

# Multi-fidelity, model-based stochastic optimization: applications in random media.

Constantin Grigo\*

Technische Universität München  
Boltzmannstr. 15, 85748 Garching b. München, Germany  
constantin.grigo@tum.de

## ABSTRACT

In various fields of engineering and applied sciences, processes can only be controlled up to a particular degree of uncertainty, be it in structural element conception [6] or in material microstructure design [5]. The design of such system using rigorous optimization tools in the presence of uncertainty poses significant computational difficulties as several solutions of the forward problem are needed to evaluate the objective function and/or its gradient. Forward solver evaluations of typical physical or engineering problems, e.g. a finite element analysis, may take up several CPU-hours. Hence, the problem of stochastic optimization quickly becomes infeasible.

This paper explores strategies that utilize multi-fidelity solvers in order to enable efficient and accurate solutions to model-based, stochastic optimization problems. To that end, we advocate probabilistic surrogate models [3, 1] which are trained on a relatively small number of forward solver solutions. Unavoidably this introduces a significant component of predictive uncertainty that should be accounted for in the formulation of the optimization problem. This leads not just to point estimates of the optima, but also confidence metrics that can in turn be used for adaptive enrichment of the training dataset. We discuss challenges related to high-dimensional problems both in terms of the random and design variables and statistical learning tools that can discover low-dimensional salient features. We finally present advanced Monte Carlo strategies [2] as well as efficient optimization algorithms tailored to noisy estimates of gradients [7, 4].

## References

- [1] I. Bilonis and N. Zabaras. Solution of inverse problems with limited forward solver evaluations: a Bayesian perspective. *Inverse Problems*, 30(1):015004, 2014.
- [2] P. Del Moral, A. Doucet, and A. Jasra. Sequential monte carlo samplers. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(3):411–436, 2006.
- [3] S. Koziel, D. Ciaurri, and L. Leifsson. Surrogatebased methods. In S. Koziel and X.-S. Yang, editors, *Computational Optimization, Methods and Algorithms*, volume 356 of *Studies in Computational Intelligence*, pages 33–59. Springer Berlin Heidelberg, 2011.
- [4] H. J. Kushner and G. G. Yin. *Stochastic Approximation and Recursive Algorithms and Applications*. 2003.
- [5] S. Sankaran and N. Zabaras. Computing property variability of polycrystals induced by grain size and orientation uncertainties. *Acta Materialia*, 55(7):2279–2290, 2007.
- [6] P. Seshadri, P. Constantine, G. Iaccarino, and G. Parks. Aggressive design : A density-matching approach for optimization under uncertainty arXiv : submit / 1074553 [ math . OC ] 24 Sep 2014. 2014.
- [7] J. C. Spall. *Introduction to Stochastic Search and Optimization*. John Wiley & Sons, Inc., 2005.