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On stochastic global optimization of one-dimensional functions

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Abstract

We consider the applicability of stochastic global optimization algorithms on test-functions whose domain of definition is a simply-connected and finite interval of real numbers. We argue on the basis of theoretical reflections of statistical physics (namely random-walk) and computer simulations that there is a decisive difference between test-problems in one and multiple dimensions pointing to the necessity to only consider test-functions in higher dimensions. We argue that only test-problems in two or more dimensions provide for the possibility to discriminate the efficiency of stochastic global optimization algorithms with respect to the complexity of the underlying physical system at all.
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1. Introduction

In such distinct fields as physics, electrical and chemical engineering or operations research the determination of the global optimum of a function or at least an

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approximation thereof is of greatest interest. Biophysicists and -chemists try to predict peptide and protein structures by minimizing a suitable energy function [1–7] and dock ligands to proteins [8–10], researchers from the fields of chemical physics and physical chemistry forecast three-dimensional structures of atomic clusters [11–17], engineers try to minimize distances on integrated circuits [18] and scientists in operations research are concerned with minimizing transport costs and production times [19,20]. Advances in this computational technique have therefore great impact on many scientific fields and are subject to ongoing research [21–28].

In several applications one encounters the problem that the optimization problem itself is NP-complete [29–31]. The computational effort to find the global optimum with certainty is therefore governed by an exponential law with respect to the size of the system under consideration [32]. This size might for example be given by the number of amino acids in a protein, the number of atoms in a cluster, or the number of components on an integrated circuit. One can only hope to give an algorithm that approaches the global optimum probabilistically in a polynomial time.

In general the computational time is related to the system size N by either

$$t_{\text{det}} = a \exp(bN) \quad \text{or} \quad t_{\text{stoch}} = \beta N^{\alpha} . \tag{1}$$

Hamacher and Wenzel [33,34] were able to distinguish the efficiency of stochastic global optimization algorithms in a generic model in chemical physics and found different scaling behavior for thermodynamical and biological-inspired approaches of global optimization.

One encounters also the one-dimensional case:

- Most processes in physical chemistry are described and best understood as a function of a reaction coordinate, like the distance of a ligand to a protein, the concentration of a compound in a mixture and several other scalars.
- High-dimensional problems can be mapped at least approximately onto a one-dimensional domain [35]. This approach was for example implemented for a geophysical problem using TRUST [36].
- One-dimensional test-functions are used to derive knowledge for applications in higher dimensions [37].

In these cases the notion of Eqs. (1) points to the reduction in the prefactor β to get an efficient algorithm.

In this paper we show that the venue of deriving knowledge from the one- to the multi-dimensional case cannot be successful due to an intrinsic characteristic of a one-dimensional search space in comparison to multi-dimensional spaces. We will argue that it is always more efficient to just sample the domain of definition randomly than to sample it by any correlated movement of a particle on the surface of the function.

The work is organized as follows: first we introduce general stochastic global optimization algorithms via the Metropolis-criterion [38]. After this brief review we describe theoretical considerations for the behavior of a general stochastic sampling algorithm in one-dimension and augment those points with results from computer