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Finding saddle points of energy landscapes: why and how?

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One way to bridge the scale between full atomistic models and more coarse-grained descriptions is to use Markov State models parameterized by the Eyring Kramers formulas. These formulas give the hopping rates between local minima of the potential energy function. They require to identify the local minima and saddle points of the potential energy function. This approach is for example used in materials science (kinetic Monte Carlo models, accelerated dynamics à la A.F. Voter and D. Perez).

In this talk, I will first present a recent result obtained in collaboration with D. Le Peutrec (Université d'Orléans) and B. Nectoux (Université Clermont Auvergne) about the mathematical foundations of this approach, by deriving these Eyring-Kramers exit rates starting from the overdamped Langevin dynamics [1]. I will then introduce a recent algorithm we proposed together with P. Parpas (Imperial College London) in order to locate saddle points [2]. I will explain why these two works both rely on concentration properties of the eigenvectors of Witten Laplacians, in the small temperature regime.

References:
[1] TL, D. Le Peutrec and B. Nectoux, Eyring-Kramers exit rates for the overdamped Langevin dynamics: the case with saddle points on the boundary, https://arxiv.org/abs/2207.09284.
[2] TL, P. Parpas /Using Witten Laplacians to locate index-1 saddle points/, https://arxiv.org/abs/2212.10135.

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Classification de Session: Challenge and Perspective