


复旦大学数学科学学院
数学综合报告会

报告题目： Active Learning for Transition State Calculation

报告人：周翔（香港城市大学）

时间：2021-10-15 星期五 13:00-14:00

地点：光华东主楼1801

报告摘要：

The transition state (TS) calculation is a grand challenge for computational intensive energy function such as potential energy surface (PES). The traditional methods need to evaluate the gradients of the energy function at a very large number of locations. To reduce the number of expensive computations of the true gradients, we propose an active learning framework for this problem consisting of a statistical surrogate model, Gaussian process regression (GPR) for the energy function, and a single-walker dynamics method: gentle accent dynamics (GAD) for saddle search. TS is detected by the GAD applied to the GPR surrogate of the gradient vector and the Hessian matrix of the original model. The active learning is our key ingredient for efficiency improvements, which sequentially designs the most informative locations and takes evaluations of the original model at these locations to train GPR. We formulate this active learning task as the optimal experimental design problem and propose a very efficient sample-based sub-optimal criterion to construct the optimal locations. We show that the new method significantly decreases the required number of energy/force evaluations of the original model.

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