Local Search and Optimization

Chapter 4

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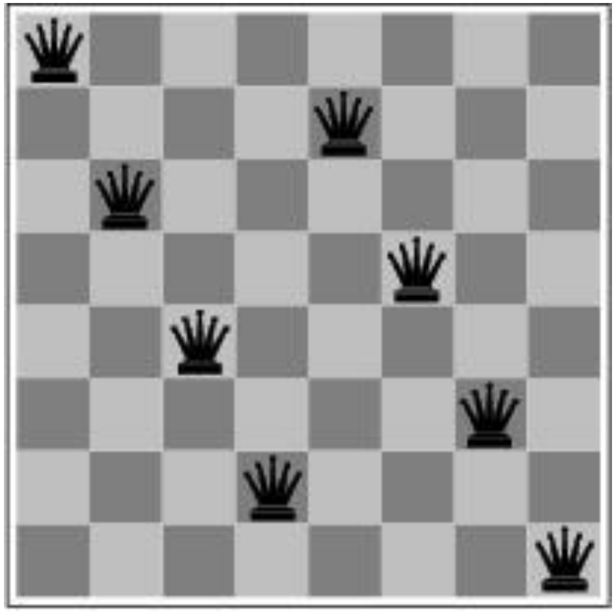
(Based on slides of Padhraic Smyth, Stuart Russell, Rao Kambhampati, Raj Rao, Dan Weld…)

Outline

- Local search techniques and optimization
  - Hill-climbing
  - Gradient methods
  - Simulated annealing
  - Genetic algorithms
  - Issues with local search

Local search and optimization

- Previous lecture: path to goal is solution to problem
  - systematic exploration of search space.
- This lecture: a state is solution to problem
  - for some problems path is irrelevant.
  - E.g., 8-queens
- Different algorithms can be used
  - Local search



Goal Satisfaction

reach the goal node
Constraint satisfaction

Optimization

optimize(objective fn)
Constraint Optimization

You can go back and forth between the two problems
Typically in the same complexity class

Local search and optimization

- Local search
  - Keep track of single current state
  - Move only to neighboring states
  - Ignore paths

- Advantages:
  - Use very little memory
  - Can often find reasonable solutions in large or infinite (continuous) state spaces.

- “Pure optimization” problems
  - All states have an objective function
  - Goal is to find state with max (or min) objective value
  - Does not quite fit into path-cost/goal-state formulation
  - Local search can do quite well on these problems.

Trivial Algorithms

- Random Sampling
  - Generate a state randomly

- Random Walk
  - Randomly pick a neighbor of the current state

- Both algorithms asymptotically complete.

Hill-climbing (Greedy Local Search) max version

function HILL-CLIMBING(*problem*) **return** a state that is a local maximum
    input: *problem*, a problem
    local variables: *current*, **a node.**
                neighbor, **a node.**

    current ← MAKE-NODE(INITIAL-STATE[*problem*])
    loop do
        neighbor ← a highest valued successor of *current*
        if VALUE [*neighbor*] ≤ VALUE[*current*] **then return** STATE[*current*]
        current ← *neighbor*

min version will reverse inequalities and look for lowest valued successor

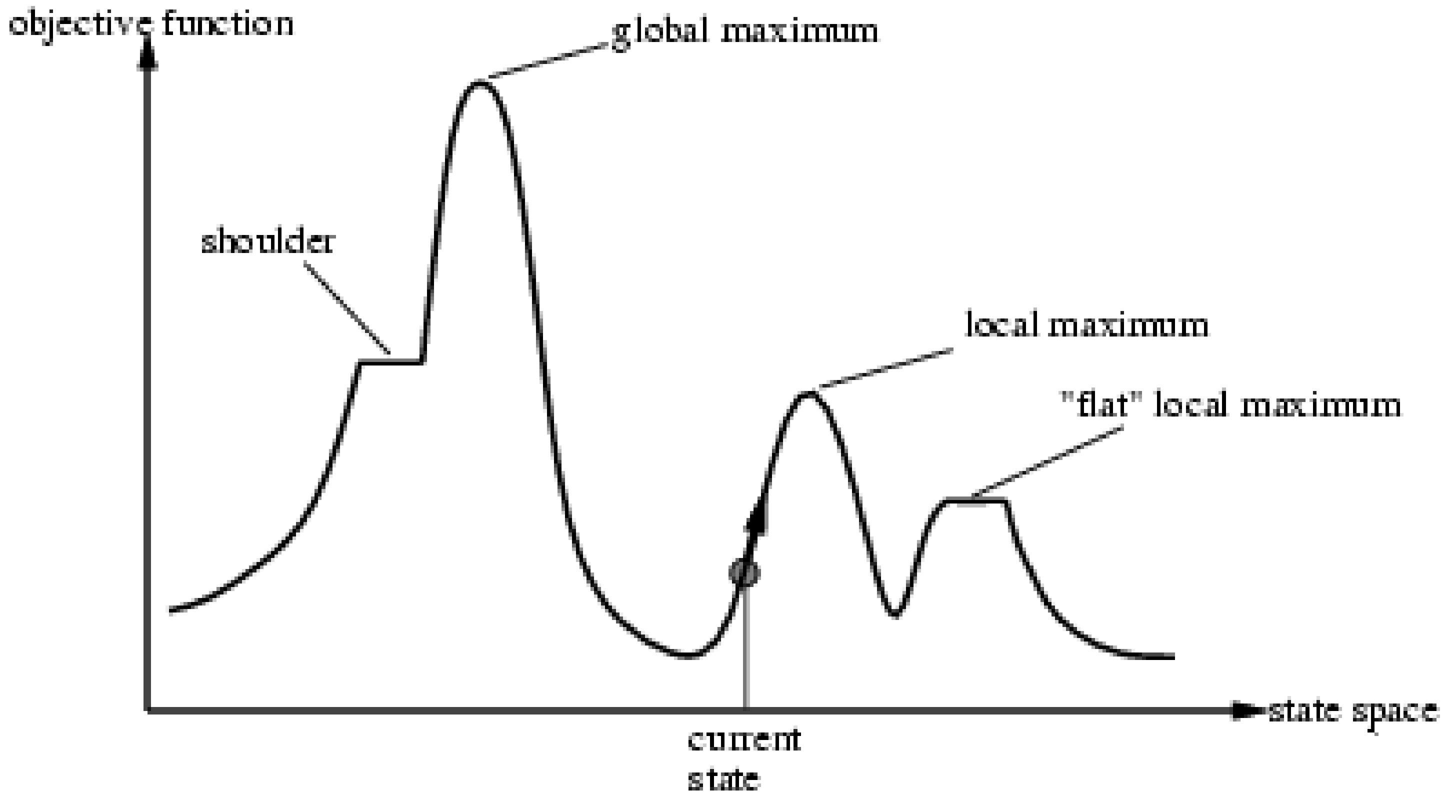
Hill-climbing search

- "a loop that continuously moves towards increasing value"
  - terminates when a peak is reached
  - Aka greedy local search
- Value can be either
  - Objective function value
  - Heuristic function value (minimized)

- Hill climbing does not look ahead of the immediate neighbors
- Can randomly choose among the set of best successors
  - if multiple have the best value

- "climbing Mount Everest in a thick fog with amnesia"

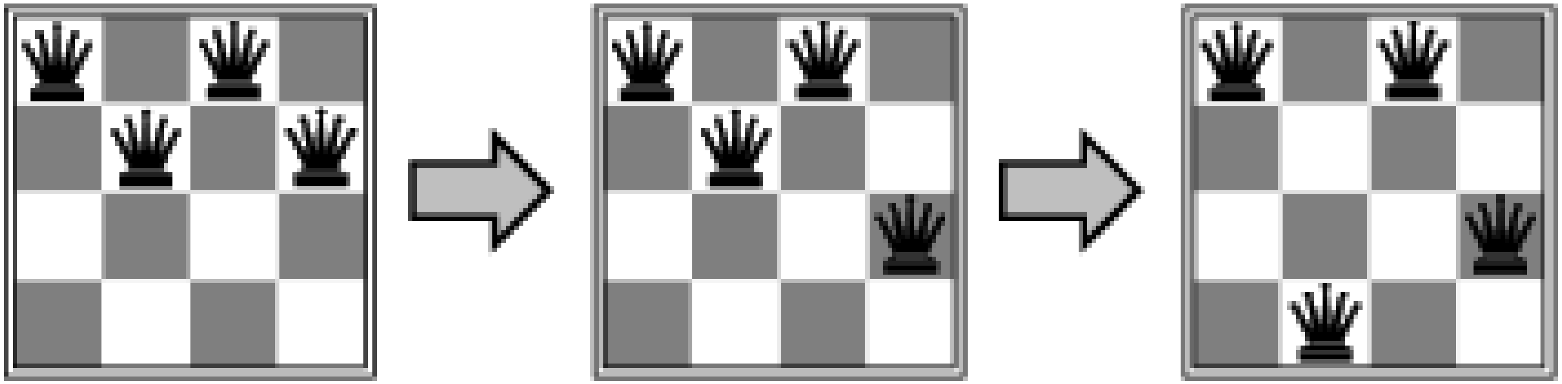
“Landscape” of search



Hill Climbing gets stuck in local minima
depending on?

Example: *n*-queens

- Put *n* queens on an *n* x *n* board with no two queens on the same row, column, or diagonal



- Is it a satisfaction problem or optimization?

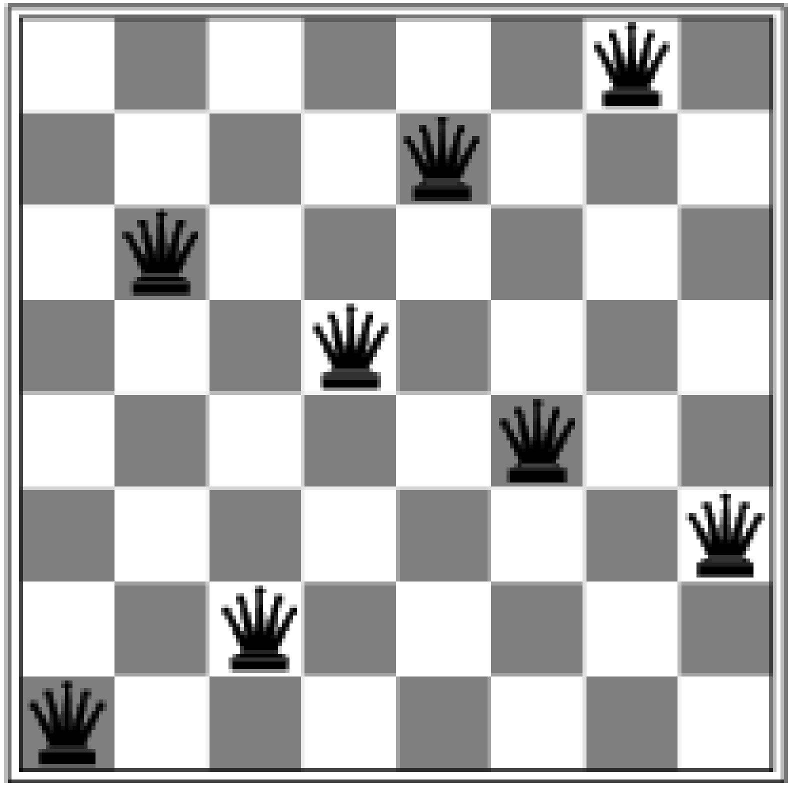
Hill-climbing search: 8-queens problem

- Need to convert to an optimization problem
- *h* = number of pairs of queens that are attacking each other
- *h = 17* for the above state

Search Space

- State
  - All 8 queens on the board in some configuration
- Successor function
  - move a single queen to another square in the same column.
- Example of a heuristic function *h(n)*:
  - the number of pairs of queens that are attacking each other
  - (so we want to minimize this)

Hill-climbing search: 8-queens problem



- Is this a solution?
- What is h?

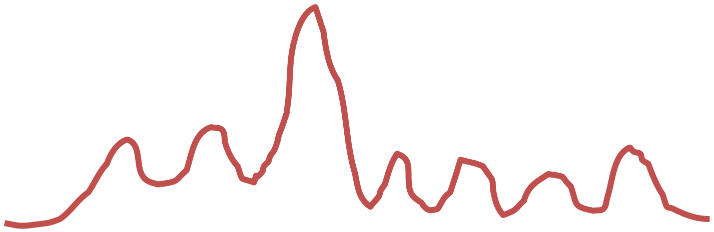
Hill-climbing on 8-queens

- Randomly generated 8-queens starting states…
- 14% the time it solves the problem
- 86% of the time it get stuck at a local minimum

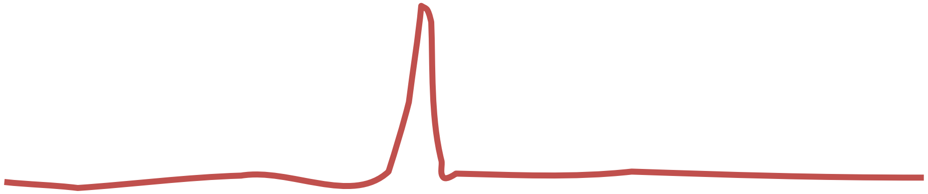
- However…
  - Takes only 4 steps on average when it succeeds
  - And 3 on average when it gets stuck
  - (for a state space with 8^8 =~17 million states)

Hill Climbing Drawbacks

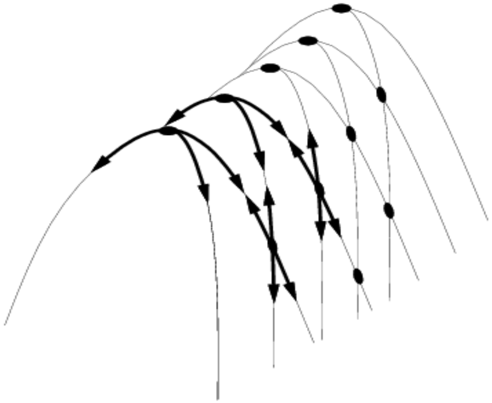
- Local maxima



- Plateaus



- Diagonal ridges



Escaping Shoulders: Sideways Move

- If no downhill (uphill) moves, allow sideways moves in hope that algorithm can escape
  - Need to place a limit on the possible number of sideways moves to avoid infinite loops
- For 8-queens
  - Now allow sideways moves with a limit of 100
  - Raises percentage of problem instances solved from 14 to 94%
  - However….
    - 21 steps for every successful solution
    - 64 for each failure

Tabu Search

- prevent returning quickly to the same state
- Keep fixed length queue (“tabu list”)
- add most recent state to queue; drop oldest
- Never make the step that is currently tabu’ed

- Properties:
  - As the size of the tabu list grows, hill-climbing will asymptotically become “non-redundant” (won’t look at the same state twice)
  - In practice, a reasonable sized tabu list (say 100 or so) improves the performance of hill climbing in many problems

Escaping Shoulders/local Optima Enforced Hill Climbing

- Perform breadth first search from a local optima
  - to find the next state with better h function
- Typically,
  - prolonged periods of exhaustive search
  - bridged by relatively quick periods of hill-climbing
- Middle ground b/w local and systematic search

Hill-climbing: stochastic variations

- Stochastic hill-climbing
  - Random selection among the uphill moves.
  - The selection probability can vary with the steepness of the uphill move.

- To avoid getting stuck in local minima
  - Random-walk hill-climbing
  - Random-restart hill-climbing
  - Hill-climbing with both

Hill Climbing: stochastic variations

→When the state-space landscape has local minima, any search that moves only in the greedy direction cannot be complete

→Random walk, on the other hand, is asymptotically complete

Idea: Put random walk into greedy hill-climbing

Hill-climbing with random restarts

- If at first you don’t succeed, try, try again!
- Different variations
  - For each restart: run until termination vs. run for a fixed time
  - Run a fixed number of restarts or run indefinitely
- Analysis
  - Say each search has probability p of success
    - E.g., for 8-queens, p = 0.14 with no sideways moves
  - Expected number of restarts?
  - Expected number of steps taken?
- If you want to pick one local search algorithm, learn this one!!

Hill-climbing with random walk

- At each step do one of the two
  - Greedy: With prob p move to the neighbor with largest value
  - Random: With prob 1-p move to a random neighbor

Hill-climbing with both

- At each step do one of the three
  - Greedy: move to the neighbor with largest value
  - Random Walk: move to a random neighbor
  - Random Restart: Resample a new current state

Simulated Annealing

- Simulated Annealing = physics inspired twist on random walk
- Basic ideas:
  - like hill-climbing identify the quality of the local improvements
  - instead of picking the best move, pick one randomly
  - say the change in objective function is δ
  - if δ is positive, then move to that state
  - otherwise:
    - move to this state with probability proportional to δ
    - thus: worse moves (very large negative δ) are executed less often
  - however, there is always a chance of escaping from local maxima
  - over time, make it less likely to accept locally bad moves
  - (Can also make the size of the move random as well, i.e., allow “large” steps in state space)

Physical Interpretation of Simulated Annealing

- A Physical Analogy:
  - imagine letting a ball roll downhill on the function surface
    - this is like hill-climbing (for minimization)
  - now imagine shaking the surface, while the ball rolls, gradually reducing the amount of shaking
    - this is like simulated annealing

- Annealing = physical process of cooling a liquid or metal until particles achieve a certain frozen crystal state
  - simulated annealing:
    - free variables are like particles
    - seek "low energy" (high quality) configuration
    - slowly reducing temp. T with particles moving around randomly

Simulated annealing

function SIMULATED-ANNEALING(*problem, schedule*) **return** a solution state
input: *problem*, a problem
schedule, a mapping from time to temperature
local variables: *current***,** a node.
*next***,** a node.
*T***,** a "temperature" controlling the prob. of downward steps

current ← MAKE-NODE(INITIAL-STATE[*problem*])
for t ← 1 to ∞ do
T ← *schedule*[*t*]
if *T = 0* **then return** *current*
next ← a randomly selected successor of *current*
ΔE ← VALUE[*next*] - VALUE[*current*]
if $\Delta E > 0$ **then** *current* ← *next*
else *current* ← *next* only with probability $e^{\Delta E / T}$

Temperature T

- high T: probability of "locally bad" move is higher
- low T: probability of "locally bad" move is lower
- typically, T is decreased as the algorithm runs longer
- i.e., there is a "temperature schedule"

Simulated Annealing in Practice

- method proposed in 1983 by IBM researchers for solving VLSI layout problems (Kirkpatrick et al, *Science*, 220:671-680, 1983).
  - theoretically will always find the global optimum

- Other applications: Traveling salesman, Graph partitioning, Graph coloring, Scheduling, Facility Layout, Image Processing, …

- useful for some problems, but can be very slow
  - slowness comes about because T must be decreased very gradually to retain optimality

Local beam search

- Idea: Keeping only one node in memory is an extreme reaction to memory problems.

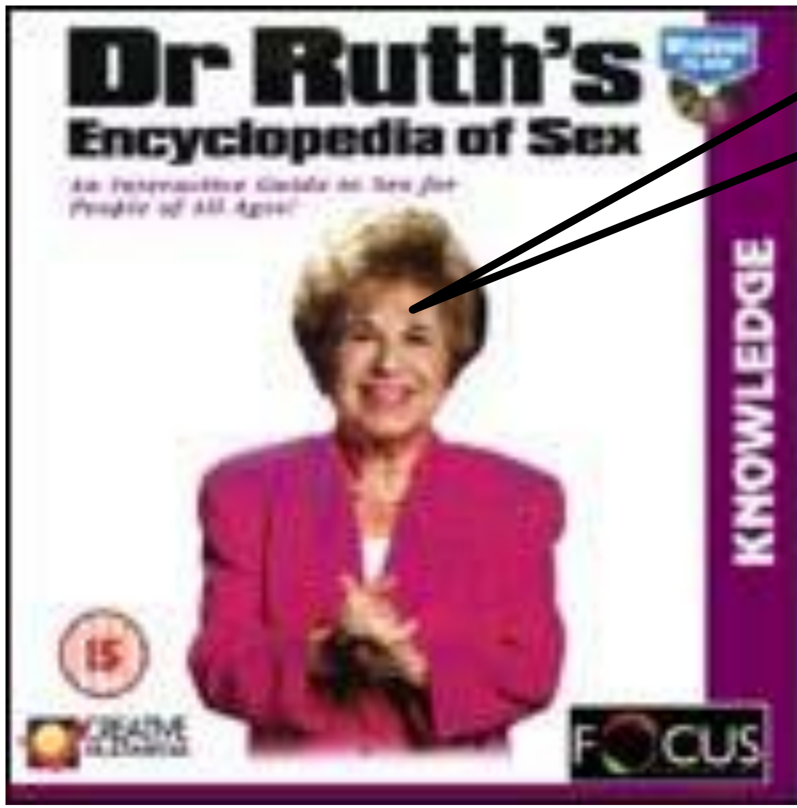
- Keep track of *k* states instead of one
  - Initially: *k* randomly selected states
  - Next: determine all successors of *k* states
  - If any of successors is goal $\rightarrow$ finished
  - Else select *k* best from successors and repeat

Local Beam Search (contd)

- Not the same as *k random-start searches run in parallel!*
- Searches that find good states recruit other searches to join them

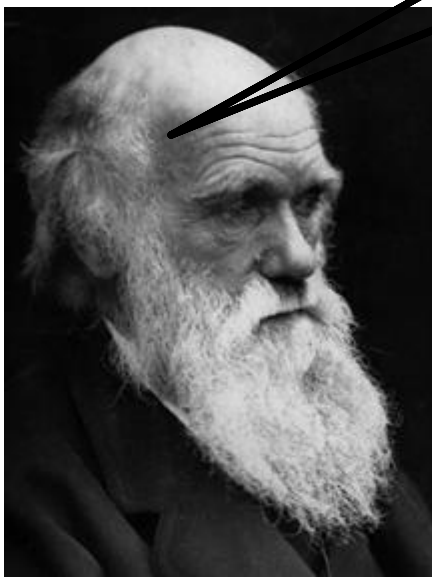
- Problem: quite often, all *k states end up on same local hill*
- Idea: Stochastic beam search
  - Choose *k successors randomly, biased towards good ones*

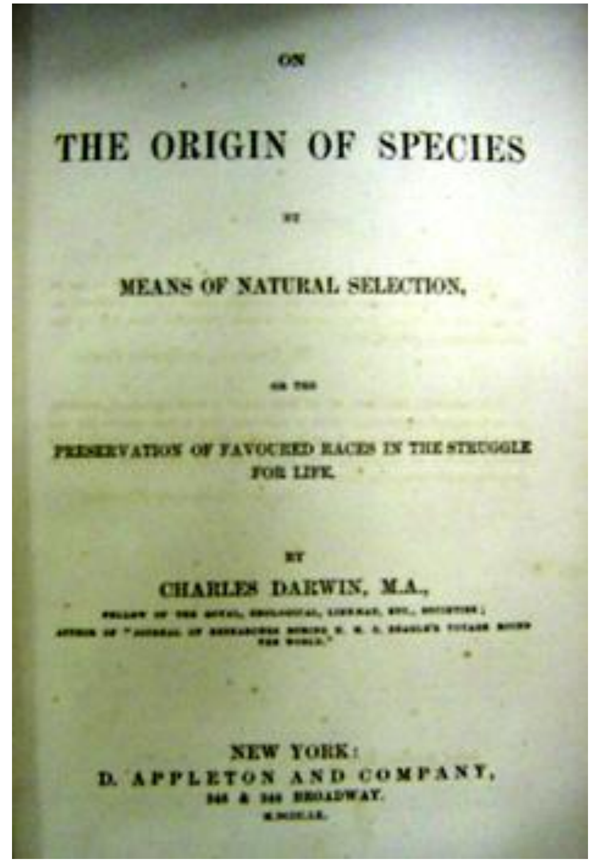
- Observe the close analogy to natural selection!



Hey! Perhaps sex can improve search?

Sure! Check out ye book.




ON

THE ORIGIN OF SPECIES

MEANS OF NATURAL SELECTION,

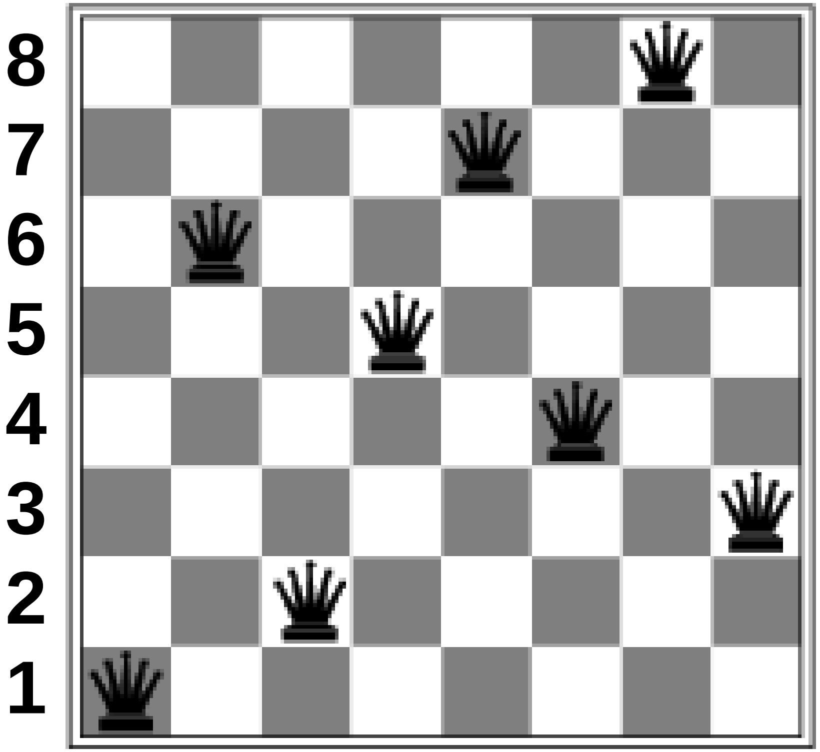
PRESERVATION OF FAVOURED RACES IN THE STRUGGLE FOR LIFE.

CHARLES DARWIN, M.A.,

NEW YORK:
D. APPLETON AND COMPANY,

Genetic algorithms

- Twist on Local Search: successor is generated by combining two parent states
- A state is represented as a string over a finite alphabet (e.g. binary)
  - 8-queens
    - State = position of 8 queens each in a column
- Start with *k* randomly generated states (population)
- Evaluation function (fitness function):
  - Higher values for better states.
  - Opposite to heuristic function, e.g., # non-attacking pairs in 8-queens
- Produce the next generation of states by "simulated evolution"
  - Random selection
  - Crossover
  - Random mutation



String representation
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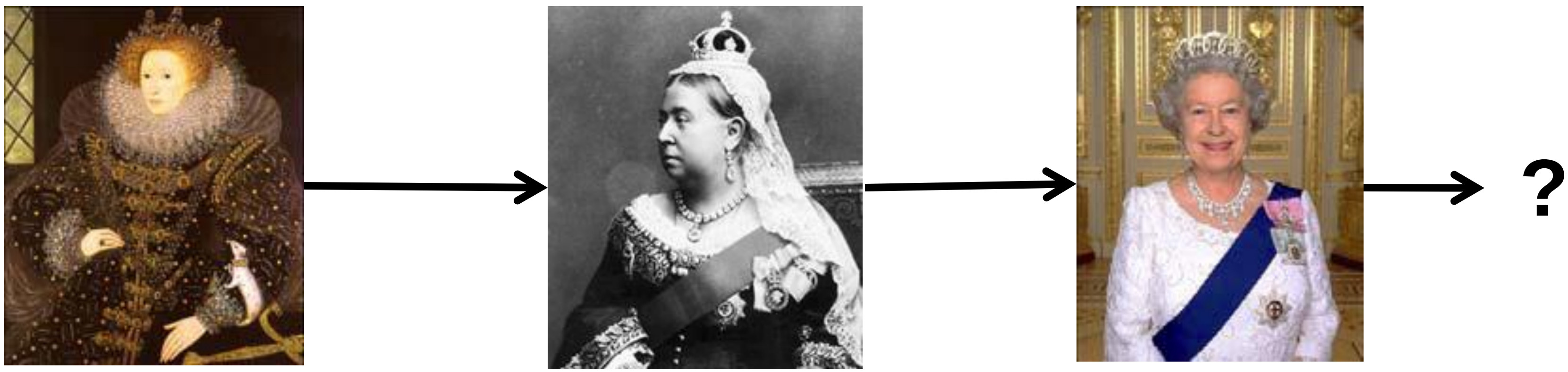
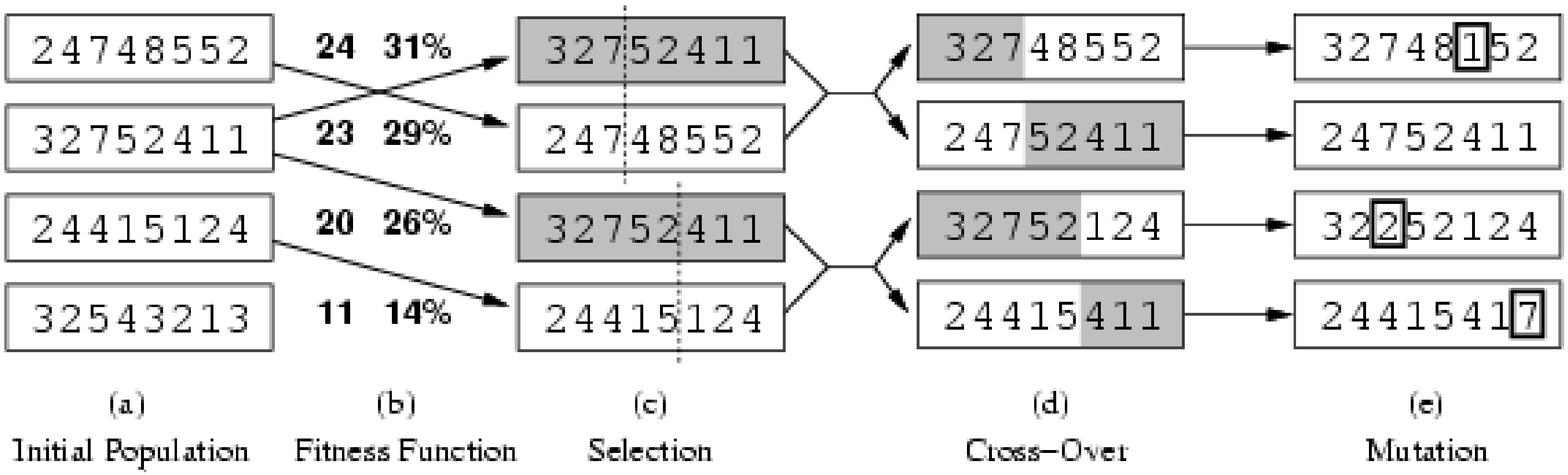
Can we evolve 8-queens through genetic algorithms?

Evolving 8-queens



Genetic algorithms



4 states for 8-queens problem

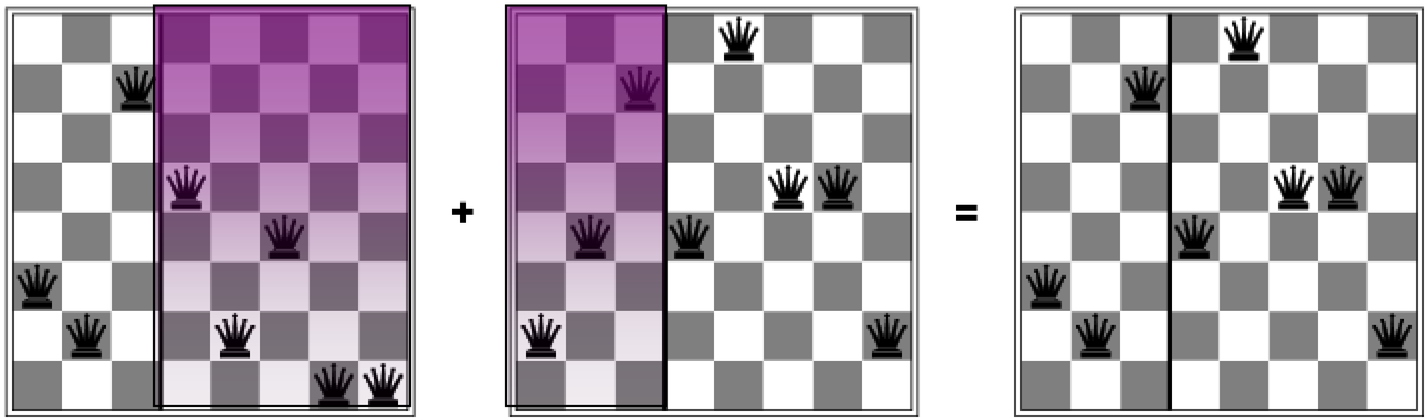
2 pairs of 2 states randomly selected based on fitness. Random crossover points selected

New states after crossover

Random mutation applied

- Fitness function: number of non-attacking pairs of queens (min = 0, max = $8 \times 7/2 = 28$)
- $24/(24+23+20+11) = 31\%$
- $23/(24+23+20+11) = 29\%$ etc

Genetic algorithms



Has the effect of "jumping" to a completely different new part of the search space (quite non-local)

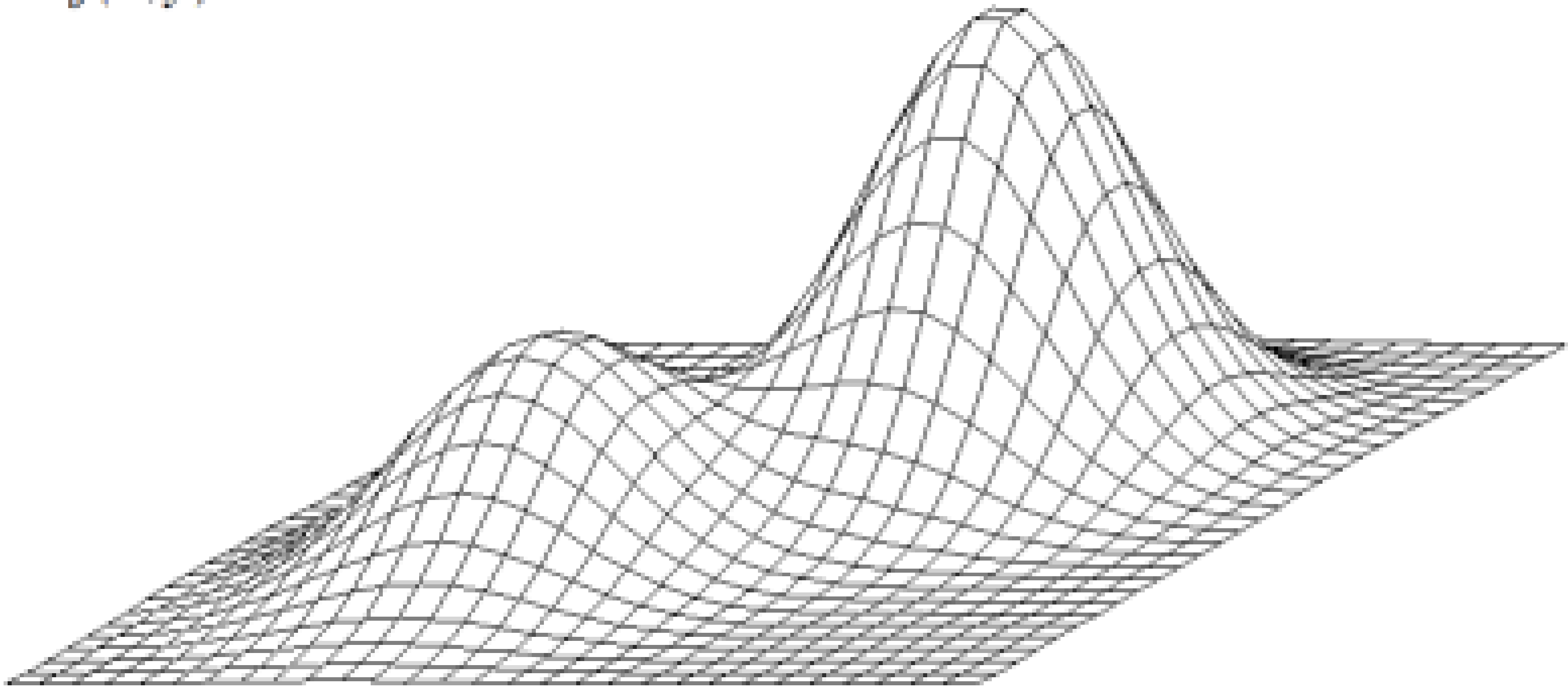
Comments on Genetic Algorithms

- Genetic algorithm is a variant of "stochastic beam search"
- Positive points
  - Random exploration can find solutions that local search can't
    - (via crossover primarily)
  - Appealing connection to human evolution
    - "neural" networks, and "genetic" algorithms are **metaphors**!
- Negative points
  - Large number of "tunable" parameters
    - Difficult to replicate performance from one problem to another
  - Lack of good empirical studies comparing to simpler methods
  - Useful on some (small?) set of problems but no convincing evidence that GAs are better than hill-climbing w/random restarts in general

Optimization of Continuous Functions

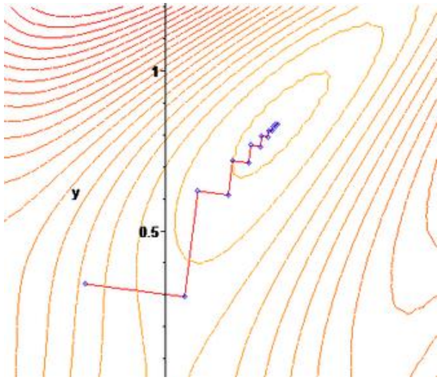
- Discretization
  - use hill-climbing
- Gradient descent
  - make a move in the direction of the gradient
    - gradients: closed form or empirical

$$f(x,y) = e^{-(x^2+y^2)} + 2e^{-((x-1.7)^2+(y-1.7)^2)}$$



Gradient Descent

Assume we have a continuous function: $f(x_1,x_2,\ldots,x_N)$
and we want minimize over continuous variables X1,X2,..,Xn

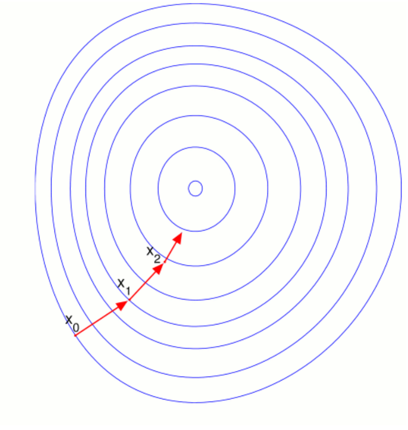


1. Compute the *gradients* for all i: $\partial f(x_1,x_2,\ldots,x_N) / \partial x_i$

2. Take a small step downhill in the direction of the gradient:

$$x_i \leftarrow x_i - \lambda \partial f(x_1,x_2,\ldots,x_N) / \partial x_i$$

3. Repeat.



- How to select λ
  - Line search: successively double
    - until *f* starts to increase again

Newton-Raphson applied to function minimization

- Newton-Raphson method: roots of a polynomial
  - To find roots of g(x), start with x and iterate
    - $x \leftarrow x - g(x)/g'(x)$
  - To minimize a function f(x), we need to find the roots of the equation f'(x)=0
    - $x \leftarrow x - f'(x)/f''(x)$
    - If x is a vector then
      - $\mathbf{x \leftarrow x - f'(x)/f''(x)}$

$\nabla f(x)$ $\qquad$ $H_f(x)$

$$X \leftarrow X - \underbrace{H_f^{-1}(X)}_{\text{Hessian}} \overbrace{\nabla f(x)}^{\text{gradient}}$$

Hessian is costly to compute (n^2 double derivative entries for an n-dimensional vector)
➔ approximations

- Equivalent to fitting a quadratic function for f in the local neighborhood of x.