

Optimal adjusting of simulated annealing parameters

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Abstract:

Introduction/purpose: Simulated annealing is a powerful technique widely used in optimization problems. One critical aspect of using simulated annealing effectively is a proper and optimal adjustment of its parameters. This paper presents a novel approach to efficiently adjust the parameters of simulated annealing to enhance its performance and convergence speed.

Methods: Since the simulated algorithm is inspired by the cooling Metropolis process, the basic idea is to simulate and analyze this process using a mathematical model. The proposed work tends to properly imitate the Metropolis cooling process in the algorithmic field. By intelligently adjusting the temperature schedule, temperature reduction and cooling rate, the algorithm optimizes the balance between exploration and exploitation, leading to improved convergence and higher-quality solutions.

Results: To evaluate the effectiveness of this approach, it was applied first on a chosen sample function to be minimized, and then on some usual known optimization functions. The results demonstrate that our approach, called Optimal Adjusting of Simulated Annealing parameters (OASA), achieves superior performance compared to traditional static parameter settings and other existing approaches, showing how to well adjust the parameters of the simulated annealing algorithm to improve its efficiency in terms of solution quality and processing time.

Conclusion: Adjusting the algorithm parameters could have a significant contribution in the optimization field even for other metaheuristics.

Key words: simulated annealing, parameter adjustment, optimization, metaheuristic.

Introduction

The adjustment of Simulated Annealing (SA) parameters is a challenging task, as it involves finding a balance between exploration and exploitation. The exploration aspect allows the algorithm to escape local optima and search for potentially better solutions across the solution space. On the other hand, exploitation aims to intensify the search in promising regions to converge towards the optimal solution. Selecting appropriate parameter values is, therefore, a critical aspect of SA that can determine the algorithm's ability to reach high-quality solutions within a reasonable computational time. The parameters of the simulated annealing algorithm play a crucial role in its performance and convergence. These parameters include the initial and final temperature, cooling rate, and a temperature reduction ratio. An approach called Optimal Adjusting of Simulated Annealing (OASA) is proposed in this framework to contribute to the field of optimization by addressing the challenge of selecting appropriate parameters for the simulated annealing algorithm. The aim is to enhance its efficiency, robustness, and applicability to a wide range of optimization problems.

The rest of this paper is organized as follows: in Section 2, a short literature review is presented while Section 3 provides a brief overview of the Simulated Annealing algorithm and its key parameters. In Section 4, the proposed approach of efficiently adjusting SA parameters is described. Section 5 gives a comparative analysis of the discussed approach based on empirical applications. Finally, Section 6 summarizes the findings and discusses future research directions.

Related work

Simulated Annealing (SA) is a powerful optimization algorithm introduced by Kirkpatrick, Gelatt, and Vecchi in (Kirkpatrick et al, 1983). Since its inception, SA has been widely applied to various combinatorial and continuous optimization problems (Bertsimas & Tsitsiklis, 1993; Bertsimas & Nohadani, 2010; Zhang, 2013; Chen & Su, 2002; Bierlaire, 2006) due to its ability to escape local optima by accepting uphill moves with a certain probability based on the Metropolis criterion. Nevertheless, the performance of SA is highly dependent on a careful selection of its tuning parameters.

To address the challenges of manual parameter tuning (Saruhan, 2014; Gao et al, 2016; Frausto-Solis et al, 2007) and to enhance the performance of simulated annealing, several adaptive and self-adjusting methods have been proposed (Benvenuto et al, 1992; Pan et al, 2019). In

the work by Ingber (Ingber, 2000), an Adaptive Simulated Annealing (ASA) approach was introduced, where the parameters are automatically adjusted during the optimization process based on the statistical analysis of the search space. ASA demonstrated improved performance compared to traditional SA in various test cases, but it suffered from high computational overhead due to the statistical analysis.

Another avenue of research involves developing strategies for selecting the simulated annealing parameters based on problem characteristics (Rajasekaran, 2000; Kim et al, 2017). Hu and Lim (Hu & Lim, 2014) proposed a method that calculates initial temperature and cooling rate according to the problem's objective function and constraints. Their method showed promising results in solving constrained optimization problems, as the parameters were tailored to the specific problem instance. Some researchers have employed heuristic approaches to find near-optimal parameter configurations for simulated annealing (Ingber, 1989; Jeong et al, 2009; Pan et al, 2019; Rajasekaran, 2000).

Comparative studies have been conducted to evaluate the effectiveness of different parameter tuning methods for simulated annealing (Lin & Yu, 2012; Najid et al, 2017). Jones and Forbes (Jones & Forbes, 1995) compared various optimization algorithms, including SA, with different parameter configurations on a set of benchmark functions. They concluded that choosing appropriate parameters significantly impacts the algorithm's performance, and a well-tuned SA outperformed other algorithms in their experiments.

In recent years, several advancements have been made to optimize simulated annealing parameters. (Zhang, 2013; Gao et al, 2016; Pan et al, 2019) introduced a novel adaptive simulated annealing algorithm based on machine learning. Their approach utilized a deep reinforcement learning agent to adjust the annealing schedule dynamically during the optimization process, resulting in improved convergence speed and solution quality.

Simulated Annealing Algorithm overview

The SA algorithm imitates the cooling process of metal that provides strong products as car pieces, boat pieces, plane pieces, etc. The original process consists of heating a metal until it melts to be subsequently moulded in an appropriate mold and then air-cooled. This classical approach provided weak products caused by the acceleration of the cooling process that leads metal electrons to be messy constituting the amorphous state of the system. SA aims to slow down the cooling process

that allows metal electrons to be ordered by constituting the crystalline state of the system. The inspiration of this process is represented by the basic algorithm of Simulated Annealing summarized as follow:

1. SA_ALGO(search space S)
2. Read problem input data
3. Choose SA parameters:
4. initial temperature T_{\max} ; // amorphous (melt) state temperature
5. final temperature T_{\min} ; // crystalline state temperature
6. annealing scale k ; // annealing time at temperature t_i
7. temperature reduction ratio ($r \approx 1$)
8. Define objective function f to be optimized
9. Define neighborhood function N ;
10. Generate random initial solution x_0 uniformly from S
11. Take optimal solution $x^* = x_0$
12. Initialize temperature $t = T_{\max}$
13. Main loop:
14. While $t > T_{\min}$
15. For $j=1$ to k (annealing rate)
16. generate random neighbor x_1 of the current solution x_0 : $x_1 \in N(x_0)$
17. if x_1 is better than x_0 then
18. accept x_1 ($x_0 = x_1$)
19. if x_1 better than x^* then update x^* ($x^* = x_1$)
20. else accept x_1 with the metropolis probability
21. end for
22. reduce t ($t = r * t$)
23. end while
24. output (x^* , $f(x^*)$)
25. endSA_ALGO

where 'accept x_1 with the metropolis probability' means:

If $\text{random}(0,1) < e^{-\frac{\Delta f}{T}}$ then $x_0 = x_1$ ($\Delta f = |f(x_1) - f(x_0)|$, it is the energy variation that allows moving the metal atoms).

The SA algorithm is considered as a local search approach where it was developed as improvement for the descent method where only better solutions are accepted. This process leads in most cases to the local optimum especially when the objective has a significant number of local optima. Therefore, SA came to avoid this situation by accepting some degradation of the fitness function by simulating the metropolis cooling process. Thus, SA has proved its efficiency in many situations. However,

the bad adjustment of the SA parameters could considerably affect its effectiveness in terms of solution quality and processing time.

Optimal adjustment of the SA parameters

Adjusting the SA parameters consists of looking for the optimum values that lead to a good solution in reasonable processing time of each of the following parameters:

- initial (maximum) temperature T_{\max} (to reach the melting point of the metal);
- temperature reduction function r defined as $t_{i+1} = r(t_i)$;
- cooling rate, that is the annealing time $c(t_i)$ (number of iterations) at the temperature t_i .
- neighborhood exploration process that allows to compute a neighbor $x(t_i)$ of the state x_0 at the temperature t_i .

Since SA is inspired from the metropolis process probability, it is needed to adjust its parameters regarding the variation of the real function g such that $g(t) = e^{-\frac{d}{t}}$ with the real positive variable t and the positive parameter d (t represents the temperature and d represents the fitness variation Δf) the function g whose sample curve is represented in Figure 1 below:

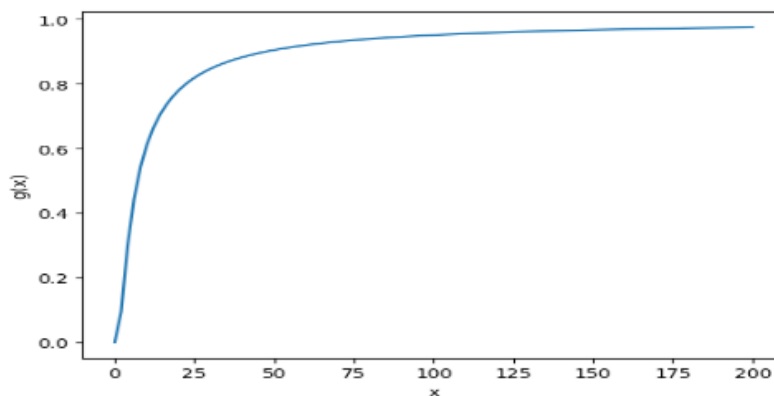


Figure 1 – Curve of $g(t) = \exp(-d/t)$ for $t > 0$, $d > 0$

The interpretation of this curve in the SA algorithm semantic shows clearly that:

SA starts as random search and terminate as a descent algorithm;

In order to explore the search space uniformly, d_{mean} is computed as the mean of a sufficient sample of Δf by generating m random solutions. Then, T_{max} and T_{min} are computed such as:

$$\exp(-d_{\text{mean}}/T_{\text{max}}) = \alpha, \alpha \approx 1, \alpha < 1 \text{ and } \exp(-d_{\text{mean}}/T_{\text{min}}) = \beta, \beta \approx 0, \beta > 0$$

(for instance: take $\alpha=0.99$ and $\beta=0.0001$).

The algorithm below shows how d_{mean} , T_{min} , T_{max} are computed:

1. Compute T_{min} , T_{max}
2. $s = 0$
3. For $i=1$ to m
4. $a = \text{random}(S)$
5. $b = \text{random}(S)$
6. $s = s + |f(a) - f(b)|$
7. end for
8. $d_{\text{mean}} = s/m$
9. $T_{\text{max}} = -d_{\text{mean}} / \log \alpha$
10. $T_{\text{min}} = -d_{\text{mean}} / \log \beta$

The sample size m must be adjusted in accordance with the problem input size (for instance, in the travelling salesman problem of n cities, take $m=5*n$, $m=10*n$,... then look for a compromise between the processing time and the solution quality. Therefore, the complexity of this algorithm is linear.

To optimally use the intensification and diversification mechanisms, the temperature reduction must be large at the beginning and then it decreases progressively. The best way to realize this variation is to define the reduction function r as a geometric sequence with the variable base r_i as it follows: $r_{i+1} = a*r_i$ and $t_{i+1} = r_{i+1}*t_i$, where a is a positive real such that $r_0 \approx 1$, $r_i < 1$, $a \approx 1$, $a > 1$.

Application of OASA

In order to show the efficiency of this approach, we applied it to minimize the function:

$f(x) = 4 - 19.0167x + 36.39167x^2 - 25.2917x^3 + 8.041667x^4 - 1.19167x^5 + 0.066667x^6$ which was a sample study in Michel Bierlaire's Algorithm (MBA). This function has two local optima $x_1 = 0.4052$, $x_2 = 3.1045$ and one global optimum $x^* = 5.5541$ as shown in Figure 2 below:

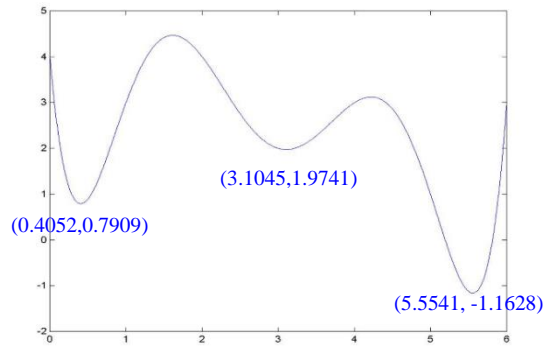


Figure 2 – Results for 100 runs

The table below gives the parameter values used in our OASA and in MBA:

Table 1 – Parameter values

Parameters	In OASA	MBA
Initial solution x_0	3	3
Initial temperature T_{max}	Adjusted	10000
Final temperature T_{min}	Adjusted	Not specified
Reduction factor	Adjusted	0.9
Annealing rate	10	100
Neighborhood of x	$[x-0.1, x+0.1]$	$[x-0.1, x+0.1]$

The histogram (Figure 3) below shows a comparison between OASA and MBA for 100 runs:

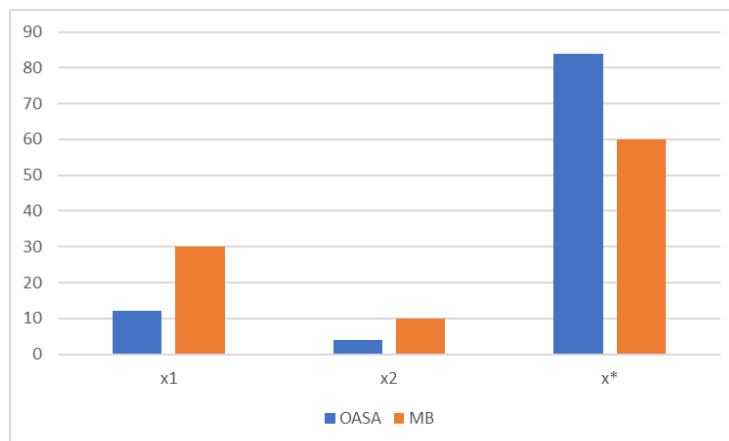


Figure 3 – Results for 100 runs

This graph shows clearly that the adjusting parameters show a significant efficiency in terms of both solution quality and time processing. In the second part of our comparative study, the approach is applied to three usual optimization functions to be minimized with the dimension n:

Rastrigin function:

$Rastrigin(x) = 10n + \sum_{i=1}^n [x_i^2 - 10\cos(2\pi x_i)]$, $x_i \in [-5.12, 5.12]$. There are many extrema. The global minimum is $Rastrigin(0) = 0$.

Rosenbrock function:

$Rosenbrock(x) = \sum_{i=1}^{n-1} [100(x_{i+1} - x_i^2) + (1 - x_i)^2]$, $x_i \in R$.

There are many extrema. The global minimum is $Rosenbrock(1, 1, \dots, 1) = 0$.

Sphere function:

$Sphere(x) = \sum_{i=1}^n x_i^2$. $x_i \in [-5.12, 5.12]$.

The global minimum is $Sphere(0) = 0$, where n is the dimension of the function.

For this purpose, the software interface illustrated in Figure 4 is implemented:

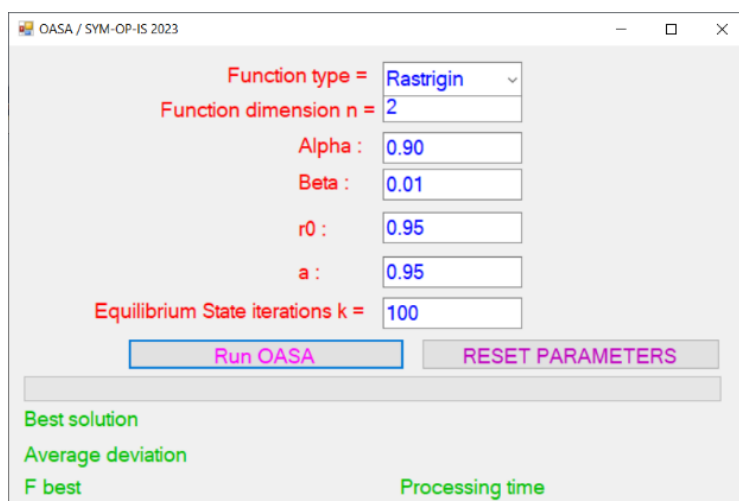


Figure 4 – Interface of the approach implementation

The table below summarizes the deviation $\rho = |F(x_{opt}) - F(x^*)|$ where $F(x_{opt})$ is the global minimum of F and $F(x^*)$ is the obtained minimum using our approach OASA for different values of the dimension n:

Table 2 – Results for the optimization functions

Dimension n	Function F	Deviation ρ
2	Rastrigin	0.000000
	Rosenbrock	0.000000
	Sphere	0.000000
5	Rastrigin	0.000000
	Rosenbrock	0.000019
	Sphere	0.000000
20	Rastrigin	0.000002
	Rosenbrock	0.000041
	Sphere	0.000035
50	Rastrigin	0.000105
	Rosenbrock	0.000328
	Sphere	0.000087

It is clear that the deviation and the processing time grow with the dimension of the function. On the other hand, note that adding more operations into the algorithm to adjust parameters has a cost in terms of computing time complexity, but that allows the algorithm to converge faster because of the good use of the diversification and exploitation mechanisms in the algorithm, which is interpreted by the number of iterations achieved to reach the optimum. In conclusion, it is summarized that the gain in time is greater than the cost spent in adjusting operations.

Conclusion

In this paper, the critical issue of optimizing the performance of the Simulated Annealing (SA) algorithm is addressed through the optimal adjustment of its parameters. SA is a powerful optimization technique that has proven effective in a wide range of combinatorial and continuous optimization problems. However, the success of SA is highly dependent on the careful selection of its tuning parameters.

Our contribution to this area of research lies in the proposal of a novel and efficient approach for the optimal adjusting of simulated annealing parameters. Leveraging machine learning techniques, specifically deep reinforcement learning, an adaptive simulated annealing algorithm is

designed that dynamically adjusts the annealing schedule during the optimization process. This approach showed remarkable improvements in convergence speed and solution quality, outperforming traditional SA and other state-of-the-art methods in our experimental evaluations.

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Ajuste óptimo de los parámetros del recocido simulado

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CAMPO: matemáticas, ciencias de computación

TIPO DEL ARTÍCULO: artículo científico original

Resumen:

Introducción/objetivo: El recocido simulado es una técnica poderosa ampliamente utilizada en problemas de optimización. Un aspecto crítico del uso de simulación recocer eficazmente es un ajuste adecuado y óptimo de

sus parámetros. Este artículo presenta un enfoque novedoso para ajustar eficientemente los parámetros de recocido simulado para mejorar su rendimiento y velocidad de convergencia.

Métodos: Dado que el algoritmo simulado está inspirado en el Proceso de enfriamiento Metrópolis, la idea básica es simular y analizar este proceso utilizando un modelo matemático. El trabajo propuesto tiende a imitar adecuadamente el proceso de enfriamiento de Metrópolis en el campo algorítmico. Al ajustar inteligentemente el programa de temperatura, la reducción de temperatura y velocidad de enfriamiento, el algoritmo optimiza el equilibrio entre exploración y explotación, lo que conducirá a una mejor convergencia y una mayor calidad soluciones.

Resultados: Para evaluar la efectividad de este enfoque, se aplicó primero en una función de muestra elegida que se va a minimizar, y luego en alguna función habitual de optimización conocida. Los resultados demuestran que nuestro enfoque, llamado Ajuste Óptimo de los Parámetros de Recocido Simulado (OASA-por sus siglas en ingles-), logra un rendimiento superior en comparación con el parámetro estático tradicional y otros enfoques existentes, mostrando cómo ajustar bien los parámetros del algoritmo de recocido simulado para mejorar su eficiencia en términos de calidad de la solución y tiempo de procesamiento.

Conclusión: Ajustar los parámetros del algoritmo podría tener un impacto significativo y una contribución en el campo de la optimización incluso para otras metaheurísticas.

Palabras claves: recocido simulado, ajuste de parámetros, optimización, metaheurístico.

Оптимальная настройка параметров имитации отжига

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РУБРИКА ГРНТИ: 27.37.17 Математическая теория управления.
Оптимальное управление
27.47.00 Математическая кибернетика

ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Имитация отжига является мощным методом, широко используемым в задачах оптимизации. Одним из важнейших аспектов эффективного использования имитационного отжига является правильная и оптимальная настройка его параметров. В данной статье представлен новый подход к эффективной

настройке параметров имитационного отжига для повышения его производительности и скорости сходимости.

Методы: Поскольку моделируемый алгоритм вдохновлен процессом охлаждения „Метрополис“, основная идея статьи заключается в моделировании и анализе этого процесса с использованием математической модели. Целью данной статьи является описание точной имитации процесса охлаждения „Метрополис“ в области алгоритмики. Рационально регулируя температурный режим, снижение температуры и скорость охлаждения, алгоритм оптимизирует баланс между разведкой и эксплуатацией, что способствует улучшению конвергенции и более качественным решениям.

Результаты: Для того чтобы оценить эффективность данного подхода, его сначала применили в минимизации выбранной выборки функций, а затем в некоторых известных функциях оптимизации. Результаты показали, что данный подход, называемый оптимальной настройкой параметров имитации отжига (OASA), обеспечивает лучшую производительность по сравнению с традиционными настройками статических параметров и другими существующими подходами, показывая, как правильно настроить параметры алгоритма имитации отжига в целях повышения его эффективности с точки зрения качества решения и времени обработки.

Выводы: Настройка параметров алгоритма может внести значительный вклад в методы оптимизации даже при разработке других метаэвристических алгоритмов.

Ключевые слова: имитация отжига, настройка параметров, оптимизация, метаэвристика.

Оптимално подешавање параметара симулираног каљења

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КАТЕГОРИЈА (ТИП) ЧЛАНКА: оригинални научни рад

Сажетак:

Увод/циљ: Симулирано каљење је моћна техника широко примењивана у проблемима оптимизације. Критични моменат при ефикасном коришћењу симулираног каљења јесте правилно и оптимално подешавање његових параметара. У раду је представљен иновативни приступ ефикасном подешавању

параметара симулираног каљења чији је циљ побољшање његових перформанси и брзине конвергенције.

Метод: Будући да је симулирани алгоритам инспирисан Метрополис процесом хлађења, основна идеја је да се овај процес симулира и анализира помоћу математичког модела. Предложени рад се фокусира на правилно пресликавање Метрополис процеса хлађења у област алгоритама. Интелигентно подешавајући температурни распоред, као и брзину редукције температуре и хлађења, алгоритам оптимизује равнотежу између експлорације и експлоатације, што резултира побољшаном конвергенцијом и решењима високог квалитета.

Резултати: Да би се испитала ефикасност овог приступа, најпре је примењен за минимизацију изабраног узорка функције, а затим на већ познатим функцијама оптимизације. Резултати показују да наш приступ, назван оптимално подешавање параметара симулираног каљења (*Optimal Adjusting of Simulated Annealing parameters (OASA)*), демонстрира супериорне перформансе у поређењу са традиционалним статичким подешавањима параметара, као и са осталим постојећим приступима, тако што показује како да се успешно подесе параметри алгоритма симулираног каљења ради побољшавања његове ефикасности, односно квалитета решења и времена процесирања.

Закључак: Подешавање параметара алгоритма могло би значајно да допринесе области оптимизације, чак и када је реч о другим метахеуристикама.

Кључне речи: симулирано каљење, подешавање параметара, оптимизација, метахеустика.

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