Multi-fidelity machine learning by the sparse grid combination technique

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Abstract

The solution of parametric partial differential equations or other parametric problems is the main component of many applications in scientific computing. Such applications include, but are not limited to, uncertainty quantification, inverse problems and optimization. To avoid the re-implementation of scientific simulation codes, the use of snapshot-based (non-intrusive) techniques for the solution of parametric problems becomes very attractive.

In this presentation, I will report on ongoing work to solve parametric problems with a higher-dimensional parameter space by means of approximation in reproducing kernel Hilbert spaces. In presence of regularization, approximation in reproducing kernel Hilbert spaces is equivalent to the so-called "kernel ridge regression", which is a classical approach in machine learning. In that sense, results on the use of machine learning for an efficient approximation of parametric problems will be discussed.

One challenge in parametric problems with high-dimensional parameter space is the high number of simulation snapshots that has to be computed in order to get a low approximation error with respect to the parameter space. If a single simulation is computationally expensive, many simulations of this kind become computationally intractable. To overcome this, we have introduced a multi-fidelity kernel ridge regression approach based on the sparse grid combination technique or multi-index approximation. In fact, this approach allows to significantly reduce the number of expensive calculations by adding coarser and coarser simulation snapshots.

The results presented in this talk include applications in quantum chemistry [1] and computational fluid mechanics [2] and are based in parts on joined work with Michael Griebel, Helmut Harbrecht, Bing Huang, Christian Rieger and Anatole von Lilienfeld (in alphabetical order).

References

[1] P. Zaspel, B. Huang, H. Harbrecht and O.A. von Lilienfeld: *Boosting quantum machine learning models with multi-level combination technique: Pople diagrams revisited*, Journal of Chemical Theory and Computation, 15(3):1546-1559, 2019; also available as arXiv:1808.02799.

[2] M. Griebel, Ch. Rieger and P. Zaspel: *Kernel-based stochastic collocation for the random two-phase Navier-Stokes equations*, Accepted for publication in International Journal for Uncertainty Quantification, April 2019; also available as arXiv:1810.11270.