Adaptive Gaussian Process Regression for Efficient Building of Surrogate Models in Inverse Problems

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Given a task where many similar inverse problems need to be solved, evaluating costly simulations is infeasible, such that replacing the model y with a fast to evaluate surrogate model y_s results in a significant speed up. The approximation quality of the surrogate model depends highly on the number, position and accuracy of the sample points. Given an additional finite computational budget hence leads to a design of (computer) experiment problem. In contrast to the selection of sample points, the accuracy-effort trade off has so fast barely been investigated systematically e.g., [1]. We therefore propose an adaptive algorithm for finding an optimal design in terms of position *and* accuracies. Following a sequential design by incrementally spending computational budget, leads to a convex and constrained optimization problem. As surrogate we construct a Gaussian process regression model. We measure the global approximation error by its impaxt on the accuracy of the identified parameter, and aim at a uniform absolute tolerance, assuming y_s being calculated by finite element computation. A priori error estimates and a coarse estimate of the computational work relates the expected improvement of the surrogate model error the computational work, which leads to the most efficient combination of sample point and evaluation tolerance. We also allow for improving the accuracy of already existing sample points by continuing previously truncated finite element solution procedures.

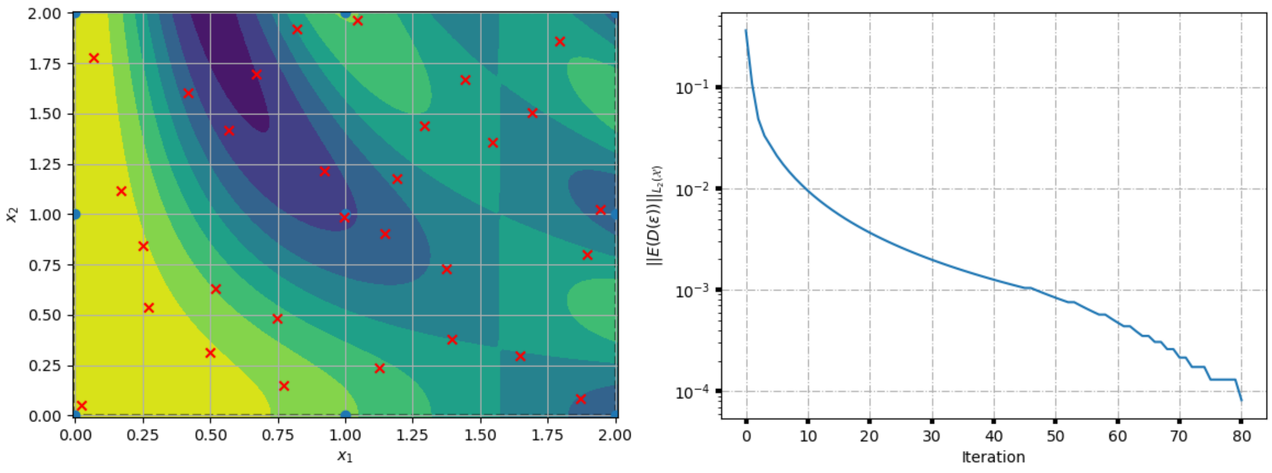

Figure 1: Left: Initial data points are indicated with blue dots. Red crosses are adaptively added data points. The color mapping indicates the isolines of y. Right: Log-plot of global error estimator over number of iterations.

References

[1] G. Sagnol, H.-C. Hege, and M. Weiser. Using sparse kernels to design computer experiments with tunable precision. In A. Colubi, A. Blanco, and C. Gatu, editors, *Proceedings of COMPSTAT 2016*, pages 397–408, 2016.