Optimization and Evolutionary Algorithms

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PoAI

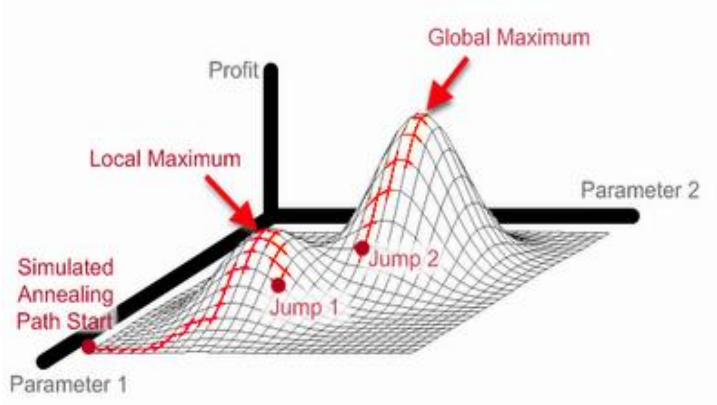
Contents

Annealing 退火

- In metallurgy, annealing is used to temper or harden metals and glass.
  在冶金学中，退火用于对金属和玻璃进行回火或硬化。
- A solid is heated in a hot bath, increasing the temperature up to a maximum value. At this temperature, all material is in liquid state and the particles arrange themselves randomly.
  将一个固体放在高温炉内进行加热，提升温度至最大值。在该温度下，所有的材料都处于液体状态，并且粒子本身随机地排列。
- As the temperature of the hot bath is cooled gradually, all the particles of this structure will be arranged in the state of lower energy.
  随着高温炉内的温度逐渐冷却，该结构的所有粒子将呈现低能状态。

Simulated Annealing 模拟退火

- Simulated annealing is a probabilistic technique for approximating the global optimum of a given function. Proposed in 1953.
  模拟退火是一种给定函数逼近全局最优解的概率方法。发表于1953年。
- Specifically, it is a meta-heuristic to approximate global optimization in a large search space.
  具体来说，是一种在大搜索空间逼近全局最优解的元启发式方法。
- Optimization and Thermodynamics 优化与热力学
  - Objective function 目标函数 ⇔ Energy level 能量极位
  - Admissible solution 可接受解 ⇔ System state 系统状态
  - Neighbor solution 相邻解 ⇔ Change of state 状态变化
  - Control parameter 控制参数 ⇔ Temperature 温度
  - Better solution 更优解 ⇔ Solidification state 凝固状态



Source: http://www.maxdama.com

Simulated Annealing Algorithm 模拟退火算法

- **Initial Solution** 初始解

  Generated using an heuristic. Chosen at random.

  使用启发式方法生成。随机选择。

- **Neighborhood** 相邻节点

  Generated randomly. Mutating the current solution.

  随机生成。当前解的变异。

- **Acceptance** 接受条件

  Neighbor has lower cost value, higher cost value is accepted with the probability p.

  相邻节点具有较低代价值，具有较高代价值的相邻节点则以概率P接受。

- **Stopping Criteria** 停止判据

  Solution with a lower value than threshold. Maximum total number of iterations.解具有比阈值低的值。已达到迭代最大总次数。

Simulated Annealing Algorithm 模拟退火算法

function SIMULATED-ANNEALING(*problem*, *schedule*) **returns** a solution state
  inputs: *problem*, a problem
    schedule, a mapping from time to "temperature"
  current ← MAKE-NODE(*problem*.INITIAL-STATE)
  for $t = 1$ **to** ∞ **do**
    $T \leftarrow schedule(t)$
    if $T = 0$ **then return** *current*
    next ← a randomly selected successor of *current*
    $\Delta E \leftarrow next.\text{VALUE} - current.\text{VALUE}$
    if $\Delta E > 0$ **then** *current* ← *next*
    else *current* ← *next* only with probability $e^{\Delta E/T}$

A version of stochastic hill climbing where some downhill moves are allowed.
Downhill moves are accepted readily early in the annealing schedule and then less often as time goes on.
一种允许部分下山移动的随机爬山法的版本。下山移动在退火调度的早期容易被接受，随着时间的推移逐步降低。

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- 4.3.1. Simulated Annealing
- 4.3.2. Genetic Algorithms

Genetic Algorithms 遗传算法

- The elements of genetic algorithms was introduced in 1960s. Became popular through the work of John Holland in early 1970s, and particularly his book *Adaptation in Natural and Artificial Systems* (1975).

  遗传算法的一些要素是1960年代提出的。通过约翰·霍兰在1970年代早期的工作，尤其是他的《神经元与人工系统的适应性》（1975年）一书，使得遗传算法流行起来。

- It is a *search heuristic* that mimics the process of natural selection.

  它是一种模仿自然选择过程的搜索启发式算法。

- The algorithm is a variant of stochastic beam search, in which successor states are generated by combining *two parent* states rather than by modifying a single state. It is dealing with *sexual reproduction* rather than asexual reproduction.

  该算法是随机束搜索的一个变型，其中后继节点是由两个父辈状态的组合而不是修改单一状态生成的。其处理过程是有性繁殖，而不是无性繁殖。

Genetic Algorithms 遗传算法

- Genetic algorithms belong to the larger class of *evolutionary algorithms*.遗传算法属于进化算法这个大分类。
- The algorithms generate solutions to optimization problems using techniques inspired by natural evolution, such as

  该算法采用自然进化所派生的技法来生成优化问题的解，例如

  - inheritance, mutation, selection, and crossover.

    遗传、突变、选择、以及杂交。
- It begin with a set of k randomly generated states, called the population.

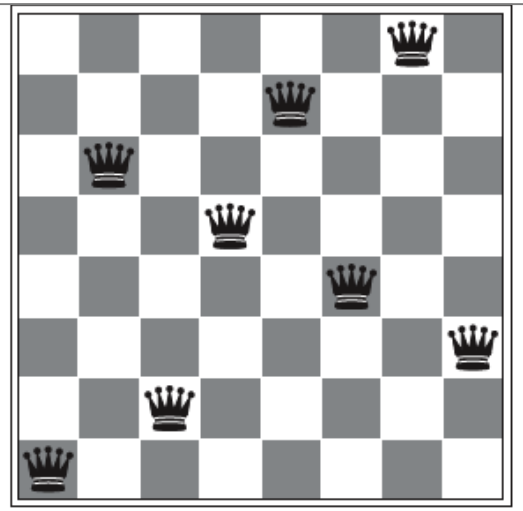
  该算法开始时具有一组k个随机生成的状态，称其为种群。
- Each state (individual) is represented as a string over a finite alphabet, most commonly, a string of 0s and 1s.

  每个状态（个体）表示为有限字母表上的一个字符串，通常是0和1的字符串。

Example: 8-queens problem 8皇后问题

- An 8-queens state must specify the positions of 8 queens, each in a column of 8 squares, the state could be represented as 8 digits, each in the range from 1 to 8.

  某8皇后状态需要指明8个皇后的位置，每个位于8个方格的一列，其状态可用8个数字表示，每个位于1到8之间。



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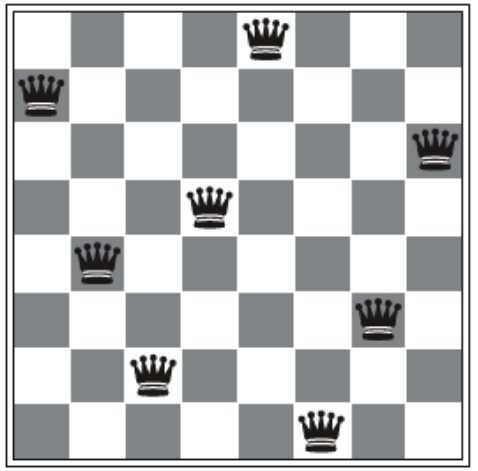

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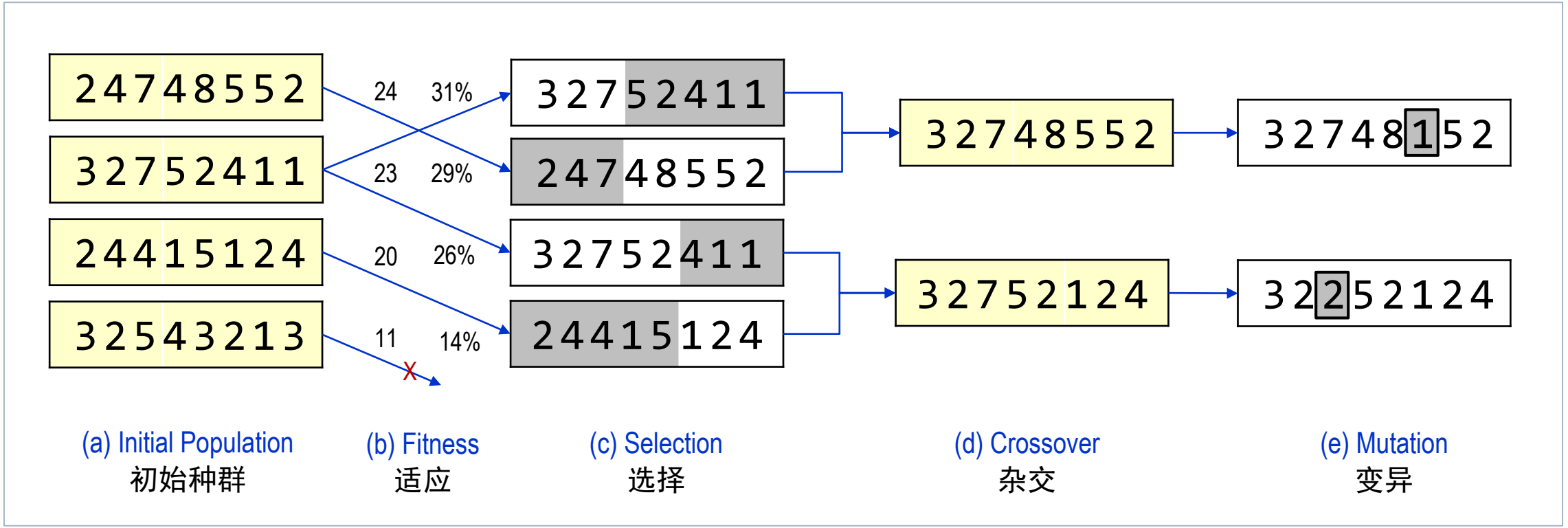
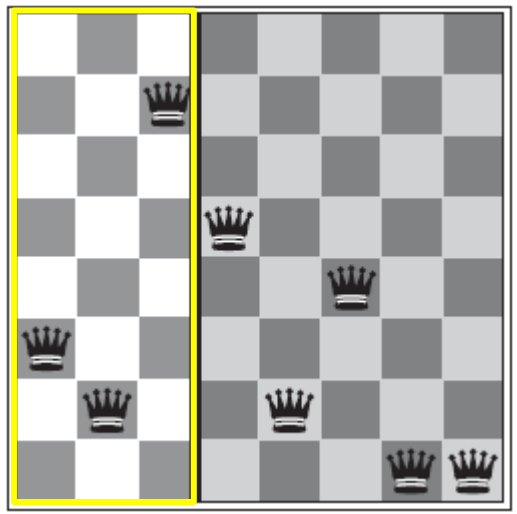
Example: 8-queens problem 8皇后问题



Digit strings representing 8-queens states. (a) the initial population, (b) ranked by the fitness function, (c) resulting in pairs for mating, (d) reproduce child, (e) subject to mutation.

数字串表示8皇后的状态。(a) 为初始种群，(b) 通过适应函数进行分级，(c) 导致交配对产生，(d) 繁殖后代，(e) 取决于突变。

Example: 8-queens problem 8皇后问题



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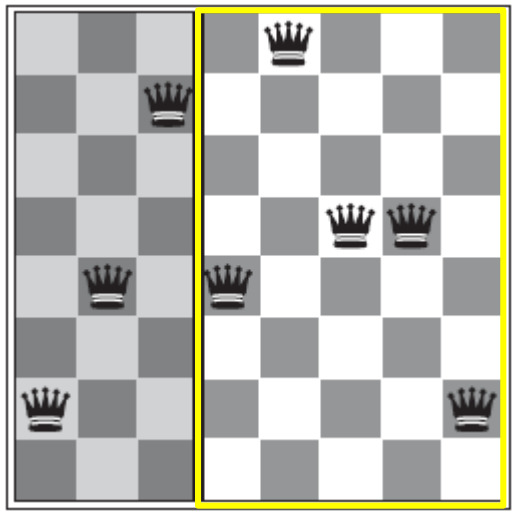

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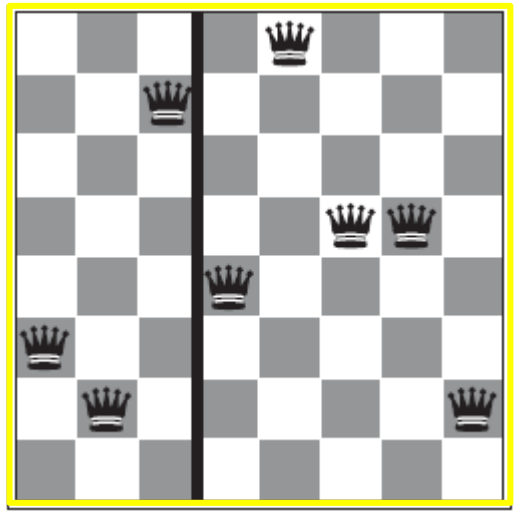

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Those three 8-queens states correspond to the first two parents in “Selection” and their offspring in “Crossover”.
The shaded columns are lost in the crossover step and the unshaded columns are retained.

这三个8皇后的状态分别对应于“选择”中的两个父辈和“杂交”中它们的后代。
阴影的若干列在杂交步骤中被丢掉，而无阴影的若干列则被保留下来。

The Genetic Algorithm 遗传算法

function GENETIC-ALGORITHM(*population*, FITNESS-FN) **returns** an individual
  inputs: *population*, a set of individuals
    FITNESS-FN, a function that measures the fitness of an individual
  repeat
    new_population ← empty set
    for *i* = 1 **to** SIZE(*population*) **do**
      x ← RANDOM-SELECTION(*population*, FITNESS-FN)
      y ← RANDOM-SELECTION(*population*, FITNESS-FN)
      child ← REPRODUCE(*x*, *y*)
      if (small random probability) **then** *child* ← MUTATE(*child*)
      add *child* to *new_population*
    population ← *new_population*
  until some individual is fit enough, or enough time has elapsed
  return the best individual in *population*, according to FITNESS-FN

Applications of Genetic Algorithms 遗传算法的应用

- bioinformatics 生物信息学
- computational science 计算科学
- engineering 工程
- economics 经济学
- chemistry 化学
- manufacturing 制造
- mathematics 数学
- physics 物理
- phylogenetics 种系遗传学
- pharmacometrics 定量药理学

Thank you for your attention!