STAT 547E: Scalable Sampling

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Schedule. February 23rd – April 6th, Mondays and Wednesdays (12 lectures over 6 weeks).
Location. ESB 4192.
Time. 16:00–17:30.
Enrolment. To enrol or audit please email `gradinfo@stat.ubc.ca`.
Office Hours. If you have any questions or want to arrange a meeting about the course please email me at `saif.syed@stat.ubc.ca`.

Overview

Many problems in science reduce to computing expectations with respect to a probability distribution. Areas such as Bayesian statistics, statistical mechanics, computational chemistry, lattice QCD and generative modelling all require us to sample from complex, high-dimensional distributions defined only up to a normalising constant. For example, in Bayesian inference we specify a prior and a likelihood, but computing the posterior mean of a parameter requires integrating over a posterior distribution whose normalising constant (the marginal likelihood) is typically intractable. The classical approach is to use Monte Carlo methods such as Markov chain Monte Carlo (MCMC) or importance sampling to estimate these quantities. But as distributions grow more challenging, with multiple isolated modes and rare transitions between metastable states, classical methods break down. Chains get trapped, importance weights collapse, and estimates become unreliable. Multi-modality is common in challenging problems: in Bayesian statistics, multiple modes correspond to multiple plausible explanations of the data; in computational chemistry, they correspond to distinct metastable conformations of a molecule.

This course develops the modern toolkit for *scalable sampling*, focusing on *annealing methods*, the dominant paradigm for overcoming multi-modality. The idea is simple: rather than attacking the target directly, we construct a sequence of intermediate distributions that interpolate from a tractable reference to the target. Annealing manifests in several frameworks: parallel tempering runs coupled chains at different temperatures; sequential Monte Carlo propagates weighted particles through the annealing schedule. Both of these frameworks can incorporate flexility with learned neural flows and diffusions. We will also examine how annealing enables estimation of normalising constants, central to Bayesian model comparison and free energy calculations, via thermodynamic integration and related techniques.

Throughout the course, the emphasis is on implementation: students will design, analyse, tune, and benchmark these algorithms on problems where naive approaches fail.

Learning Objectives

1. Understand the fundamental Monte Carlo algorithms used for statistical inference.
2. Design robust sampling algorithms scalable to modern hardware.
3. Learn to how efficiently implement these algorithms to tackle modern inference problems.

Prerequisites

- A course in probability theory (measure theory is an asset but not required).
- Proficiency in a scientific programming language (Julia, Python, R, or similar).

Requirements and Grades

- **Homework.** One or two assignments due during the term.

- **Final Project.** A comparative report between two methods from the course. You should implement both methods, apply them to a common problem, and critically analyse their strengths and weaknesses. The project includes a write-up and a short presentation with Q&A.

Syllabus

Classical Inference. Overview of classical Monte Carlo methods including MCMC (Metropolis–Hastings algorithms, Gibbs sampling, MALA, HMC, slice sampler), importance sampling, normalising flows, and Langevin dynamics.

Parallel Annealing. Parallel/simulated tempering. Reversible versus non-reversible parallel tempering, index process and adaptive tuning of temperature schedules.

Sequential Annealing. Annealed importance sampling (AIS). Sequential Monte Carlo (SMC) samplers. Resampling strategies and degeneracy. Adaptive tempering in SMC.

Normalising Constants and Free Energy Methods. Thermodynamic integration. Normalising constant estimators from SMC and parallel tempering. Bridge sampling, BAR, and MBAR.

Neural Samplers. Normalising flows for sampling. Flow-based proposals in SMC and parallel tempering. Diffusion-based samplers and score matching. Connections to generative modelling.

References

- Neal. "Annealed Importance Sampling." *Statistics and Computing*, 2001.
- Del Moral, Doucet, and Jasra. "Sequential Monte Carlo Samplers." *JRSS-B*, 2006.
- Syed, Bouchard-Côté, Deligiannidis, and Doucet. "Non-Reversible Parallel Tempering: A Scalable Highly Parallel MCMC Scheme." *JRSS-B*, 2022.
- Gelman and Meng. "Simulating Normalizing Constants: From Importance Sampling to Bridge Sampling to Path Sampling." *Statistical Science*, 1998.
- Chopin and Papaspiliopoulos. *An Introduction to Sequential Monte Carlo.* Springer, 2020.