

Monte Carlo Adjoints

Target group

M.Sc. Mathematics

Description of the topic

Context. When solving optimization problems constrained by high-dimensional PDEs, Monte Carlo particle methods are often the most practical approach to simulate the PDE. These methods produce approximate solutions to the given PDEs with a stochastic error. Consequently, producing noisy evaluations of the objective functional. This noise causes challenges in the numerical computation of gradients of the objective function to the parameter being optimized.

Adjoint Monte Carlo. A suitable approach to compute gradients in this setting is the adjoint method. This method works by deriving an adjoint PDE through which the gradient can be computed. In the Monte Carlo setting, the discretization of this adjoint PDE results in time-reversed particle simulations, to compute a numerical gradient.

Challenges. To achieve good convergence behavior in the optimization loop, one must simulate the same trajectories in both the Monte Carlo solver used to evaluate the objective functional. Ideally, one wishes to do so without requiring the excessive storage of these paths in memory. Hence, clever techniques are required to perform such computations efficiently.

Helpful prerequisites

Helpful prerequisites for working on this topic:

- Monte Carlo simulation / stochastic simulation
- Optimization theory
- Knowledge of a relevant model, e.g., kinetic models, financial SDEs, rendering equation, ...
- Programming: C++ is a bonus, Python is also possible

Exemplary questions

- How can existing methods in adjoint Monte Carlo be applied to new problems?
- How can one reduce the memory requirement of simulations through the use of specialized random number generators that can be used to re-compute Monte Carlo trajectories backwards in time?
- How do these reversible random number generators compare with alternative approaches to compute adjoints.

Contact

Computational Science and Mathematical Methods <https://www.scc.kit.edu/forschung/csmm.php>
Dr. Emil Løvbak (emil.loevbak@kit.edu)