模 拟 退 火
Simulated Annealing

王 凌　　教授
清华大学自动化系 中央主楼427A
wangling@tsinghua.edu.cn

Purpose of Lecture

1 What is SA?

2 Why use SA?

3 How to use SA?

4 How to improve SA?

- 优化的定位
  - 优化技术是一种以数学为基础，用于求解各种工程问题优化解的应用技术。任何控制与决策问题本质上都是优化问题！
- 优化问题的三要素
  - 决策变量
  - 约束条件
  - 目标函数
- 优化问题的分类
  - 函数优化/连续优化

$$
\begin{aligned}
&\min f(x), x \in R^n \\
&s.t. \quad g_i(x) \le 0, 1 \le i \le l \\
&\qquad h_i(x) = 0, l+1 \le i \le m \\
&\qquad lb \le x \le ub
\end{aligned}
$$

结构设计
参数估计

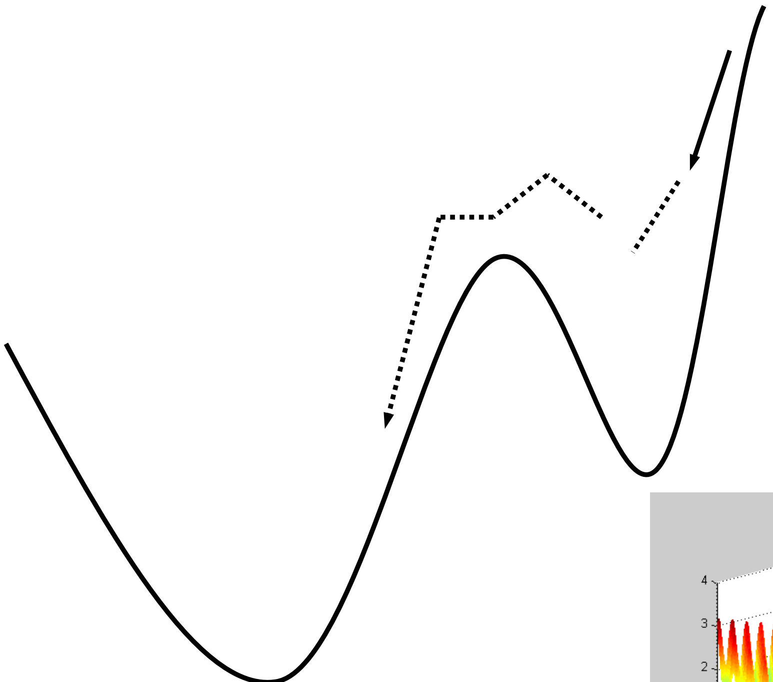
  - 组合优化/离散优化

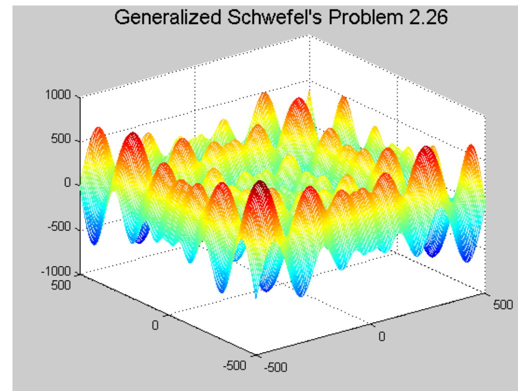
$$
\text{Find } s^*, \forall s \in \Omega, C(s^*) = \min C(s), \quad \Omega = \{s_1, s_2, \ldots, s_n\}
$$

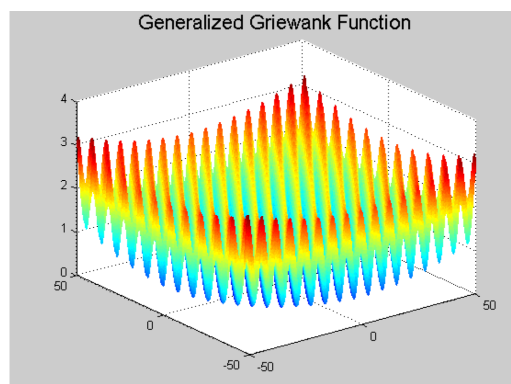
物流、背包、调度

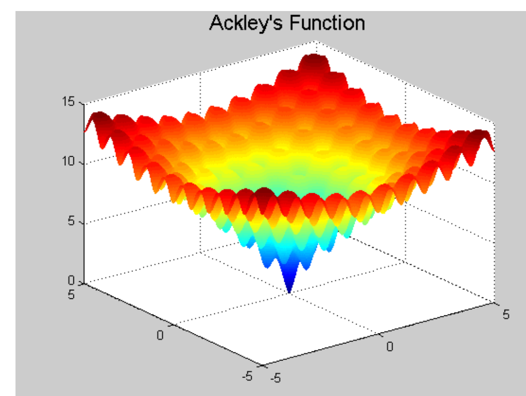
$$\min f(x),\ x \in \boldsymbol{R}$$

梯度下降 $x(k+1)=x(k)-\alpha \times \mathrm{d}f/\mathrm{d}x$，$k=0,1,\ldots$

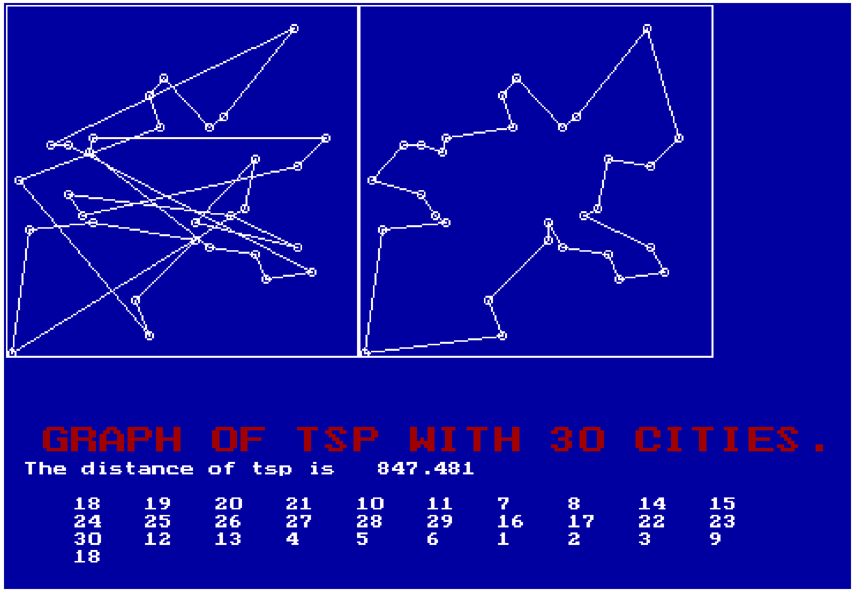


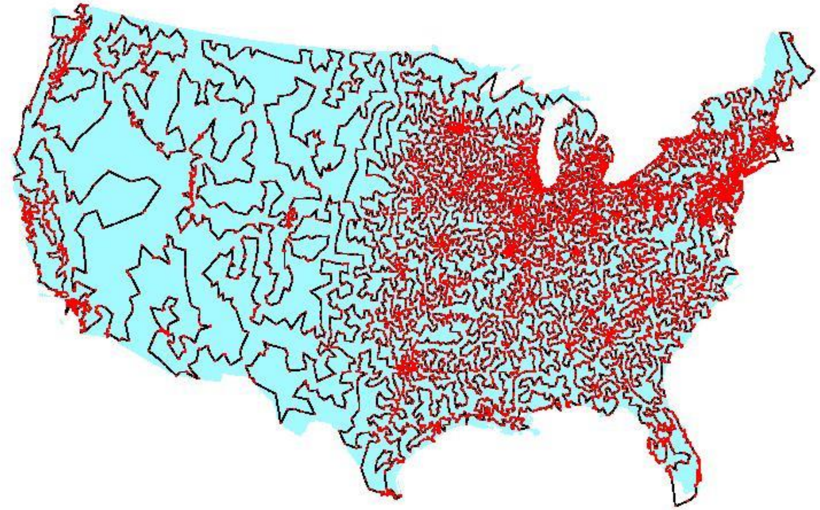






搜索过程易陷入局部极小





$30! > 2.65*10^{32}$

面临维数灾

从30!个解中寻找最优解，若计算机1秒列举1亿个解，则穷举需要约$8.4*10^{16}$年！若穷举20！个解也需要771年多时间！(从元朝就得开始)

城市数	24	25	26	27	28	29	30	31
计算时间	1 sec	24 sec	10 min	4.3 hour	4.9 day	136.5 day	10.8 year	325 year

ARTICLES

Optimization by Simulated Annealing

S. Kirkpatrick[1], C. D. Gelatt Jr.[1], M. P. Vecchi[2]

[1]Research staff members at IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598

[2]Instituto Venezolano de Investigaciones Cientificas, Caracas 1010A, Venezuela

– Hide authors and affiliations

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Abstract

There is a deep and useful connection between statistical mechanics (the behavior of systems with many degrees of freedom in thermal equilibrium at a finite temperature) and multivariate or combinatorial optimization (finding the minimum of a given function depending on many parameters). A detailed analogy with annealing in solids provides a framework for optimization of the properties of very large and complex systems. This connection to statistical mechanics exposes new information and provides an unfamiliar perspective on traditional optimization problems and methods.

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Optimization by Simulated Annealing

S. Kirkpatrick, C. D. Gelatt, Jr., M. P. Vecchi

In this article we briefly review the central constructs in combinatorial optimization and in statistical mechanics and then develop the similarities between the two fields. We show how the Metropolis algorithm for approximate numerical simulation of the behavior of a many-body system at a finite temperature provides a natural tool for bringing the techniques of statistical mechanics to bear on optimization.

We have applied this point of view to a number of problems arising in optimal design of computers. Applications to partitioning, component placement, and wiring of electronic systems are described in this article. In each context, we introduce the problem and discuss the improvements available from optimization.

Of classic optimization problems, the traveling salesman problem has received the most intensive study. To test the power of simulated annealing, we used the algorithm on traveling salesman problems with as many as several thousand cities. This work is described in a final section, followed by our conclusions.

Combinatorial Optimization

The subject of combinatorial optimization (*1*) consists of a set of problems that are central to the disciplines of computer science and engineering. Research in this area aims at developing efficient techniques for finding minimum or maximum values of a function of very many independent variables (*2*). This function, usually called the cost function or objective function, represents a quantitative measure of the "goodness" of some complex system. The cost function depends on the detailed configuration of the many parts of that system. We are most familiar with optimization problems occurring in the physical design of computers, so examples used below are drawn from that context. The number of variables involved may range up into the tens of thousands.

The classic example, because it is so simply stated, of a combinatorial optimization problem is the traveling salesman problem. Given a list of N cities and a means of calculating the cost of traveling between any two cities, one must plan the salesman's route, which will pass through each city once and return finally to the starting point, minimizing the total cost. Problems with this flavor arise in all areas of scheduling and design. Two subsidiary problems are of general interest: predicting the expected cost of the salesman's optimal route, averaged over some class of typical arrangements of cities, and estimating or obtaining bounds for the computing effort necessary to determine that route.

All exact methods known for determining an optimal route require a computing effort that increases exponentially with N, so that in practice exact solutions can be attempted only on problems involving a few hundred cities or less. The traveling salesman belongs to the large class of NP-complete (nondeterministic polynomial time complete) problems, which has received extensive study in the past 10 years (*3*). No method for exact solution with a computing effort bounded by a power of N has been found for any of these problems, but if such a solution were found, it could be mapped into a procedure for solving all members of the class. It is not known what features of the individual problems in the NP-complete class are the cause of their difficulty.

Since the NP-complete class of problems contains many situations of practical interest, heuristic methods have been developed with computational requirements proportional to small powers of N. Heuristics are rather problem-specific: there is no guarantee that a heuristic procedure for finding near-optimal solutions for one NP-complete problem will be effective for another.

There are two basic strategies for heuristics: "divide-and-conquer" and iterative improvement. In the first, one divides the problem into subproblems of manageable size, then solves the subproblems. The solutions to the subproblems must then be patched back together. For this method to produce very good solutions, the subproblems must be naturally disjoint, and the division made must be an appropriate one, so that errors made in patching do not offset the gains

Summary. There is a deep and useful connection between statistical mechanics (the behavior of systems with many degrees of freedom in thermal equilibrium at a finite temperature) and multivariate or combinatorial optimization (finding the minimum of a given function depending on many parameters). A detailed analogy with annealing in solids provides a framework for optimization of the properties of very large and complex systems. This connection to statistical mechanics exposes new information and provides an unfamiliar perspective on traditional optimization problems and methods.

S. Kirkpatrick and C. D. Gelatt, Jr., are research staff members and M. P. Vecchi was a visiting scientist at IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598. M. P. Vecchi's present address is Instituto Venezolano de Investigaciones Cientificas, Caracas 1010A, Venezuela.

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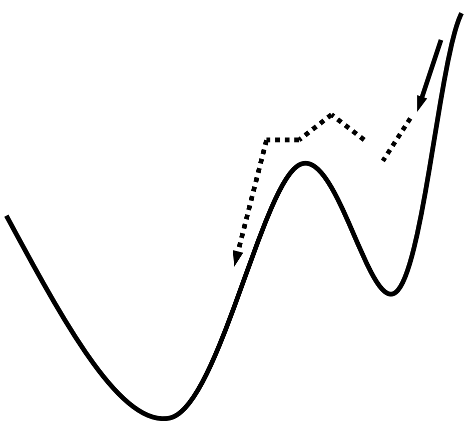
What is Simulated Annealing?

MICHAEL W. TROSSET
Department of Mathematics, College of William & Mary, P.O. Box 8795, Williamsburg, VA 23187-8795, USA; Department of Computational & Applied Mathematics, Rice University, 6100 Main Street, Houston, TX 77005-1892, USA

提出背景

- NP问题(Non-deterministic Polynomial)获得最优解的计算量随问题规模呈指数性增长，计算时间难以承受——质量与效率需均衡
- 模型建立与求解难度大——数据驱动迭代寻优
- 邻域搜索过程陷入局部极小——初值依赖性需削弱

- Inspired from: 统计力学与多变量或组合优化的联系



优化与物理退火的类比

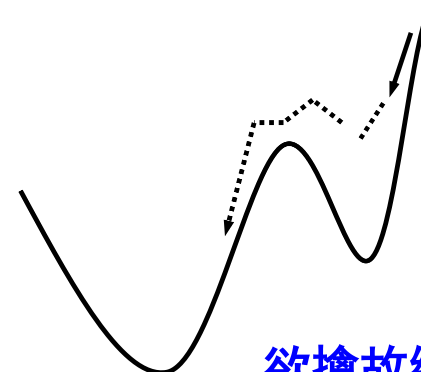
优 化	物理退火
解	状态
最优解	能量最低状态
初温	熔化
Metropolis抽样	等温过程
降“温”	冷却
目标函数	能量

- **加温**：增强粒子热运动，偏离平衡态，熔解消除原先非均匀态
- **等温**：与周围环境交换热量而温度不变的封闭系统，状态的自发变化总是朝自由能减少的方向进行，直至达到平衡态
- **冷却**：使粒子的热运动减弱并渐趋有序，系统能量逐渐下降

Metropolis 抽样(重要性采样法)

- 模拟等温过程的Monte Carlo方法需大量采样以使系统达到平稳态
- 概率接受：

$$\begin{array}{ccc} x & \longrightarrow & x' \\ \downarrow & & \downarrow \\ E_x & & E_{x'} \end{array}$$

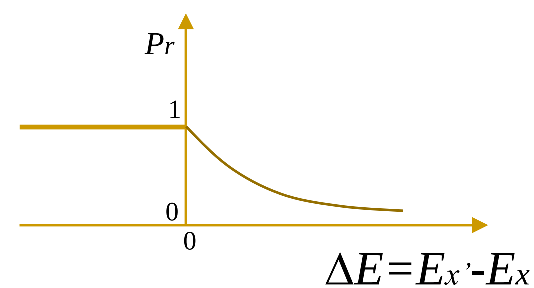


欲擒故纵

$$P_r = \min\{1, \exp[-(E_{x'} - E_x)/kt]\}$$

$$\xi \sim random[0,1)$$

$$\xi < P_r \Rightarrow x = x'$$



Q1: ΔE不变，若t1>t2，则Pr1和Pr2的大小关系？

Q2: t变小，接受曲线如何变化？

Exploration-Exploitation

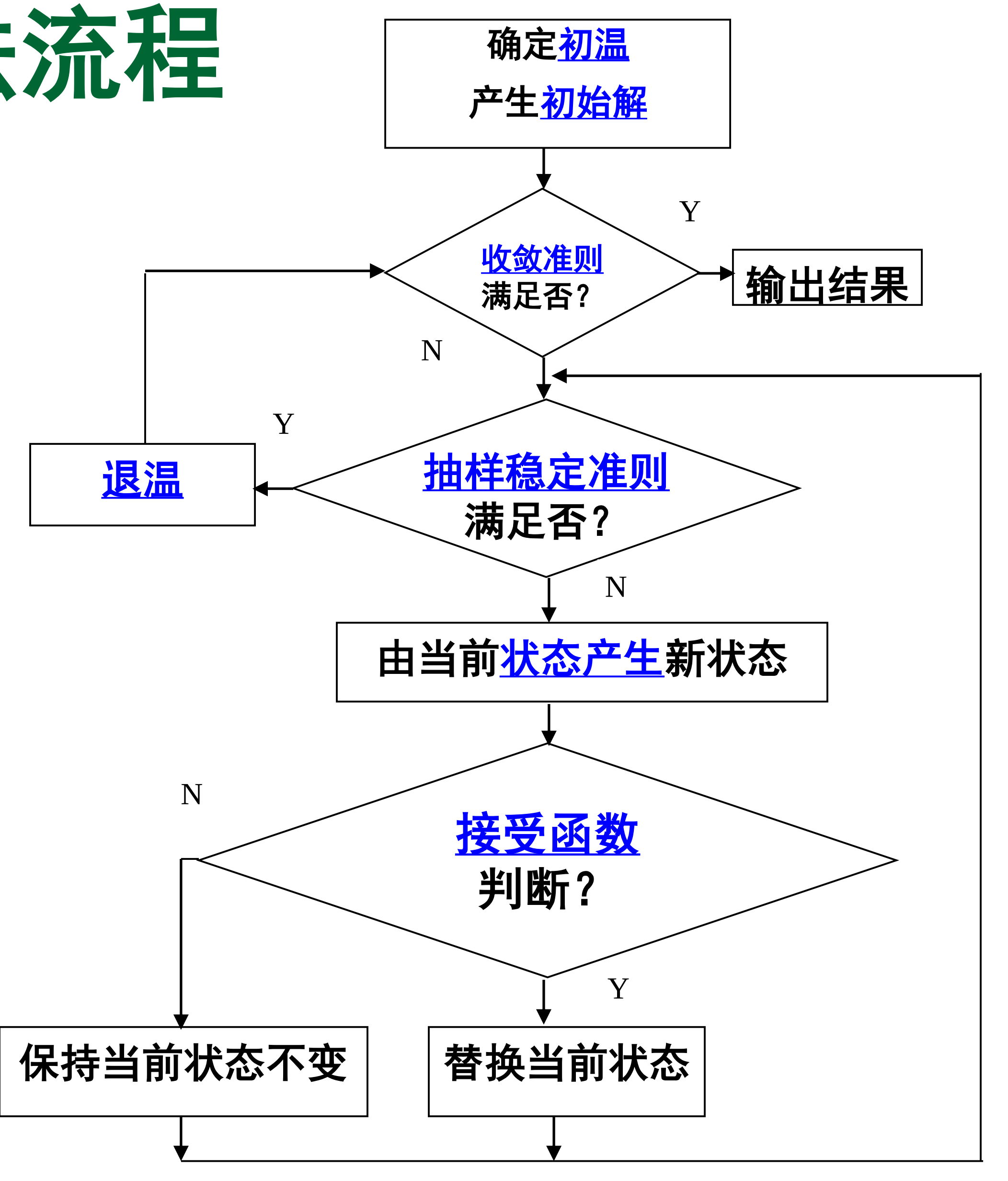
模拟退火优化机制

- **SA算法是基于Monte Carlo迭代求解策略的一种随机寻优算法，其机制来源于基于物理退火过程与组合优化之间的相似性，算法从较高初温开始，利用具有概率突跳特性的Metropolis抽样策略在解空间中进行随机邻域搜索，伴随温度的不断下降重复抽样过程，最终获得问题的全局最优解或满意解。**

模拟退火算法流程

关键环节

- 初温、初始解
- 状态产生操作
- 状态接受判断
- 退温操作
- 抽样稳定准则
- 收敛准则



模拟退火收敛性

- **马氏链模型**

$$\forall i, j \quad p_{i,j}(t) = \begin{cases} g_{i,j} \cdot a_{i,j}(t) & j \in N_i \ \ and \ \ j \neq i \\ 0 & j \notin N_i \ \ and \ \ j \neq i \\ 1 - \sum_{k \in N_i} p_{i,k}(t) & j = i \end{cases}$$

通常， $a_{i,j} = \min\{1, \exp[-(E_j - E_i)/t]\}$

非时齐马氏链模型的收敛定理

令 $S_m = \{i \in V \mid C(j) \le C(i), \forall j \in N_i\}$ 为状态空间中目标函数局部极大的点集，$r = \min\limits_{i \in V - S_m} \max\limits_{j \in V} d(i, j)$ 为图 G 的半径，其中 $d(i, j)$ 为图 G 中由顶点 i 到达顶点 j 的最少边数，$L = \max\limits_{i \in V} \max\limits_{j \in N_i} |C(i) - C(j)|$。若 $t_0 > t_1 > \cdots > t_n$，$\lim\limits_{n \to \infty} t_n = 0$，当存在正整数 k_0 使得式 $\sum\limits_{k=k_0}^{\infty} \exp(-rL / T_{kr-1}) = \infty$ 成立，则马氏链强遍历，即 SA 算法依概率 1 收敛到问题的全局最优解。

注：为满足上述定理的条件，可设计退温函数 $t_k = \alpha / \ln(k + m), k = 0,1,\ldots$，其中 $2 \le m < \infty$，则当 $\alpha \ge rL$ 时，SA 算法依概率 1 收敛到全局最优解。

模拟退火算法设计

- 初始解、初温
- 状态产生操作
- 状态接受判断
- 退温操作
- 抽样稳定准则
- 收敛准则

初始解、初温

- 初始解通常随机产生，或分析landscape后针对性产生。
- 非时齐SA收敛理论，初温由退温函数中的a决定，但求解实际问题时难以确定。
- 时齐SA收敛理论，没有对初温给出限制，但根据与物理退火过程的类比，初温应充分大，使得几乎所有产生的候选解都能被接受，才能保证最终收敛。
- 实验表明，初温越大，获得高质量解的几率越大，但花费计算时间将增加。因此，初温的确定应折衷考虑优化质量和优化效率。
  - 根据经验设定
  - 均匀抽样一组状态，以各状态目标值的方差为初温
  - 均匀随机产生一组状态，确定两两状态间的最大目标值差$|\Delta_{max}|$，设定最差状态相对最佳状态的接受概率p_r，然后根据下式确定初温$t_0 = |\Delta_{max}| / \ln(1/p_r)$。

✓ 考虑解之间的相对性能

✓ p_r设定比较直观

状态产生操作

- 搜索的引擎，一方面要保证新解的全空间分布，另一方面要考虑局部的密度，即E&E。
- 产生新解的方式
  - 离散优化由问题的特性决定
    - 背包问题、调度问题
  - 连续优化 $x(k+1)=x(k)+\eta\cdot\xi$ ξ 为随机变量
    - 均匀分布、正态分布、指数分布、柯西分布等

$$f(\xi)=\frac{1}{\pi}\cdot\frac{a}{a^2+\xi^2}\quad -\infty<\xi<\infty$$

$$f(\xi)=\frac{1}{\sqrt{2\pi\sigma}}\exp[-\xi^2/(2\sigma)]\quad -\infty<\xi<\infty$$

$$f(\xi)=\begin{cases}1/(b-a) & \xi\in[a,b]\\ 0 & else\end{cases}$$

状态产生操作

a为最大值一半处的一半宽度的尺度参数

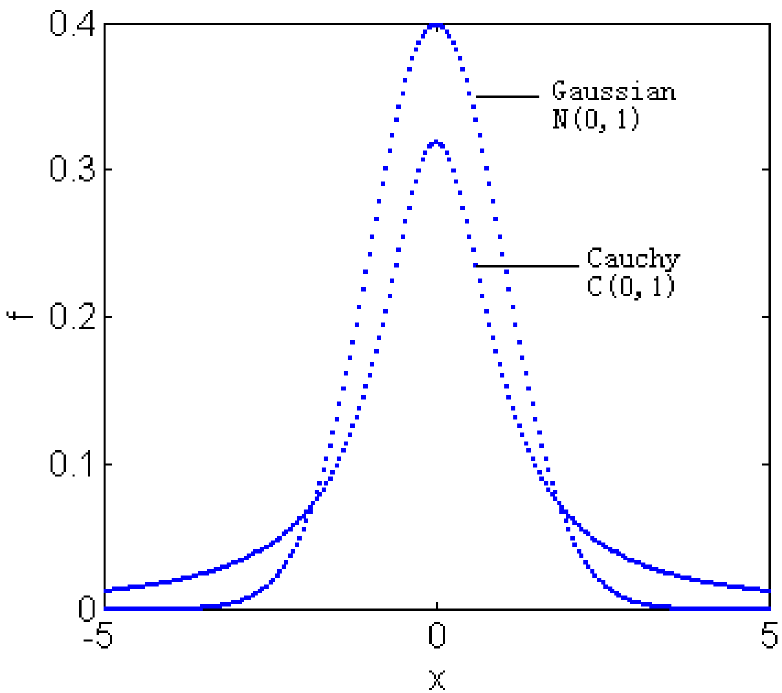


Fig 1. Comparison of Cauchy and Gaussian distribution

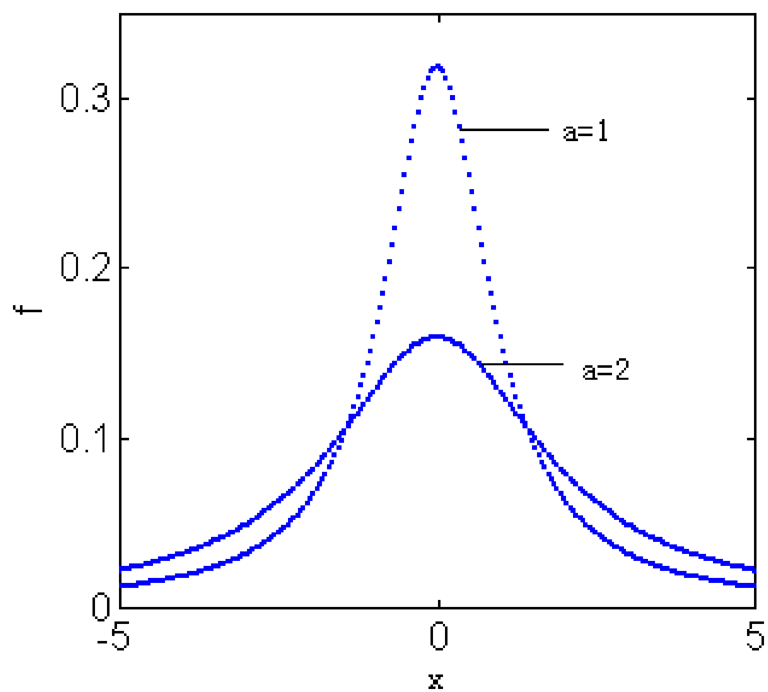


Fig 2. Cauchy distribution with different scale parameter

Q1: **柯西分布与高斯分布的差异？**

Q2: **尺度参数的变化有何影响？**

Q：尺度参数的自适应变化，如何变？

Exploration-->Exploitation

针对置换串的搜索行为分析

- 譬如：TSP、FSP、VRP　　非对称\对称

互换(SWAP): 随机交换串中两个不同位置的基因
逆序(INV): 将两个不同位置间的子串逆序
插入(INS): 随机选择某一位置的基因插入到另一随机位置

- 两随机位置相邻
  - SWAP(3\2), INV(3\2), INS(3\2)
- 两随机位置间隔一基因
  - SWAP(4\2), INV(4\2), INS(3\3)
- 两随机位置间隔k(k>1)基因以上
  - SWAP(4\4), INV(k+3\2), INS(3\3)
- 给定状态串长度，计算期望行为
  - 明显的，中大规模TSP状态串很长，上述第三种情况发生概率最大

状态接受判断

- 状态接受判断常以概率方式给出，不同判断方式的差别主要是接受概率的形式不同。
- 设计状态接受判断条件，应该遵循以下原则：
  - 在同一温度下，接受使目标值下降的候选解的概率要大于使目标值上升的候选解的概率；
  - 随温度的下降，接受使目标值上升的解的概率要逐渐减小；
  - 当温度趋于零时，只能接受目标值下降的解。
- 状态接受判断的引入是SA实现全局搜索的关键因素，但实验表明其形式对性能的影响不显著。
- 最通常方式： $a_{i,j} = \min\{1, \exp[-(E_j - E_i)/t]\}$

退温操作

- 非时齐SA收敛理论
  - 采用$t_k=a/\log(k+k_0)$，温度与退温步数的对数成反比，温度下降速度很慢。当a较大时，温度下降到较小值需很长计算时间。
  - 采用$t_k=a/(1+k)$，温度下降加快，但单纯快速降温不能保证算法快速收敛。事实上，快速退温下的SA不具备全局收敛性。
- 时齐SA算法收敛理论
  - 要求温度最终趋于零，对温度下降速度没有限制。这并不意味着温度可以下降很快，因为收敛条件要求各温度下产生的候选解数目无穷大，实际应用无法实现。
- 通常，各温度下产生候选解增多，降温速度可适度加快。
- 常用退温函数为指数退温$t_k=\lambda\times t_{k-1}$
  - λ为降温速率，其值越大表示退温越慢。

抽样稳定准则

- **Metropolis抽样稳定准则，用于决定在各温度下产生的候选解数目。**
  - 非时齐SA算法理论，在每个温度下只产生一个或少量候选解，不存在选择内循环终止准则的问题。
  - 时齐SA算法理论，收敛性条件要求在每个温度下产生候选解数目趋于无穷大，以使相应的马氏链达到平稳概率分布。现实无法做到。
- **常用设计：**
  - 连续若干步的目标值变化小于预设阈值
  - 固定步数抽样

收敛准则

- 算法终止准则，即判断终止算法的条件。
- 设置温度终值是一种简单的方法。
  - SA算法收敛性理论要求温度终值趋于零，这显然不切实际。
- 基于时间的准则
  - 设置终止温度的阈值
  - 设置外循环迭代次数
- 基于性能的准则
  - 搜索到的最优值连续若干步变化微小（不变）
  - 系统熵趋于稳定

程序演示、应用举例

- 函数优化：见演示 智能优化算法演示软件V2.0、Opt_test
- TSP：见演示 TspClientV2.0软件、Opt_test
- 模型参数辨识/控制器设计
- 车间调度

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An effective hybrid optimization strategy for job-shop scheduling problems

Ling Wang*, Da-Zhong Zheng

Department of Automation, Tsinghua University, Beijing, 100084, People's Republic of China

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非最小相位系统控制器的优化设计[1)]

王 凌 李文峰 郑大钟

(清华大学自动化系 北京 100084)

(E-mail: wangling@mail.tsinghua.edu.cn)

摘 要 抑制非最小相位系统的右半平面零点所造成的负调至今仍是个开放问题. 以同时抑制非最小相位系统的超调、负调和调整时间为目的, 合理融合遗传算法的并行搜索结构和模拟退火的可控性概率突跳, 提出了设计一类 PID 控制器的混合优化策略. 基于典型系统的数值仿真验证了混合策略的有效性和对系统的适应性, 以及所设计控制器的优越性.

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非线性系统参数估计的一类有效搜索策略[1)]

王 凌 李令莱 郑大钟

(清华大学自动化系 北京 100084)

(E-mail: wangling@mail.tsinghua.edu.cn)

摘 要 结合模拟退火的随机概率突跳性搜索和单纯形法的凸多面体几何搜索, 提出了非线性系统参数估计的一类有效搜索策略. 通过对多种非线性定常系统的多维参数估计和非线性时变水箱系统的参数与时滞在线联合估计的仿真研究, 验证了该方法的可行性、有效性及其一定的抗噪声能力.

算法改进-内部环节

- 在确保一定优化质量的基础上，提高SA的搜索效率是对改进SA的主要目标。
- 设计合适的初始化环节，包括参数、状态。
- 设计合适的状态产生操作，或者是多操作的融合使用，使其根据搜索进程的需要强调全空间分散性或局部区域性。
- 设计高效的退火历程，尤其是温度控制策略。
- 避免状态的迂回搜索。
- 采用并行搜索结构。
- 设计合适的算法终止准则。

算法改进-外部环节

- 增加升温或重升温过程。择机将温度适当提高，以激活各状态的接受概率，避免陷入当前状态。
- 增加记忆功能，譬如保优、访问频次。
- 增加补充搜索过程，譬如局部增强搜索、规则（知识）性调整。
- 对当前状态，采用多次搜索策略，以概率接受区域内的最优状态，而单次比较方式。
- 结合基于其他搜索机制的寻优算法，如遗传算法，更好地平衡E&E。
- 多种方案的综合应用。

变型-Noising Method

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Theory and Methodology

The noising methods: A generalization of some metaheuristics

Irène Charon, Olivier Hudry *
Departement d'Informatique et Réseaux, École nationale supérieure des télécommunications, 46 Rue Barrault, 75634 Paris cedex 13, France

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Application of the noising method to the travelling salesman problem

Irène Charon, Olivier Hudry *
École nationale supérieure des télécommunications, 46 rue Barrault, 75634 Paris Cedex 13, France

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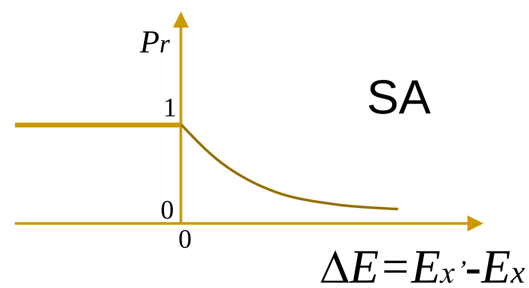
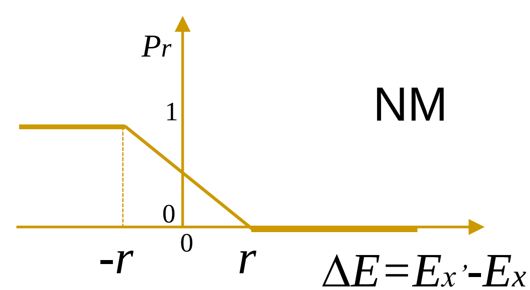
- Compute an initial solution C
- $best\_sol \leftarrow C$
- $r \leftarrow r_{max}$
- $nb\_it \leftarrow 0$
- repeat the following steps:
  - * $nb\_it \leftarrow nb\_it + 1$
  - * let C' be a neighbour of C: $C' \in N(C)$
  - * draw a random number ρ in $[-r, r]$ uniformly
  - * compute $\Delta f(C, C')$ and $\Delta f_{noised}(C, C') = \Delta f(C, C') + \rho$
  - * if $\Delta f_{noised}(C, C') < 0$, then $C \leftarrow C'$
  - * if $f(C) < f(best\_sol)$, then $best\_sol \leftarrow C$
  - * if $nb\_it \equiv 0 \pmod{nb\_it\_at\_fixed\_rate}$, then decrease r
- until $nb\_it = total\_nb\_it$
- return $best\_sol$.

Fig. 1. A scheme of the noising method.





Q: r变小，接受曲线如何变化？

Exploration-Exploitation

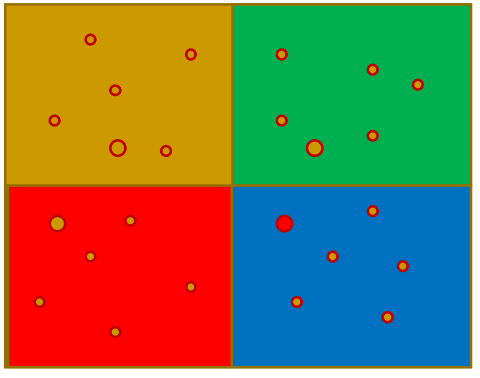
并行SA：进程并行

- 全过程并行、子进程并行
- 全过程并行：算法首先产生一组初始状态，然后将各状态发送给不同的处理机，各处理机独立进行整个SA搜索过程，最后汇总比较得到最终结果。
  - 利用空间资源弥补单机串行搜索的不足，非真正并行。
- 子进程并行：由多个处理机同时独立执行算法的某些进程，综合后继续执行算法的其他环节。譬如，多个处理机分别对当前状态执行抽样过程，当所有抽样过程结束后，综合得到新的当前状态。各处理机可采用不同的状态产生操作、接受准则，甚至不同的控制参数，从而增强灵活性，发挥各处理机的作用，实现并行策略的优越性。

并行SA：空间并行

- **Divide and conquer**

- **空间并行性：将整个搜索空间分解成若干个子区域，各子区域分别由不同的处理机执行模拟退火的搜索过程，最后综合得到最终的优化结果。**
- **由于各处理机的搜索空间缩小，对各子问题的搜索效率和可靠性得以提高，可改善对原问题的优化质量与效率。然而，当问题不适合分解或分解不当时，子问题的独立优化将难以反映问题的整体特性。**



大规模TSP举例
- ✓ **解空间分解**
- ✓ **点空间分解**

嵌套分区 NP

- **Nested Partitions**

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computers & operations research

New parallel randomized algorithms for the traveling salesman problem

Leyuan Shi*[,1], Sigurdur Ólafsson[2], Ning Sun[3]
Department of Industrial Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA

Received March 1997; received in revised form February 1998

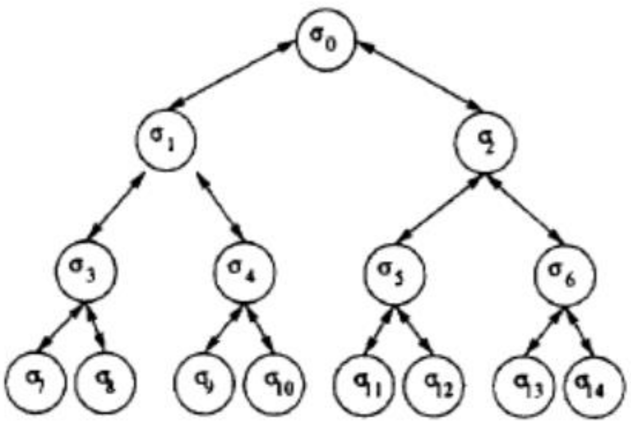
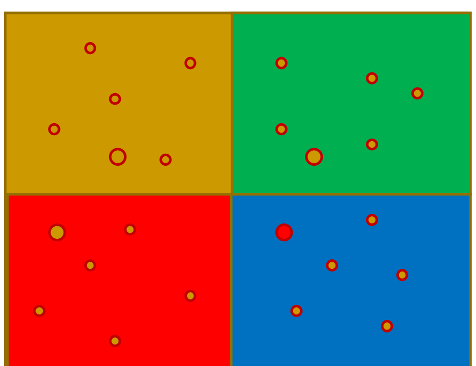
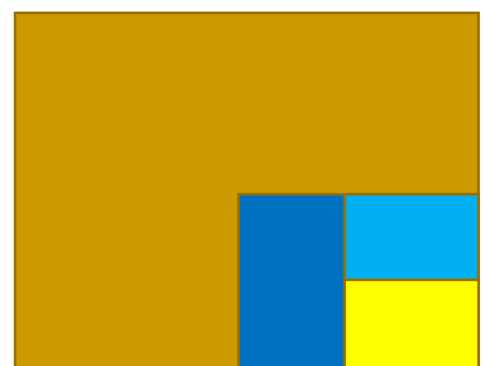


Fig. 1. Example of a partitioning generated by the NP method.

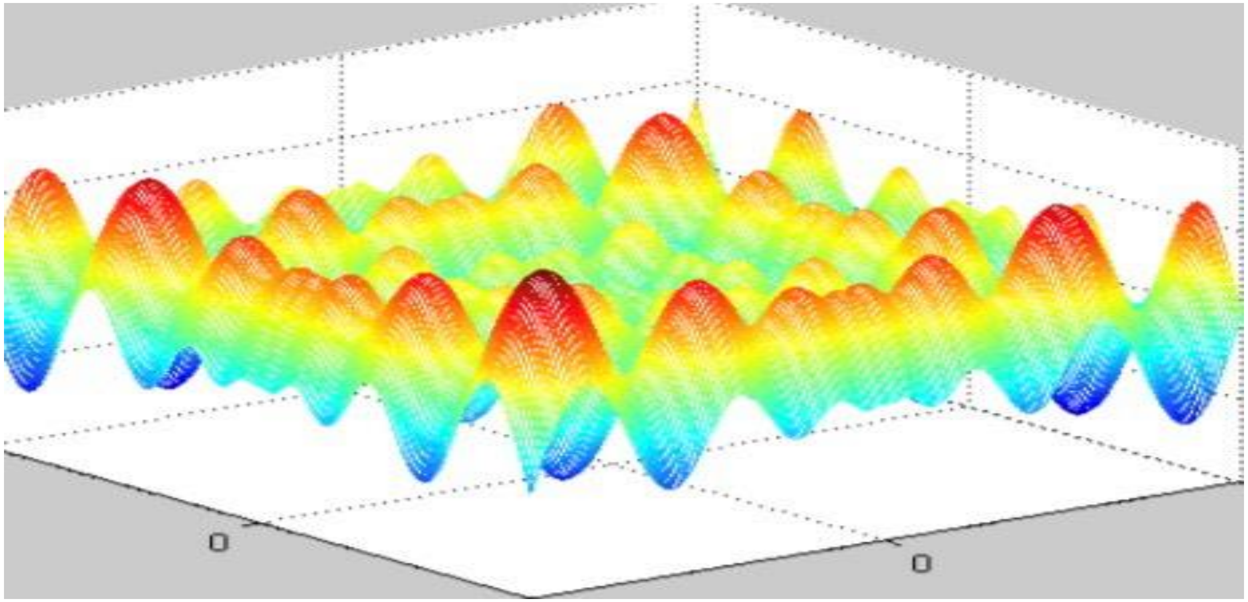




坐观云卷云舒
静看花开花谢
任凭潮起潮落
梦想始终如一

那就是理想中的全局最优！

欲擒故纵



退一步海阔天空