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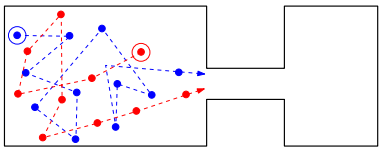
Master internship proposal



On the convergence of iterative sampling methods and the detection of meta-stable states in dynamical systems

Keywords: dynamical systems, meta-stable states, Monte Carlo Markov Chain, two-sample tests, high dimensional geometry, molecular conformations.

Context. In the theory of dynamical systems, loosely speaking, a *meta-stable state* is a region in phase or conformational space where the system remains sufficiently long before jumping to another such state, via some *transition* which is in general a *rare* event. Equivalently, such a state may be characterized by *local* ergodicity, meaning that for such a region and at the relevant time scale, spatial averages equal time averages [1]. A key difficulty for complex systems, for example a molecule undergoing conformational changes, is to understand the multiple scales at which the system is meta stable.

In statistics, the convergence of iterative methods in general and Monte Carlo Markov chains in particular relies on techniques related to r-hat ($\hat{R}$) and effective sample sizes [2]. In the theory of statistical hypothesis testing [3], a two-sample test is a statistical test aiming at detecting whether two collections of samples (*e.g.* in a high dimensional space, on a manifold, etc) have the same underlying distribution [4].

Goals. The goal of this master internship is to develop a novel approach for the detection of meta-stable states in dynamical systems, using ideas from geometry [5], information theory [6, 7], and statistical hypothesis testing [4]. Tests will be conducted on classical test systems [8], as well as on proteins undergoing conformational changes [9].

The work envisioned encompasses the design and mathematical analysis of algorithms, their coding (C++ and python), as well their experimental evaluation.

Training. Master 2 or equivalent degree in Computer science (algorithms) or machine learning or statistics or statistical physics.

Misc. Internship with *gratification*. Possibility to follow-up with a **PhD thesis**.

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