Chapter 2
Theory and Background

Abstract This chapter describes the theoretical concepts and background required to understand the new nature inspired optimization method based on the paradigm of chemical reactions.

Keywords Chemical reactions • Chemistry • Nature inspired optimization

This chapter overviews the background and main definitions and basic concepts, useful to the development of this investigation work.

2.1 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 (of mathematical nature), there is more than one path to arrive to a correct solution and that's where the optimization algorithms come into play. As mentioned before, for some problems, deterministic algorithms are not suitable, due the complexity and/or large dimension of the search space; probabilistic algorithms on the other hand, deal with this problem 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.

Most of these novel optimization paradigms inspired by nature were conceived by merely observation of an existing process. These insights were embodied as computational algorithms and were later applied to solve diverse kinds of problems.

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The advantage when doing this is that –at least at the beginning-, no mathematical equations are involved. It's later, -when these techniques are widely explored-, that the theory, concepts and applications can be widely described.

Some examples of these algorithms are the Genetic Algorithms [1], Ant Colony Optimization [2], Particle Swarm Optimization [3], DNA computing [4], among others.

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 [5]. 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 [6].

Particle Swarm Optimization, was introduced by Kennedy and Eberhart [3]. 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. The position, or site, of a particle in a swarms is the vector of optimizations parameters x in PSO. Particles in a swarm cooperate by sharing knowledge. This has been shown to be critical idea behind the success of the particle PSO algorithm.

DNA computing, introduced by Adleman [4], 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.

The operations that can be applied in this methodology are: synthesis, denaturing, annealing and ligation.

2.2 Artificial Chemistry

2.2.1 The Set of Molecules S

The set of molecules $S = \{s_1, \ldots s_i, \ldots s_n\}$, where n might be infinite, describes all valid molecules that may appear in an artificial chemistry. A molecule's representation is often referred to as its structure and is set in contrast to its function, which is given by the reaction rules R. The description of valid molecules and their structure is usually the first step in the definition of an AC. This step is analogous to the part of chemistry that describes what kind of atomic configurations form stable molecules and how these molecules appear.

2.2.2 The Set of Rules R

The set of reaction rules R describes the interactions between molecules. A rule can be written according to the chemical notation of reaction rules in the form:

$$s_1 + s_2 + \ldots s_n \tag{2.1}$$

A reaction rule determines the *n* components (objects, molecules) on the left-hand side that can react and subsequently be replaced by the *m* components on the right-hand side. *n* may be called the *order* o the reaction. Note that the "+" sign is not necessarily an operator here, but only separates the components on either side.

2.2.3 Reactor Algorithm A–Dynamics

An algorithm determines how the set *R* of rules is applied to a collection of molecules *P*, called *reactor*; *soup, reaction vessel or Pool.* Note that *P* cannot be identical to *S* since some molecules might be present in many exemplars, others not at all.

Algorithm *A* depends on the representation of P. In the simplest case, without a spatial structure in *P*, the collection of molecules can be represented explicitly as a multi set or implicitly as a concentration vector.

2.3 Fuzzy Logic

Zadeh introduced the term fuzzy logic in his work "fuzzy sets", where he described the mathematics of the fuzzy set theory in 1965.

Fuzzy logic gives the opportunity to model conditions that are defined with imprecision.

The tolerance of the fuzzy in the process of human rezoning suggests that most of the logic behind the human rezoning is not the traditional bi-valued logic, or even the multi-valued, but the logic with fuzzy values, with fuzzy connections and fuzzy rules or inferences.

2.3.1 Fuzzy Sets

Fuzzy sets are an extension of the classic set theory and, as it name implies it, it is a set with boundaries not well defined, this means that the transition of belonging or not belonging to certain set is gradual, and this smooth transition is characterized by grades of membership that gives the fuzzy sets flexibility in modeling linguistic expressions commonly used, such as "the weather is cold" or "Gustavo is tall".

2.3.2 Fuzzy Logic Controller

Fuzzy control is a control method based on fuzzy logic. Just as fuzzy logic can be described simply as "computing with words rather than numbers" fuzzy control can be described simply as "control with sentences rather than equations".

The collection of rules is called a *rule base*. The rules are in the familiar if–then format, and formally the "if" side is called the *antecedent* and the "then" side is called the *consequent*.

Fuzzy controllers are being used in various control schemes; the most used is the *direct control*, where the fuzzy controller is in the forward path in a feedback control system. The process output is compares with a reference, and if there is a deviation, the controller takes action according to the control strategy.

In a *feed forward control* a measurable disturbance is being compensated, it requires a good model, but if a mathematical model is difficult or expensive to obtain, a fuzzy model may be useful. Fuzzy rules are also used to correct tuning parameters. If a nonlinear plant changes operating point it may be possible to change the parameters of the controller according to each operating point. This is called *gain scheduling* since it was originally used to change process gains.

A gain scheduling controller contains a linear controller whose parameters are changed as a function of the operating point in a preprogrammed way. It requires thorough knowledge of the plant, but it is often a good way to compensate for nonlinearities and parameter variations. Sensor measurements are used as *scheduling variables* that govern the change of the controller parameters, often by means of a table look-up.

2.4 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, by assigning kinetic coefficients, defining molecule representation and focusing on an efficient energy conservation state.

The main difference between these metaheuristics is the parameter representation, which can be explicit or implicit.

A review of scientific work in artificial chemistry can be found in [7]. Chemical inspired paradigms can be differenced by their parameter representation, which can be explicit or implicit. A DNA based algorithm is applied in [8] to solve the small hitting set problem. This NP-complete problem takes exponential time to solve it and it was demonstrated that when using DNA-based supercomputing, only polynomial time is needed to solve it.

In [9] 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 [10], 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.

A chemical reaction optimization was applied to the grid scheduling problem in [11], where molecules interact with each other aiming to reach the minimum state of free potential and kinetic energies.

The main difference of the proposed chemical optimization algorithm with respect to the previous mentioned approaches is that it has a simpler parameter representation and yet it is proven to be efficient. Since only the general schema of the chemical reactions is taken into consideration, the initial set of elements is simply represented and no extra parameters (such as mass, kinetic coefficient, etc.) are added.

The selected elements react to obtain new compounds and vice versa, and as mentioned before, no previous validation is performed; this improves efficiently the execution rate of the algorithm and ensures a broad exploration of the search space in every iteration, otherwise if the selected parents don't comply with the validation rules then no new products are generated, reducing the possibilities of fully exploring the complete search space.

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