Mathematics, Statistics, and Computer Science **@ UIC**

## Statistics and Data Science Seminar

*A method for computing transition pathways of conformational changes of a biomolecule*

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**Abstract:** Molecular dynamics (MD) is a computer simulation method for studying the physical movement of atoms and molecules. It has broad applications in many fields of sciences. In this talk, I will discuss how we use MD to compute transition pathways of conformational change, given two different metastable states of a biomolecule. In particular, we proposed an efficient algorithm, Maximum Flux Transition Paths, to compute such a path and applied the method to the Src tyrosine kinase family, which has long been implicated in the development of cancer.

Maximum Flux Transition Paths relies on efficiently computing the free energy and proto-diffusion tensor, which are computed as the conditional expectations of some "observable'' A(x) that depend on random states x drawn from distributions that are known except for their normalizing factor. Vast amounts of computer time are used to compute these expectations. Markov chain Monte Carlo methods are very popular for computing these expectations. In this talk, I will also discuss the challenge of this method and how to estimate the accuracy of these expectations.

Wednesday, March 7 at 4:00 PM in SEO 636