Monte Carlo Methods

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Monte Carlo methods are computational methods that use random numbers. They are central to many parts of computational science such as phase transitions in statistical physics, electronic structure in computational chemistry and materials science, mechanisms for chemical reactions, etc. Emerging applications include uncertainty quantification and reliability, Bayesian statistics, and nonlinear filtering. There is a strong relationship between theoretical analysis and development of novel algorithms.

This is an introduction to Monte Carlo methods with an emphasis on areas of active interest, both from a practical and a theoretical point of view. We focus on four related active research areas: finding good samplers, theoretical analysis of their convergence rates, rare event simulation, filtering and optimization.

Tentative weekly schedule

1. Introduction
   (a) Monte Carlo, curse of dimensionality, integration, simulation
   (b) Some examples:
      i. Gibbs Boltzmann distributions
      ii. Bayesian posteriors (not swimsuits in Barbados)
      iii. Iterated integrals
   (c) Random number generators
   (d) Direct samplers, mapping.
   (e) Direct samplers, rejection
   (f) Direct Gaussian samplers
   (g) The central limit theorem, and error bars
2. Markov Chain Monte Carlo – MCMC
   (a) The failure of static samplers in high dimensions
   (b) The Perron Frobenius theorem and the ergodic theorem
   (c) Balance and detailed balance
   (d) Partial resampling, heat bath, Gibbs samplers
   (e) Metropolis Hastings
   (f) Measures of convergence and error bars
   (g) Startup and total variation convergence of measures
   (h) Autocovariance, the Kubo formula, autocorrelation time

3. Examples of slow Markov chains
    (a) Random walk in a double well potential
    (b) Analysis of linear Gaussian processes,
        i. Hermite polynomials, Wick's theorem, Fock space, polynomial chaos
        ii. The discrete Laplacian
    (c) Collective modes in non-Gaussian problems
4. Filtering
    (a) Dynamic Bayesian estimation
    (b) The linear Gaussian case: Kalman filtering
    (c) Ensemble methods
        i. Particle filtering, reweighting, resampling
        ii. Examples in low and high dimensions
        iii. The extended Kalman filter
5. Quantum Monte Carlo
    (a) The Schrödinger eigenvalue problem
    (b) Variational methods
        i. Constructing trial functions
        ii. Estimating the Rayleigh Schrödinger integrals
    (c) Diffusion Monte Carlo, splitting and deleting.
    (d) Green's functions and first passage acceleration of diffusions
    (e) The fermion sign problem (briefly)
6. MCMC convergence estimates, direct methods
    (a) A coupling argument for the discrete Perron Frobenius theorem
    (b) Random walk on a hypercube
    (c) The Propp and Wilson construction
7. MCMC convergence rate theorems, Cheeger's inequality
    (a) Cheeger's constant (conductance) for a Markov chain
    (b) Total variation convergence and conductance, after Lovasz and Simonovits
    (c) Diffusion and bottlenecks
    (d) Convex analysis and isoparametric inequalities
8. MCMC convergence rate theorems, Poincare and log Sobolev inequalities

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9. Multiscale methods and collective mode acceleration strategies
   (a) Multigrid Monte Carlo
   (b) The Swendsen Wang algorithm
   (c) Langevin and hybrid Monte Carlo
   (d) Sequential sampling

10. Ensembles and state space enrichment strategies
    (a) The multi-histogram method
    (b) Simulated tempering, simulated annealing
    (c) Parallel tempering, temperature and multiscale versions
    (d) Local wells

11. Rare event simulation
    (a) Introduction to large deviation theory and the critical path
    (b) Importance sampling with large deviation theory
    (c) Transition path sampling

12. Discretization of continuous processes
    (a) Time stepping for stochastic differential equations
        i. Euler, Milstein, Runge Kutta methods
        ii. Notions of accuracy
    (b) Discretization of path integrals, renormalization approach

13. Stochastic approximation and optimization
    (a) Sensitivity analysis
        i. The pathwise differentiation (same paths) method
        ii. The likelihood ratio (score function) method
    (b) The Robbins Monro method and "online learning"
    (c) The SSA method