Sampling methods in statistical physics and Bayesian inference
Isaac Newton Institute, Cambridge, 18 July 2017

09:30 Registration

10:10 Welcome

10:20 Joris Bierkens, Warwick

Title: Piecewise deterministic Markov processes and efficiency gains through exact subsampling for MCMC

Abstract: Markov chain Monte Carlo methods provide an essential tool in statistics for sampling from complex probability distributions. While the standard approach to MCMC involves constructing discrete-time reversible Markov chains whose transition kernel is obtained via the Metropolis-Hastings algorithm, there has been recent interest in alternative schemes based on piecewise deterministic Markov processes (PDMPs). One such approach is based on the Zig-Zag process, introduced in Bierkens and Roberts (2016), which proved to provide a highly scalable sampling scheme for sampling in the big data regime (Bierkens, Fearnhead and Roberts (2016)). In this talk we will present a broad overview of these methods along with some theoretical results.

11:00 Robert Jack, Bath

Title: How does breaking detailed balance accelerate convergence to equilibrium?

Abstract: A number of recent results show that irreversible Markov chains (which lack detailed balance) tend to converge faster to their steady states, compared to reversible ones (where detailed balance holds). We analyse this convergence in terms of large deviations of time-averaged quantities. For interacting-particle systems which have hydrodynamic limits with diffusive behaviour, we present a geometrical interpretation of this acceleration, on the hydrodynamic scale [1]. We also discuss how this geometrical structure originates in the underlying (microscopic) Markov models.

[1] M Kaiser, RL Jack, and J Zimmer, "Acceleration of convergence to equilibrium in Markov chains by breaking detailed balance", J. Stat. Phys., in press (2017).

11:40 Coffee break

12:10 Manon Michel, Orange Labs

Title: Event-chain algorithms: taming randomness in Monte Carlo methods through irreversibility, factorization and lifting

Abstract: I will first present the irreversible and rejection-free Monte Carlo methods recently developed in Physics under the name Event-Chain. They have proven to produce clear acceleration over standard Monte Carlo methods, thanks to the reduction of their random-walk behavior. Their irreversible nature relies on three key ingredients: the factorized filter, the generalized lifting framework and the infinitesimal moves.

Then, I will focus on the new Forward Event-Chain version that allows to reduce the randomization needed for ergodicity, leading to a striking speed-up.

Finally, I will explain how the factorized filter may be the key to subsampling in Monte Carlo methods.

12:50 Michela Ottobre, Heriot-Watt

Title: Sampling with non-reversible dynamics

Abstract: In recent years the observation that "irreversible processes converge to equilibrium faster than their reversible counterparts" has sparked a significant amount of research to exploit irreversibility within sampling schemes, thereby accelerating convergence of the resulting Markov Chains. It is now understood how to design irreversible continuous-time dynamics with prescribed invariant measure. However, for sampling/simulation purposes, such dynamics still need to undergo discretization and, as it is well known, naive discretizations can completely destroy all the good properties of the continuous-time process.

In this talk we will i) give some background on irreversibility ii) present some pros and cons of using irreversible proposals within reversible schemes (Joint work with K. Spiliopoulos and N. Pillai).

13:30 Lunch break

15:00 Tony Maggs, CNRS and ESPCI Paris

Title: Multi-scale algorithms for simple fluids

Abstract: We consider multi-scale algorithms for the simulation of dense simple fluids based on both Monte Carlo sampling and molecular dynamics algorithms. We pay particular attention to the imposition of detailed balance and show that a proper choice of hierarchical sampling almost completely eliminates hydrodynamic slowing down.

We also link to recent algorithms for accelerating the simulation of hydrodynamic interactions in polymeric systems and present ideas on how to attack,more efficiently, long-ranged electrostatic interactions.

15:40 Andrew Duncan, Sussex and the Alan Turing Institute

Title: Measuring Sample Discrepancy with Diffusions

Abstract: In many applications one often wishes to quantify the discrepancy between a sample and a target probability distribution. This has become particularly relevant for Markov Chain Monte Carlo methods, where practitioners are now turning to biased methods which trade off asymptotic exactness for computational speed. While a reduction in variance due to more rapid sampling can outweigh the bias introduced, the inexactness creates new challenges for parameter selection. The natural metric in which to quantify this discrepancy is the Wasserstein or Kantorovich metric. However, the computational difficulties in computing this quantity has typically dissuaded practitioners. To address this, we introduce a new computable quality measure based on Stein's method that quantifies the maximum discrepancy between sample and target expectations over a large class of test functions. We demonstrate this tool by comparing exact, biased, and deterministic sample sequences and illustrate applications to hyperparameter selection, convergence rate assessment, and quantifying bias-variance tradeoffs in posterior inference.