Multigrid Monte Carlo Revisited: Fast Sampling of Gaussian Random Fields

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Abstract

The fast simulation of Gaussian random fields plays a pivotal role in Uncertainty Quantification, data science and spatial statistics. In theory, it is a well understood problem, but in practice the efficiency and performance of traditional sampling procedures degenerates quickly when the random field is discretised on a fine grid. Most existing algorithms, such as Cholesky factorisation samplers, do not scale well on large-scale parallel computers. On the other hand, stationary, iterative approaches such as the Gibbs sampler become extremely inefficient at high grid resolution since they perform inherently local updates. In the late 1980s Goodman & Sokal [1] showed that the Gibbs sampler can be accelerated using multigrid ideas. The key observation is the intricate connection of random samplers, such as the Gibbs method, with iterative solvers for linear systems also pointed out in [2]: both methods have very similar convergence properties. Based on this observation, Goodman & Sokal proposed the so-called multigrid Monte Carlo (MGMC) method for hierarchical sampling and applied it to problems in quantum physics. However, MGMC does not overcome critical slowing down in simulations of field theories near phase transitions.

In [3] we extend the MGMC algorithm to the important setting of a Gaussian random field conditioned on noisy data via a Bayesian approach; in this case, the precision matrix is a finite-rank perturbation of some differential operator. By using a bespoke variant of the Gibbs sampler with a low-rank update on each level of the multigrid hierarchy we are able to generate Markov chains with a fixed, grid-independent integrated autocorrelation time. Our theoretical analysis is confirmed by numerical experiments for sampling rough Gaussian random fields in two and three dimensions. At high resolution MGMC is able to produce independent samples at a faster rate than a Cholesky sampler. We also extend MGMC to a purely algebraic setting to handle problems formulated on graphs and unstructured grids; in this case our implementation leverages existing building blocks from the well-established PETSc iterative solver library.

References

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