ to the trend, pick the meta-model with the lowest leave-one-out error as the PC-Kriging model.

Behaviour of PC-Kriging illustrated on the Rastrigin function (128 samples):



Exact function — Ordinary Kriging — PCE — PC-Kriging

Validation: Relative generalization error (L_2-error) of the Rastrigin function (LHS design, varying experimental design (DOE), 50 replications (boxplot)):



Ordinary Kriging — PCE — SPC-Kriging — OPC-Kriging

Conclusion

Comparing the three meta-modelling techniques on analytical meta-modelling benchmark functions led us to the conclusions:

- PC-Kriging combines the advantages of the single approaches: the set of polynomials approximates the global behaviour whereas the correlation part interpolates the local variabilities.
- OPC-Kriging is preferable to SPC-Kriging, despite the increased computational effort.
- PC-Kriging performs better than PCE and Kriging according to the relative generalization error (L_2-error), especially for small experimental designs.
- For large experimental designs, PC-Kriging converges to PCE.
- PC-Kriging is suitable for **reliability analysis** and **design optimization**, *i.e.* adaptive designs, due to the stochastic nature of the Kriging predictor.

References

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