CS 4700: Foundations of Artificial Intelligence



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Cornell University

Informed Search Recap

A*: Summary



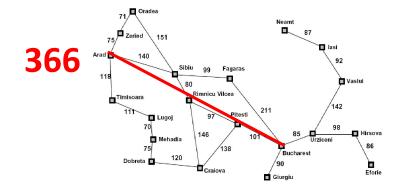
A*: Summary

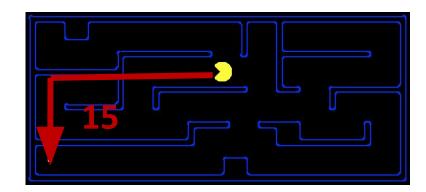
- A* uses both backward costs and (estimates of) forward costs
 - f(n) = g(n) + h(n)
 - = cost-so-far + heuristic-estimate-of-distance-to-goal
- A* is optimal with admissible / consistent heuristics
- Heuristic design is key: often use relaxed problems



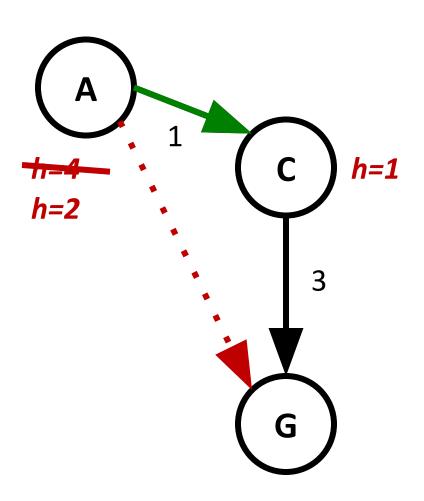
Creating Admissible Heuristics

- Most of the work in solving hard search problems optimally is in coming up with admissible heuristics
- Often, admissible heuristics are solutions to relaxed problems, where new actions are available





Creating Admissible+Consistent Heuristics



- Main idea: estimated heuristic costs ≤ actual costs
 - Admissibility: heuristic cost ≤ actual cost to goal
 h(A) ≤ actual cost from A to G
 - Consistency: heuristic "arc" cost ≤ actual cost for each arc
 h(A) h(C) ≤ cost(A to C)
- Consequences of consistency:
 - A* graph search is optimal

Tree Search Pseudo-Code

```
function Tree-Search(problem, fringe) return a solution, or failure

fringe ← Insert(make-node(initial-state[problem]), fringe)

loop do

if fringe is empty then return failure

node ← remove-front(fringe)

if goal-test(problem, state[node]) then return node

for child-node in expand(state[node], problem) do

fringe ← insert(child-node, fringe)

end

end
```

Graph Search Pseudo-Code

```
function Graph-Search (problem, fringe) return a solution, or failure
   closed \leftarrow an empty set
   fringe \leftarrow Insert(make-node(initial-state[problem]), fringe)
   loop do
       if fringe is empty then return failure
       node \leftarrow \text{REMOVE-FRONT}(fringe)
       if GOAL-TEST(problem, STATE[node]) then return node
       if STATE[node] is not in closed then
          add STATE[node] to closed
          for child-node in EXPAND(STATE[node], problem) do
              fringe \leftarrow INSERT(child-node, fringe)
          end
   end
```

Local search



Plan for today

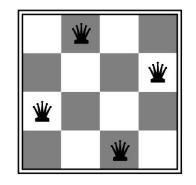
Overview of local search algorithms

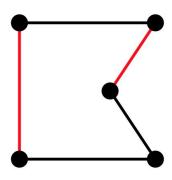
Gradient descent

Genetic algorithms at Cornell

Local search algorithms

- In many optimization problems, path is irrelevant; the goal state is the solution
- Then state space = set of "complete" configurations; find configuration satisfying constraints, e.g., n-queens problem; or, find optimal configuration, e.g., travelling salesperson problem





- In such cases, can use iterative improvement algorithms: keep a single "current" state, try to improve it
- Constant space, suitable for online as well as offline search
- More or less unavoidable if the "state" is yourself (i.e., learning)

Hill Climbing

Simple, general idea:

Start wherever

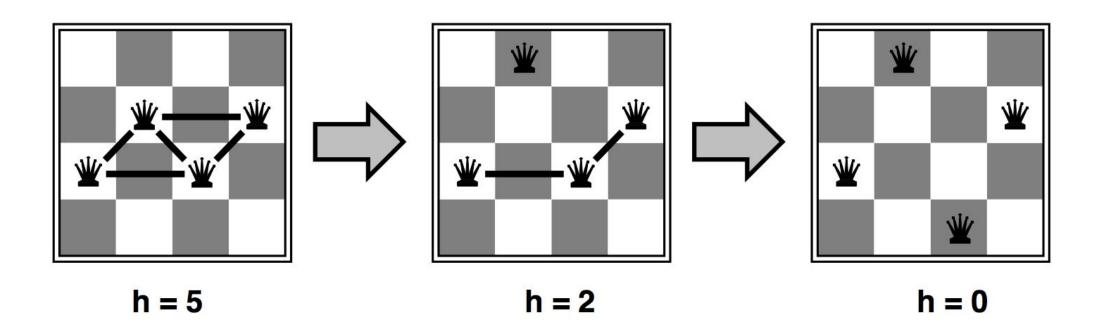
Repeat: move to the best neighboring state

• If no neighbors better than current, quit



Heuristic for *n*-queens problem

- Goal: n queens on board with no conflicts, i.e., no queen attacking another
- States: n queens on board, one per column
- Actions: move a queen in its column
- Heuristic value function: number of conflicts

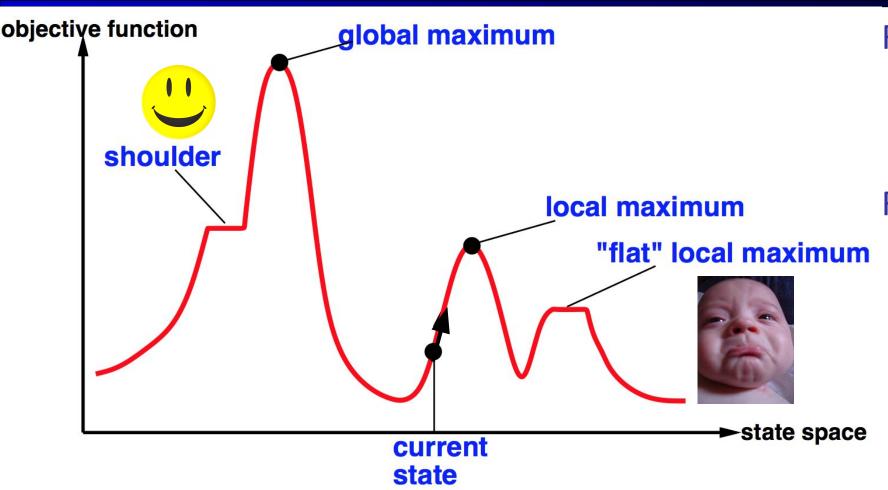


Hill-climbing algorithm

```
function HILL-CLIMBING(problem) returns a state
  current ← make-node(problem.initial-state)
  loop do
      neighbor ← a highest-valued successor of current
      if neighbor.value ≤ current.value then
           return current.state
      current ← neighbor
```

"Like climbing Everest in thick fog with amnesia"

Global and local maxima



Random restarts

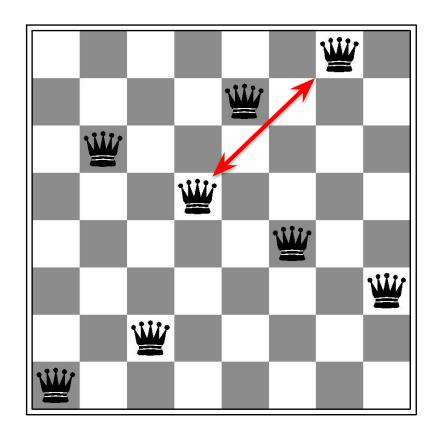
- find global optimum
- duh

Random sideways moves

- Escape from shoulders
- Loop forever on flat local maxima

Hill-climbing on the 8-queens problem

- No sideways moves:
 - Succeeds w/ prob. 0.14
 - Average number of moves per trial:
 - 4 when succeeding, 3 when getting stuck
 - Expected total number of moves needed:
 - $-3(1-p)/p + 4 = ^2 22 \text{ moves}$
- Allowing 100 sideways moves:
 - Succeeds w/ prob. 0.94
 - Average number of moves per trial:
 - 21 when succeeding, 65 when getting stuck
 - Expected total number of moves needed:
 - -65(1-p)/p + 21 = 25 moves



Moral: algorithms with knobs to twiddle are irritating

Simulated annealing

- Resembles the annealing process used to cool metals slowly to reach an ordered (low-energy) state
- Basic idea:
 - Allow "bad" moves occasionally, depending on "temperature"
 - High temperature => more bad moves allowed, shake the system out of its local minimum
 - Gradually reduce temperature according to some schedule
 - Sounds pretty flaky, doesn't it?

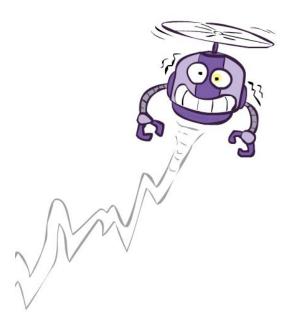
Simulated annealing algorithm

```
function SIMULATED-ANNEALING(problem, schedule) returns a state
current ← problem.initial-state
for t = 1 to \infty do
     T \leftarrow schedule(t)
     if T = 0 then return current
     next ← a randomly selected successor of current
     \Delta E \leftarrow next.value - current.value
     if \Delta E < 0 then current \leftarrow next
                else current \leftarrow next only with probability e^{-\Delta E/T}
```



Simulated Annealing

- Theoretical guarantee:
 - Stationary distribution (Boltzmann): $P(x) \propto e^{-E(x)/T}$
 - If *T* decreased slowly enough, will converge to optimal state!



Simulated Annealing

- Is this convergence an interesting guarantee?
- Sounds like magic, but reality is reality:
 - The more downhill steps you need to escape a local optimum, the less likely you are to ever make them all in a row
 - "Slowly enough" may mean exponentially slowly
 - Random restart hillclimbing also converges to optimal state...
- Simulated annealing and its relatives are a key workhorse in VLSI layout and other optimal configuration problems



Local beam search

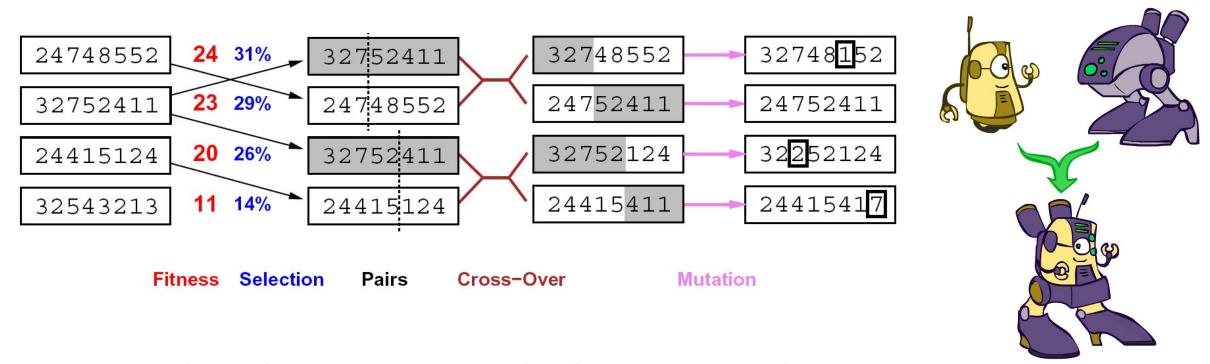
- Basic idea:
 - K copies of a local search algorithm, initialized randomly
 - For each iteration

Or, K chosen randomly with

- a bias towards good ones
 Generate ALL successors from K current states
- Choose best K of these to be the new current states
- Why is this different from K local searches in parallel?
 - The searches communicate! "Come over here, the grass is greener!"
- What other well-known algorithm does this remind you of?
 - Evolution!

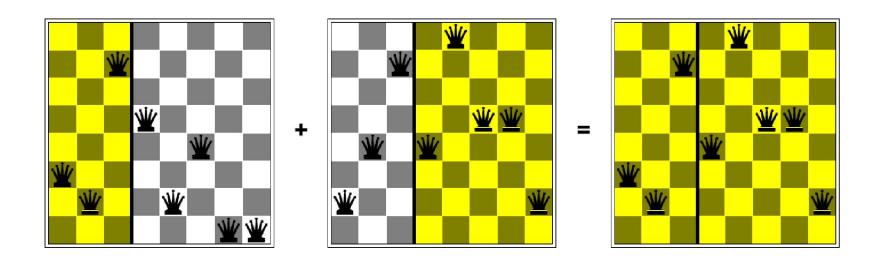


Genetic algorithms



- Genetic algorithms use a natural selection metaphor
 - Resample K individuals at each step (selection) weighted by fitness function
 - Combine by pairwise crossover operators, plus mutation to give variety

Example: N-Queens



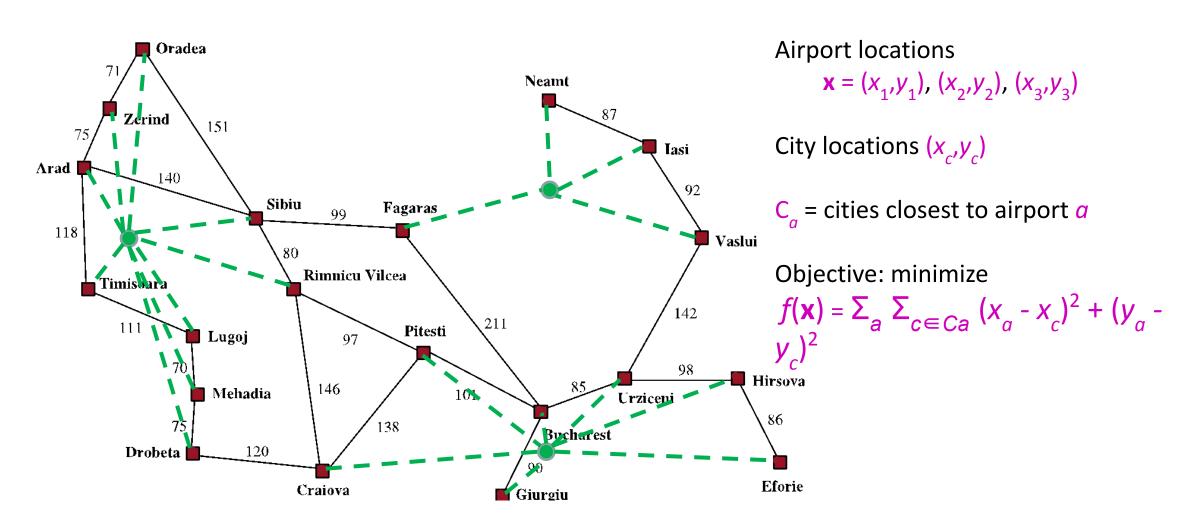
- Does crossover make sense here?
- What would mutation be?
- What would a good fitness function be?

Local search in continuous spaces



Example: Siting airports in Romania

Place 3 airports to minimize the sum of squared distances from each city to its nearest airport

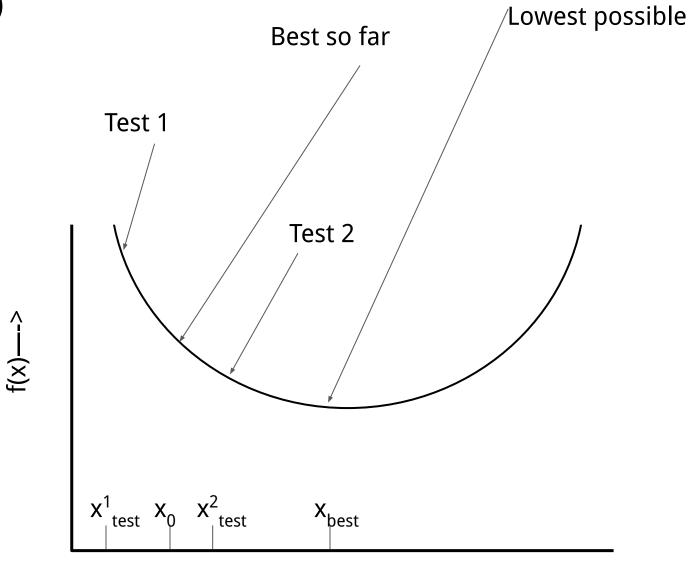


Handling a continuous state/action space

Discretize it!

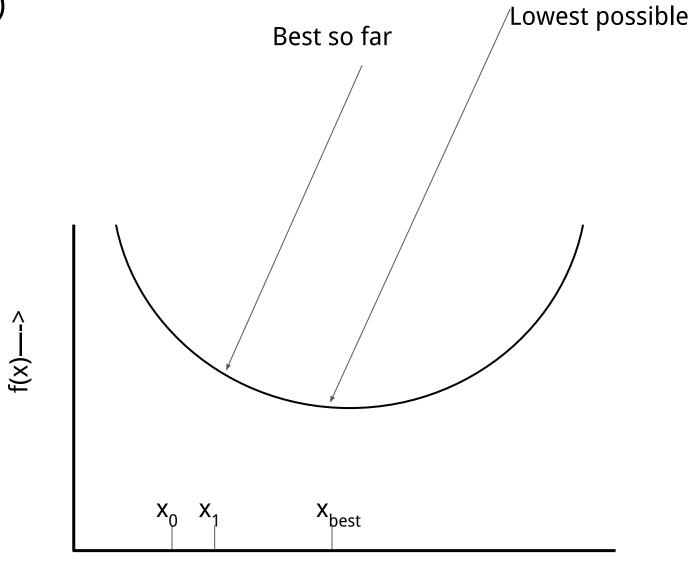
- Define a grid with increment δ , use any of the discrete algorithms
- 2. Choose random perturbations to the state
 - a. First-choice hill-climbing: keep trying until something improves the state
 - b. Simulated annealing
- 4. Compute derivatives of f(x) analytically

x= argmin f(x) x∈ℝ^D

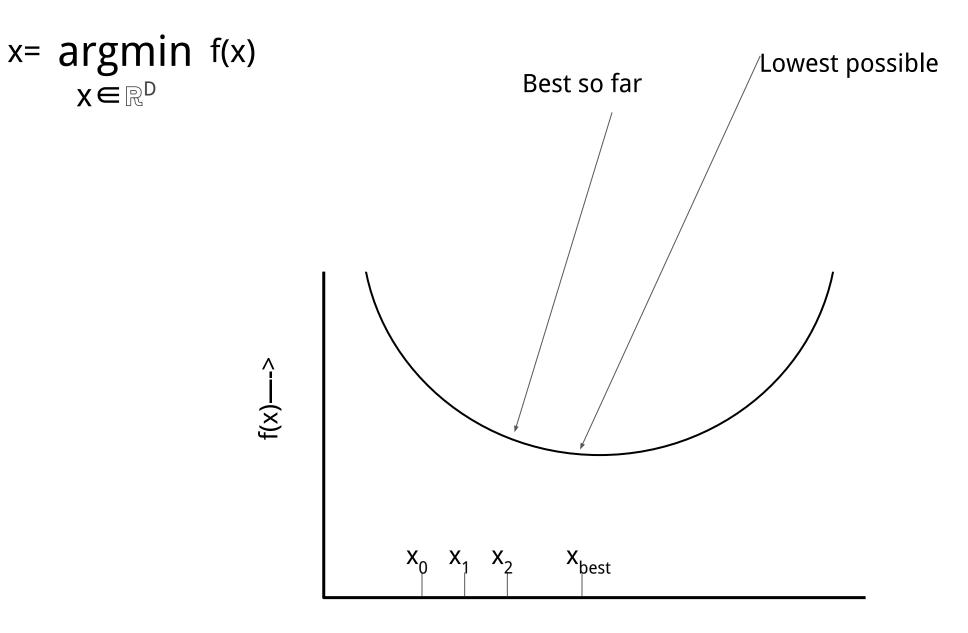


Test 2 gives lower f(x)

x= argmin f(x) x∈ℝ^D



Test 2 gives lower



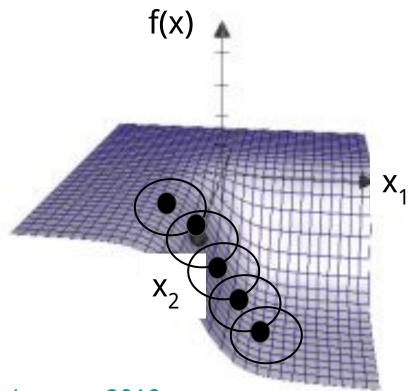
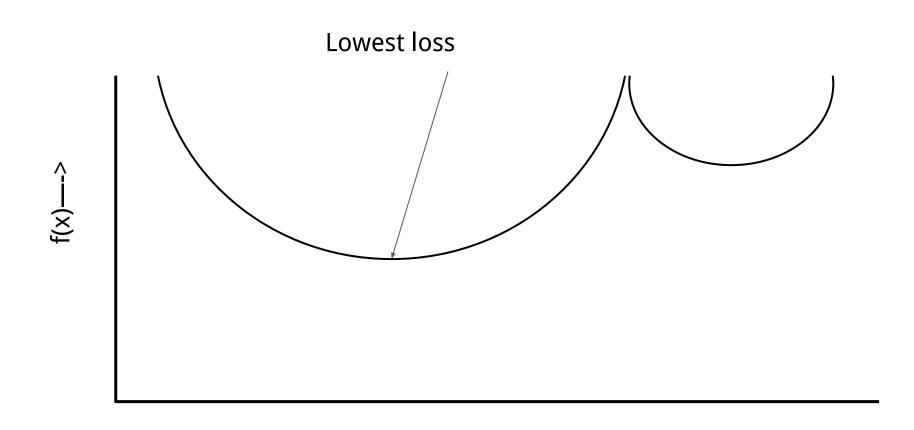


Figure from <u>Chaudhuri & Solar-Lezama 2010</u>

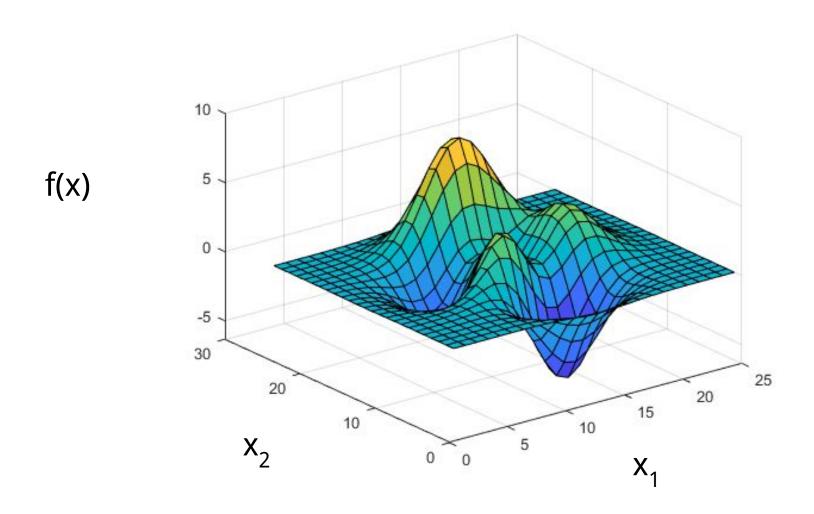
Continuous Local Search

```
x = a random vector in \mathbb{R}^D
Loop:
   Make small perturbations to x
   Call these perturbations x_{test}^{1} x_{test}^{2} x_{test}^{2} \dots
   Compute f(x_{test}^1), f(x_{test}^2), \dots
   x = the x_{test}^{i} with lowest f(x_{test}^{i})
```

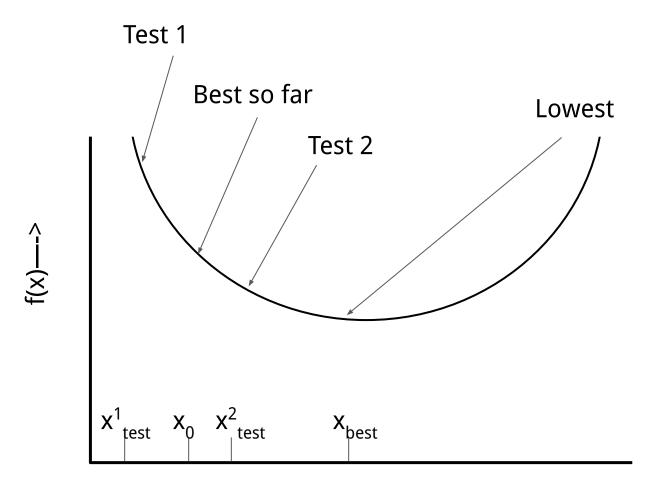
Does this local search always work?



Does This Local Search Always Work?



From here to gradient descent

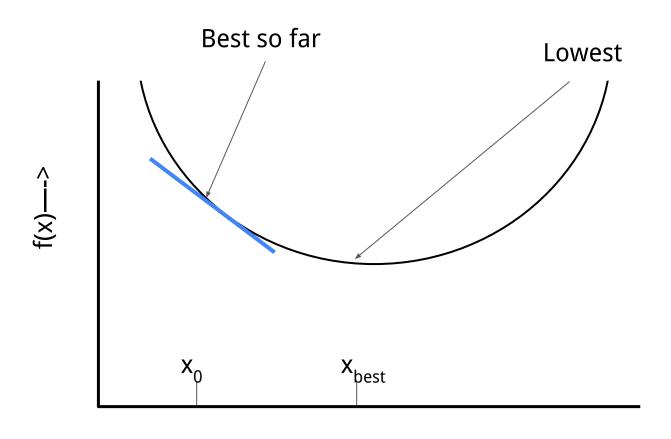


We decided to move right (increase x)

Did we need to make the test points to figure out that we should move right?



From here to gradient descent

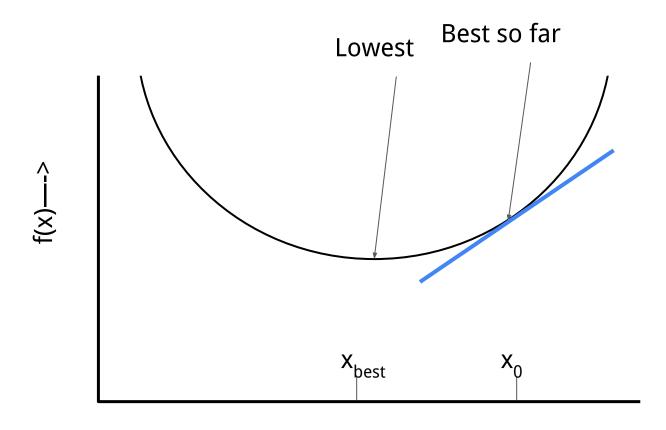


$$\left. \frac{d}{dx} f(x) \right|_{x=x_0} < 0$$

Negative derivative, increase x to decrease f(x)



From here to gradient descent



$$\frac{d}{dx}f(x)\Big|_{x=x_0} > 0$$

Positive derivative, decrease x to decrease f(x)



Gradient Descent, 1 Dimension

$$\frac{d}{dx}f(x) > 0$$

DECREASE x

$$x + = -\lambda \frac{d}{dx} f(x)$$

 $\frac{a}{a}f(x) < 0$

INCREASE x

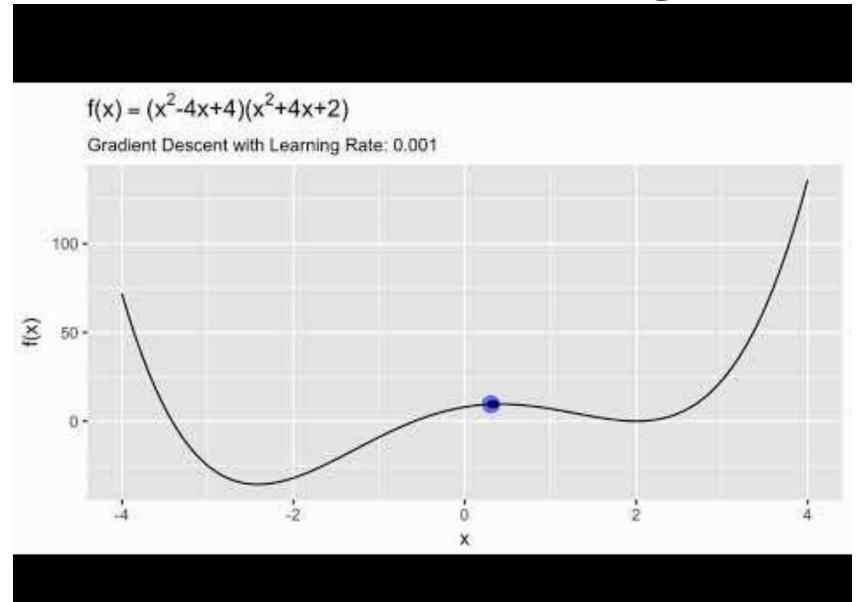
Gradient Descent, 1-dimension

 λ = a small positive number (like 0.001), called the "learning rate" x = a random number

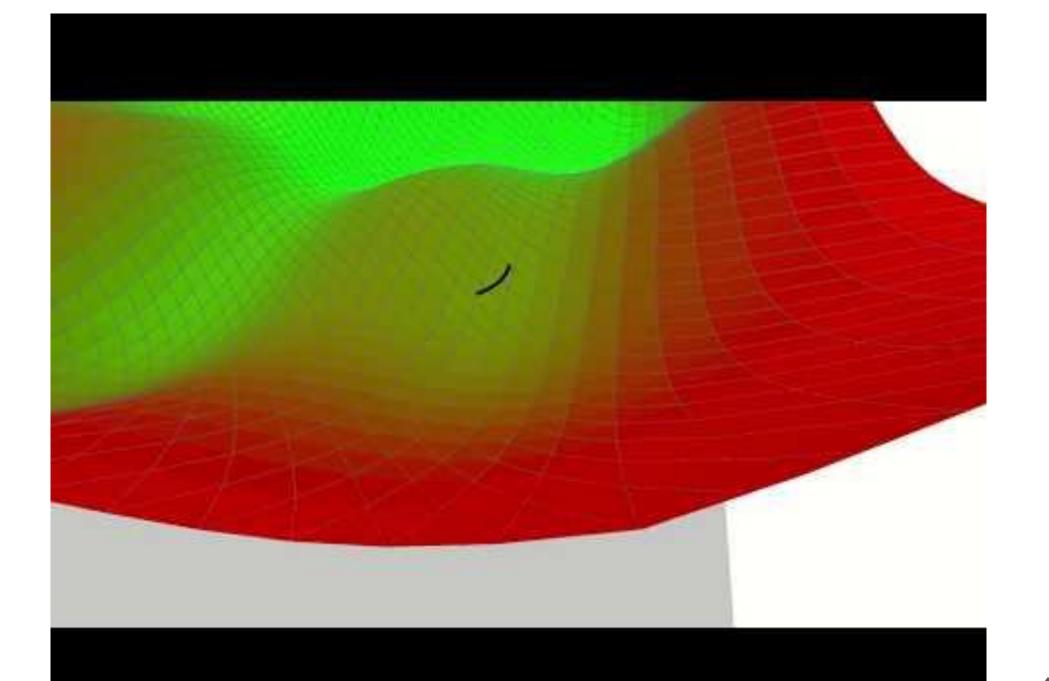
Loop:

$$x \leftarrow x - \lambda \times \frac{d}{dx} f(x)$$

Gradient Descent ~ Falling Downhill



Higher dimensions?



Gradient Descent, 2 Dimensions

x in
$$\mathbb{R}^2$$

x = (x₁, x₂)
f(x) = f(x₁, x₂)

$$\frac{d}{dx_1}f(x_1,x_2)>0 \qquad \text{DECREASE x}_1$$

$$\frac{d}{dx_1}f(x_1,x_2)<0 \qquad \text{INCREASE x}_1$$

$$\frac{d}{dx_2}f(x_1,x_2)>0 \qquad \text{DECREASE x}_2$$

$$\frac{d}{dx_2}f(x_1,x_2)<0 \qquad \text{INCREASE x}_2$$

Gradient Descent

 λ = a small positive number (like 0.001), called the "learning rate"

 $x = a random vector in \mathbb{R}^D$

Loop:

Compute:

$$g_i = \frac{d}{dx_i} f(x)$$
, for i from 1 to D

For each dimension *i* ranging from 1 to D:

$$x_i \leftarrow x_i - \lambda \times g_i$$

Summary

- Many configuration and optimization problems can be formulated as local search
- General families of algorithms:
 - Hill-climbing, continuous optimization
 - Simulated annealing (and other stochastic methods)
 - Local beam search: multiple interaction searches
 - Genetic algorithms: break and recombine states

Many machine learning algorithms are local searches

Example: Discovering Natural Laws

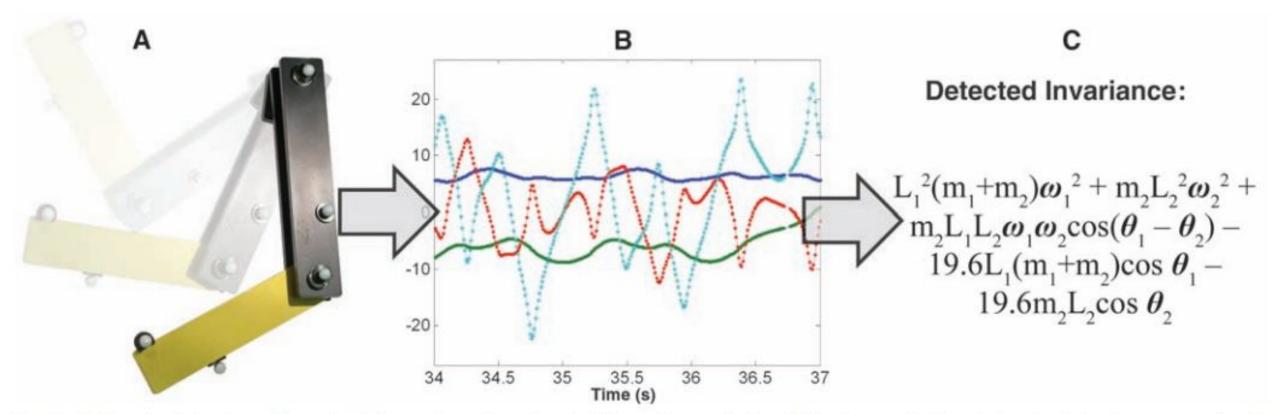


Fig. 1. Mining physical systems. We captured the angles and angular velocities of a chaotic double-pendulum (**A**) over time using motion tracking (**B**), then we automatically searched for equations that describe a single natural law relating

these variables. Without any prior knowledge about physics or geometry, the algorithm found the conservation law (C), which turns out to be the double pendulum's Hamiltonian. Actual pendulum, data, and results are shown.



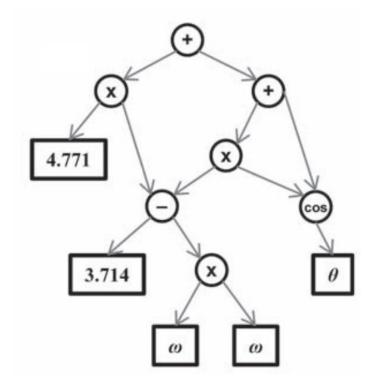
Genotype:

Mutation and crossover operate over this

```
(0) <- load [3.714]
(1) <- load [ω]
(2) <- mul (1), (1)
(3) <- sub (0), (2)
(4) <- load [θ]
(5) <- cos (4)
(6) <- mul (3), (5)
(7) <- load [4.771]
(8) <- mul (7), (3)
(9) <- add (8), (5)
(10) <- add (9), (6)
```

Phenotype:

Fitness operates over this

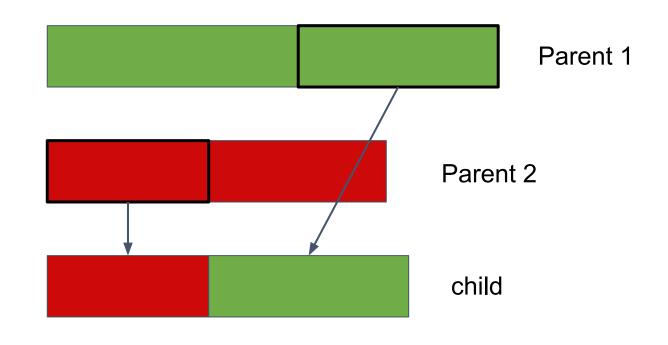






Crossover randomly exchanges prefix/suffix of parents

```
(0) <- load [3.714]
(1) <- load [ω]
(2) <- mul (1), (1)
(3) <- sub (0), (2)
(4) <- load [θ]
(5) <- cos (4)
(6) <- mul (3), (5)
(7) <- load [4.771]
(8) <- mul (7), (3)
(9) <- add (8), (5)
(10) <- add (9), (6)
```



Fitness for physical laws

Very subtle:

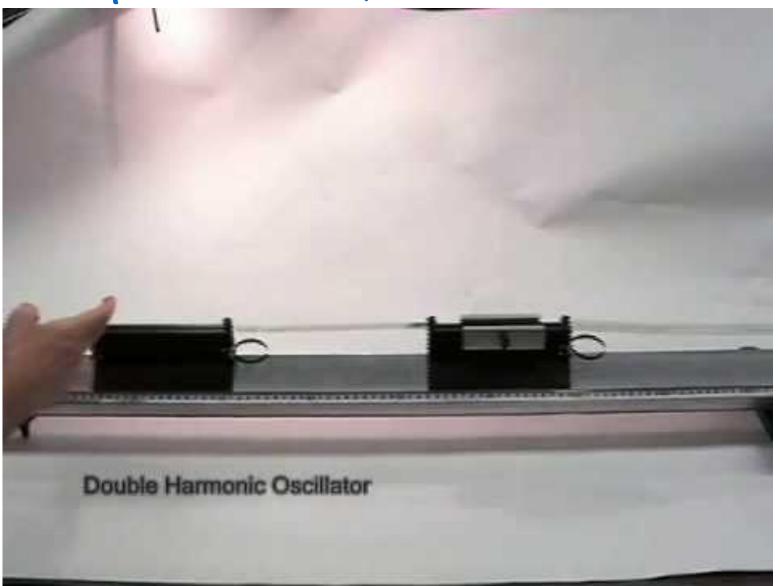
Want to discover equations that capture conserved invariants, like energy or momentum

Main physics insight goes into design of "fitness" for a candidate invariant that is being evolved

Done at Cornell!

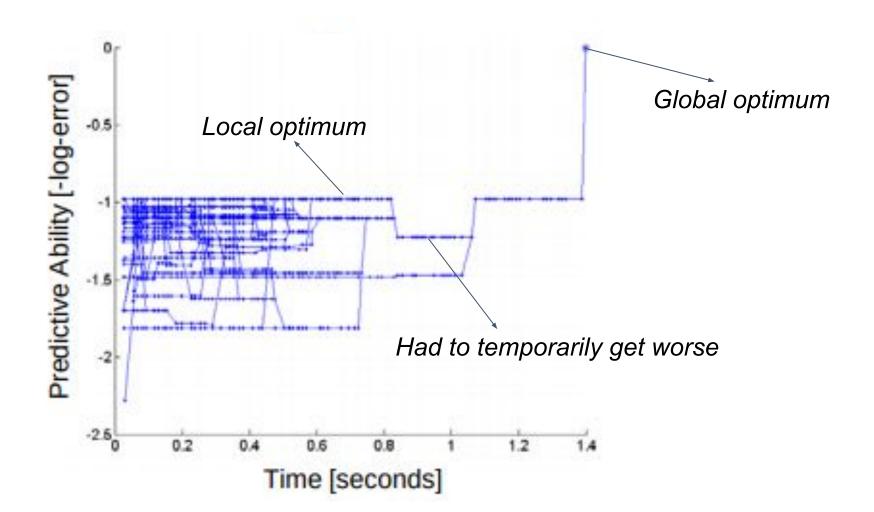
Example: Discovering Natural Laws (Schmidt & Lipson 2009)











Done at Cornell!



"Island" evolution model:

Separate evolving populations that occasionally exchange solutions Promotes diversity, more parallel

