南京大学
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Lecture 6: Search 5

General Solution Space Search & CSP

Constraint satisfaction problems (CSPs)

Constraint satisfaction problems (CSPs)

Standard search problem:

state is a "black box"—any old data structure
that supports goal test, eval, successor

CSP:

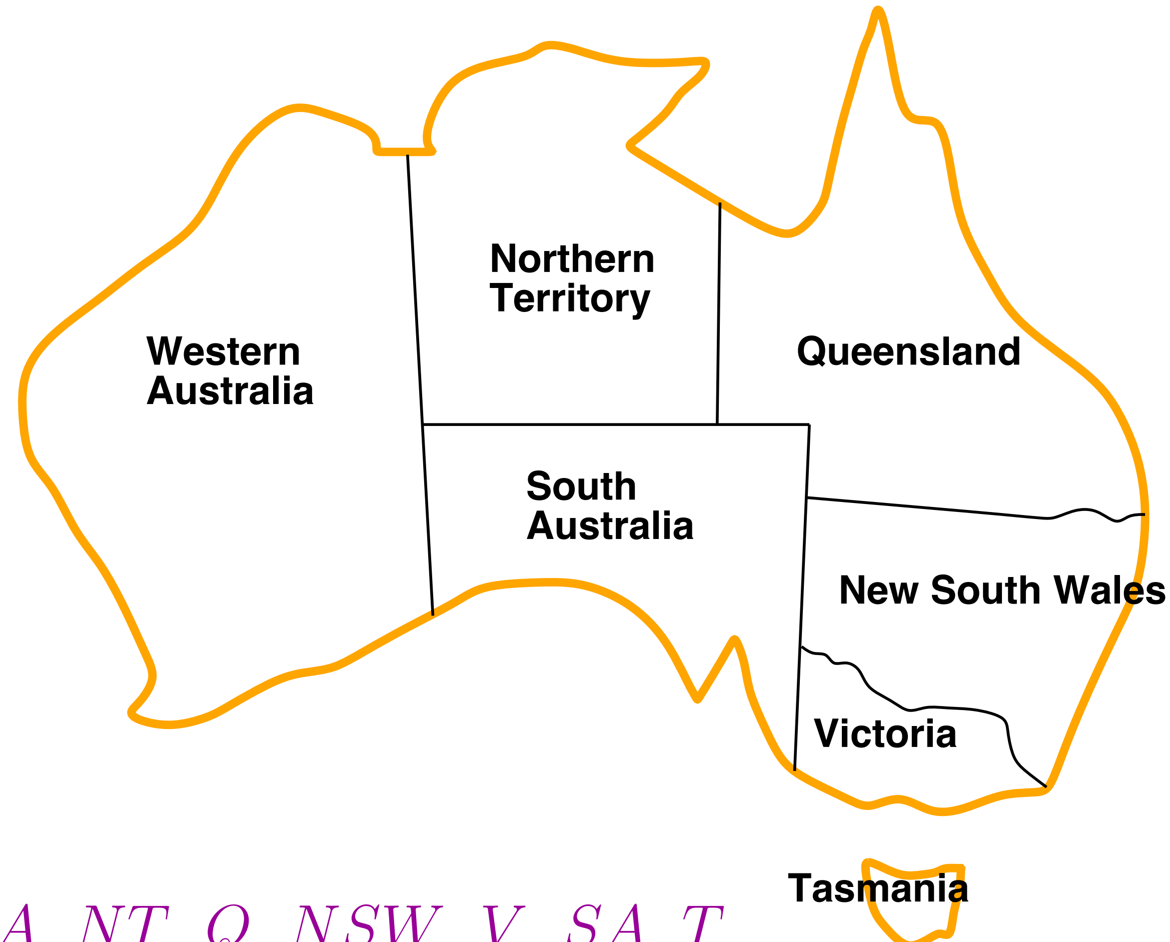
state is defined by variables X_i with values from domain D_i

goal test is a set of constraints specifying
allowable combinations of values for subsets of variables

Simple example of a **formal representation language**

Allows useful **general-purpose** algorithms with more power than standard search algorithms

Example: Map-Coloring



Variables WA, NT, Q, NSW, V, SA, T

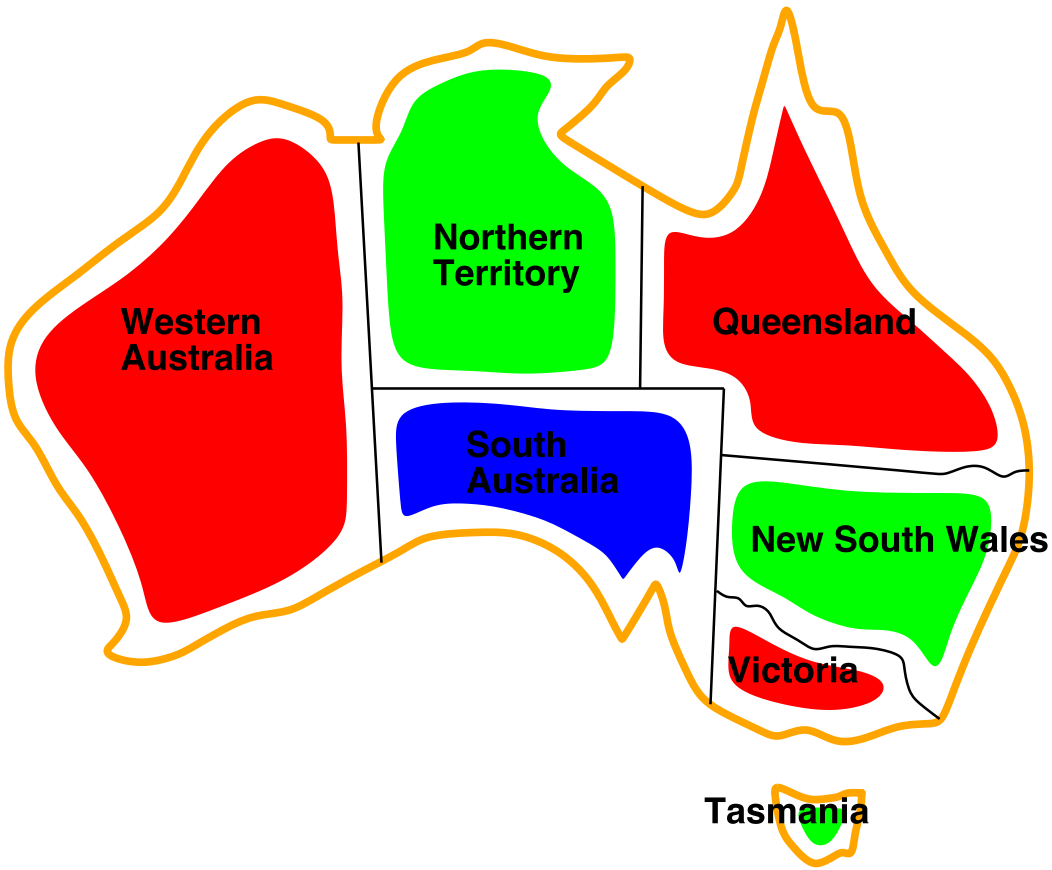
Domains $D_i = \{red, green, blue\}$

Constraints: adjacent regions must have different colors

e.g., $WA \neq NT$ (if the language allows this), or

$(WA, NT) \in \{(red, green), (red, blue), (green, red), (green, blue), \ldots\}$

Example: Map-Coloring



Solutions are assignments satisfying all constraints, e.g.,
$\{WA = red, NT = green, Q = red, NSW = green, V = red, SA = blue, T = green\}$

Standard search formulation (incremental)

Let's start with the straightforward, dumb approach, then fix it

States are defined by the values assigned so far

- ♢ Initial state: the empty assignment, $\{\,\}$
- ♢ Successor function: assign a value to an unassigned variable that does not conflict with current assignment.
  $\Rightarrow$ fail if no legal assignments (not fixable!)
- ♢ Goal test: the current assignment is complete

1) This is the same for all CSPs!
2) Every solution appears at depth n with n variables
   $\Rightarrow$ use depth-first search
3) Path is irrelevant, so can also use complete-state formulation
4) $b = (n - \ell)d$ at depth ℓ, hence $n!d^n$ leaves!!!!

Backtracking search

Variable assignments are commutative, i.e.,

$[WA = red$ then $NT = green]$ same as $[NT = green$ then $WA = red]$

Only need to consider assignments to a single variable at each node

$\Rightarrow \quad b = d$ and there are d^n leaves

Depth-first search for CSPs with single-variable assignments
is called backtracking search

Backtracking search is the basic uninformed algorithm for CSPs

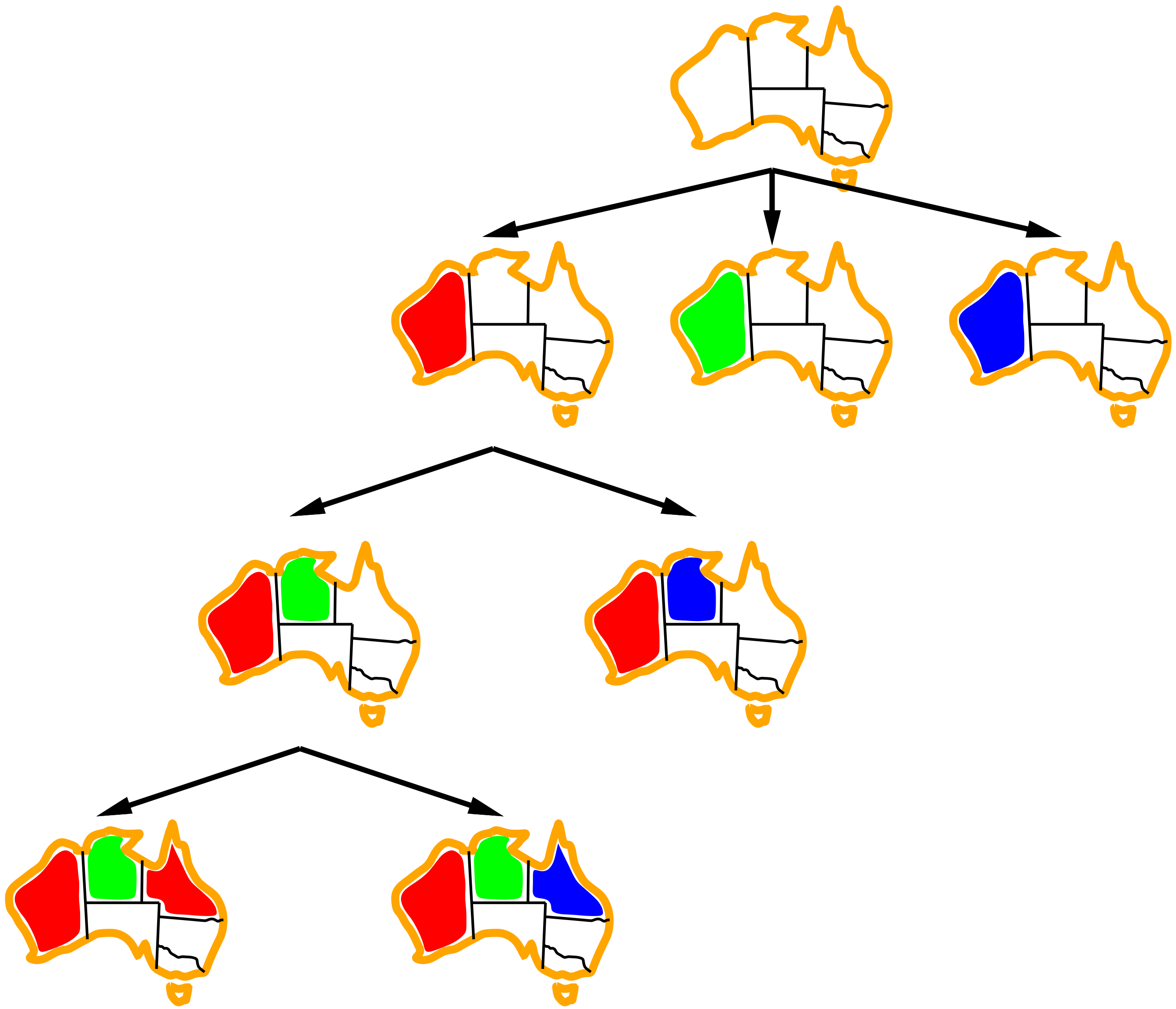
Can solve n-queens for $n \approx 25$

Backtracking search

```
function BACKTRACKING-SEARCH(csp) returns solution/failure
    return RECURSIVE-BACKTRACKING({ }, csp)

function RECURSIVE-BACKTRACKING(assignment, csp) returns soln/failure
    if assignment is complete then return assignment
    var ← SELECT-UNASSIGNED-VARIABLE(VARIABLES[csp], assignment, csp)
    for each value in ORDER-DOMAIN-VALUES(var, assignment, csp) do
        if value is consistent with assignment given CONSTRAINTS[csp] then
            add {var = value} to assignment
            result ← RECURSIVE-BACKTRACKING(assignment, csp)
            if result ≠ failure then return result
            remove {var = value} from assignment
    return failure
```

Backtracking search example



Improving backtracking efficiency

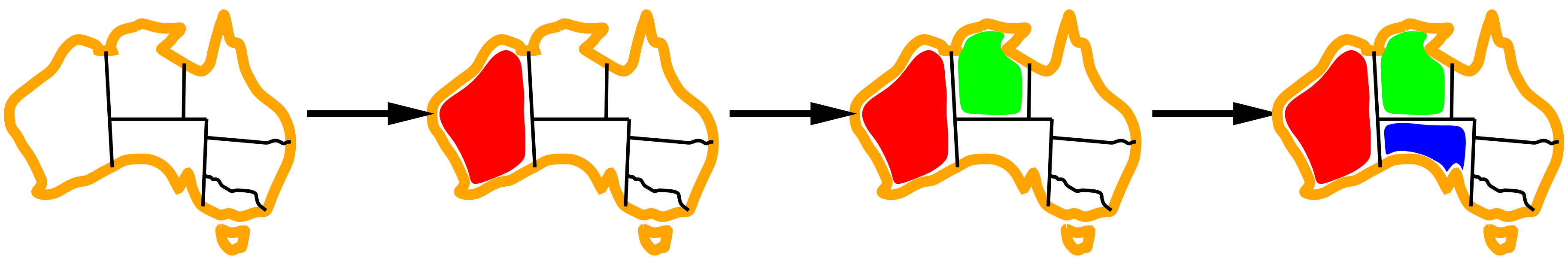
backtracking is uninformed
make it more informed

General-purpose methods can give huge gains in speed:

1. Which variable should be assigned next?
2. In what order should its values be tried?
3. Can we detect inevitable failure early?
4. Can we take advantage of problem structure?

Minimum remaining values

Minimum remaining values (MRV):
choose the variable with the fewest legal values

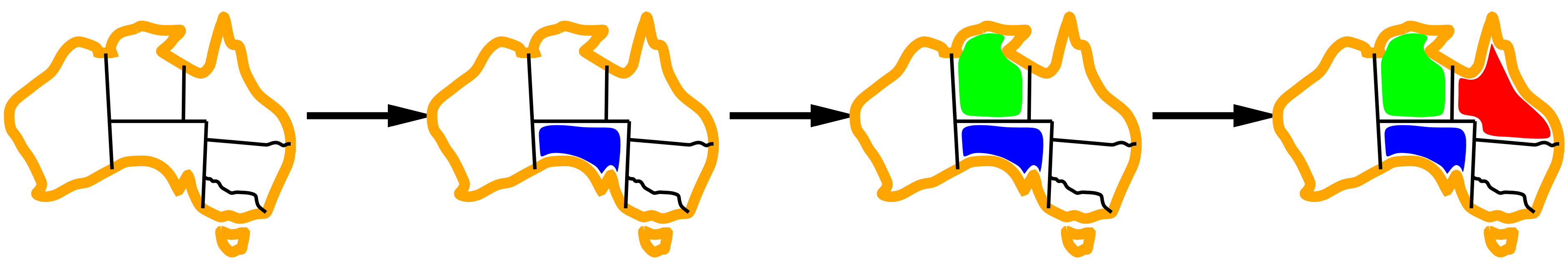


Degree heuristic

Tie-breaker among MRV variables

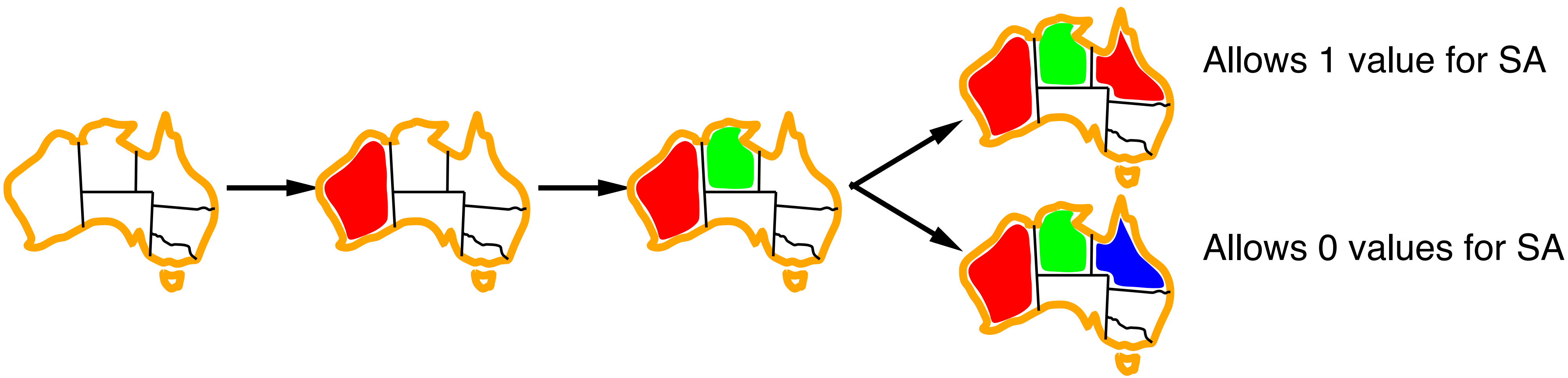
Degree heuristic:

choose the variable with the most constraints on remaining variables



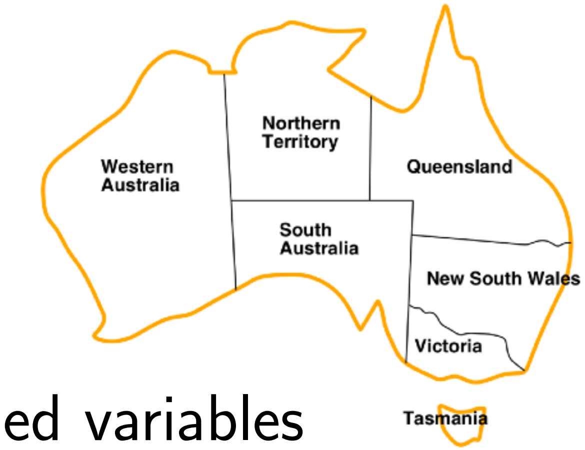
Least constraining value

Given a variable, choose the least constraining value:
the one that rules out the fewest values in the remaining variables

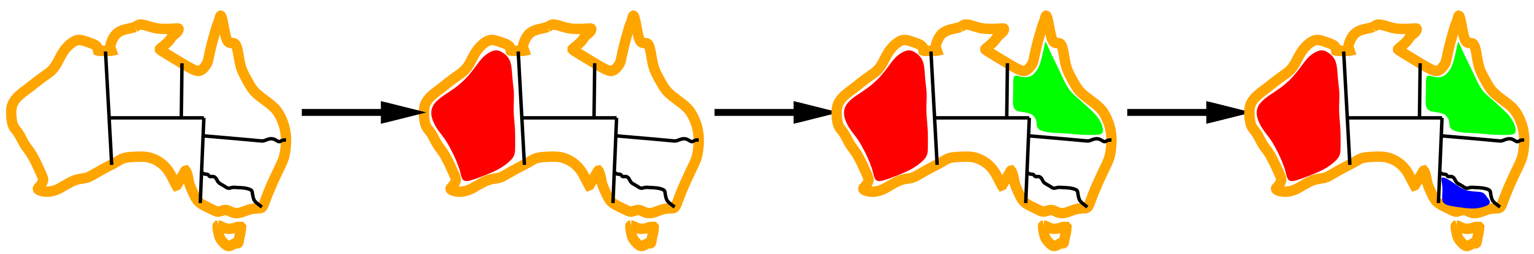


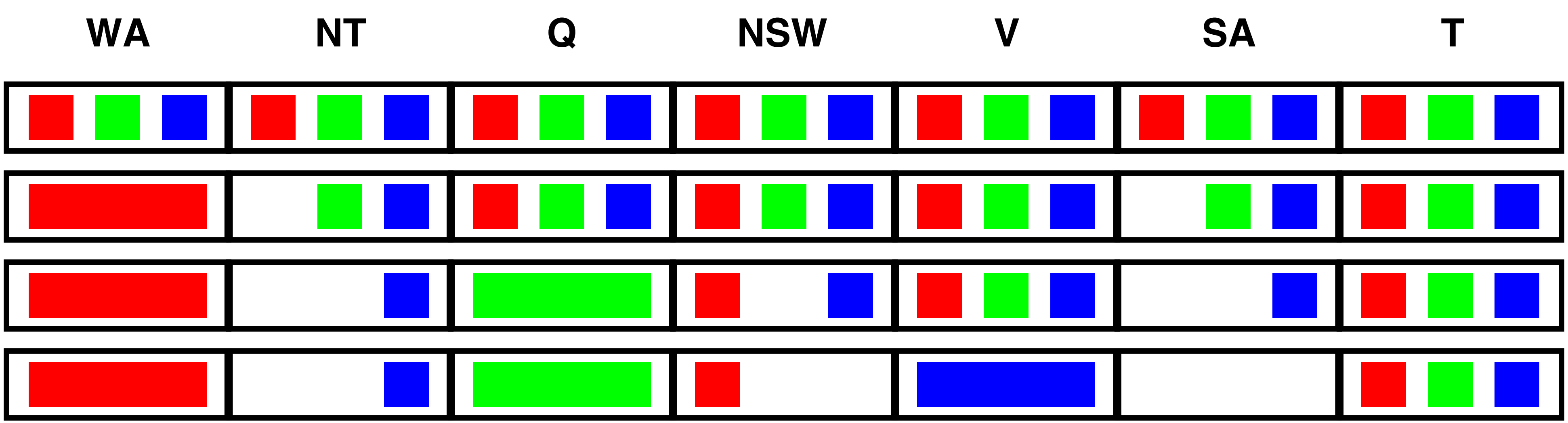
Combining these heuristics makes 1000 queens feasible

Forward checking



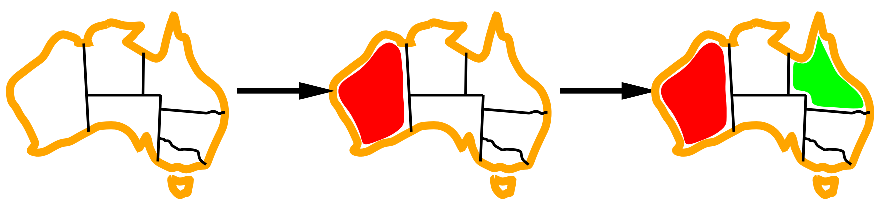
Idea: Keep track of remaining legal values for unassigned variables
Terminate search when any variable has no legal values

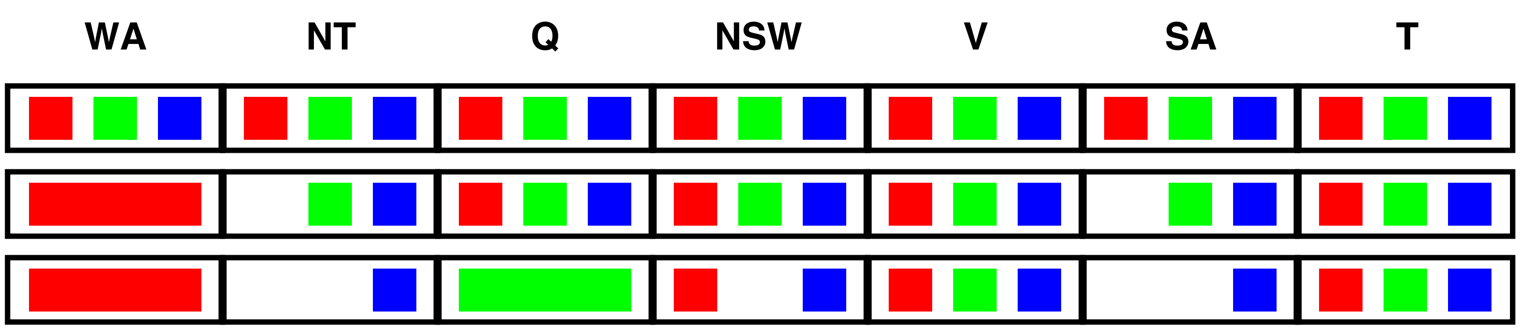




Constraint propagation

Forward checking propagates information from assigned to unassigned variables, but doesn't provide early detection for all failures:





NT and SA cannot both be blue!

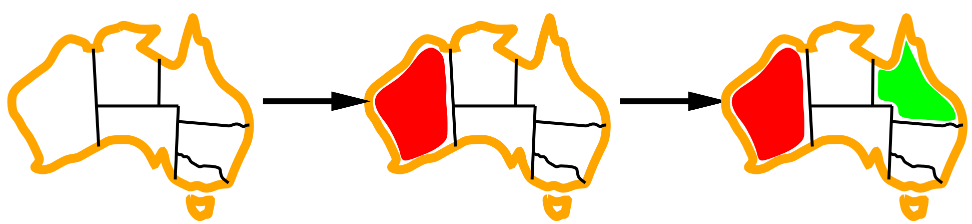
Constraint propagation repeatedly enforces constraints locally

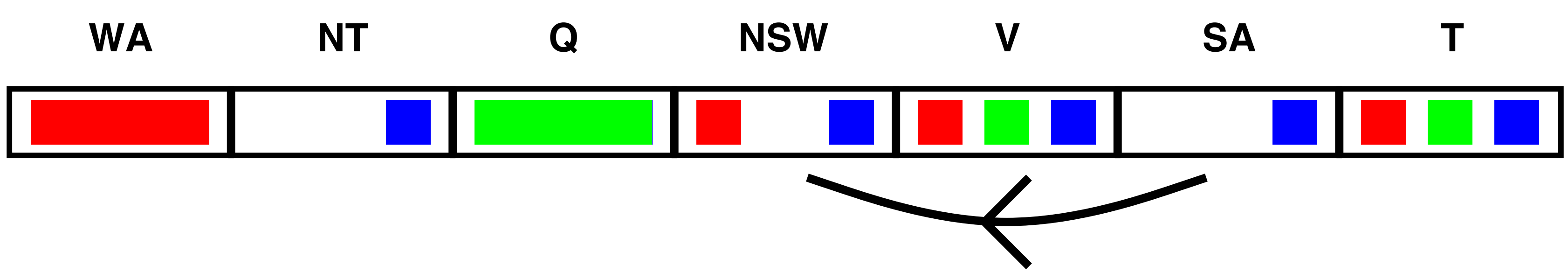
Arc consistency

Simplest form of propagation makes each arc consistent

$X \rightarrow Y$ is consistent iff

for **every** value x of X there is **some** allowed y



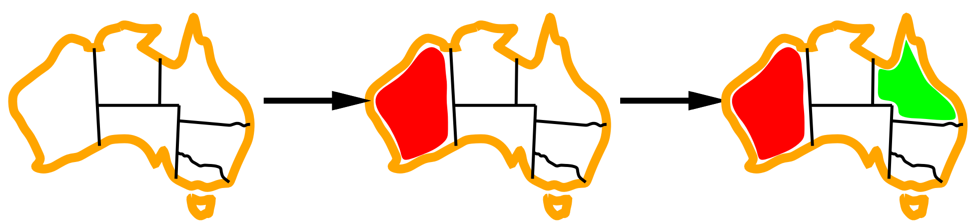


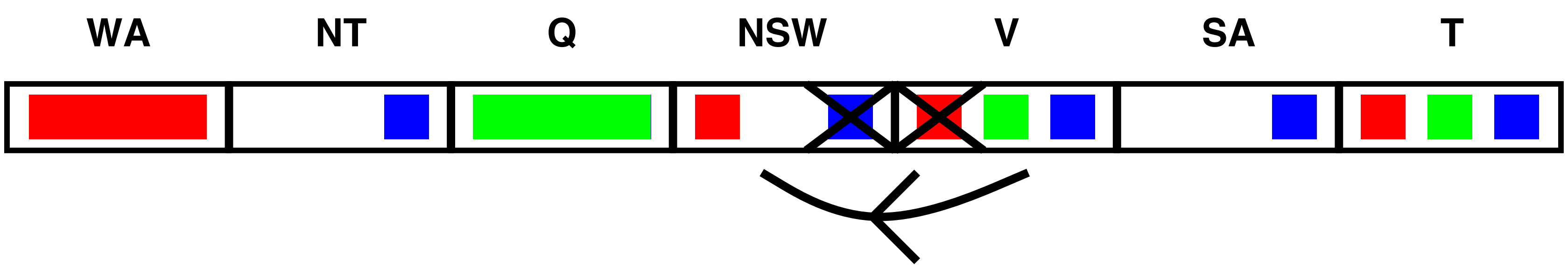
Arc consistency

Simplest form of propagation makes each arc consistent

$X \to Y$ is consistent iff

for **every** value x of X there is **some** allowed y





If X loses a value, neighbors of X need to be rechecked

Arc consistency

Simplest form of propagation makes each arc consistent

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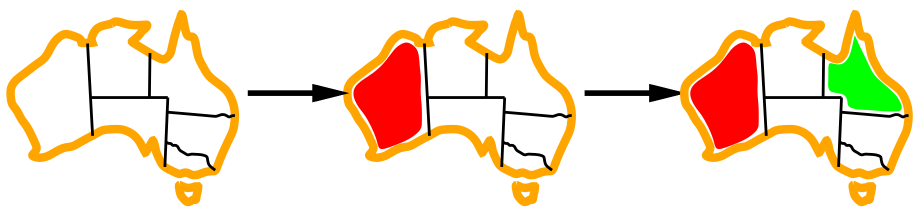
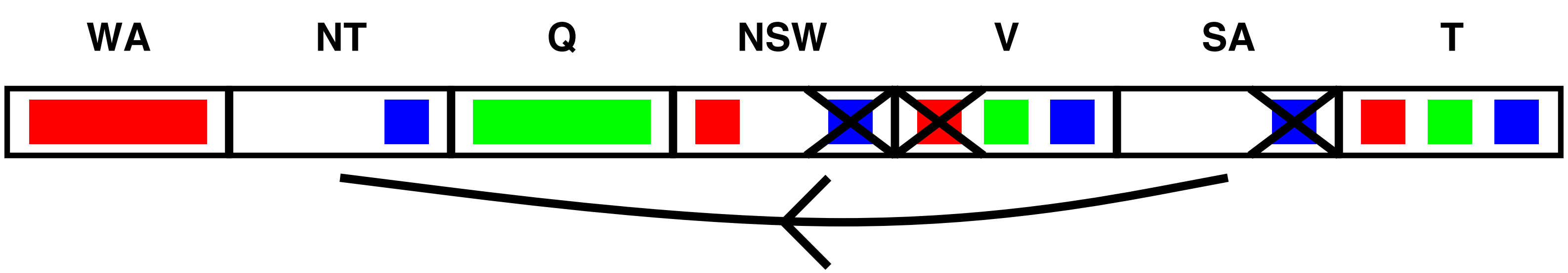




If X loses a value, neighbors of X need to be rechecked

Arc consistency detects failure earlier than forward checking

Can be run as a preprocessor or after each assignment

Arc consistency

function AC-3(*csp*) **returns** the CSP, possibly with reduced domains
  inputs: *csp*, a binary CSP with variables $\{X_1, X_2, \ldots, X_n\}$
  local variables: *queue*, a queue of arcs, initially all the arcs in *csp*

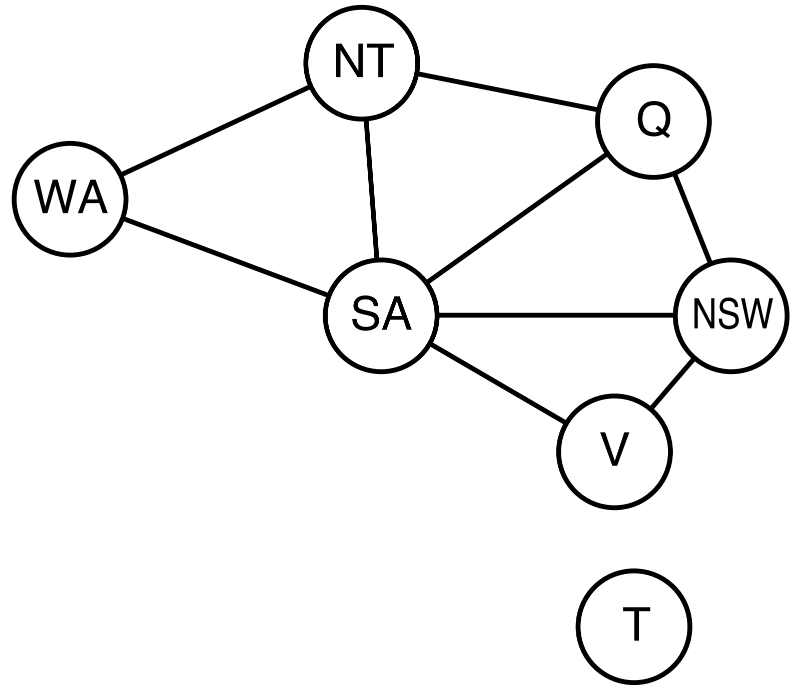
  while *queue* is not empty **do**
    $(X_i, X_j) \leftarrow$ REMOVE-FIRST(*queue*)
    if REMOVE-INCONSISTENT-VALUES(X_i, X_j) **then**
      for each X_k **in** NEIGHBORS$[X_i]$ **do**
        add (X_k, X_i) to *queue*

---

function REMOVE-INCONSISTENT-VALUES(X_i, X_j) **returns** true iff succeeds
  removed $\leftarrow$ *false*
  for each x **in** DOMAIN$[X_i]$ **do**
    if no value y in DOMAIN$[X_j]$ allows (x,y) to satisfy the constraint $X_i \leftrightarrow X_j$
      then delete x from DOMAIN$[X_i]$; *removed* $\leftarrow$ *true*
  return *removed*

$O(n^2d^3)$, can be reduced to $O(n^2d^2)$ (but detecting **all** is NP-hard)

Problem Structure



Tasmania and mainland are independent subproblems

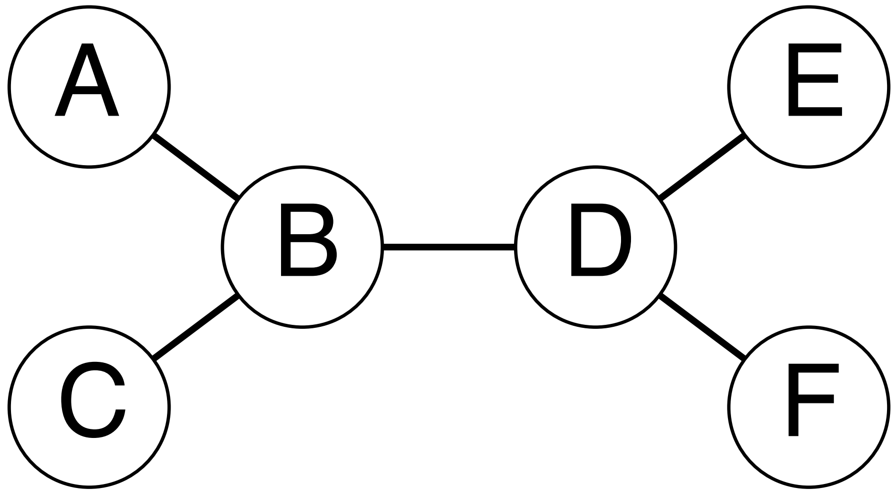
Identifiable as connected components of constraint graph

Suppose each subproblem has c variables out of n total

Worst-case solution cost is $n/c \cdot d^c$, **linear** in n

E.g., $n=80$, $d=2$, $c=20$
2^{80} = 4 billion years at 10 million nodes/sec
$4 \cdot 2^{20}$ = 0.4 seconds at 10 million nodes/sec

Tree-structured CSPs



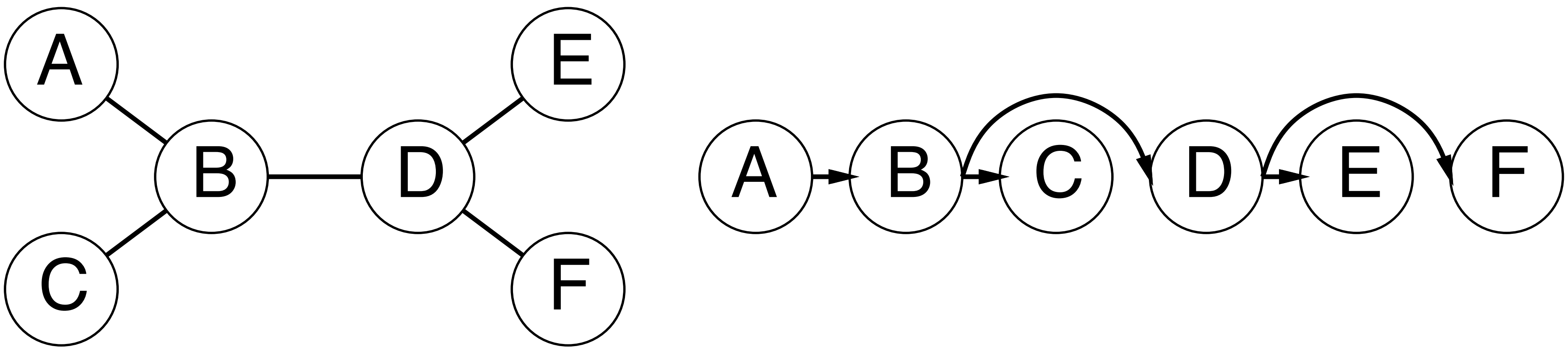
Theorem: if the constraint graph has no loops, the CSP can be solved in $O(n\,d^2)$ time

Compare to general CSPs, where worst-case time is $O(d^n)$

This property also applies to logical and probabilistic reasoning:
an important example of the relation between syntactic restrictions
and the complexity of reasoning.

Algorithm for tree-structured CSPs

1. Choose a variable as root, order variables from root to leaves such that every node's parent precedes it in the ordering

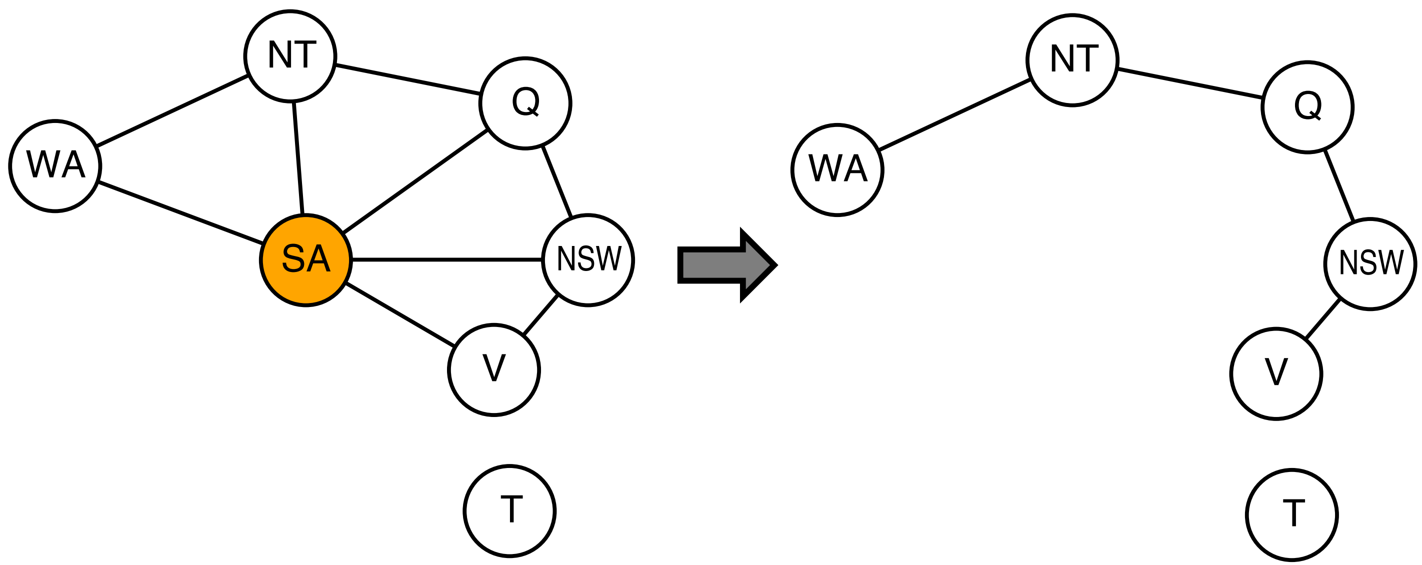


2. For j from n down to 2, apply $\textsc{RemoveInconsistent}(Parent(X_j), X_j)$

3. For j from 1 to n, assign X_j consistently with $Parent(X_j)$

Nearly tree-structured CSPs

Conditioning: instantiate a variable, prune its neighbors' domains



Cutset conditioning: instantiate (in all ways) a set of variables such that the remaining constraint graph is a tree

Cutset size c $\Rightarrow$ runtime $O(d^c \cdot (n-c)d^2)$, very fast for small c

Iterative algorithms for CSPs

Hill-climbing, simulated annealing typically work with "complete" states, i.e., all variables assigned

To apply to CSPs:
- allow states with unsatisfied constraints
- operators **reassign** variable values

Variable selection: randomly select any conflicted variable

Value selection by min-conflicts heuristic:
- choose value that violates the fewest constraints
- i.e., hillclimb with $h(n)$ = total number of violated constraints

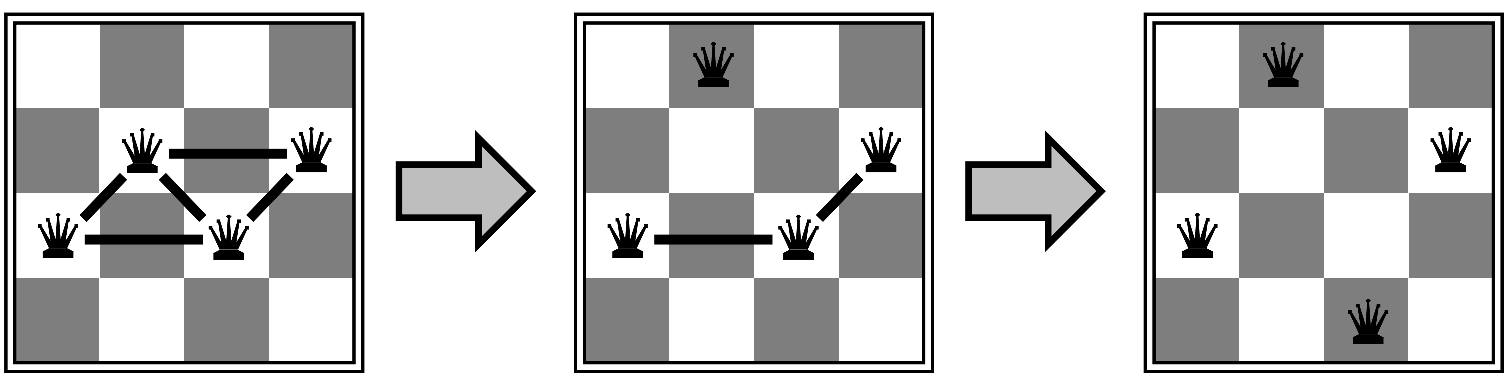
Example: 4-Queens

States: 4 queens in 4 columns ($4^4 = 256$ states)

Operators: move queen in column

Goal test: no attacks

Evaluation: $h(n)$ = number of attacks



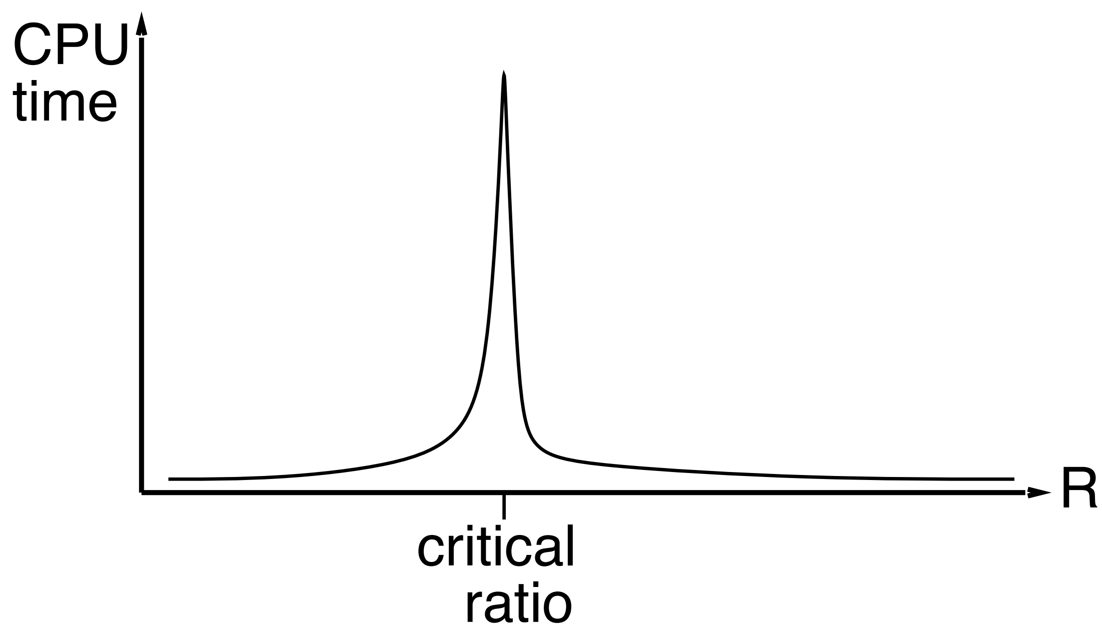
h = 5 **h = 2** **h = 0**

Performance of min-conflicts

Given random initial state, can solve n-queens in almost constant time for arbitrary n with high probability (e.g., $n = 10{,}000{,}000$)

The same appears to be true for any randomly-generated CSP **except** in a narrow range of the ratio

$$R = \frac{\text{number of constraints}}{\text{number of variables}}$$



Varieties of CSPs

Discrete variables

- finite domains; size $d \Rightarrow O(d^n)$ complete assignments
  - ♢ e.g., Boolean CSPs, incl. Boolean satisfiability (NP-complete)
- infinite domains (integers, strings, etc.)
  - ♢ e.g., job scheduling, variables are start/end days for each job
  - ♢ need a constraint language, e.g., $StartJob_1 + 5 \leq StartJob_3$
  - ♢ linear constraints solvable, nonlinear undecidable

Continuous variables

- ♢ e.g., start/end times for Hubble Telescope observations
- ♢ linear constraints solvable in poly time by LP methods

Varieties of CSPs

Unary constraints involve a single variable,
  e.g., $SA \neq green$

Binary constraints involve pairs of variables,
  e.g., $SA \neq WA$

Higher-order constraints involve 3 or more variables,
  e.g., cryptarithmetic column constraints

Preferences (soft constraints), e.g., red is better than $green$
often representable by a cost for each variable assignment
  $\rightarrow$ constrained optimization problems

Real-world CSPs

Assignment problems
  e.g., who teaches what class

Timetabling problems
  e.g., which class is offered when and where?

Hardware configuration

Spreadsheets

Transportation scheduling

Factory scheduling

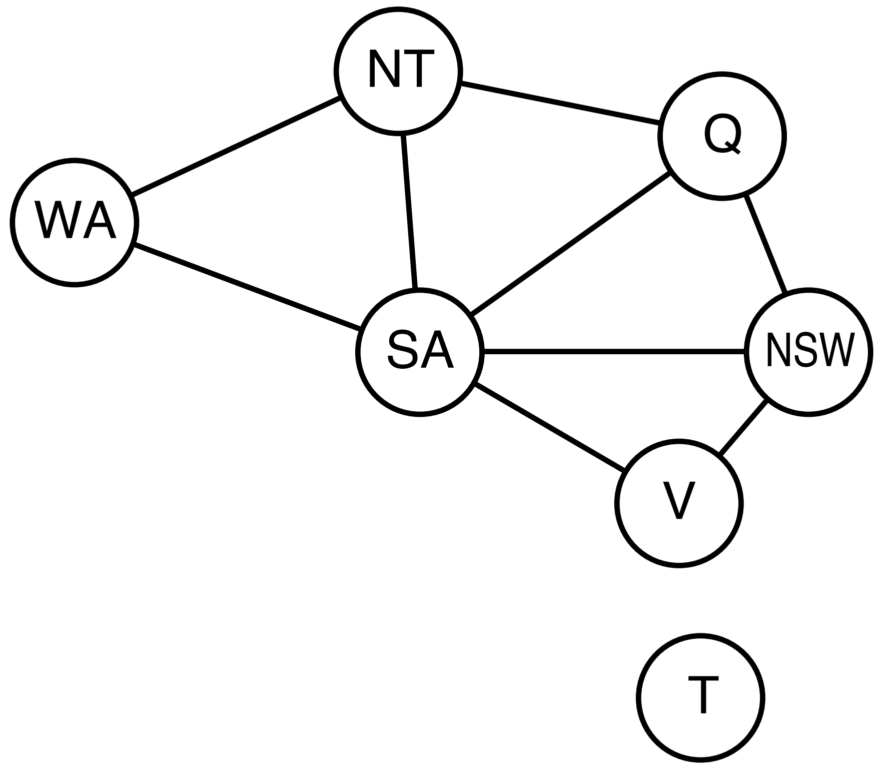
Floorplanning

Notice that many real-world problems involve real-valued variables

Constraint graph

Binary CSP: each constraint relates at most two variables

Constraint graph: nodes are variables, arcs show constraints



General-purpose CSP algorithms use the graph structure
to speed up search. E.g., Tasmania is an independent subproblem!

Convert higher-order to binary

A higher-order constraint can be converted to binary constraints with a *hidden-variable*

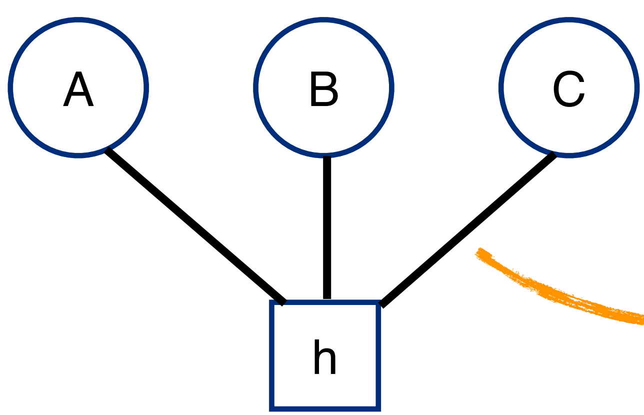
variable: A, B, C   domain: {1,2,3}   constraint: A+B=C

all possible assignments: (A,B,C) = (1,1,2), (1,2,3), (2,1,3)

hidden-variable: h with domain: {1,2,3}

(each value corresponds to an assignment)

the constraint graph:

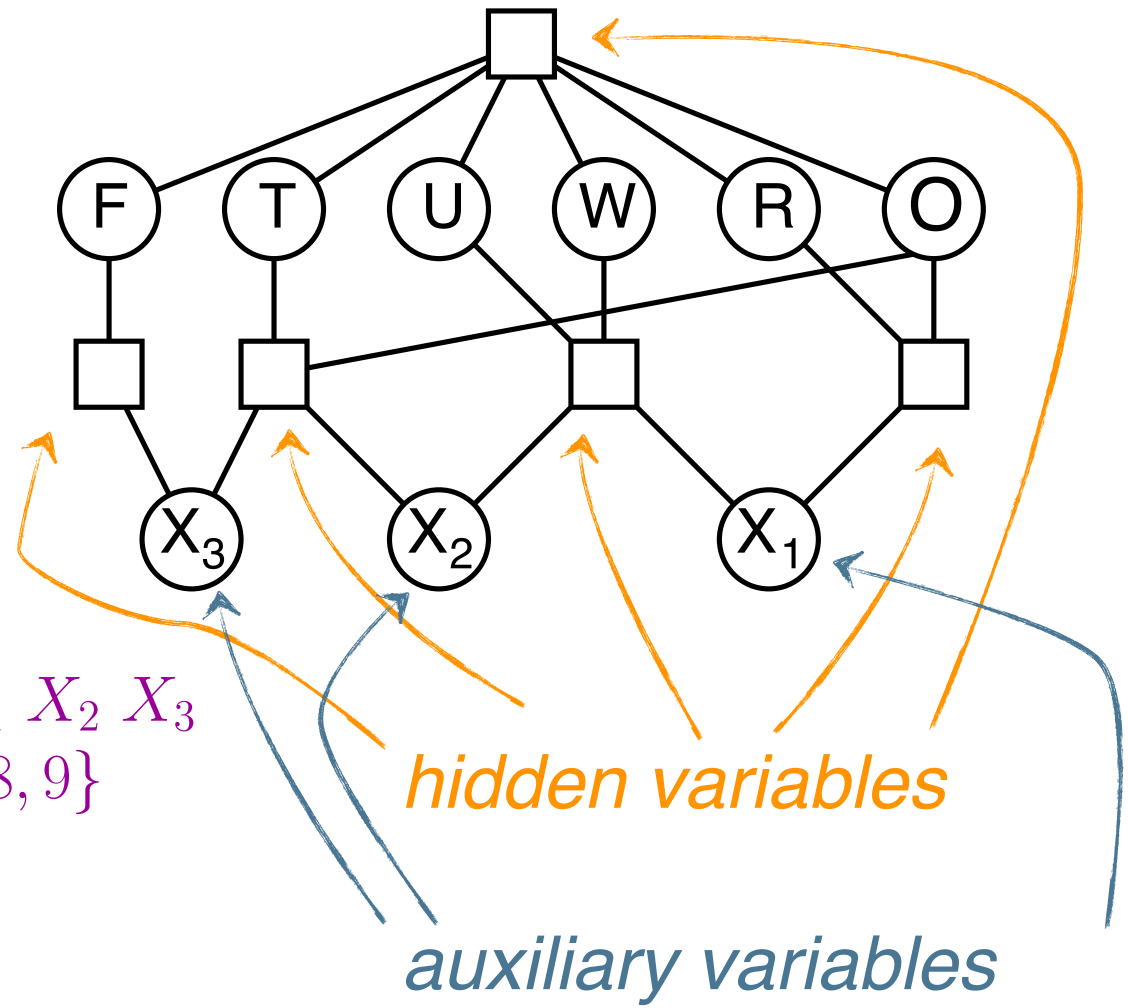


constraint:
h=1, C=2
h=2, C=3
h=3, C=3

from the definition of h

Example: Cryptarithmetic

$$
\begin{array}{r}
T\ W\ O \\
+\ T\ W\ O \\
\hline
F\ O\ U\ R
\end{array}
$$



Variables: $F\ T\ U\ W\ R\ O\ X_1\ X_2\ X_3$

Domains: $\{0,1,2,3,4,5,6,7,8,9\}$

Constraints

alldiff(F,T,U,W,R,O)

$O+O=R+10\cdot X_1$, etc.

Summary of CSP

CSPs are a special kind of problem:
  states defined by values of a fixed set of variables
  goal test defined by constraints on variable values

Backtracking = depth-first search with one variable assigned per node

Variable ordering and value selection heuristics help significantly

Forward checking prevents assignments that guarantee later failure

Constraint propagation (e.g., arc consistency) does additional work to constrain values and detect inconsistencies

The CSP representation allows analysis of problem structure

Tree-structured CSPs can be solved in linear time

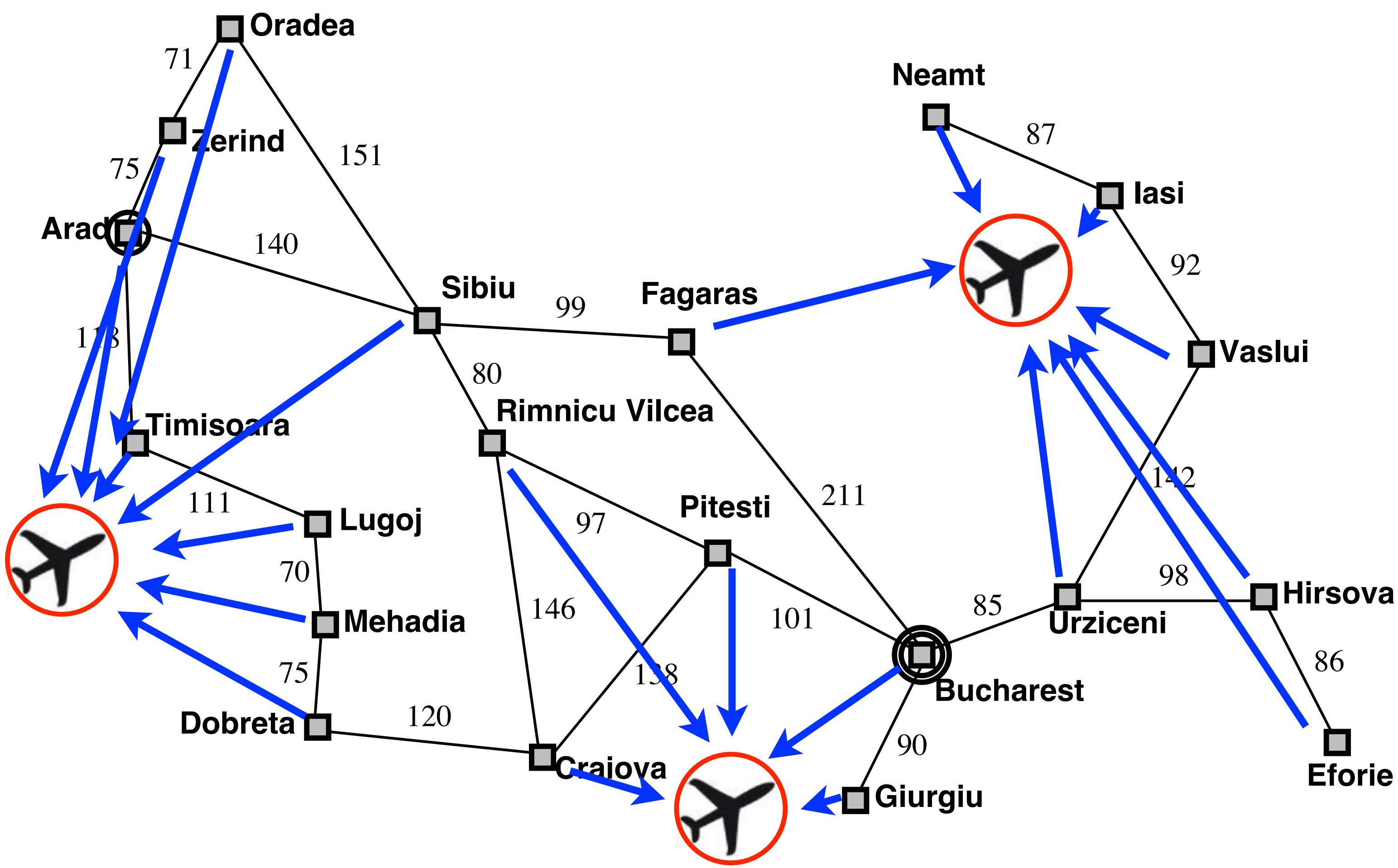
Iterative min-conflicts is usually effective in practice

General (Iterative) Solution Space Search

Greedy idea in continuous space

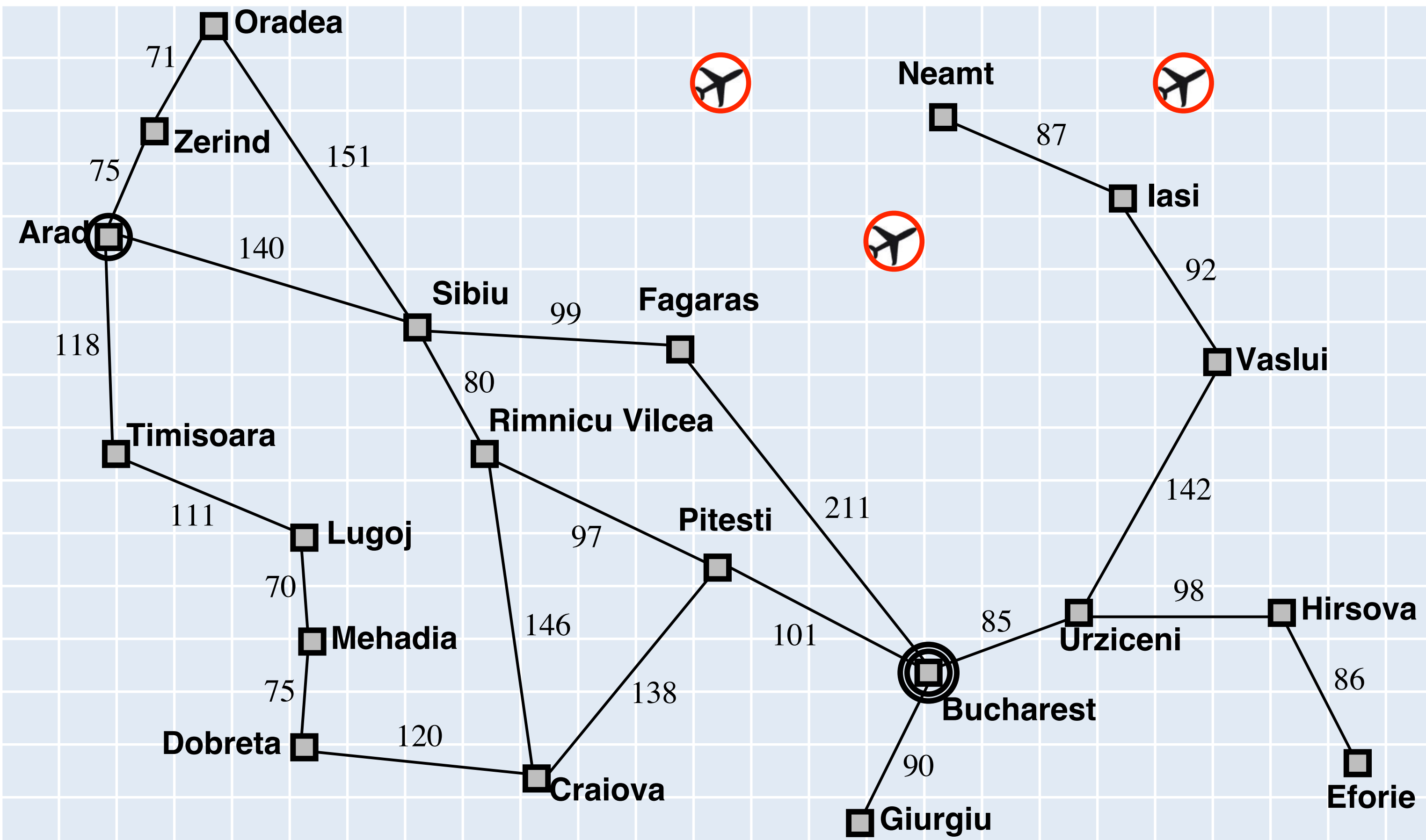
Suppose we want to site three airports in Romania:

- 6-D state space defined by (x_1, y_2), (x_2, y_2), (x_3, y_3)
- objective function $f(x_1, y_2, x_2, y_2, x_3, y_3) =$
  sum of squared distances from each city to nearest airport



Greedy idea in continuous space

discretize and use hill climbing



Hill climbing

```
function HillClimb_Step(double[] solution)
    double value = Eval(solution)
    List neighbors = Neighbors(solution)
    double bestv = value
    double[] bestc = none
    for each candidate in neighbors do
        double candivalue = eval(candidate)
        if candivalue < bestv then
            bestv = candivalue
            bestc = candidate
        end if
    end for
return bestc
```

Greedy idea in continuous space

gradient decent

- 6-D state space defined by (x_1, y_2), (x_2, y_2), (x_3, y_3)
- objective function $f(x_1, y_2, x_2, y_2, x_3, y_3) =$
  sum of squared distances from each city to nearest airport

Gradient methods compute

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial y_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial y_2}, \frac{\partial f}{\partial x_3}, \frac{\partial f}{\partial y_3}\right)$$

to increase/reduce f, e.g., by $\mathbf{x} \leftarrow \mathbf{x} + \alpha \nabla f(\mathbf{x})$

1-order method

Greedy idea in continuous space

gradient decent

- 6-D state space defined by (x_1, y_2), (x_2, y_2), (x_3, y_3)
- objective function $f(x_1, y_2, x_2, y_2, x_3, y_3) =$
  sum of squared distances from each city to nearest airport

Sometimes can solve for $\nabla f(\mathbf{x}) = 0$ exactly (e.g., with one city).
Newton–Raphson (1664, 1690) iterates $\mathbf{x} \leftarrow \mathbf{x} - \mathbf{H}_f^{-1}(\mathbf{x})\nabla f(\mathbf{x})$
to solve $\nabla f(\mathbf{x}) = 0$, where $\mathbf{H}_{ij} = \partial^2 f / \partial x_i \partial x_j$

2-order method

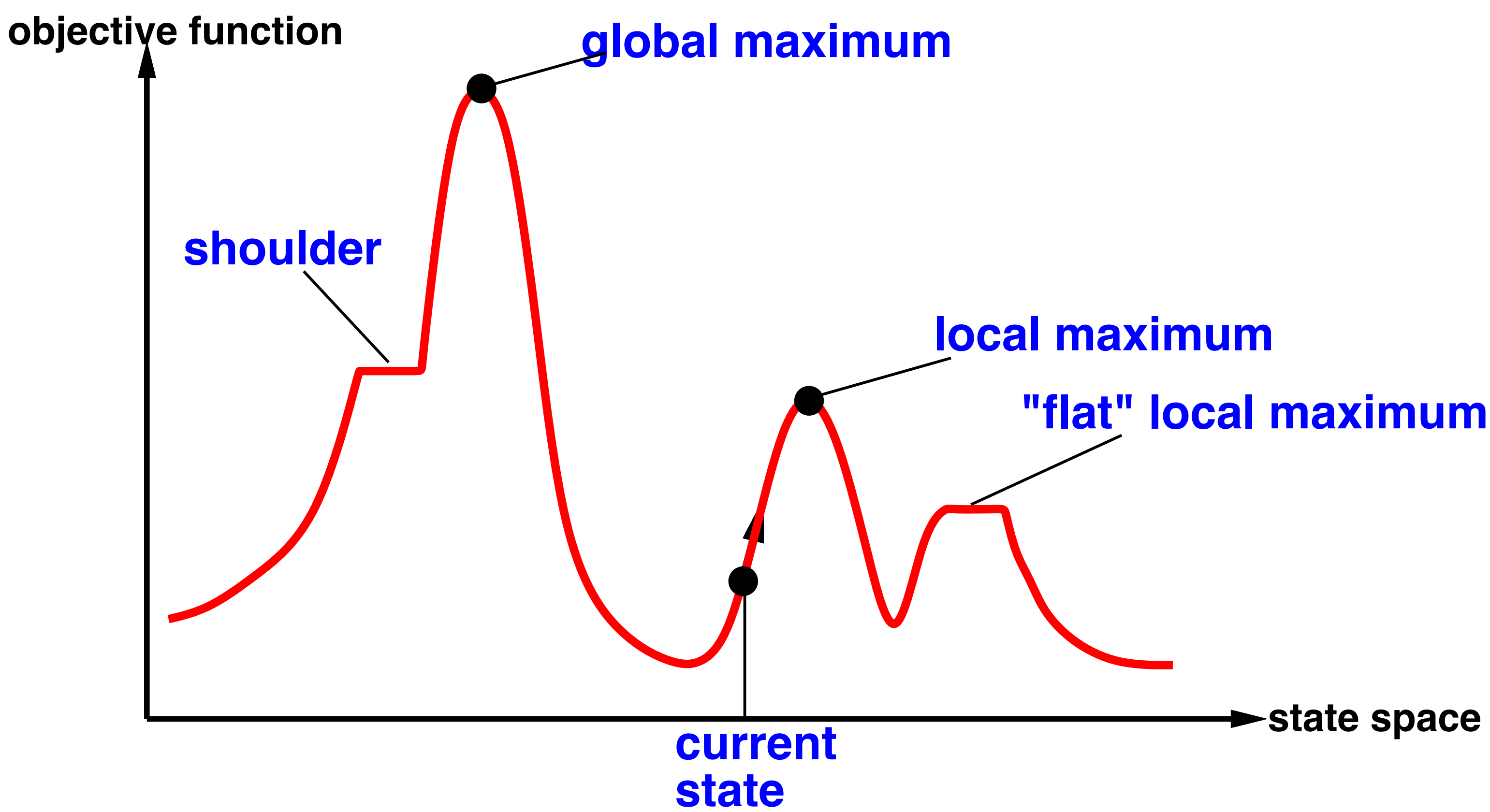
Taylor's series:

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2} f''(a) + \cdots = \sum_{i=0}^{\infty} \frac{(x-a)^i}{i!} f^{(i)}(a).$$

Greedy idea

1st and 2nd order methods may not find global optimal solutions

they work for convex functions



Purely random search

```
function RandomSearch_Step(double[] solution)
    double value = Eval(solution)
    double[] rsol = RandomSolution()
    double vr = Eval(rsol)
    if vr < value then
        return rsol
    end if
return none
```

optimal after infinite steps! why?

can be more smart? replace RandomSolution

Hill climbing vs. Pure random search

```
function HillClimb_Step(double[] solution)
    double value = Eval(solution)
    List neighbors = Neighbors(solution)
    double bestv = value
    double[] bestc = none
    for each candidate in neighbors do
        double candivalue = eval(candidate)
        if candivalue < bestv then
            bestv = candivalue
            bestc = candidate
        end if
    end for
return bestc
```

```
function RandomSearch_Step(double[] solution)
    double value = Eval(solution)
    double[] rsol = RandomSolution()
    double vr = Eval(rsol)
    if vr < value then
        return rsol
    end if
return none
```

exploitation vs. exploration

locally optimal vs. globally optimal

Meta-heuristics

“problem independent
“black-box
“zeroth-order method
...

and usually inspired from nature phenomenon

Simulated annealing

temperature from high to low

when high temperature, form the shape
when low temperature, polish the detail

Simulated annealing

Idea: escape local maxima by allowing some "bad" moves
but gradually decrease their size and frequency

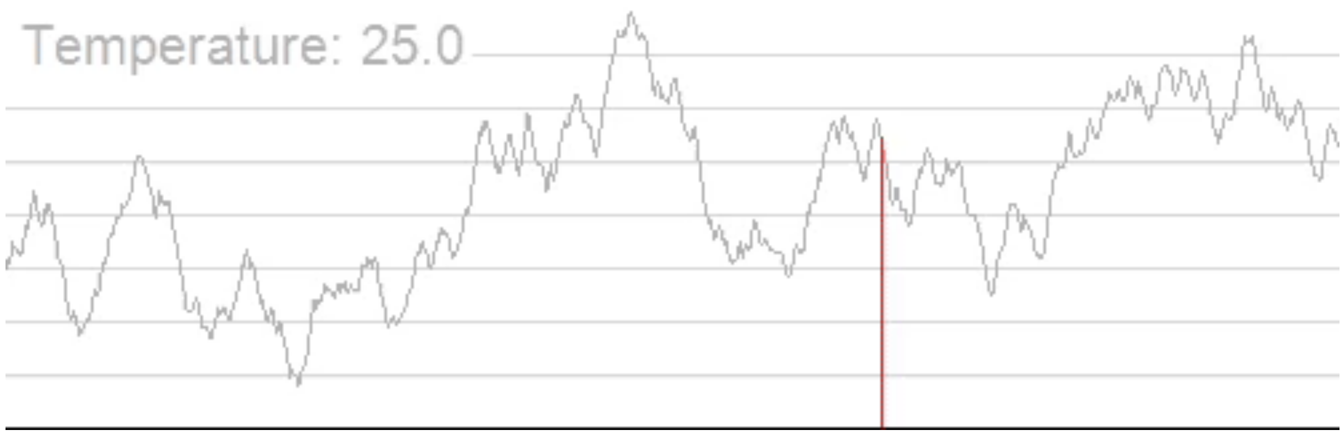
```
function SIMULATED-ANNEALING(problem, schedule) returns a solution state
    inputs: problem, a problem
            schedule, a mapping from time to "temperature"
    local variables: current, a node
                     next, a node
                     T, a "temperature" controlling prob. of downward 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 ΔE > 0 then current ← next
        else current ← next only with probability e^(ΔE/T)
```

the neighborhood range shrinks with T

the probability of accepting a bad solution decreases with T

Simulated annealing

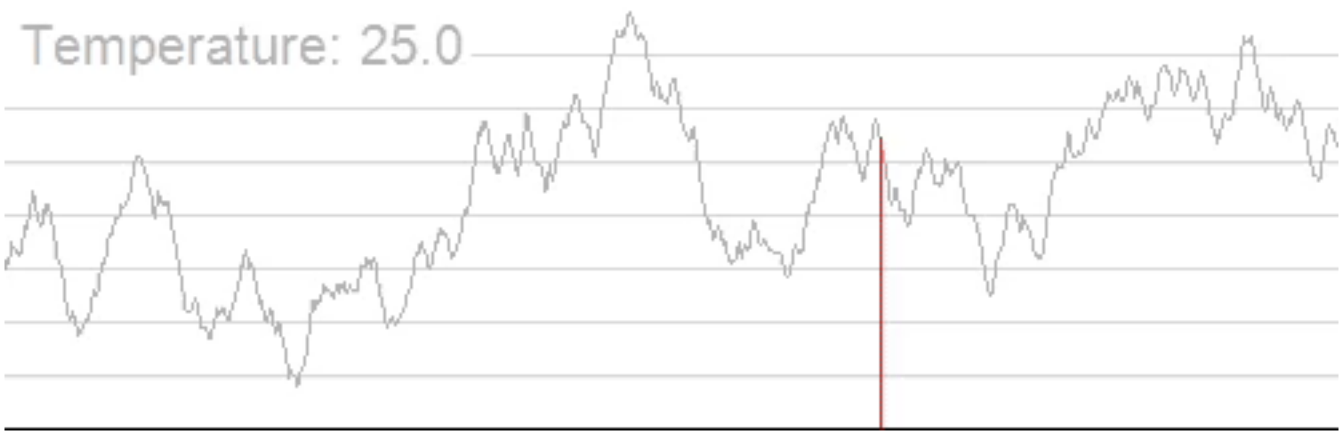
a demo



graphic from http://en.wikipedia.org/wiki/Simulated_annealing

Simulated annealing

a demo



graphic from http://en.wikipedia.org/wiki/Simulated_annealing

Local beam search

Idea: keep k states instead of 1; choose top k of all their successors

Not the same as k 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

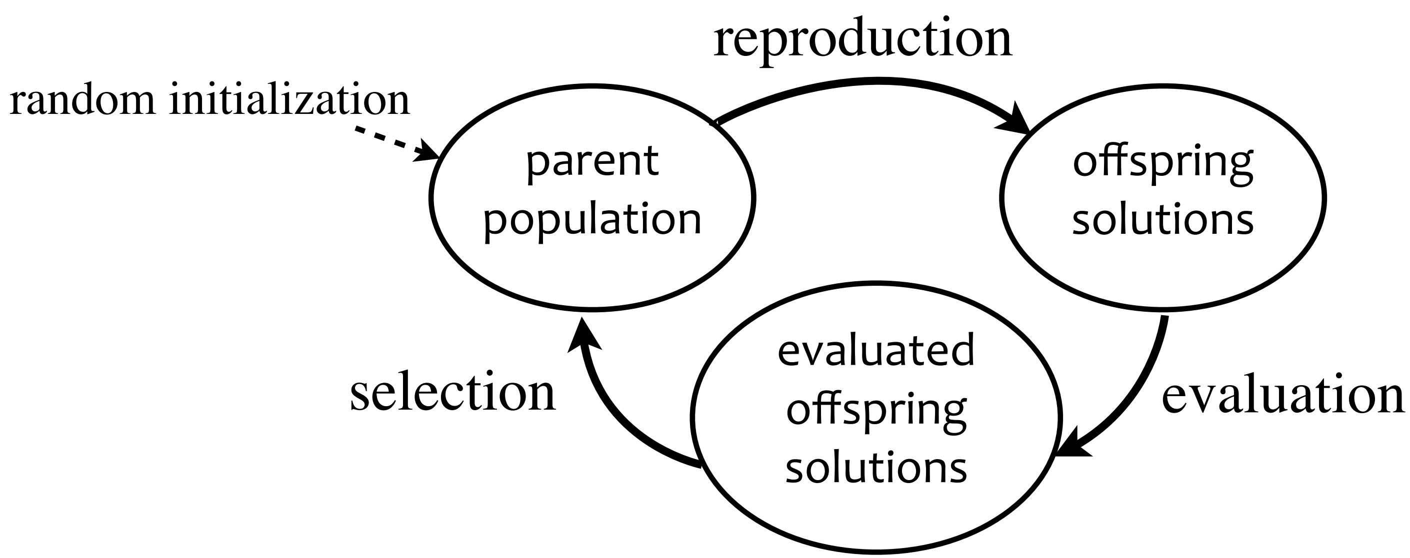
Idea: choose k successors randomly, biased towards good ones

Observe the close analogy to natural selection!

Genetic algorithm

a simulation of Darwin's evolutionary theory
(more generally: evolutionary algorithm)

– over-reproduction with diversity
– nature selection



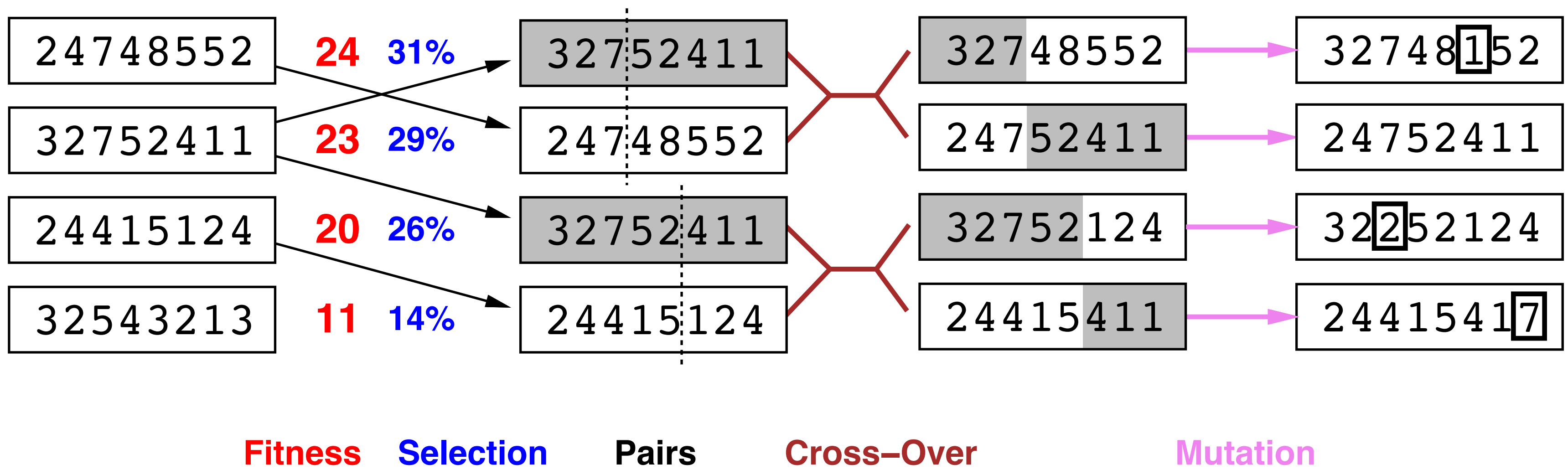
Genetic algorithm

Encode a solution as a vector,

$Pop \leftarrow n$ randomly drawn solutions from $\mathcal{X}$
for t=1,2,... **do**
    $Pop^m \leftarrow \{mutate(s) \mid \forall s \in Pop\}$, the mutated solutions
    $Pop^c \leftarrow \{crossover(s_1, s_2) \mid \exists s_1, s_2 \in Pop^m\}$, the recombined solutions
    evaluate every solution in Pop^c by $f(s)(\forall s \in Pop^c)$
    $Pop^s \leftarrow$ selected solutions from Pop and Pop^c
    $Pop \leftarrow Pop^s$
    terminate if meets a stopping criterion
end for

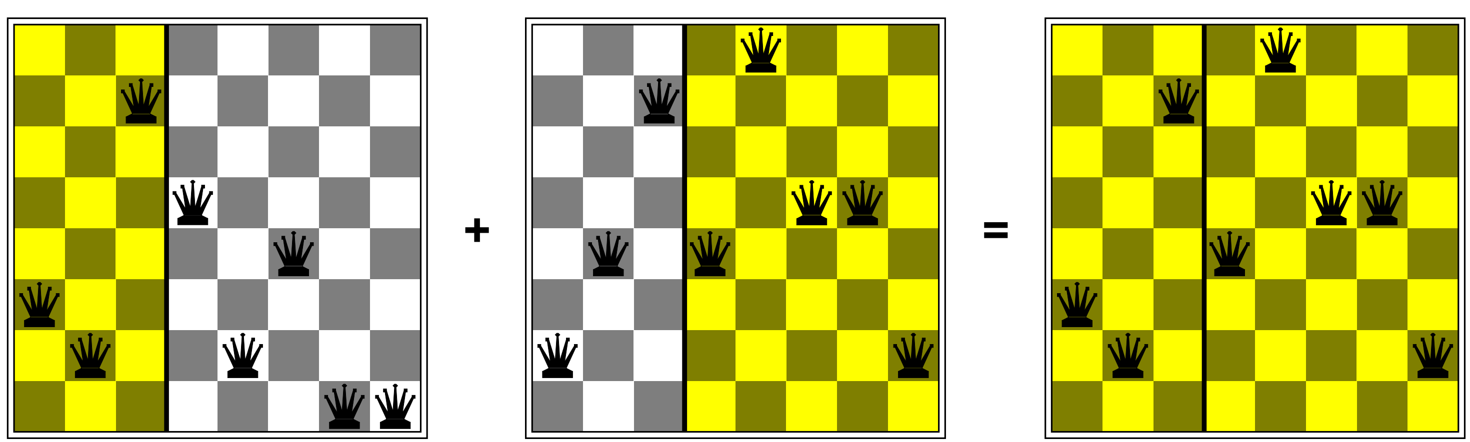
mutation: some kind of random changes
crossover: some kind of random exchanges
selection: some kind of quality related selection

Genetic algorithm

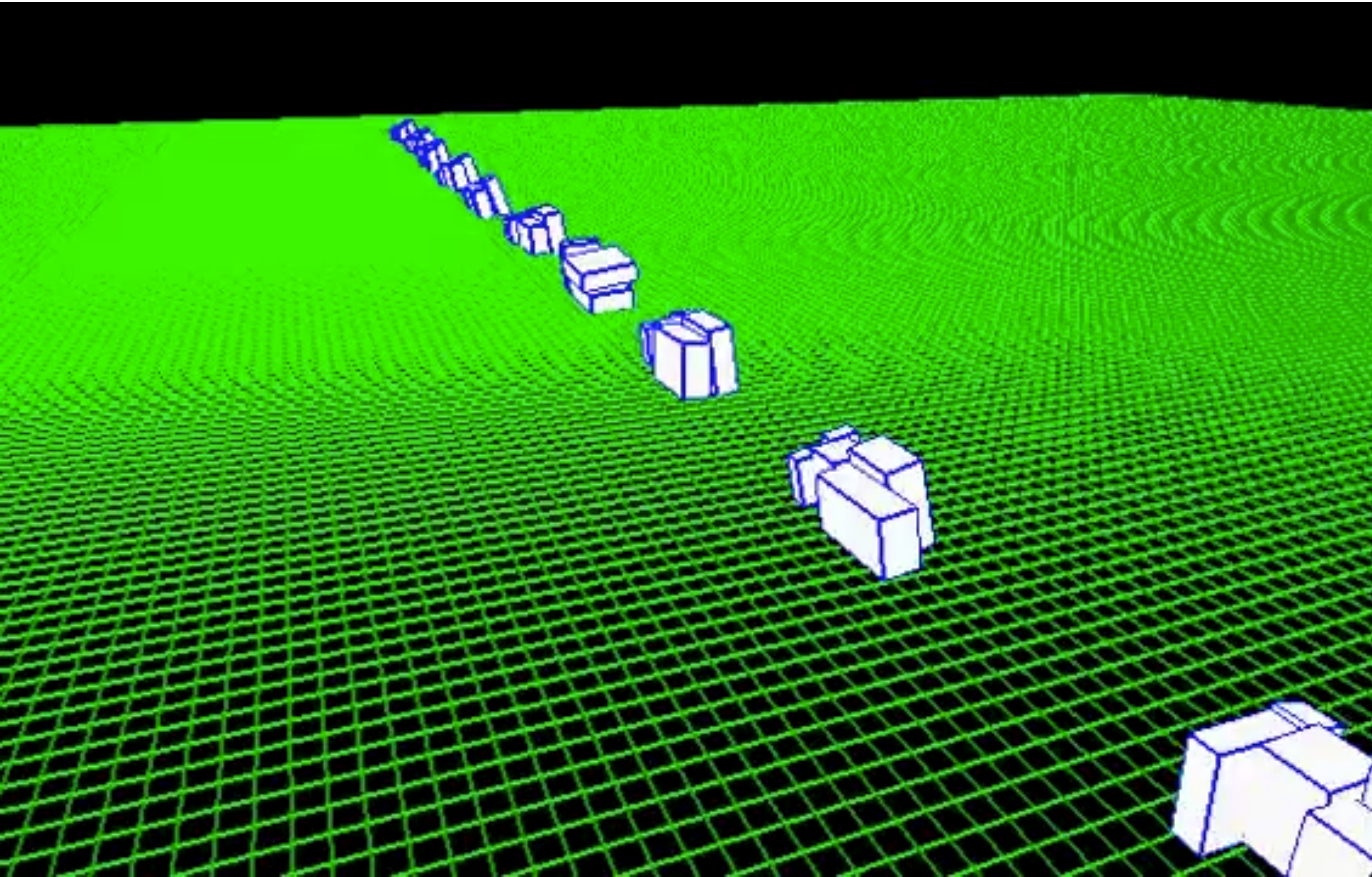


GAs require states encoded as strings (GPs use programs)

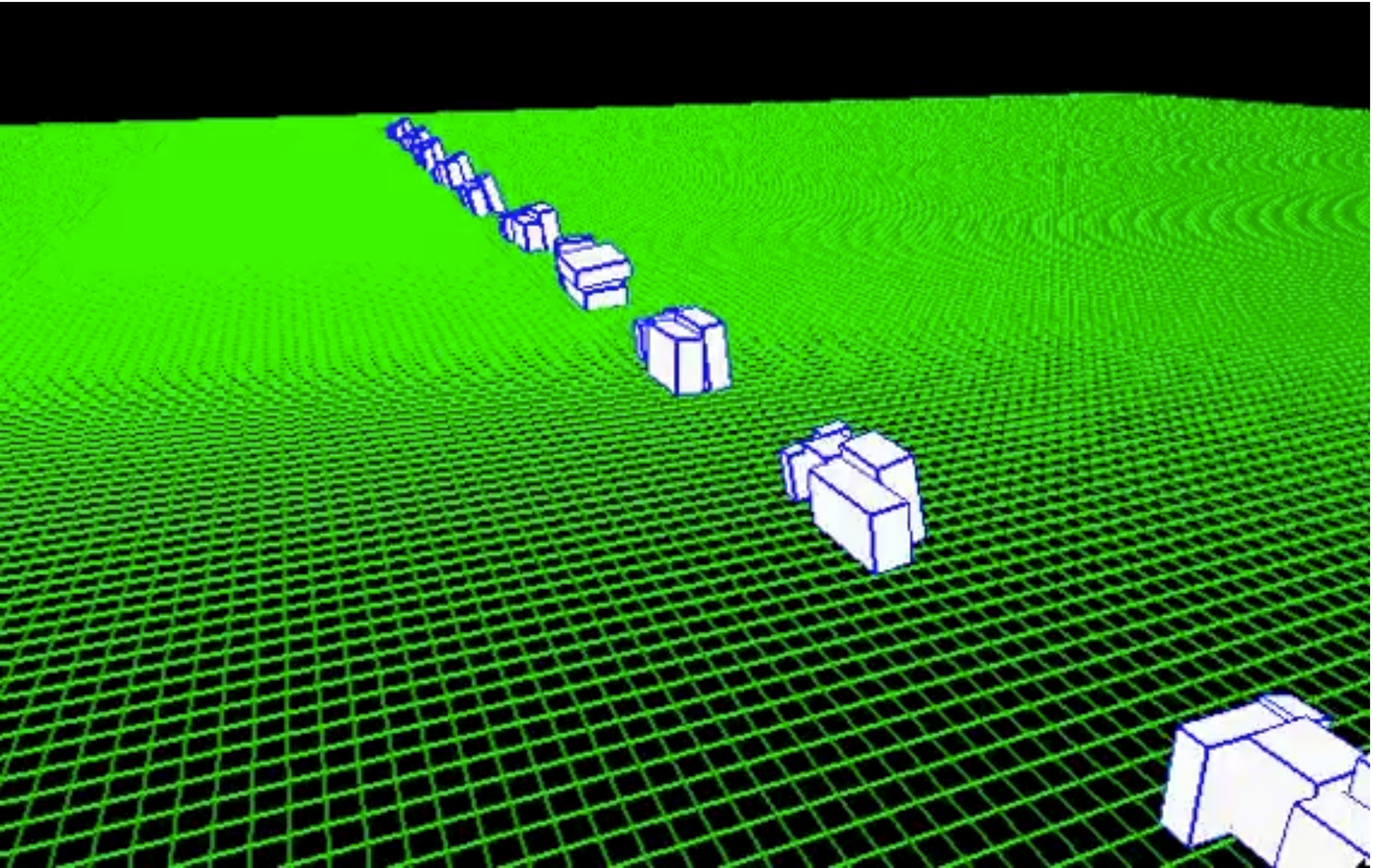
Crossover helps **iff substrings are meaningful components**



An evolutionary of virtual life



An evolutionary of virtual life



Example

hard to apply traditional optimization methods
but easy to test a given solution

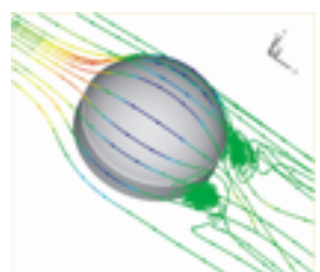
Representation:

parameterize

represented as a vector of parameters

Fitness:

x_i



$f(x_i)$

test by simulation/experiment

Example

Series 700

Series N700

Technological overview of the next generation Shinkansen high-speed train Series N700

M. Ueno[1], S. Usui[1], H. Tanaka[1], A. Watanabe[2]

[1]*Central Japan Railway Company, Tokyo, Japan,* [2]*West Japan Railway Company, Osaka, Japan*

Abstract

In March 2005, Central Japan Railway Company (JR Central) has completed prototype

waves and other issues related to environmental compatibility such as external noise. To combat this, an aero double-wing-type has been adopted for nose shape (Fig. 3). This nose shape, which boasts the most appropriate aerodynamic performance, has been newly developed for railway rolling stock using the latest analytical technique (i.e. genetic algorithms) used to develop the main wings of airplanes. The shape resembles a bird in flight, suggesting a feeling of boldness and speed

On the Tokaido Shinkansen line, Series N700 cars save 19% energy than Series 700 cars, despite a 30% increase in the output of their traction equipment for higher-speed operation (Fig. 4).

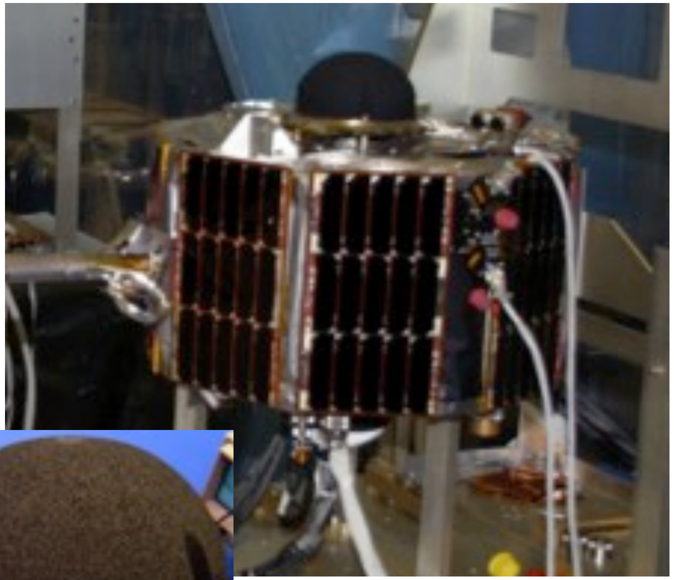
This is a result of adopting the aerodynamically excellent nose shape, reduced running resistance thanks to the drastically smoothened car body and under-floor equipment, effective

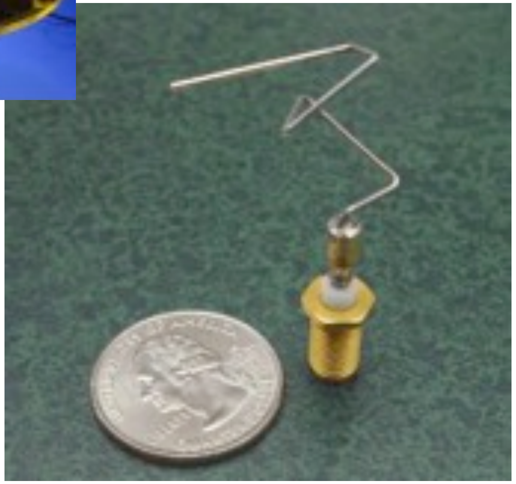
this nose ... has been newly developed ... using the latest analytical technique (i.e. **genetic algorithms**)

N700 cars save **19%** energy ... **30%** increase in the output... This is a result of adopting the ... nose shape

Example

NASA ST5 satellite

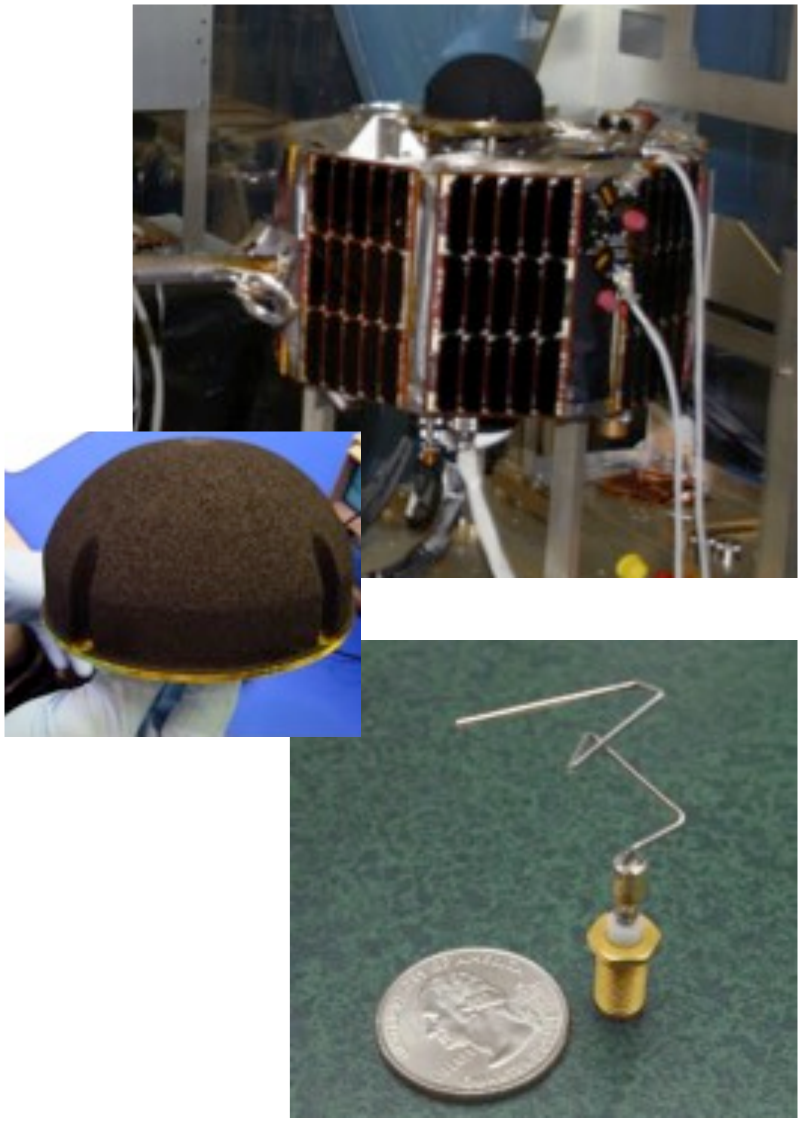




hard to apply traditional optimization methods

Example

NASA ST5 satellite



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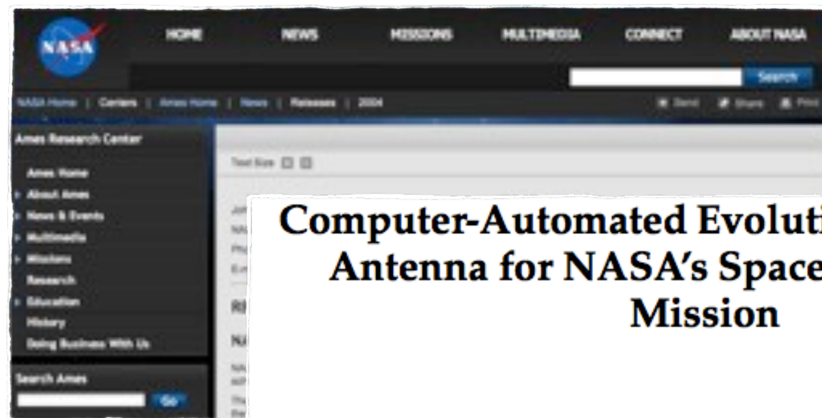

Computer-Automated Evolution of an X-Band Antenna for NASA's Space Technology 5 Mission

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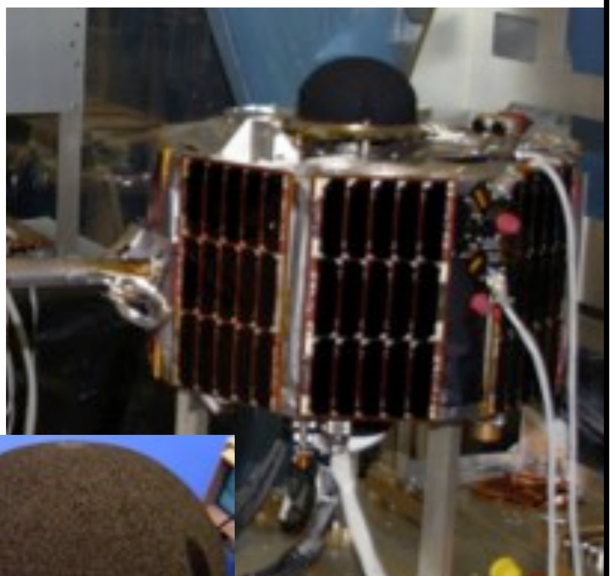
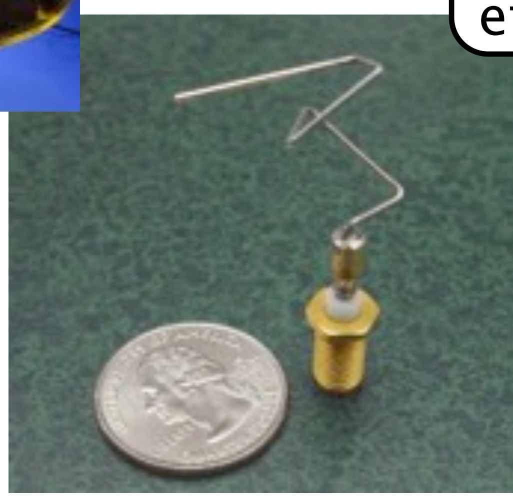
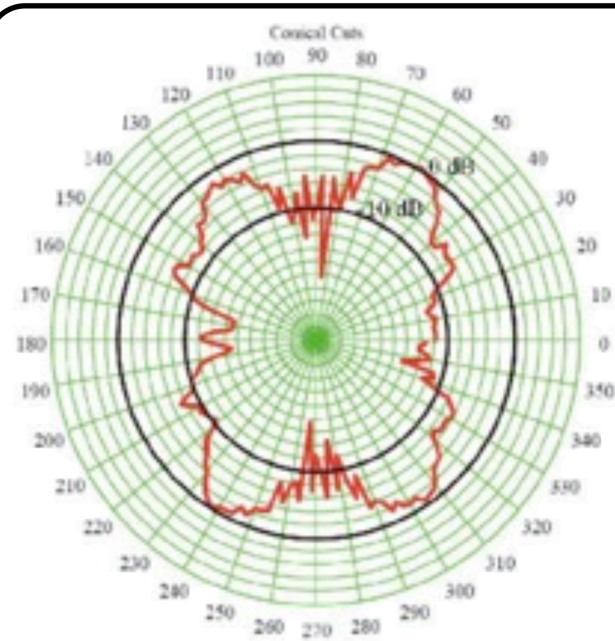
Since there are two antennas on each spacecraft, and not just one, it is important o measure the overall gain pattern with two antennas mounted on the spacecraft. For this, different combinations of the two evolved antennas and the QHA were tried on the the ST5 mock-up and measured in an anechoic chamber. With two QHAs 38% efficiency was achieved, using a QHA with an evolved antenna resulted in 80% efficiency and using two evolved antennas resulted in 93% efficiency. Here "efficiency" means how much power is being radiated versus how much power is being eaten up in resistance, with greater efficiency resulting in a stronger signal and greater range. Figure 11

Example

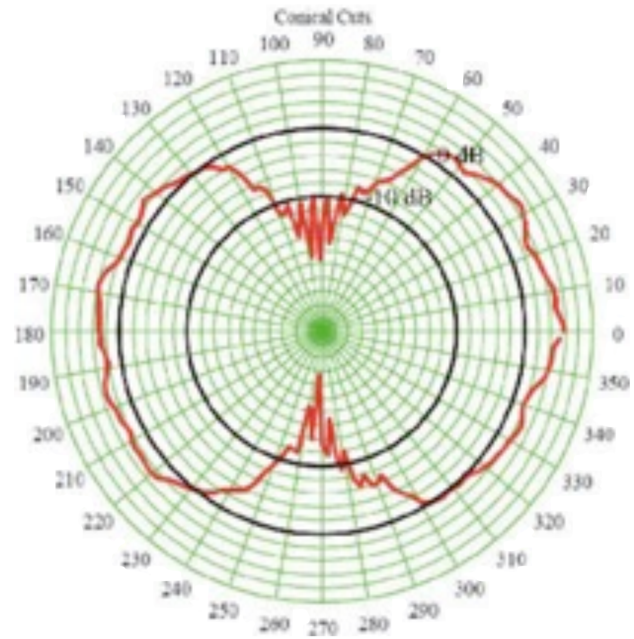
NASA ST5 satellite







QHAs(人工设计) 38% efficiency



evolved antennas resulted in 93% efficiency

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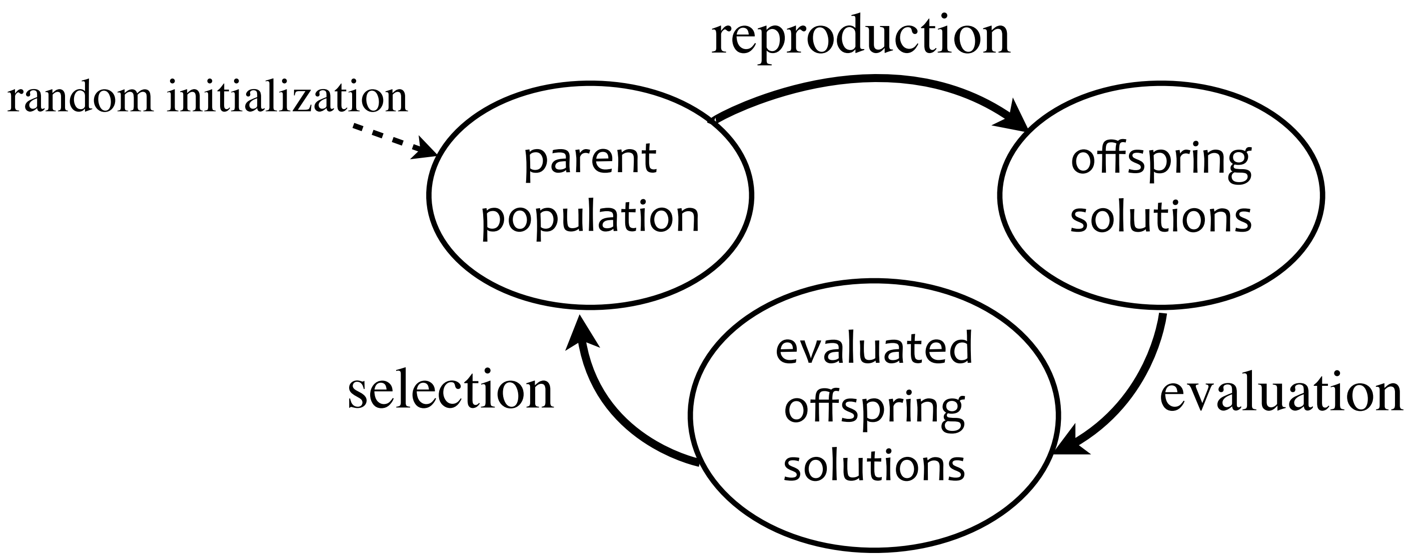
Properties of meta-heuristics



zeroth order

do not need differentiable functions

convergence

will find an optimal solution if
or $P(x \text{->} x_1 \text{->} \ldots \text{->} x_k \text{->} x^*)>0$

$P(x^* \mid x)>0$

Which is the best algorithm?

a search algorithm A, objective f, m solutions
arbitrary measure of the objective values of the m solutions:

$$\Phi(\boldsymbol{y}_m \mid f, m, A)$$

assume no replicates

Over all objectives $f : \mathcal{X} \to \{1, 2, \ldots, Y\}$

Overall performance assessment (for arbitrary k):

$$\sum_f I[k = \Phi(\boldsymbol{y}_m | f, m, A)]$$

$$\sum_{f} I[k = \Phi(\boldsymbol{y}_m | f, m, A)] = \sum_{f} I[k = \Phi(f(A(m)))]$$

$$\sum_f I[k = \Phi(\boldsymbol{y}_m | f, m, A)] = \sum_f I[k = \Phi(f(A(m)))]$$

$$= \sum_f \sum_{\boldsymbol{y}_m} I[k = \Phi(\boldsymbol{y}_m)] I[\boldsymbol{y}_m = f(A(m))]$$

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$$= \sum_{\boldsymbol{y}_m} I[k = \Phi(\boldsymbol{y}_m)] Y^{|\mathcal{X}|-m}$$

$$\sum_f I[k = \Phi(\boldsymbol{y}_m | f, m, A)] = \sum_f I[k = \Phi(f(A(m)))]$$

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all algorithms have the same average performance

[Wolpert & Macready, 97]

No Free Lunch Theorem

$$\sum_f I[k = \Phi(\boldsymbol{y}_m | f, m, A)] = \sum_f I[k = \Phi(f(A(m)))]$$

$$= \sum_f \sum_{\boldsymbol{y}_m} I[k = \Phi(\boldsymbol{y}_m)] I[\boldsymbol{y}_m = f(A(m))]$$

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all algorithms have the same average performance

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