An Overview on Simulated Annealing Vs Adaptive Mutation Simulated Annealing

Srijeeta Talukder*

ABSTRACT

Stochastic optimization algorithms are the global search engine that can find the global minima unequivocally. Most of such algorithms are based on some physical processes or natural phenomena. Simulated Annealing (SA) is one of the very popular stochastic search techniques, which has been applied in different domains of science for problem-solving. For chemists, the most common use of SA or any other stochastic optimizers is to find the geometry of molecules to which the optimizer needs to explore the very rugged multi-minima surface. Searching such surfaces to find global minima (which indicates the most stable geometry of the molecule) is not a trivial job. Generally, SA has a tendency to premature convergence, however, if one incorporates an adaptive mutation technique to get the step length for each search steps the optimizer would work in a much better way. This kind of SA is named as Adaptive Mutation Simulated Annealing (AMSA). The present paper portray an overview on SA and AMSA and a comparison on their workability is also be presented.

I. Introduction

Optimization is something that we are doing continuously knowingly or unknowingly to place ourselves in a best possible situation. Apart from the philosophical aspect, as a chemist we always need optimization algorithm to find molecular structure as we know that the stable molecular structures are none other than a minimum in potential energy surface (PES). The dimension of a potential energy surface is quite large even for a small molecule as we know that for a molecular system of N atom the dimensionality of PES is 3N-6 (for non-linear system). These multi-dimensional PES is constists of many number of minima. The stable molecular structure has most resemblance with the global minimum or deepest minimum sturucture on the PES. Thus to get the deepest minimum structure is not a trivial job. There are many optimization techniques available and a useful way to catgorise them is to divide them as deterministic approach or stochastic search processes. Deterministic approaches [1] are initial point dependents and generally fail to get the global minimum for a multi-dimentional multi-minima surface, whereas in stochastic search processes algorithm has some in-build property by which it can surmount the potential barrier to find global solution.

The stochastic optimization algorithms are generally algorithmic replica of a natural processes. There are plenty numbers of such optimizers. Some popular stochstic optimizers are Monte Carlo based algorithm [2], Particle swam opotimization [3] etc.

In the presernt study I want to portray an overview Simulated Annealing [4,5], a Monte Carlo algorithm based stochastic optimizer and its comparison with Adaptive Mutation Simulated Annealing [6].

Department of Chemistry,
Adamas University, Kolkata, 20016, India.
**Corresponding email:*
srijeeta1.talukder@adamasuniversity.ac.in