Monte Carlo methods
Syllabus, schedule (tentative)

Course description

The theory and practice of Monte Carlo methods. Random number generators and direct sampling methods, visualization and error bars. Variance reduction methods, including multi-level methods and importance sampling. Markov chain Monte Carlo (MCMC), detailed balance, non-degeneracy and convergence theorems. Advanced MCMC, including Langevin and MALA, Hamiltonian, and affine invariant ensemble samplers. Theory and estimation of auto-correlation functions for MCMC error bars. Rare event methods including nested sampling, milestoning, and transition path sampling. Multi-step methods for integration including Wang Landau and related thermodynamic integration methods. Application to sampling problems in physical chemistry and statistical physics and to Bayesian statistics.

Prerequisites

Necessary

- A good probability course at the level of *Theory of Probability* (math, undergrad) or *Fundamentals of Probability* (math, masters level)
- Linear algebra: Factorizations (especially Cholesky), subspaces, solvability conditions, symmetric and non-symmetric eigenvalue problem and applications
- Working knowledge of a programming language such as Python, Matlab, C++, Fortran, etc.
- Familiarity with numerical computing at the level of *Scientific Computing*

Desirable

- Numerical methods for ODE
- *Applied Stochastic Analysis*
- Familiarity with an application area, either basic statistical mechanics (Gibbs Boltzmann distribution) or Bayesian statistics.

Workload and grading

The grade will be based on bi-weekly computing and analysis assignments and on a final project. The project can be individual or with a small group. There will be project presentations during finals week.

Schedule (tentative, weekly)

1. Using random numbers, simulation, random number generators, histograms, scatterplots, triangleplots, error bars.
2. Direct sampling methods. CDF inversion, mappings, rejection, multivariate normal (Cholesky, inverse Cholesky), (sequential Monte Carlo??)
3. Variance reduction. control variates (with multi-level?), importance sampling/rare events
4. MCMC. Perron Frobenius (for discrete Markov chains?), detailed balance, symmetric proposal Metropolis (gaussian proposal?), composition of "moves" and the Gibbs sampler.
5. Auto-correlation, Kubo formula and auto-correlation time, spectral gap (min acceptance probability), MCMC error bar.
6. Statistical estimates of the auto-correlation function and auto-correlation time
7. Samplers with gradients, Langevin and MALA samplers. Hamiltonian
8. Application to Bayesian uncertainty quantification (UQ), estimating model parameters from data.
9. Application to Gibbs Boltzmann distributions, local update methods, introduction to multi-scale samplers.
10. Bayesian model selection and criteria for avoiding over-fitting.
11. Evidence integrals and partition functions. Thermodynamic integration methods including nested sampling, the Wang Landau method and some relatives.
12. Further methods for rare events and transition rates, transition paths and checkpoints/ milestones.
13. MCMC theory – small sets, Lovasz Simonovich function, coupling .