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Performance Analysis of Simulated Annealing Using Adaptive Markov Chain Length

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Abstract. In the Simulated Annealing (SA) algorithm, the Metropolis algorithm is applied to generate a sequence of solutions in the search space, known as the Markov chain. Usually, the algorithms employ the same Markov Chain Length (MCL) in the Metropolis cycle for each temperature. However, SA can use adaptive methods to compute the MCL. This work aims to analyze the effect of using different MCL strategies in SA behavior. This experimentation considers the Water Distribution Network Design (WDND) problem, a multimodal and NP-hard problem interesting to optimize. The results indicate that the use of adaptive MCL strategies improves the solution quality versus the static one.

Keywords: Simulated Annealing, Markov Chain Length, Water Distribution Network Design, Optimization

1 Introduction

Stochastic search optimization methods are widely used in various disciplines, such as science, engineering, management, modern statistical, machine-learning applications, to mention some. Many stochastic algorithms are inspired by a biological or physical process with some heuristic manners to find the global optimum [1]. The most common methods are simulated annealing, genetic algorithms, differential evolution, particle swarm optimization, among others [2]. In this work we focus on Simulated Annealing (SA) [3,4] due to its popularity as a search procedure because of its simple concepts, good speed, and easy implementation. SA is applied to solve NP-hard problems where it is difficult to find the optimal solution or even near-to-optimum solutions [5,6].

The Simulated Annealing algorithm is based on the principles of statistical thermodynamics. The SA simulates the energy changes in a system subjected to a cooling process until it converges to an equilibrium state (steady frozen state), where the material states correspond to problem solutions, the energy of a state to a solution cost, and the temperature to a control parameter.

The SA cooling process consists of initial and final temperatures, the cooling function, and the length of the Markov chain established by the Metropolis algorithm [7]. For each value of the temperature, the SA algorithm achieves

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a certain number of Metropolis decisions. In this way, the SA consists of two cycles: one external for temperatures and the other internal, named Metropolis. Most SA literature proposals use a static Markov Chain Length (MCL) in the Metropolis cycle for each temperature [8]. But adaptive strategies to dynamically establish each MCL for the SA algorithm are also present in the literature [9,10].

The main contribution of our research is to enlarge the knowledge concerning the MCL influence on the efficiency and efficacy of a SA when solving optimization problems. In particular, we tackle the Water Distribution Network Design (WDND), which was defined as a multi-period, single-objective, and gravity-fed design optimization problem [11]. A hybrid SA (HSA), presented in [12], was used as a starting point to consider the different strategies to compute the MCL. Accordingly, research questions (RQs) arise out: Can the adaptive MCL strategies modify or improve the HSA performance in contrast with the static one? If they can, how do variable MC lengths affect the HSA behavior? To answer these RQs, we conduct experiments by applying HSA with different configurations on publicly available [13] and real-world [14] instances of the WDND problem. Furthermore, we analyze and compare these results considering the published ones in the literature.

This article is organized as follows. First, we give in Section 2 a description of the SA algorithm. In the next section, we address the strategies for computing MCL. Then, we describe the experimental design and the methodology used in Section 4. We analyze and compare the HSA behavior when solving the WDND problems in Section 5. Finally, we summarize our most important conclusions and sketch out our future work.

2 Simulated Annealing

The Simulated Annealing [3] is an efficient trajectory-based metaheuristic with the capacity of escape from local optimum. The SA generates a sequence of changes (chain) between states generated by transition probabilities, which are calculated involving the current temperature. Therefore, the SA can be modeled mathematically by Markov chains, and consists of two cycles:

- an external one, named temperature, slowly reduces the temperature to decrease defects, thus minimizing the system energy.
- an internal cycle, named Metropolis [7], generates a new potential solution (or neighbor of the current state) to the considered problem by altering the current state, according to a predefined criterion.

For each temperature, the Markov chain length usually remains without changes in the Metropolys cycle.

Figure 1 shows the general scheme of a SA algorithm, highlighting these two cycles. The SA begins with the initialization of the temperature, T, and the generation of a feasible initial solution, S_0, for the target problem. After that the two overlapping cycles begin. A new trial solution, S_1, is obtained by applying a move to the current solution, S_0, to explore other areas of the search space. At this point, S_1 is accepted with the Boltzmann probability. This process

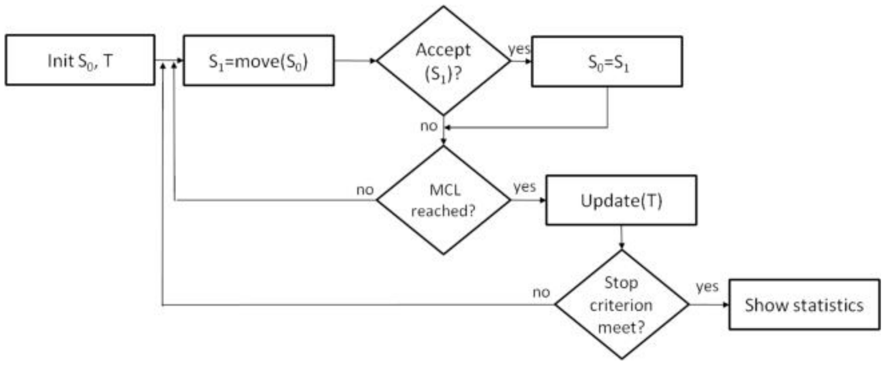

Fig. 1. Scheme of the SA algorithm.

generates a Markov chain, which is repeated until a number of steps denominated as Markov chain length. After that, the temperature in the SA algorithm is sequentially lowered until the system freezes by a cooling schedule. Finally, the SA ends the search when the total evaluation number or the temperature equilibrium ($T = 0$) is achieved.

The search space exploration is strengthened when the temperature (T) is high. But at low temperatures, the algorithm only exploits a promising region of the solution space, intensifying the search. The annealing procedure involves taking enough steps at each temperature (internal cycle). The number of steps aims to keep the system close to equilibrium until the system approaches the ground state. Traditionally, the equilibrium can be achieved by maintaining the temperature constant for a limited number of iterations; but adaptive strategies can be considered. The main objective of this work is to identify how sensitive the SA can be to the number of these iterations, by considering different strategies to compute the Markov chain length to solve NP-hard problems.

3 Markov Chain Length

The SA starts by constructing a sequence of temperatures T_1, T_2 and so on. At each step of this sequence, SA does a set of k moves to neighboring positions. Such a stochastic sequence construction is called a Markov chain, and the number of moves k is denominated Markov chain length. There are few researches in literature concerning to the effect of the MCL on the solution quality and annealing speed [9,10].

The MCL can be determined experimentally and considered static throughout the search, but also MCL can set adaptively depending on the optimization function variation. The static strategy (MCLs) assumes that each T value is held constant for a fixed number of iterations, defined before the search starts. In this work, each T value is held constant for $k = 30$ iterations, a widely used number in the scientific community. For the adaptive strategies, which depend on the characteristics of the search, we consider two different alternatives:

1. MCLa1. Cardoso et al. [9] consider that the equilibrium state is not necessarily attained at each temperature. Here, the cooling schedule is applied as soon as an improved candidate (neighbor) solution is generated. In this way, the computational effort can be drastically reduced without compromising the solution quality.
2. MCLa2. This strategy, proposed by Ali et al. [10], uses both the worst and the best solutions found in the Markov chain (inner loop) to compute the next MCL. MCLa2 increases the number of function evaluations at a given temperature if the difference between the worst and the best solutions increases. But if an improved solution is found, the MCL remains unchanged.

4 Experimental Design

In this section, we explain the experimental design tests to study the behavior of the SA introduced in [12], named HSA, using different MCL strategies to solve the WDND problem. The upcoming paragraphs briefly describe the target test problem, followed by the methodology and the parameters used.

Multi-Period Water Distribution Network Design. The mathematical formulation of the WDND is often treated as the least-cost optimization problem. The decision variables are the diameters for each pipe in the network. The problem can be characterized as simple-objective, multi-period, and gravity-fed. Two restrictions are considered: the limit of water speed in each pipe and the demand pattern that varies in time. The network can be modeled by a connected graph, which is described by a set of nodes $N = \{n_1, n_2, ...\}$, a set of pipes $P = \{p_1, p_2, ...\}$, a set of loops $L = \{l_1, l_2, ...\}$, and a set of commercially available pipe types $T = \{t_1, t_2, ...\}$. The objective of the WDND problem is to minimize the Total Investment Cost (TIC) in a water distribution network design. The TIC value is obtained by the formula shown in Equation 1.

$$\min TIC = \sum_{p \in P} \sum_{t \in T} L_p IC_t x_{p,t} \tag{1}$$

where IC_t is the cost of a pipe p of type t, L_p is the length of the pipe, and $x_{p,t}$ is the binary decision variable that determines whether the pipe p is of type t or not. The objective function is constrained by: physical laws of mass and energy conservation, minimum pressure demand in the nodes, and the maximum speed in the pipes, for each time $\tau \in \mathcal{T}$.

Methodology and Experimental Setup. To answer the *RQs* formulated in Section 1, we need the empirical verification provided by testing the HSA in a WDND test set of varying complexity. The static (MCLs) and the two adaptive (MCLa1 and MCLa2) MCL strategies are considered. Therefore, three new HSA configurations arise. The stop condition is to reach 1,500,000 evaluations of the objective function to make a fair comparison with the literature algorithms. The HSA uses the random cooling scheme [15] and 100 as seed temperature (see [16] for a justification of this parameter selection). Moreover, the testing includes 50 HydroGen instances [13] of WDND optimization problem grouped

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Table 1. The best known TIC values found by our proposals and ILS.

Network	MCLs	MLCa1	MLCa2	ILS
HG-MP-1	**298000**	**298000**	**298000**	**298000**
HG-MP-2	245330	245330	245330	**245000**
HG-MP-3	310899	310706	**310493**	318000
HG-MP-4	592048	**590837**	592036	598000
HG-MP-5	**631000**	**631000**	**631000**	**631000**
HG-MP-6	617821	**609752**	614917	618000
HG-MP-7	648372	644568	**639932**	653000
HG-MP-8	795996	792436	**790037**	807000
HG-MP-9	716944	715863	**712450**	725000
HG-MP-10	730916	**712847**	727818	724000
GP-Z2-2020	355756	366684	358717	**347596**

by five different distribution networks, named as HG-MP-i with $i \in [1, 10]$, and GP-Z2-2020, a real-world case [14].

Since we deal with stochastic algorithms, we have performed 30 independent runs per WDND instance and for each HSA configuration. We have carried out a statistical analysis of the results that consists of the following steps. Before performing the statistical tests, we first check whether the data follow a normal distribution by applying the Shapiro-Wilks test. Where the data are distributed normally, we later apply an ANOVA test. Otherwise, we use the Kruskal–Wallis (KW) test. These statistical studies allow us to assess whether or not there are meaningful differences between the compared algorithms with $\alpha = 0.05$. These pairwise algorithm differences are determined by carrying out a post hoc test, as is the case of the Wilcoxon test if the KW test is used.

5 HSA Result Analysis

The result analysis is carried out considering the performance and internal behavior of the proposed HSA configurations (MCLs, MCLa1, and MCLa2).

5.1 HSA Performance

The HSA performance is analyzed considering the solutions found by each configuration, the effort required by the search, and the comparison of HSA results against the ILS ones [17], a well-known WDND solver.

To study the solution quality, we present Table 1 with the minimum TIC values for the HSA considering the three MCL strategies. Furthermore, the last column shows the TIC values corresponding to ILS. To complete the solution quality analysis, we use the relative distance between the best-known TIC value and the best TIC value of each HSA configuration as the error measure. The figures 2 and 3.a) show the distribution of the HSA errors grouped by the Hydrogen and GP-Z2-2020 networks and MCL strategies. Boxplots with different colors mean statistically different behaviors. From these results, we observe that adaptive HSA configurations improve the static one in 7 of 11 network groups. For HG-MP-i with $i \in [7, 10]$ and GP-Z2-2020 networks, the MCLs behavior is

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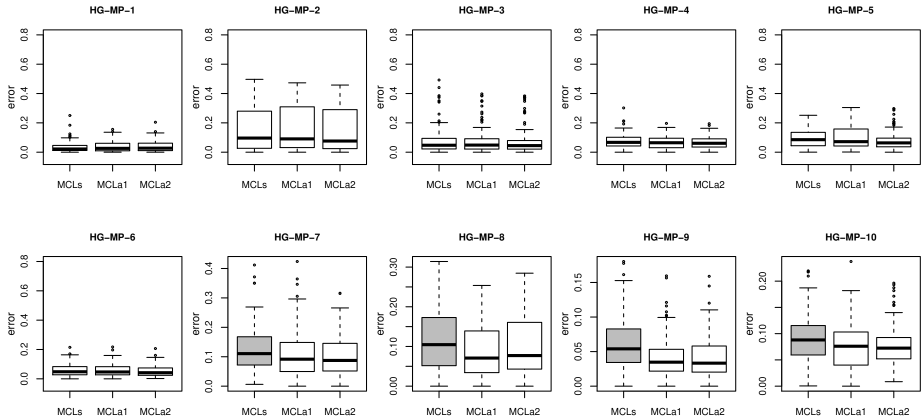

Fig. 2. BoxPlots of TIC error values found by HSA and each MCL strategies for WDND networks.

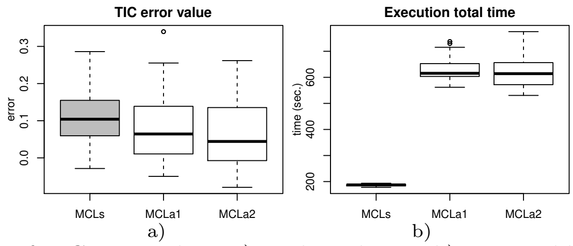

Fig. 3. BoxPlots of TIC error values, a), and total time, b), required by HSA and each MCL strategies for WDND real network (GP-Z2-2020).

significantly different (gray boxplot) to MCLa1 and MCLa2, which keep similar behavior for all cases (white boxplots). In this way, the first RQ is positively answered because the adaptive MCL strategies improve the HSA performance versus the static one, regarding efficiency and efficacy.

The following analysis is devoted to study each HSA configuration with more detail, considering the computational effort measured with the required time to execute the whole search process. Figures 4 and 3.b) show the distribution of these measures grouped by Hydrogen and GP-Z2-2020 networks and MCL strategies. First, we observe that the HSA run times grow as the instance complexity increases for all configurations. Second, MCLs is the quickest strategy for all networks, whereas adaptive HSA configurations increment significantly the total runtime. However, the MCLa1 runtimes are significantly less than the required ones by MCLa2 for HG-MP-i with $i \in [1, 4]$ networks.

Finally, we compare our results with ILS (see Table 1) from the quality point of view. In this sense, we also detect that the three HSA configurations find better average TIC values than ILS for 7 of 11 networks. Besides, all algorithms reach the same result in two cases.

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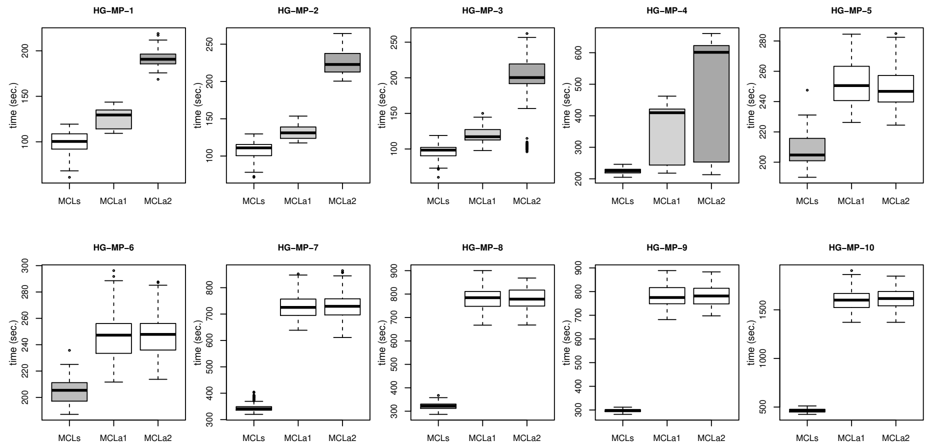

Fig. 4. BoxPlots of the total time (in seconds) required by HSA and each MCL strategies to solve the WDND networks.

5.2 HSA internal behavior

The idea behind the HSA's internal behavior analysis is to discover if the MCL strategies affect the solution quality or the temperature schedules.

Figures 5, 6, and 7 show the upper triangular matrix of scatter plots, where the correlation between the variables TIC values, MC lengths, and temperatures are graphically presented, for each HSA configuration. The Spearman's correlation coefficient, R, is calculated in every comparison and measures the linear correlation between two data sets. R belongs to the range $[-1, 1]$ and expresses the strength of association between two variables. If $R > 0$ indicates a positive relationship between the two variables (as values of one variable increase, values of the other variable also increase). When $R < 0$ indicates a negative relationship (as values of one variable increase, values of the other variable decrease). A $R = 0$ means that no linear correlation exists between the variables.

The MCLs strategy maintains constant (equal to 30) the MC length during the whole search process. Consequently, no linear correlation exists between this length and the solution quality ($R = 0$), as Fig. 5 shown. Instead, the temperature reduction is related to the solution quality because the network costs decrease during the annealing process ($R = 0.46$).

As we explain in Section 3, the adaptive strategies calculate on runtime the MC length according to different criteria. The lengths computed by MCLa1 vary in the range [730, 2850] and the calculated ones by MCLa2 belongs to [730, 3320], becoming a factor that impacts positively in the solution quality (R=0.82 and R=0.2, respectively). As figures 6 and 7 show, this impact is different when the first adaptive strategy is used, because only MCLa1 enable to decrease the MC length. Consequently, when HSA uses MCLa1 can reduce the temperature more times during the search process. This situation allows reaching a better

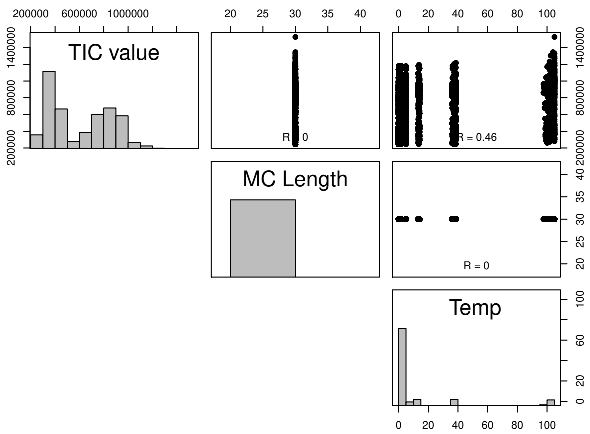

Fig. 5. Scatter plots of correlation for MCLs strategy.

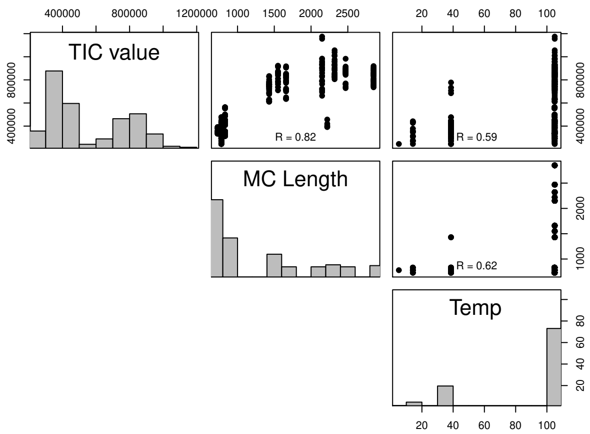

Fig. 6. Scatter plots of correlation for MCLa1 strategy.

equilibrium between exploration and exploitation in the search space, leading to a solution quality improvement.

Finally, we analyze the temperature behavior in more detail. As we can observe in the above paragraph, the variability of the MC length also affects the temperature schedule, but this relationship differs according to the adaptive strategy used. MCLa1 maintains a positive correlation (R=0.62), indicating that a diminution in the lengths is associated with a temperature reduction. Instead, these variables are inversely (R=-0.45) correlated when HSA uses MCLa2 because this strategy never decreases the MC length, but HSA always reduces the temperature after each MC ends. According to this analysis, the second *RQ* is also satisfactorily answered because HSA modifies its behavior with the MC length variability.

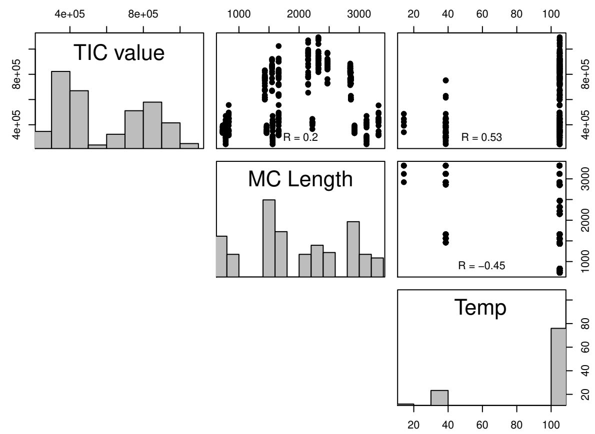

Fig. 7. Scatter plots of correlation for MCLa2 strategy.

6 Conclusions

The Simulated Annealing algorithms usually employ static Markov chain lengths in the Metropolis cycle for each temperature. However, adaptive strategies, which depend on the optimization function variability, to compute this length are also available. In this work, we contrast the static versus adaptive ones by studying the influence on the efficiency and efficacy of a SA when solving NP-hard optimization problems.

We enhance the concerning knowledge by solving several instances and real-world cases of the Water Distribution Network Design problem with a hybrid SA, in which MCL is computed by a static (MCLs) and two adaptive (MCLa1 and MCLa2) strategies. The experimentation results allowed us affirmatively to answer our research questions. The adaptive MCL strategies improve the SA performance versus the static one, modifying its behavior with the MC length variability. MCLa1 is a good trade-off between efficiency and efficacy.

A future research line consists of finding a new MCL strategy based on MCLa1 to reduce the execution time for almost all test cases. The analysis of the parallel SA behavior considering the adaptive MCL strategies for solving high-dimensional NP-hard problems is another interesting research line.

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