Πανεπιστημιο Κρητης

Τμημα Μαθηματικων και Εφαρμοσμενων Μαθηματικων

Ομιλιες Στατιστικης και Πιθανοτητων

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Αίθουσα A-303

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Bayesian Uncertainty Quantification in Pharmacodynamics and Molecular Dynamics

Bayesian computations, such Bayesian Uncertainty Quantification (BUQ), benefit today from the availability of large scale data as well as new efficient sampling algorithms and powerful supercomputers. In this presentation, I will discuss all the stages of BUQ, from the development of a novel sampling algorithm to the application in computationally demanding applications.

In the first part of the talk I will present a novel method for the effective sampling of the posterior distributions in Bayesian inference problems. The algorithm combines the local search capabilities of the Manifold Metropolis Adjusted Langevin transition kernels with the advantages of global exploration by a population based sampling algorithm. The capabilities of our method will be demonstrated in sampling a challenging posterior distribution resulting from a Pharmacodynamics inference problem. In the second part I will present an application of BUQ in Molecular Dynamics: we reconsider the repulsive exponent in the Lennard-Jones potential, traditionally set to 12. For this purpose, we will employ a Hierarchical Bayesian method and use experimental data from the radial distribution function of argon for various thermodynamic conditions. I will demonstrate that the inferred exponents are close to 6 and are able to simulate the system in a bigger variety of thermodynamic conditions.