Fall, 2022

MATH 6395: Stochastic Computations and Monte Carlo Methods

by Wei Cai

Objectives: To present probabilistic computational methods for finding PDEs solutions and Monte Carlo methods for high dimensional integrals and integral equations and quantum many body problems.

Reference books:

[F] Daan Frenkel, Understanding Molecular Simulation: From Algorithms to Applications, 2nd Edition, 2001

[GT] Carl Graham and Denis Talay, Stochastic simulation and Monte Carlo Methods, Springer, 2012.

[K] F. Klebaner, Introduction to Stochastic Calculus with application, 3rd edition, World Scientific Publishing Company; 2012.

[P] Tao Pang, Introduction to Quantum Monte Carlo, IOP Concise Physics, 2016.

[Pa] Pavliotis G**.** Stochastic Processes and Applications, Springer, 2014

[R] Christian Robert, George Casella Monte Carlo Statistical Methods, 2nd Edition, 2004.

[RK]* (main text) **R. Rubinstein and D. Kroese, Simulation and the Monte Carlo Method, third edition, Wiley, 2017**.

Outline of lecture topics:

Part I – Probabilistic methods for PDEs

1. Basics of probability (conditional probability some distributions, limit theorem, Poisson process, Gauss process, invariant distribution of Markov process, Shannon entropy, Kullback-Leibler cross entropy) [**RK**] Ch. 1
2. Simulation of typical distribution, Poisson, Beta, Uniform, Gaussian [**RK**] 2.2-2.9
3. Acceptance-rejection method [**RK**] 2.3.4
4. Generator of semi-group of Markov processes, forward (Fokker-Planck) and backward Kolmogorov equations **[Pa]** 2.5
5. Stochastic differential equations (SDEs) and Ito formula [**K**] 4.6
6. Feynman-Kac formula for IVP of parabolic problem, exit time, Dynkin formula and Feynman-Kac formula for BVP of elliptic problems [**K]** Ch. 6
7. Boundary integral equation and walk-on-spheres (BIE-WOS) for Dirichlet Problems (paper)
8. Feynman-Kac formula for Neumann problem and local time L(t) (paper)
9. BIE-WOS iterative method for Neumann Problem (paper)
10. Forward backward SDE and quasilinear PDEs (paper), FBSDE Deep neural networks for high dimensional PDEs (paper)

Part II – Monte Carlo method and Markov Chain Monte Carlo (MCMC)

11. Euler and Milstein methods for SDEs [**GT**] 7.2
12. Basics of Monte Carlo, integral [**R**] 3.2
13. Controlling variance of Monte Carlo method [**RK**] ch. 5,
14. Control variable, Conditional MC **[RK]** 5.3, 5.4
15. Stratified Sampling, Multi-level Monte Carlo, ([**RK**] 5.5, 5.6
16. Importance Sampling [**RK**] 5.7
17. Sequential Importance Sampling, [**RK**] 5.8
18. Invariant measure of Markov chain [**R**] 6.5
19. Markov chain Monte Carlo (MCMC) **[RK]** 6.1 Convergence **[R]** 6.6, 6.7
20. Metropolis-Hasting algorithms and convergence **[RK]** 6.2
21. Gibbs sampler, Slice sampler, reversable jump sampler **[RK]** 6.4, 6.7
22. Stimulated annealing **[RK]** 6.4
23. Monte Carlo for thermodynamics and different ensembles [**F**]

Part III – Quantum Monte Carlo Method*

24. Variational method and wave functions for N-body quantum system (Fermions and Bosons), Slater determinant, Jastrow factor
25. Variational quantum Monte Carlo (VMC), **[P]** Machine learning algorithm FermiNET (paper)
26. Diffusion Monte Carlo (DMC) **[P]**
27. Path integral Monte Carlo (PIMC) **[P]**