Aalto University

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Machine learning tools for chemistry: statistical methods for finding saddle points and minimum energy paths

Title of the dissertation	Algorithms for Finding Saddle Points and Minimum Energy Paths Using Gaussian Process Regression
Contents of the dissertation	Chemical reactions and other transitions involving rearrangements of atoms can be studied theoretically by analyzing a potential energy surface defined in a high-dimensional space of atom coordinates. Local minimum points of the energy surface correspond to stable states of the system, and minimum energy paths connecting these states characterize mechanisms of possible transitions. Of particular interest is often the maximum point of the minimum energy path, which is located at a first-order saddle point of the energy surface and can be used to estimate the activation energy and rate of the particular transition. Minimum energy paths and saddle points have been traditionally searched with iterative methods guided by imaginary forces based on gradient vectors of the potential energy surface. Since accurate evaluation of the gradient vector is often computationally expensive, the information obtained from previous iterations should be utilized as efficiently as possible to decrease the number of iterations. Using statistical models, an approximation to the energy surface can be constructed, and a minimum energy path or a saddle point can be searched on the approximate surface. The accuracy of the solution can be checked with further evaluations, which can be then used to update the model for following iterations. In this dissertation, machine learning algorithms based on Gaussian process regression are developed to enhance searches of minimum energy paths and saddle points. Based on simple test examples, the methods utilizing Gaussian processes may reduce the number of evaluations to a fraction of what is required by conventional methods.
Field of the dissertation	Computational science
Doctoral candidate	Olli-Pekka Koistinen, M.Sc.(Tech.)
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Opponent	Prof. Thomas Bligaard, Technical University of Denmark
Custos	Prof. Aki Vehtari, Aalto University School of Science, Dept. of Computer Science
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Doctoral candidate's contact information	Olli-Pekka Koistinen, Dept. of Computer Science olli-pekka.koistinen@aalto.fi, p. +358400246285