





# Metaheuristics for Smart Manufacturing 6. Simulated Annealing

Thomas Weise · 汤卫思

twe ise @hfuu.edu.cn + http://iao.hfuu.edu.cn

Hefei University, South Campus 2 合肥学院 南艳湖校区/南2区 Faculty of Computer Science and Technology Institute of Applied Optimization 230601 Shushan District, Hefei, Anhui, China Econ. & Tech. Devel. Zone, Jinxiu Dadao 99 经济技术开发区 锦绣大道99号

# Introduction

- What is "Annealing"?
- Simulated Annealing for Optimization

# Experiment and Analysis

The slides are available at <u>http://iao.hfuu.edu.cn/155</u>, the book at <u>http://thomasweise.github.io/aitoa</u>, and the source code at <u>http://www.github.com/thomasWeise/aitoa-code</u>





### An Introduction to Optimization Algorithms



The contents of this course are available as free electronic book *"An Introduction to Optimization Algorithms"*<sup>[1]</sup> at <u>http://thomasweise.github.io/aitoa</u> in pdf, <u>html, azw3</u>, and <u>epub</u> format, created with our bookbuildeR tool chain.







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- Simulated Annealing for Optimization
- 4 Experiment and Analysis





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- We found that we can utilize this variance of the result quality by restarting the optimization process when it could not improve any more.
- Such a restart is costly, as it forces the local search to start completely from scratch (while we, of course, remember the best-ever solution in a variable hidden from the algorithm).





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- But maybe there is a less-costly way?



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  - The probability also decreases with the number of performed search steps.



# Introduction

# What is "Annealing"?

3 Simulated Annealing for Optimization

4 Experiment and Analysis





#### Metaheuristics for Smart Manufacturing

#### Thomas Weise



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- An initial, brittle crystal structure is transformed to a much better configuration by stepping over good and bad states







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- With each such state, there is an energy *E* associated: If many of the particles move around quickly or are in an unfavourable position, the energy *E* is high and if they form a nice crystal and don't move, the energy is low
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$$k_b = 1.380650524 * 10^{-27} J/K$$
 is the Boltzmann constant (1)



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- A system at temperature T has the probability  $e^{-\frac{E}{k_B*T}}$  to be in a macro state with energy E.
- In other words: The higher the temperature, the higher the chance to be in a high-energy state



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•  $P(\Delta E)$  is the probability that the new state  $s_2$  will be accepted



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  - In the end, the system usually arrives at a very good solution.
- Wait. Could we just... ... and so Simulated Annealing was invented.





# 2 What is "Annealing"?

#### Simulated Annealing for Optimization

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- If the new solution is worse ( $\Delta E > 0$ ), the acceptance probability then gets smaller the larger  $\Delta E$  is and gets smaller the smaller the so-called "temperature"  $T \ge 0$  is.



• The temperature T>0 and the objective value difference  $\Delta E>0$ enter the equation in an exponential term  $e^{-\frac{\Delta E}{T}}$  and it holds that  $e^{-a} < e^{-b} \forall a > b$  and  $e^{-a} \in [0,1] \forall a > 0$ .



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- As the process "cools" down, the search tends to accept fewer and fewer worse solutions and more likely such which are only a bit worse.
- Eventually, at temperature T = 0, the algorithm only accepts better solutions.
- T is actually a monotonously decreasing function  $T(\tau)$  called the "temperature schedule" and it holds that  $\lim_{\tau\to\infty} T(\tau) = 0$ .



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$$T(\tau) = \frac{T_s}{\ln\left(\epsilon(\tau - 1) + e\right)}$$
(6)



#### Listing: Abstract Class for Temperature Schedules.

public abstract class TemperatureSchedule {

public abstract double temperature(long tau);

#### }



#### Listing: Exponential Temperature Schedule.



#### Listing: Logarithmic Temperature Schedule.

```
public class Logarithmic extends TemperatureSchedule {
```



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- We make the following choices...



















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  - if it is better: it becomes the new current solution
  - if it is worse: accept it as current solution with probability  $P(\Delta E, \tau)$ (which gets smaller over time and also the smaller the worse the new solution is) or otherwise reject it.
  - 🏮 go back to 🧶 (until the time is up)



# Introduction

- 2 What is "Annealing"?
- Simulated Annealing for Optimization
- 4 Experiment and Analysis



• We test the following configurations



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  - $\blacksquare$  sa\_e\_20\_2e-7\_1swap: Simulated Annealing with Exponential Schedule at  $T_s=20$  with  $\epsilon=2*10^{-7}$



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  - Sa\_e\_20\_8e-7\_1swap: Simulated Annealing with Exponential Schedule at  $T_s = 20$  with  $\epsilon = 8 * 10^{-7}$
  - sa\_l\_10\_1swap: Simulated Annealing with Logarithmic Schedule at  $T_s=10$  with  $\epsilon=1$



		makespan			last improvement		
I	algo	best	mean	med	sd	med(t)	med(FEs)
abz7	ea4096_1swap_5	680	712	712	10	20s	4'145'924
	sa_e_20_2e-7_1swap	663	673	672	5	92s	22'456'822
	sa_e_20_4e-7_1swap	658	674	675	5	55s	13'388'301
	sa_e_20_8e-7_1swap	663	675	675	6	36s	8'625'161
	sa_l_10_1swap	659	672	671	4	86s	21'271'077
1a24	ea4096_1swap_5	945	976	975	15	4s	1'601'925
	sa_e_20_2e-7_1swap	938	949	946	8	27s	12'358'941
	sa_e_20_4e-7_1swap	935	949	946	9	16s	7'135'423
	sa_e_20_8e-7_1swap	935	951	950	8	9s	4'044'217
	sa_l_10_1swap	938	953	950	11	7s	3'210'824
swv15	ea4096_1swap_5	3413	3543	3539	66	169s	22'266'887
	sa_e_20_2e-7_1swap	2937	2990	2988	28	148s	21'949'073
	sa_e_20_4e-7_1swap	2941	2993	2993	28	128s	18'244'751
	sa_e_20_8e-7_1swap	2936	3000	3002	28	111s	16'029'528
	sa_l_10_1swap	2964	3021	3018	30	141s	21'252'052
yn4	ea4096_1swap_5	1034	1068	1068	18	37s	5'943'196
	sa_e_20_2e-7_1swap	973	985	985	5	113s	20'676'041
	sa_e_20_4e-7_1swap	971	987	986	7	68s	12'193'934
	sa_e_20_8e-7_1swap	972	988	988	7	58s	10'178'219
	sa_l_10_1swap	975	997	996	11	108s	19'850'143

Metaheuristics for Smart Manufacturing



ea4096\_1swap\_5: (4096 + 4096) EA with 5% crossover









Metaheuristics for Smart Manufacturing

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### So what do we get?



ea4096\_1swap\_5: (4096 + 4096) EA with 5% crossover



#### So what do we get?



sa\_e\_20\_4e-7\_1swap: SA with exp. Schedule ( $T_s = 20, \epsilon = 4 * 10^{-7}$ )























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  - The Simulated Annealing algorithm allows for a smooth transition of a random search behavior towards a hill climbing behavior over time.
  - Compared to the hill climber with restarts, it offers a "softer" way to escape from local optima which sacrifices less solution information.





# 谢谢 Thank you

Thomas Weise [汤卫思] tweise@hfuu.edu.cn http://iao.hfuu.edu.cn

Hefei University, South Campus 2 Institute of Applied Optimization Shushan District, Hefei, Anhui, China

Thomas Weise





## **Bibliography I**



- Thomas Weise. An Introduction to Optimization Algorithms. Institute of Applied Optimization (IAO), Faculty of Computer Science and Technology, Hefei University, Hefei, Anhui, China, 2019-06-25 edition, 2018–2019. URL http://thomasweise.github.io/aitoa/. see also<sup>[6]</sup>.
- Scott Kirkpatrick, C. Daniel Gelatt, Jr., and Mario P. Vecchi. Optimization by simulated annealing. Science Magazine, 220 (4598):671–680, May 13, 1983. doi: 10.1126/science.220.4598.671. URL http://citeseer.ist.psu.edu/viewdoc/summary7doi=10.1.1.18.4175.
- Vladimír Černý. Thermodynamical approach to the traveling salesman problem: An efficient simulation algorithm. Journal of Optimization Theory and Applications, 45(1):41-51, January 1985. doi: 10.1007/BF00940812. URL http://mkweb.bcgcs.ca/papers/cerny-travelingsalesman.pdf.
- Dean Jacobs, Jan Prins, Peter Siegel, and Kenneth Wilson. Monte carlo techniques in code optimization. ACM SIGMICRO Newsletter, 13(4):143–148, December 1982. Proceedings of the 15th Annual Workshop on Microprogramming (MICRO 15), October 5–7, 1982, Palo Alto, CA, USA, New York, NY, USA: ACM.
- Martin Pincus. Letter to the editor a monte carlo method for the approximate solution of certain types of constrained optimization problems. *Operations Research*, 18(6):1225–1228, November–December 1970. doi: 10.1287/opre.18.6.1225.
- Thomas Weise. Global Optimization Algorithms Theory and Application. it-weise.de (self-published), Germany, 2009. URL http://www.it-weise.de/projects/book.pdf.
- James C. Spall. Introduction to Stochastic Search and Optimization, volume 6 of Estimation, Simulation, and Control Wiley-Interscience Series in Discrete Mathematics and Optimizationn. Wiley Interscience, Chichester, West Sussex, UK, April 2003. ISBN 0-471-33052-3. URL https://www.jhuapl.edu/ISS0/.
- F. J. Humphreys and M. Hatherly. Recrystallization and Related Annealing Phenomena. Pergamon Materials Series. Amsterdam, The Netherlands: Elsevier Science Publishers B.V., 2004. ISBN 0080441645 and 9780080441641. URL http://books.google.de/books?id=52Glao7HxGaC.
- Nicholas Metropolis, Arianna W. Rosenbluth, Marshall Nicholas Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of state calculations by fast computing machines. *The Journal of Chemical Physics*, 21(6):1087–1092, June 1953. doi: 10.1063/1.1699114. URL http://sc.fsu.edu/~beerli/mcmc/metropolis-et-al-1953.pdf.