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Bayesian Optimization for Conformational Energy Minimization

Consideration of the conformation of chemical systems is a highly important initial step of a reaction modeling investigation in computational chemistry, since the error introduced due to a higher energy conformer can be on the order of, or greater than, the energy differences that explain reaction mechanisms and selectivities. Unfortunately, computationally cheap, low levels of theory that are required to perform a conformational search can provide unreliable approximations of the higher-level quantum mechanical conformational energies, and it is very difficult ahead of time to know if such a low-level method will accurately select the lowest energy conformers. In addition, the large computational cost of more accurate quantum chemistry calculations means that in general it is highly impractical to compute the energies of all conformers of a chemical system, and thus one cannot normally be confident that the lowest energy conformation has been accurately modeled. To address this, we develop a Bayesian optimization algorithm which, after an initial conformational search, uses its surrogate machine learning model to select conformers that are to be modeled with high-level quantum chemistry calculations, with the aim of locating the global minimum energy conformation. Our results find that the algorithm is very efficient; on average only approximately 13 conformers were sampled before the minimum was found and typically no more than 36 were required. This represents a very large saving in terms of computational cost, considering that even medium sized organic molecules may have tens or hundreds of conformers each. Importantly, our algorithm was also equally efficient for finding the lowest energy conformers of complex hydrogen bond-donating catalyst transition states, despite the large size and complexity of these systems. This idea promises broad application in mechanistic modeling with computational chemistry, potentially allowing for computational costs substantially lower than that associated with full conformational treatment, whilst allowing for greater confidence that errors due to conformation are reduced as far as is practical.

Primary author(s) : Mr. LEWIS-ATWELL, Toby (University of Bath)

Co-author(s) : Dr. FARRAR, Elliot H. E. (University of Bath); Dr. GRAYSON, Matthew N. (University of Bath)

Presenter(s) : Mr. LEWIS-ATWELL, Toby (University of Bath)