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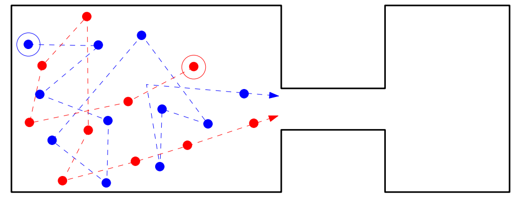

PhD thesis proposal

Online detection of meta-stable states in dynamical systems: a two-sample test based approach

Keywords: dynamical systems, meta-stable states, two-sample tests, high dimensional geometry, deep learning, Bayesian models, protein structures.

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 a *local* ergodicity property, 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 protein molecular undergoing conformational changes, or a dynamical system modeling the climate, is to understand the multiple scales at which the system is meta stable.

In the theory of statistical hypothesis testing [2], 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. The test is termed *online* if the number of samples is not fixed a priori, but the test accommodates two sources of data providing samples online.

Goals. The goal of this PhD thesis is to develop a novel approach for the detection of meta-stable states in dynamical systems, using ideas from geometry, information theory, and statistical hypothesis testing [3, 4, 5]. Two applications will be considered. The first one is the problem of sampling protein conformations using advanced *proposals* or *move sets* studied [6], an especially challenging case since protein motions span 15 orders of magnitude in time scales [7][8]. The second one is the assessment of the convergence of MCMC processes used in machine learning to learn generative models, including Boltzmann samplers [9] and Bayesian models [10, 11], to make such models more robust and sustainable.

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.

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