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Introduction to an optimization algorithm based on the chemical reactions

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ABSTRACT

In this paper, a novel optimization method inspired by a paradigm from nature is introduced. Chemical reactions are used as a paradigm to propose an algorithm that can be considered as a general purpose optimization technique. The proposed algorithm is described in detail and then a set of typical complex benchmark functions is used to evaluate the performance of the algorithm. Simulation results show that the proposed optimization algorithm can outperform other methods in a set of benchmark functions.

1. Introduction

Optimization is an activity carried out in almost every aspect of our life, from planning the best route in our way back home from work to more sophisticated approximations at the stock market, or the parameter optimization for a wave solder process used in a printed circuit board assembly manufacturing process; optimization theory has gained importance over the last decades, from science to applied engineering (to name a few), there is always something to optimize and of course, more than one way to do it.

In a generic definition, we may say that optimization aims to find the "best" available solution among a set of potential solutions in a defined search space. For almost every problem exists a solution, not necessarily the best, but we can always find an approximation to the "ideal solution".

When the complexity and the dimension of the search space make a problem unsolvable by a deterministic algorithm, probabilistic algorithms deal with this problem by going through a diverse set of possible solutions or candidate solutions.

Over the past years, there has been a growing interest in solving optimization problems by means of algorithms inspired on natural paradigms [1,5,7,10]. These techniques have been applied to the optimization of complex computational problems including forecasting [2], control [14,15], pattern recognition [9,16] and trajectory planning [6,13] among others, and have demonstrated not only to comply with their objectives, but they also promote the creation of new ways to give solutions to these complex problems and improve the actual methods as well [8,18,19,23].

In this paper, the main objective is to introduce a new optimization algorithm based on the chemical reactions existing on nature. In this work, we are considering the process in which the different elements existing in nature are created, behave and interact with each other to form chemical compounds. The main contribution of the paper is the introduction of the

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proposed chemical optimization algorithm that incorporates four types of chemical reactions existing in nature to achieve the goals of exploration and exploitation of the search space.

The rest of the paper is organized as follows. Theory and background are presented in Section 2. In Section 3 some of the related work is presented. In Section 4, we describe the proposed method, its characteristics and main objectives. Section 5 shows the results obtained in this paper and finally in Section 6 some conclusions and current/future work are presented.

2. Nature-inspired metaheuristics

The importance of dealing with optimization theory has grown due to the large variety of fields where optimization is applied (mathematics, computer science, engineering, etc.).

For most problems, there is more than one path to arrive to a correct solution and that's where the optimization algorithms come into play. When a deterministic algorithm is not suitable, due its complexity and/or large dimension of the search space; probabilistic algorithms come into place by going through a diverse set of possible solutions or candidate solutions. Many metaheuristic algorithms can be considered probabilistic, while they apply probability tools to solve a problem, metaheuristic algorithms seek good solutions by mimicking natural processes or paradigms. In [26] a brief history of metaheuristics can be found, including an overview of the "no free lunch theorems for optimization" by D.H. Wolpert and W.G. also, a description of the major modern metaheuristic algorithms such as genetic algorithms (GA) [10], ant colony optimization (ACO) [5], particle swarm optimization (PSO) [11], simulated annealing (SA), harmony search (HS), differential evolution (DE), the firefly algorithm (FA), cuckoo search (CS), and bat-inspired algorithm (BA), these tree last were introduced by the same author.

Note that there is a vast approach of these algorithms in the literature and in this paper we briefly described just a few.

A genetic algorithm is a stochastic global search method that mimics the metaphor of natural biological evolution. This Darwinian evolution theory is a well known paradigm that has been proved to be robust when applied to search and optimization problems [3]. Evolution is determined by a natural selection of individuals (based on their fitness); which, is expected to be better throughout a determined number of generations by means of recombination and mutation operations.

Simulated annealing is a probabilistic metaheuristic algorithm that imitates the annealing process in metallurgy, a technique that involves the slow cooling of a physical system to find low-energy states [20].

Particle swarm optimization was introduced by Kennedy and Eberhart [11]. As it name implies, it was inspired by the movement and intelligence of swarms. A swarm is a structured collection of interacting organisms such as bees, ants, or birds. Each organism in a swarm is a particle or agent. Particles and swarms in PSO are equivalent to individuals and populations in other evolutionary algorithms. Particles in a swarm cooperate by sharing knowledge. This has been shown to be a critical idea behind the success of the PSO algorithm.

DNA computing, introduced by Adleman [1], appeared in 1994 as a form of computation whose main characteristic is the use of molecular biology instead of the traditional silicon-based computer. In DNA computing, the information is represented by sequences of bases in DNA molecules called *strings* and each molecule encodes a potential solution to the problem. The main advantage when using this optimization paradigm is the inherent parallelism.

We can observe that novel metaheuristics include the representation of social behaviors, biological systems, evolution, and artificial chemistries; the algorithm presented in this paper belongs to this last group. The operations that can be applied in this methodology are: synthesis, denaturing, annealing and ligation.

3. Related work

Optimization based on chemical processes is a growing field that has been satisfactorily applied to several problems. Artificial chemistry algorithms intend to mimic as close as possible a real chemistry process, in some cases by assigning kinetic coefficients, defining molecule representation and focusing on an efficient energy conservation state.

A very accurate review of scientific work in artificial chemistry can be found in [4], where some general characteristics of the algorithms are presented and a classification is made based on their parameter representation, which can be explicit or implicit.

To name a few, a DNA based algorithm is applied in [22] to solve the small hitting set problem. This NP-complete problem takes exponential time to solve it and it was demonstrated that only polynomial time is needed to solve it when using DNA-based supercomputing. In [25] a catalytic search algorithm is explored, where some physical laws such as mass and energy conservation are taken into account. The disadvantage of this algorithm is its slow growth rates and weak selection pressure. In [17], the potential roles of energy in algorithmic chemistries are illustrated. An energy framework is introduced, which keeps the molecules within a reasonable length bounds, allowing the algorithm to behave thermodynamically and kinetically similar to real chemistry. In [12] a tutorial of the chemical reaction optimization approach introduced by Albert Y.S. Lam is presented; in this metaheuristic, the potential and kinetic energies and the energies of the surroundings are symbolically represented by the central energy buffer; the basic unit in CRO is the molecule, which is treated as an agent with certain attributes, e.g. potential and kinetic energies, molecular structures, etc.; viewed from this perspective, this molecule can be successfully described by a class and methods define the elementary reaction types (*on wall ineffective collision, decomposition, inter-molecular ineffective collision and synthesis*), making it suitable to program in with an object-oriented