Sparse polynomial chaos expansions: Benchmark of compressive sensing solvers and experimental design techniques

Nora Lüthen
ETH Zurich, Switzerland

Supervisor(s): Prof. Bruno Sudret (ETH Zurich)

Ph.D. expected duration: Apr. 2018 - Apr. 2022

Adress: Stefano-Franscini-Platz 5, 8093 Zurich

Email: luethen@ibk.baug.ethz.ch

Abstract: Polynomial chaos expansions (PCE) are a well-known and popular surrogate modelling technique that expands the model response in terms of orthogonal polynomial functions of the input random variables. While PCEs work well for low input dimensions, the accurate computation of their coefficients becomes challenging in high dimensions, because the number of basis functions (and hence coefficients) grows exponentially with the dimension. The same holds for the case when polynomials of high degree are required to achieve a good approximation. At the same time, traditional methods for computing the coefficients of a PCE, such as projection or least-squares regression, require a number of model evaluations that is larger than the number of basis functions. Both challenges limit the applicability of such PCE methods to high-dimensional, costly models.

Fortunately, these issues can be addressed by using the Compressive Sensing framework to compute a sparse PCE, i.e., one for which only few of the coefficients are nonzero. Here, the regression problem is modified by adding a constraint on the sparsity of the solution. Sparse PCEs perform well if the model is compressible, i.e., if the coefficients of a high-dimensional PC approximation to the model decay sufficiently fast. This is usually the case for real-world models. Moreover, sparse PCEs need by far less model evaluations than traditional methods, which enables their use in high-dimensional and high-degree settings.

In recent years, a large number of articles has been published that propose efficient methods for computing sparse PCEs from a small number of model evaluations, using ideas from Compressive Sensing. Many of these contributions have good theoretical guarantees as well as superior performance on example problems. However, comparisons are often only made with respect to standard methods, not to other recent developments. Also, the methods vary considerably in computational demand. For engineers who want to apply sparse PCE to their problems but not read and evaluate the large literature on the topic, a guideline is needed to decide which method shall be used in a given situation.

Our contribution is a literature review together with extensive numerical benchmarking. We collect and explain the available methods and analyse their behavior on various analytical and numerical examples. We also propose a general modular framework for adaptive sparse PCE computations, in which most of the methods put forward in the literature can be fit. In particular, the main modules are basis adaptivity, sampling or enrichment of the experimental design, and computing a solution to the sparse regression problem. The adaptive sparse PCE procedure consists of the repeated execution of these modules.

For each of the modules, many methods have been proposed in the literature. As an example, for creating the experimental design there are

- space-filling methods such as Sobol sequences and Latin hypercube sampling (LHS);

- random methods such as Monte Carlo sampling and coherence-optimal sampling [4]; and
- methods based on optimizing a scalar function of the PC evaluation matrix over a pool of candidate samples, such as D-optimal [2], S-optimal [3] and near-optimal [1] sampling.

Likewise, many methods have been proposed for the solution of the sparse regression problem. The clear structuring of the sparse PCE procedure into modules naturally leads to a few new combinations of methods that have not yet been considered in the literature. Numerical results on example problems are presented that help guide the decision about which method shall be used in which situation.

Figure 1 shows exemplary results for surrogating the Ishigami function with a sparse PCE, using a number of different ED sampling techniques and a basis of total degree 20 (with 1771 candidate regressors). LAR is used to solve the sparse regression problem.

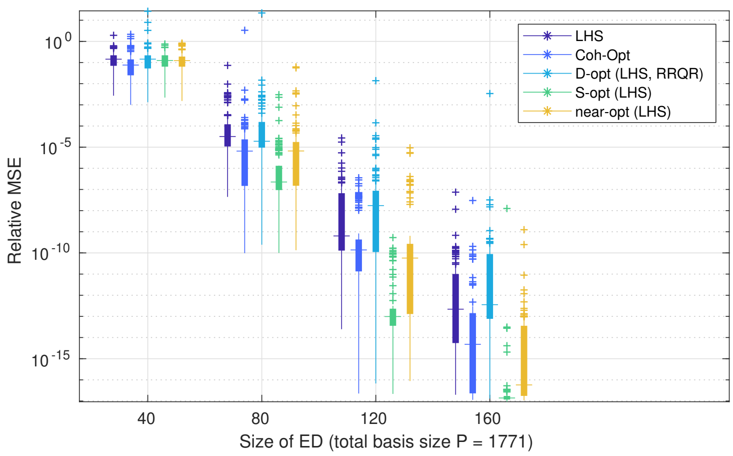

Figure 1: Surrogating the Ishigami function with sparse PCE: Plot of relative MSE against number of design points for different ED sampling techniques (sparse solver: LAR, basis: total degree ≤ 20, 100 replications).

References

[1] N. Alemazkoor and H. Meidani. A near-optimal sampling strategy for sparse recovery of polynomial chaos expansions. *J. Comp. Phys.*, 371:137–151, 2018.

[2] P. Diaz, A. Doostan, and J. Hampton. Sparse polynomial chaos expansions via compressed sensing and D-optimal design. *Comput. Methods Appl. Mech. Engrg.*, 336:640–666, 2018.

[3] N. Fajraoui, S. Marelli, and B. Sudret. Sequential design of experiment for sparse polynomial chaos expansions. *SIAM/ASA J. Unc. Quant.*, 5(1):1061–1085, 2017.

[4] J. Hampton and A. Doostan. Compressive sampling of polynomial chaos expansions: Convergence analysis and sampling strategies. *J. Comp. Phys.*, 280:363–386, 2015.

Short biography – Nora has studied mathematics with an emphasis on numerical mathematics at the University of Bonn, Germany. Since 2018, she is PhD student in Prof. Sudret's Chair of Risk, Safety and Uncertainty Quantification at ETH Zurich in Switzerland. Her PhD is part of the project "Surrogate modelling for stochastic simulators" funded by the Swiss National Science Foundation.