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

Analysis and Applied Mathematics Seminar

Sampling from Rough Energy Landscapes

Gideon Simpson (Drexel University)

Abstract: Rough energy landscapes appear in a variety of applications including disordered media and soft matter. In this work, we examine challenges to sampling from Boltzmann distributions associated with rough energy landscapes. Here, the roughness will correspond to highly oscillatory, but bounded, perturbations of a fundamentally smooth landscape. Through a combination of numerical experiments and asymptotic analysis, we demonstrate that the performance of Metropolis Adjusted Langevin Algorithm can be severely attenuated as the roughness increases. In contrast, we prove, rigorously, that Random Walk Metropolis is insensitive to such roughness. We also formulate two alternative sampling strategies that incorporate large scale features of the energy landscape, while resisting the impact of roughness; these also outperform Random Walk Metropolis. Numerical experiments on these landscapes are presented that confirm our predictions. Open analysis questions and numerical challenges are also highlighted.

This is joint work with P. Plechac (Delaware).

Monday, March 4 at 4:00 PM in 636 SEO