The New York Times

I'm a Congressman Who Codes. A.I. Freaks Me Out.

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Physics Mathematics Biology Computer Science Topics Archive

GRAPH THEORY

Finally, a Fast Algorithm for Shortest Paths on Negative Graphs

ChatGPT – calm down everyone

- Q: which is bigger? an elephant or a cat?
- A: An elephant is bigger than a cat.
- Q: which is not bigger than the other? an elephant or a cat?
- A: Neither an elephant nor a cat is bigger than the other.
- Q: what is the largest even number?
- A: The largest even number is 9,999,999,998.
- Q: I started with 20 dollars and gave 10 dollars to my friend. How much do we have in total?
- A: You and your friend have a total of 30 dollars.

Recap

- A* expands the fringe node with lowest f value where
 - $\bullet f(n) = g(n) + h(n)$
 - g(n) is the cost to reach n
 - h(n) is an admissible estimate of the least cost from n to a goal node:
 0 ≤ h(n) ≤ h*(n)
- A* tree search is optimal
- Its performance depends heavily on the heuristic h

Creating Heuristics



Creating Admissible Heuristics

Often, admissible heuristics are solutions to *relaxed problems*, where new actions are available





- Problem P_2 is a relaxed version of P_1 if $\mathcal{A}_2(s) \supseteq \mathcal{A}_1(s)$ for every s
- Theorem: $h_2^*(s) \le h_1^*(s)$ for every *s*, so $h_2^*(s)$ is admissible for P_1

Example: 8 Puzzle



Start State

Actions



Goal State

- What are the states?
- How many states?
- What are the actions?
- What are the step costs?

8 Puzzle I

- Heuristic: Number of tiles misplaced
- Why is it admissible?
- h(start) = 8







Start State

Goal State

	Average nodes expanded when the optimal path has			
	4 steps	8 steps	12 steps	
UCS	112	6,300	3.6 x 10 ⁶	
A*TILES	13	39	227	

Statistics from Andrew Moore

8 Puzzle II

- What if we had an easier 8-puzzle where any tile could slide any direction at any time, ignoring other tiles?
- Total Manhattan distance
- Why is it admissible?
- h(start) = 3 + 1 + 2 + ... = 18





Start State

Goal State

	Average nodes expanded when the optimal path has		
	4 steps	8 steps	12 steps
A*TILES	13	39	227
A*MANHATTAN	12	25	73

Combining heuristics

• Dominance: $h_1 \ge h_2$ if

$\forall n \ h_1(n) \geq h_2(n)$

- Roughly speaking, larger is better as long as both are admissible
- The zero heuristic is pretty bad (what does A* do with h=0?)
- The exact heuristic is pretty good, but usually too expensive!
- What if we have two heuristics, neither dominates the other?
 - Form a new heuristic by taking the max of both:

 $h(n) = \max(h_1(n), h_2(n))$

Max of admissible heuristics is admissible and dominates both!

Example: Knight's moves

Minimum number of knight's moves to get from A to B?

- h₁ = (Manhattan distance)/3
 - $h_1' = h_1$ rounded up to correct parity (even if A, B same color, odd otherwise)
- h₂ = (Euclidean distance)/V5 (rounded up to correct parity)
- h₃ = (max x or y shift)/2 (rounded up to correct parity)
- $h(n) = \max(h_1'(n), h_2(n), h_3(n))$ is admissible!



Optimality of A* Graph Search



This part is a bit fiddly, sorry about that

Quiz: State Space Graphs vs. Search Trees

Consider a rectangular grid:



How many states within *d* steps of start?

How many states in search tree of depth *d*?

Basic idea of graph search: don't re-expand a state that has been expanded previously

A* Graph Search Gone Wrong?







Simple check against expanded set blocks C Fancy check allows new C if cheaper than old but requires recalculating C's descendants

Consistency of Heuristics



- Main idea: estimated heuristic costs ≤ actual costs
 - Admissibility: heuristic cost ≤ actual cost to goal h(A) ≤ h^{*}(A)
 - Consistency: heuristic "arc" cost ≤ actual cost for each arc h(A) - h(C) ≤ c(A,C)

or $h(A) \le c(A,C) + h(C)$ (triangle inequality)

- Note: h* <u>necessarily</u> satisfies triangle inequality
- Consequences of consistency:
 - The *f* value along a path never decreases:

 $h(A) \le c(A,C) + h(C) \implies g(A) + h(A) \le g(A) + c(A,C) + h(C)$

A* graph search is optimal

Optimality of A* Graph Search

- Sketch: consider what A* does with a consistent heuristic:
 - Fact 1: In tree search, A* expands nodes in increasing total f value (f-contours)
 - Fact 2: For every state s, nodes that reach s optimally are expanded before nodes that reach s suboptimally
 - Result: A* graph search is optimal



Optimality

- Tree search:
 - A* is optimal if heuristic is admissible
- Graph search:
 - A* optimal if heuristic is consistent
- Consistency implies admissibility
- Most natural admissible heuristics tend to be consistent, especially if from relaxed problems



But...

- A* keeps the entire explored region in memory
- => will run out of space before you get bored waiting for the answer
- There are variants that use less memory (Section 3.5.5):
 - IDA* works like iterative deepening, except it uses an *f*-limit instead of a depth limit
 - On each iteration, remember the smallest *f*-value that exceeds the current limit, use as new limit
 - Very inefficient when *f* is real-valued and each node has a unique value
 - RBFS is a recursive depth-first search that uses an *f*-limit = the *f*-value of the best alternative path available from any ancestor of the current node
 - When the limit is exceeded, the recursion unwinds but remembers the best reachable *f*-value on that branch
 - SMA* uses all available memory for the queue, minimizing thrashing
 - When full, drop worst node on the queue but remember its value in the parent



A*: Summary

- A* orders nodes in the queue by f(n) = g(n) + h(n)
- A* is optimal for trees/graphs with admissible/consistent heuristics
- Heuristic design is key: often use relaxed problems





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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



h = 5

h = 0

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



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 =~ 22 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





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** \leftarrow 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!
- Proof sketch
 - Consider two adjacent states x, y with E(y) > E(x) [high is good]
 - Assume $x \rightarrow y$ and $y \rightarrow x$ and outdegrees D(x) = D(y) = D
 - Let P(x), P(y) be the equilibrium occupancy probabilities at T
 - Let $P(x \rightarrow y)$ be the probability that state x transitions to state y



Occupation probability as a function of *T*



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

Or, K chosen randomly with

- Basic idea:
 - K copies of a local search algorithm, initialized randomly
 - For each iteration
 - a bias towards good ones
 Generate ALL successors from K current states
 - Choose best K of these to be the new current states

Beam search example (K=4)



Local beam search

- 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

1. 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
- 3. Compute gradient of $f(\mathbf{x})$ analytically

Finding extrema in continuous space

- Gradient vector $\nabla f(\mathbf{x}) = (\partial f / \partial x_1, \partial f / \partial y_1, \partial f / \partial x_2, ...)^{\mathsf{T}}$
- For the airports, $f(\mathbf{x}) = \sum_{a} \sum_{c \in C_a} (x_a x_c)^2 + (y_a y_c)^2$
- $\partial f/\partial x_1 = \sum_{c \in C_1} 2(x_1 x_c)$
- At an extremum, $\nabla f(\mathbf{x}) = 0$
- Can sometimes solve in closed form: $x_1 = (\sum_{c \in C_1} x_c) / |C_1|$
- Is this a local or global minimum of *f*?
- Gradient descent: $\mathbf{x} \leftarrow \mathbf{x} \alpha \nabla f(\mathbf{x})$
 - Huge range of algorithms for finding extrema using gradients

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