Monte Carlo Methods
Kevin Lin

Description: Monte Carlo (MC) methods are numerical algorithms for generating samples from probability distributions. They are widely used in scientific, engineering, and statistical computing, in problems ranging from statistical physics to Bayesian inference.

This introductory course is suitable for graduate students in both the mathematical sciences (Mathematics, Applied Mathematics, Statistics / Data Science) as well as in computer science, engineering, and physical and biological sciences. The course aims to strike a balance among

(i) key concepts and basic principles;

(ii) practical algorithms and methods; and

(iii) theoretical analysis that provides useful insights and guarantees.

Topics to be covered include:

- Brief review of probability theory
- Direct sampling methods
- Markov chains & Markov chain Monte Carlo (MCMC)
- Basic Monte Carlo error analysis
- Variance reduction
- Importance sampling

Time permitting, I will cover additional topics. Possibilities include (but are not limited to)

- Sequential Monte Carlo, data assimilation, filtering
- Rare event simulation
- Gillespie & related algorithms
- Methods for stochastic differential equations
- Exact sampling

Sample applications may be drawn from statistical physics, chemistry, Bayesian statistics, etc., depending in part on student interest. However, no background in these areas is assumed.

Learning outcomes. Students will master the basic principles of Monte Carlo algorithm design and error / convergence analysis, and be able to correctly implement, diagnose, and apply Monte Carlo algorithms to concrete problems in science and engineering.

Prerequisites: students should have mastery of probability at the advanced undergraduate-level, e.g., Math 464/564 or equivalent. A solid grounding in linear algebra (e.g., Math 410 or equivalent) and ordinary differential equations (Math 355 or equivalent) is essential. Prior exposure to stochastic processes, especially the theory of Markov chains, is helpful. Some additional topics may benefit from knowledge of, e.g., numerical analysis or advanced linear algebra. Some of this material may be reviewed as needed, and references will be provided to students. Interested students without this background are encouraged to see the instructor prior to registering for the course.

In addition to mathematical prerequisites, the ability (or willingness to learn) to program in a high level programming environment such as Matlab, Python, R, Java, Julia, etc., is assumed, as students will be given programming assignments. There is, however, no "standard" language for this course.

Grading: grading will be based on a small number of problem sets and a semester project, resulting in a paper and short talk.

Textbook: none required. I plan to follow a variety of sources, some of which are listed below. I will also provide lecture notes as needed.

General MC references:

1. J M Handscomb and D C Hammersley, _Monte Carlo Methods_, Methuen 1965

2. M H Kalos and P A Whitlock, _Monte Carlo Methods_, Wiley 2008

3. J S Liu, _Monte Carlo Strategies in Scientific Computing_, Springer 2008

4. A B Owen, _Monte Carlo theory, methods and examples_, 2013

More specialized references:

5. A Asmussen and P W Glynn, _Stochastic Simulation: Algorithms and Analysis_, Springer 2007

6. A D Sokal, "Monte Carlo methods in statistical mechanics: foundations and new algorithms," Functional Integration (Carg\'ese, 1996), 131–192, NATO Adv. Sci. Inst. Ser. B Phys., 361, Plenum, New York, 1997

Useful reference for the probability we need:

7. A J Chorin and O H Hald, _Stochastic Tools in Mathematics and Science_, Springer 2009

Approximate schedule:

* Week 1: Introduction
- What are Monte Carlo methods, and why use them?
  - Curse of dimensionality
  - Examples
- Monte Carlo integration
  - Error bars and Central Limit Theorem.

* Week 2: Transform methods
- Transform methods in 1d
- Multivariate transform methods
- Review multivariate gaussian distributions
- Sampling independent normals

* Week 3: Direct sampling
- Rejection sampling
- Examples
- Analysis

* Week 4: Markov chains and MCMC
- Review Markov chains
  - Stationary distribution
  - Perron-Frobenius
  - Detailed balance
- Metropolis-Hastings

* Week 5: Anslysis of MCMC
- Ergodic theorem
- Estimator variance and the Kubo formula
- Autocorrelation times
- Initialization bias

* Week 6: More on MCMC
- Batch means
- Metropolis-Hastings for continuous state spaces
- Gibbs sampling

* Week 7: Variance reduction
- Factors that slow convergence of MCMC
- Control variates
- Antithetic variates

* Week 8: variance reduction continued

- Stratified sampling
- Examples
- Introduction to importance sampling

* Week 9: Importance sampling
- Importance sampling
- Application to rare event simulation & Cramer's theorem

* Week 10: Importance sampling continued
- rare events continued
- implicit sampling

* Week 11: Hamiltonian Mone Carlo
- Brief review of Hamiltonian dynamics
- Numerical integration of Hamilton's equations
- Hamiltonian Monte Carlo
- Metropolis-Adjusted LAngevin (MALA)

* Week 12: nonlinear filtering and data assimilation
- Sequential Monte Carlo and particle filters
- Implicit sampling revisited

* Week 13: Kalman filters
- Ensemble Kalman filter

* Week 14: more on data assimilation
- Variational methods

* Week 15: student project presentations