Chapter 7
Insights Into Simulated Annealing

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ABSTRACT

Simulated annealing is a probabilistic local search method for global combinatorial optimisation problems allowing gradual convergence to a near-optimal solution. It consists of a sequence of moves from a current solution to a better one according to certain transition rules while accepting occasionally some uphill solutions in order to guarantee diversity in the domain exploration and to avoid getting caught at local optima. The process is managed by a certain static or dynamic cooling schedule that controls the number of iterations. This meta-heuristic provides several advantages that include the ability of escaping local optima and the use of small amount of short-term memory. A wide range of applications and variants have hitherto emerged as a consequence of its adaptability to many combinatorial as well as continuous optimisation cases, and also its guaranteed asymptotic convergence to the global optimum.

INTRODUCTION

Combinatorial optimisation purpose is basically to find optimal, or at least best reached, solutions out of a finite set. When the set of solutions get larger, the combinatorial optimisation is faced to an exhaustive search which is rather memory and computing time consuming. Due to the failure of exact methods to provide optimal solutions within economical computing time and memory allocation, problem-independent (or generic) methods called meta-heuristics were introduced in the 1940s, around which a wide range of studies have been emerged on account of the ease of application and implementation for many optimisation problems, despite the solid mathematical foundations behind. Meta-heuristics includes three main categories, namely evolutionary optimisation that includes genetic algorithms; swam intelligence that includes stochastic diffusion search (Bishop, 1989), ant colony optimisation (Dorigo, 1992), and Particle swarm optimisation (Kennedy & Eberhart, 1995); and local search optimisation that includes hill climbing, tabu search (Glover, 1986), and simulated annealing (Kirkpatrick, Gelatt, & Vecchi, 1983).

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Simulated annealing is a local search method for global combinatorial optimisation problems introduced by Kirkpatrick et al. (1983). This meta-heuristic consists at each iteration of generating a candidate solution that will be whether accepted as a result of a comparison with a current one. It aims at improving the current solution (in the context of minimisation, as presented herein) by means of a certain transition rule while accepting occasionally some uphill solutions in order to guarantee diversity in the domain exploration and to avoid getting caught at local optima. The process is managed by a certain cooling schedule which can be static or dynamic whereby the number of iterations is controlled. Many variants have been introduced in the literature in order to fasten the simulated annealing execution and to simplify the tuning of the different parameters. Furthermore, an extension to the multi-objective case has been developed that allows a construction of near-Pareto optimal solutions. It consists basically of using an archive that catches the non-dominated solutions while exploring the feasible domain.

This chapter provides insights into simulated annealing. It presents the fundamentals of the meta-heuristic as well as an understanding of the choice and the design of its different parameters and discusses many related concerns.

PRINCIPLES OF SIMULATED ANNEALING

Local search represents a main category of meta-heuristics that includes hill climbing, tabu search (Glover, 1986), simulated annealing (Kirkpatrick et al., 1983), and variable neighbourhood search (Mladenovic & Hansen, 1997). Local search algorithm is based on the idea consisting of starting at a given feasible solution and making, at each iteration, a sequence of moves from the current solution to a neighbouring one that improve the objective function. A neighbouring solution is determined according to a certain defined neighbourhood structure. For instance, for a solution consisting of a vector of a certain length, all vectors differing from by one component would be considered as neighbouring solutions. The iterative process is continuously repeated until reaching a (global) optimal solution or a near-optimal one if a time or iteration bound was erected. This heuristic has been initially known as hill climbing or iterative improvements. The subsequent meta-heuristics within this category have been developed with the aim to deal with some identified issues relevant to the search loop size and being caught at local optima.

Simulated annealing has been introduced based on the Metropolis algorithm (Metropolis, Rosenbluth, Rosenbluth, Teller, & Teller, 1953) introduced in equilibrium statistical mechanics. It mimics the metallurgical process of careful annealing which consists of heating a metal or alloy to a high temperature until the molecules become melted. A slow cooling is applied thereafter until the molecules coalesce into a crystalline form called the ground state. As long as the cooling is perfectly slow, the ground state is reached, which corresponds to the most solid state of the considered metal or alloys. The simulated annealing terms, summarized in Table 1, derive from both the physical mechanics and the optimisation nomenclatures. From a combinatorial optimisation perspective, simulated annealing has extended the hill climbing algorithm by introducing an occasional acceptance mechanism of uphill solutions guaranteeing thereby diversity in the domain exploration and avoiding getting caught at local optima. The process is managed by a certain, either static or dynamic, cooling schedule. The algorithm is practically expected to stop when no significant improvement still be possible or when a cooling limit is reached. Figure 1 represents the flowchart of the algorithm pointing out its two main components, namely the neighbouring solutions generation and the energy improvement evaluation.