The University of Chicago

Departments of Computer Science,
Mathematics, and Statistics

Scientific and Statistical Computing Seminar

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Transition Paths of Conformational Change at Minimal Cost

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133 Eckhart Hall, 5734 S. University Avenue.

ABSTRACT

Given two meta-stable states of a biomolecular system, the problem is to compute a path that well represents an ensemble of trajectories connecting the states. This is potentially an extremely CPU-intensive computation. Considered here is the question of how to get a high quality result with minimal computational (and programming) effort. These considerations, and the application of transition path theory of E & Vanden-Eijnden (2006), lead to what is termed a Maximum Flux Transition Path. This turns out to be a generalization of the minimum resistance path of Berkowitz et al (1983), for which there is an implementation, MaxFlux, proposed by Huo & Straub (1997). Presented are the underlying assumptions, theoretical properties, and comparisons to other minimal cost approaches. The numerical calculation of involves 3 components: discretization, sampling, and minimization, each presenting significant challenges.

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