Algorithms help to find minimum energy paths and saddle points more effectively

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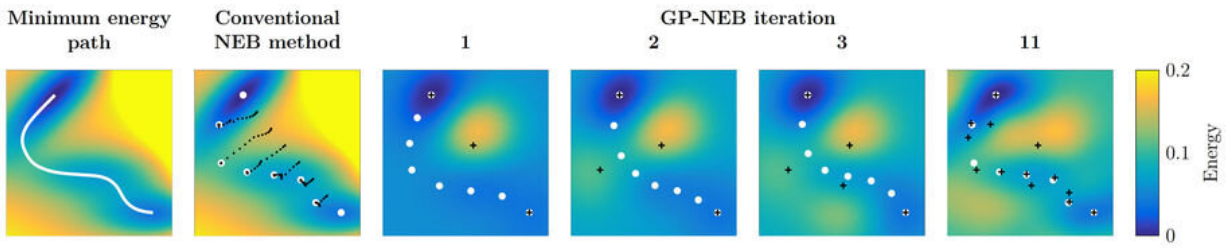

Credit: J. Chem. Phys. 147, 152720 (2017), AIP Publishing

Olli-Pekka Koistinen, doctoral candidate at Aalto University, developed machine-learning algorithms based on Gaussian process regression to enhance searches of minimum energy paths and saddle points, and tested how well the algorithms work.

In theoretical chemistry, finding minimum energy paths and saddle points is among the problems that consume the most time and computational resources. The bottleneck is the accurate evaluation of energy and forces for each atomic configuration, which typically needs to be performed at hundreds of points in the configuration space.

Algorithms using machine learning can reduce the number of observation points and expensive energy evaluations to a fraction of what is required by conventional methods, and thus speed up the

computation.

Minimum energy paths lie on a potential energy surface that describes the energy of a particular system—a molecule, for example—in terms of particular parameters. Usually, these parameters show the locations of the atoms. The local minimum points of the energy surface correspond to the stable states of the system. The minimum energy paths connect these points and describe possible reaction mechanisms.

"As an orienteer, I see this energy surface as a map. The stable atom configurations are shown as depressions on the map, and the minimum energy path is a route between two such depressions. It stays as low as possible all along the way. The highest point of the path is at a saddle point where you can get from one depression into another one staying as low as possible," Koistinen explains.

Traditionally, researchers have searched for minimum energy paths and saddle points using iterative methods that proceed on an energy surface with small steps. With the help of machine learning and statistical models, previous observations can be used to model the energy surface, and the goal can be reached with significantly fewer iterations.

Therefore, machine learning offers a more effective, lighter and thus cheaper and more ecological option. It can also open new possibilities for studying problems that have not been feasible with traditional methods. "This is another example of a research topic in which machine learning methods can be helpful," Koistinen says.

More information: The dissertation is available online: aaltodoc.aalto.fi/handle/123456789/41794