(Stochastic) Local Search

Computer Science cpsc322, Lecture 5

(Textbook Chpt 4.8-4.9)

May, 22, 2012

Course Announcements

Posted on WebCT

- Assignment2 on CSPs (due on Thurs!)

If you are confused about basic CSPs….. Check learning goals at the end of lectures. Please come to office hours

- **Work on CSPs Practice Ex:**
  - Exercise 4.A: arc consistency
  - Exercise 4.B: constraint satisfaction problems
  - Exercise 4.C: SLS for CSP

- **MIDTERM: Mon May 28th – 3PM (room TBA)**

Systematically solving CSPs: Summary

- Build Constraint Network
- Apply Arc Consistency
  - One domain is empty → no sol
  - Each domain has a single value → unique sol
  - Some domains have more than one value → ?!
    may or may not have a solution
- Apply Depth-First Search with Pruning
- Split the problem in a number of disjoint cases
  - Apply Arc Consistency to each case

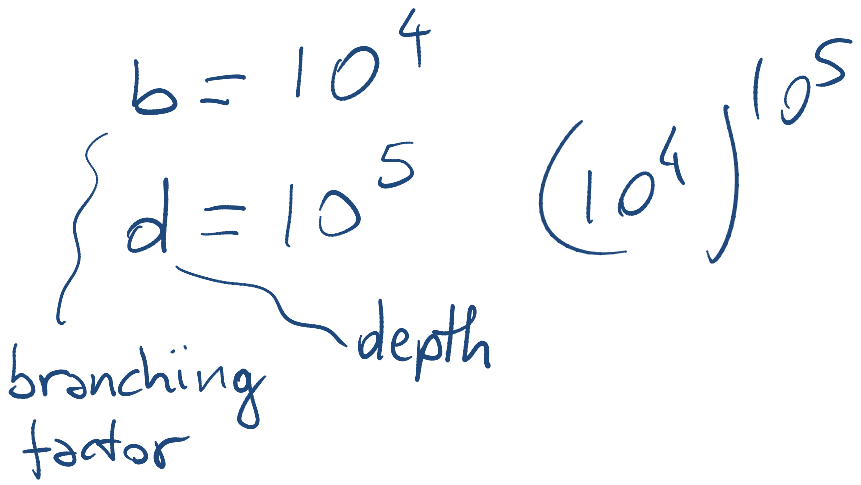
Lecture Overview

- Local search
  - Constrained Optimization
  - Greedy Descent / Hill Climbing: Problems
- Stochastic Local Search (SLS)
  - Comparing SLS algorithms
  - SLS variants
    - ✓Tabu lists
    - ✓Simulated Annealing
  - Population Based
    - ✓Beam search
    - ✓Genetic Algorithms

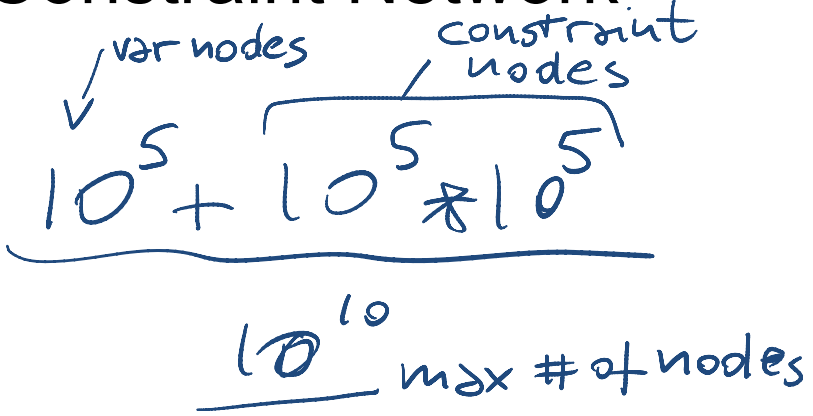
Local Search motivation: Scale

- Many CSPs (scheduling, DNA computing, more later) are simply too big for systematic approaches
- If you have 10^5 vars with $dom(var_i) = 10^4$

- Systematic Search



- Constraint Network



  - but if solutions are densely distributed……

Local Search: General Method

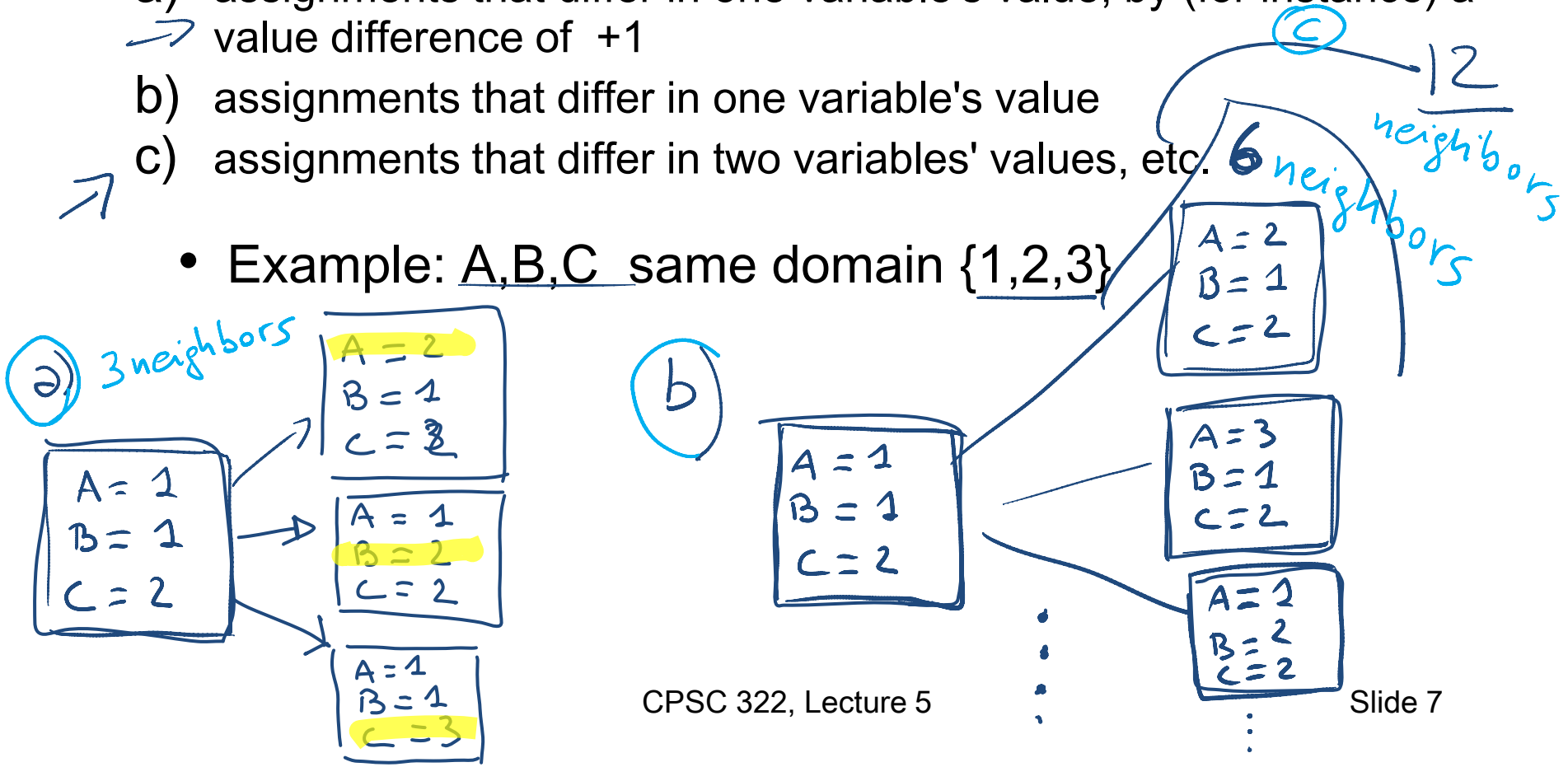
Remember , for CSP a solution is…?.. possible world (not a path)

- Start from a possible world
- Generate some neighbors ("similar" possible worlds)
- Move from the current node to a neighbor, selected according to a particular strategy
  - Example: A,B,C same domain {1,2,3}

Local Search: Selecting Neighbors

How do we determine the neighbors?

- Usually this is simple: some small incremental change to the variable assignment
  - a) assignments that differ in one variable's value, by (for instance) a value difference of +1
  - b) assignments that differ in one variable's value
  - c) assignments that differ in two variables' values, etc.
    - Example: A,B,C same domain {1,2,3}



Iterative Best Improvement

- How to determine the neighbor node to be selected?
- Iterative Best Improvement:
  - select the neighbor that optimizes some evaluation function
- Which strategy would make sense? Select neighbor with …

Maximal number of constraint violations

Similar number of constraint violations as current state

No constraint violations

Minimal number of constraint violations

Iterative Best Improvement

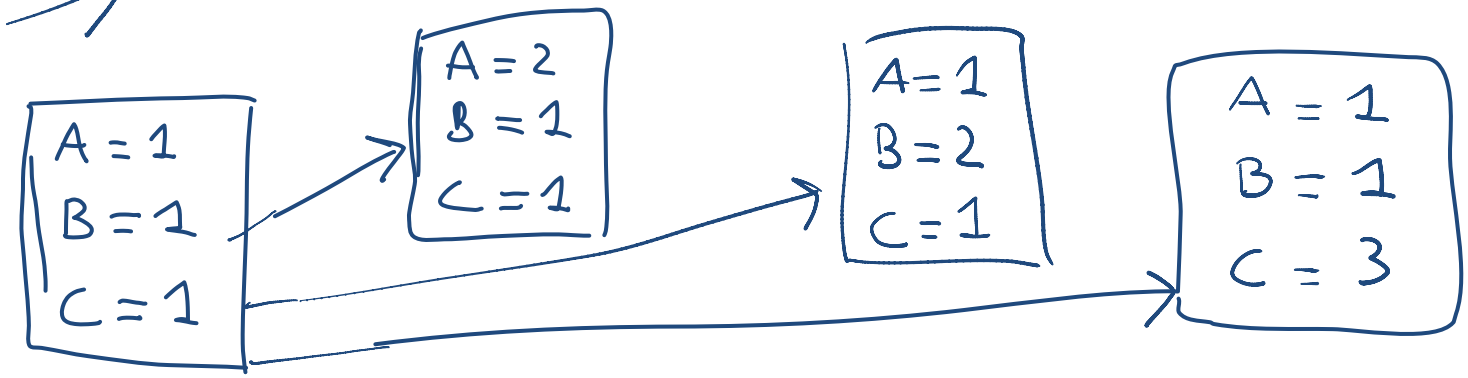
- How to determine the neighbor node to be selected?
- Iterative Best Improvement:
  - select the neighbor that optimizes some evaluation function
- Which strategy would make sense? Select

Minimal number of constraint violations

- Evaluation function:
  h(n): number of constraint violations in state n
- Greedy descent: evaluate h(n) for each neighbour, pick the neighbour n with minimal h(n)
- Hill climbing: equivalent algorithm for maximization problems
  - Here: maximize the number of constraints satisfied

Selecting the best neighbor

- Example: A,B,C same domain {1,2,3} , (A=B, A>1, C≠3)



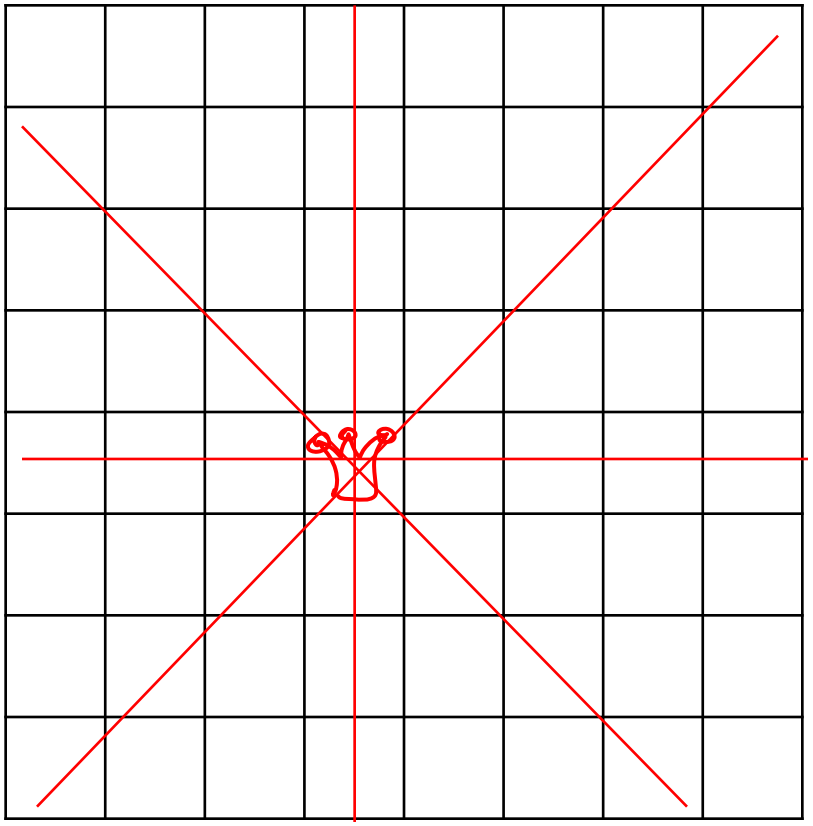
A common component of the scoring function (heuristic) => select the neighbor that results in the ……

- the **min conflicts** heuristics

Example: N-Queens

- Put n queens on an n × n board with no two queens on the same row, column, or diagonal (i.e attacking each other)

- Positions a queen can attack



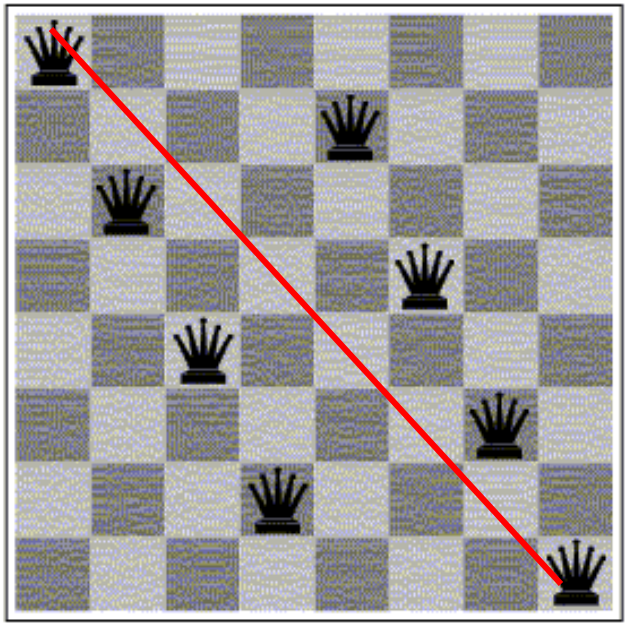
Example: N-queen as a local search problem

CSP: N-queen CSP

- One variable per column; domains {1,…,N} => row where the queen in the i^{th} column seats;
- Constraints: no two queens in the same row, column or diagonal

Neighbour relation: value of a single column differs

Scoring function: number of constraint violations (i..e, number of



Example: *n*-queens

Put *n* queens on an *n* × *n* board with no two queens on the same row, column, or diagonal (i.e attacking each other)

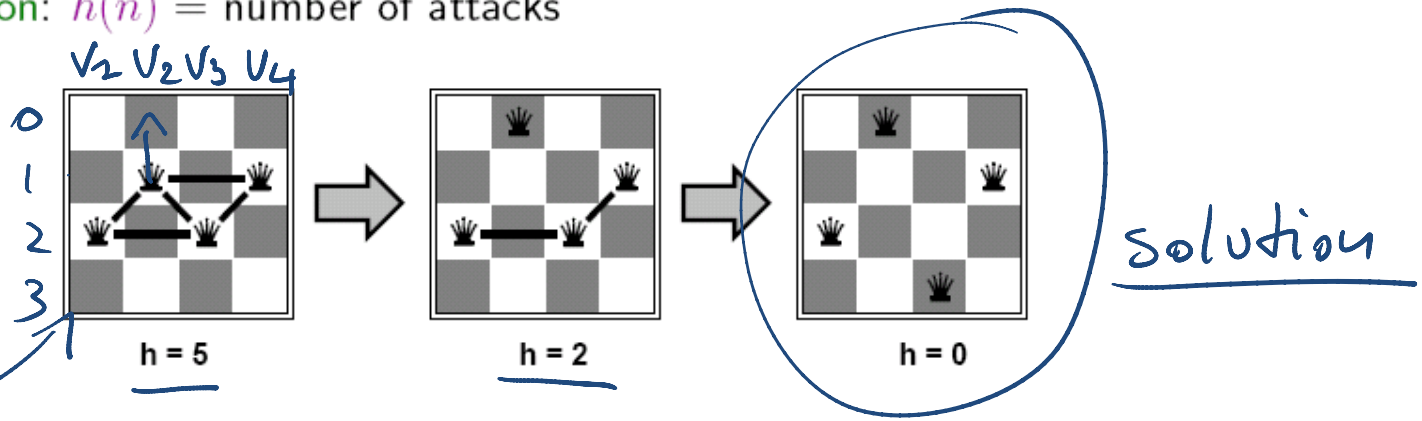
Example: 4-Queens

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

Operators: move queen in column (to generate neighbors)

Goal test: no attacks

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



$V_1 = 2$
$V_2 = 1$
$V_3 = 2$
$V_4 = 1$

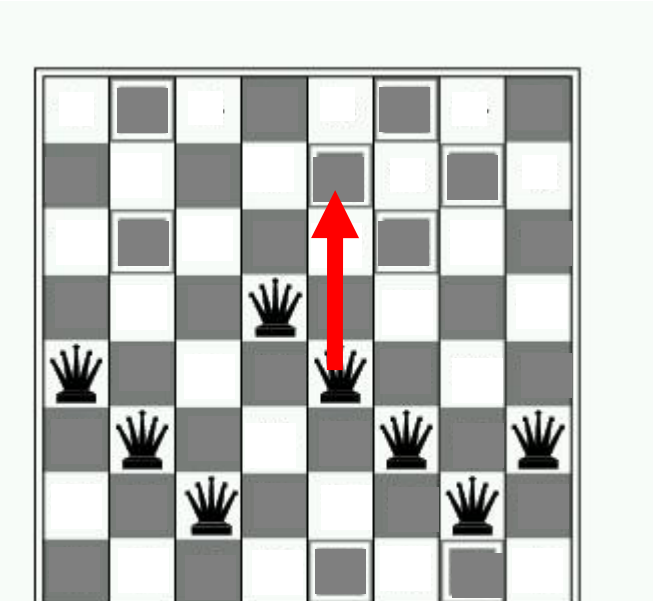
Example: Greedy descent for N-Queen

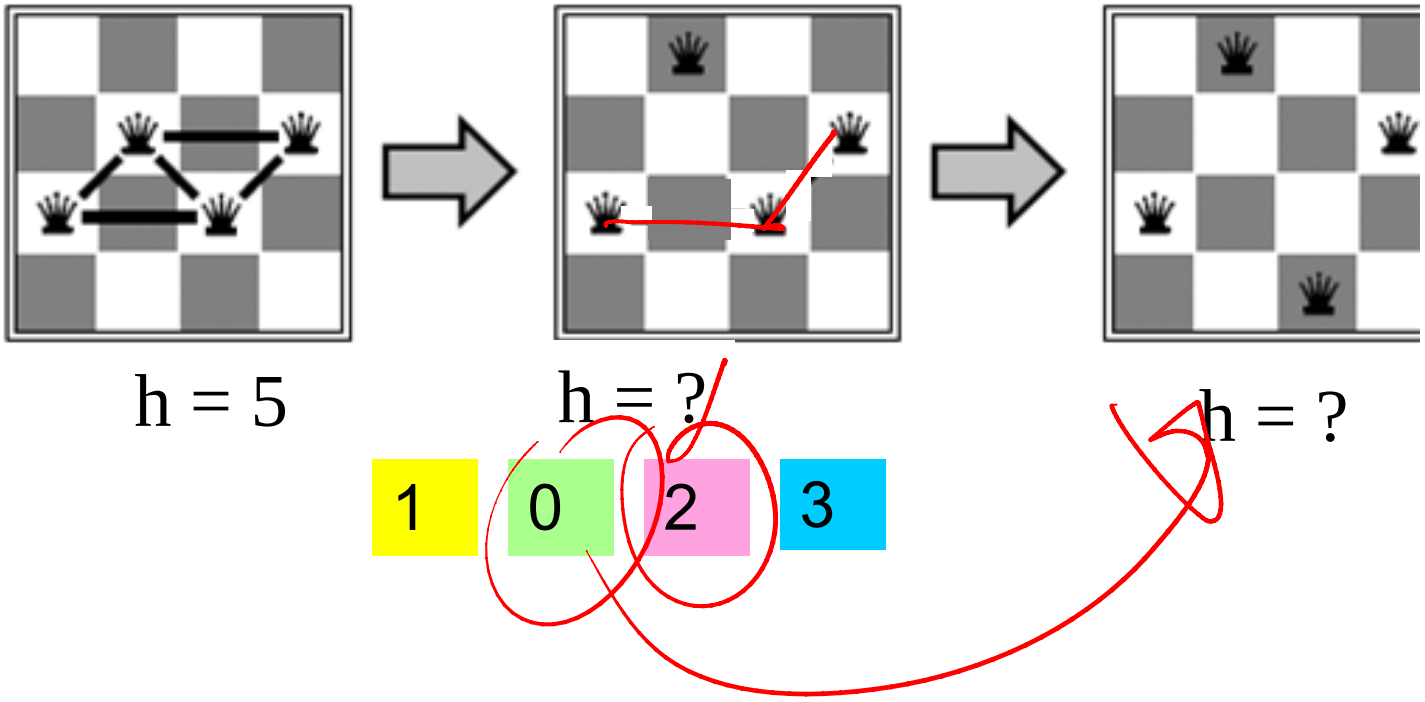
For each column, assign randomly each queen to a row
(a number between 1 and N)

Repeat

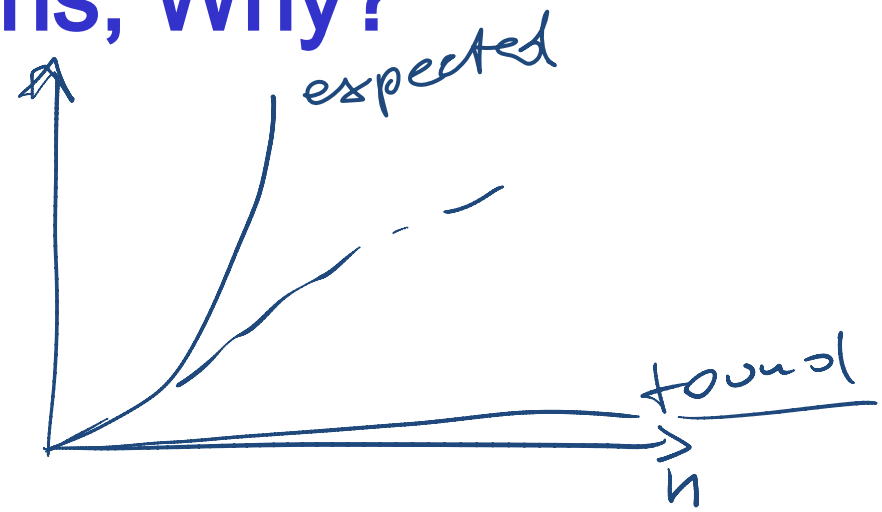
- For each column & each number: Evaluate how many constraint violations changing the assignment would yield
- Choose the column and number that leads to the fewest violated constraints; change it

Until solved




h = 5
h = ?
h = ?
1
0
2
3

n-queens, Why?



Why this problem?

Lots of research in the 90' on local search for CSP was generated by the observation that the run-time of local search on n-queens problems is **independent of problem size**!

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

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Constrained Optimization Problems

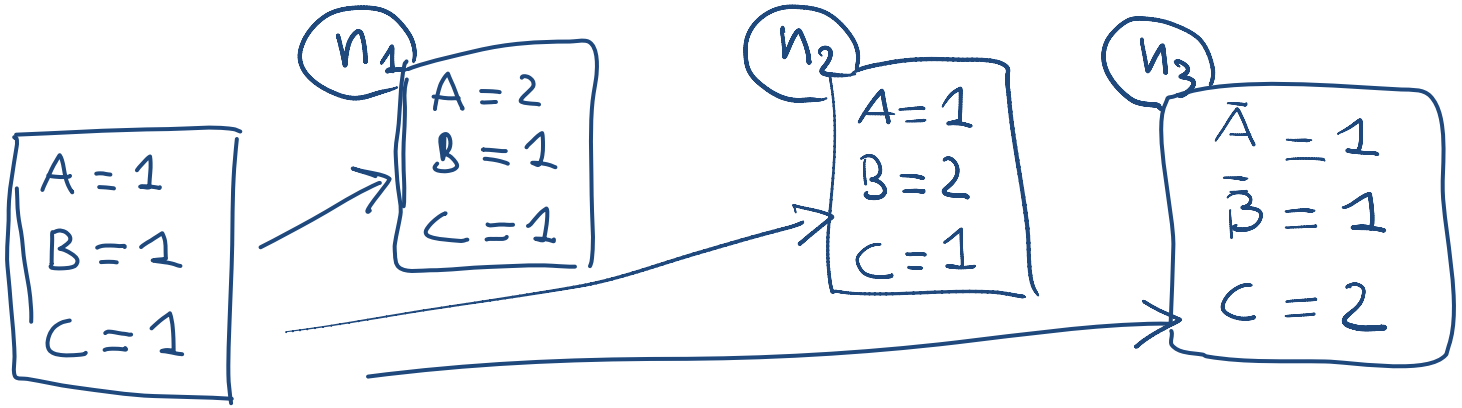
So far we have assumed that we just want to find a possible world that satisfies all the constraints.

But sometimes solutions may have different values / costs

- We want to find the optimal solution that
  - maximizes the value or
  - minimizes the cost

Constrained Optimization Example

- Example: A,B,C same domain {1,2,3} , (A=B, A>1, C≠3)
- Value = (C+A) so we want a solution that maximize that



The scoring function we'd like to maximize might be:

f(n) = (C + A) + #-of-satisfied-const

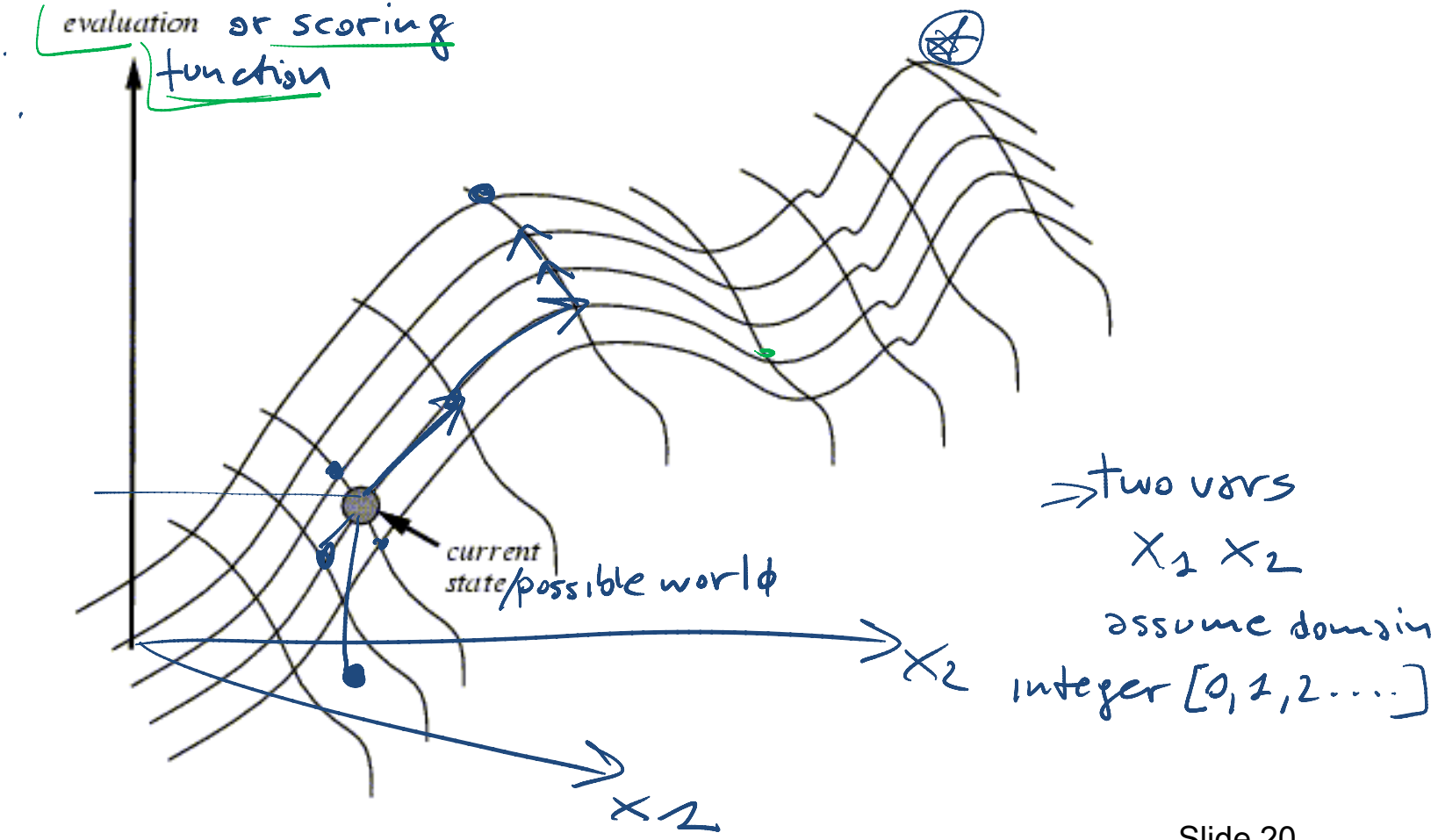
n_1: (1+2)+2 n_2: (1+1)+1 n_3: (2+1)+2

Hill Climbing means selecting the neighbor which best improves a (value-based) scoring function.

Greedy Descent means selecting the neighbor which minimizes a (cost-based) scoring function. cost + # of conflicts

Hill Climbing

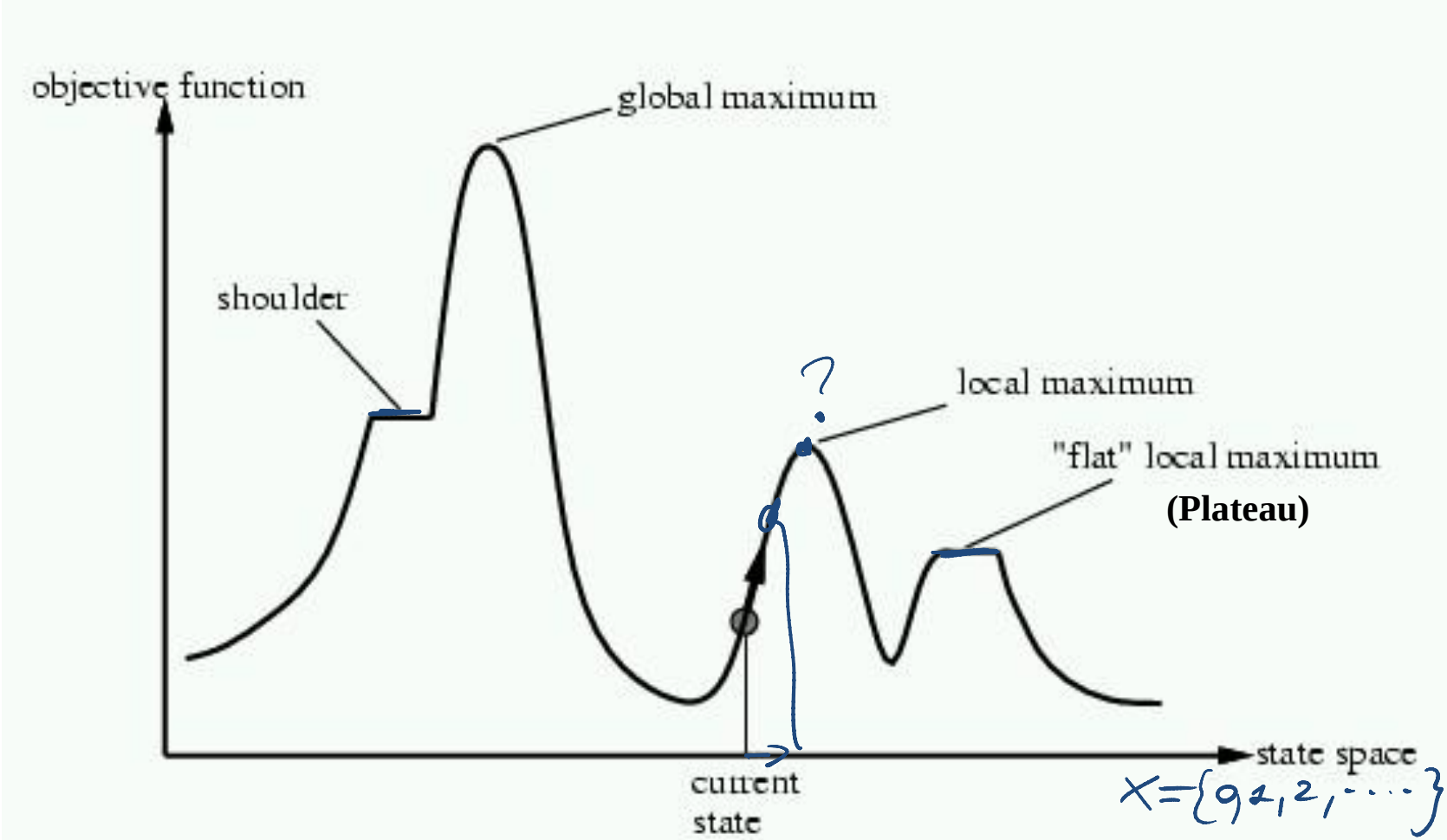
NOTE: Everything that will be said for Hill Climbing is also true for Greedy Descent



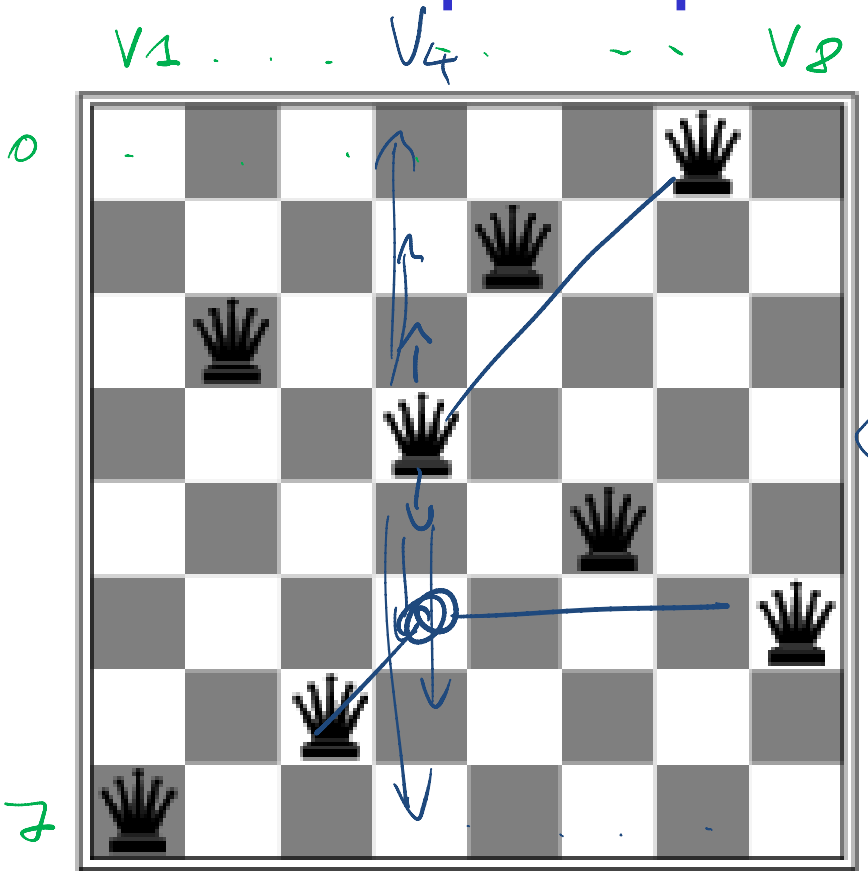
Problems with Hill Climbing

Local Maxima.

Plateau - Shoulders



Corresponding problem for GreedyDescent
Local minimum example: 8-queens problem



for all the moves (neighbors)

$h > 1$

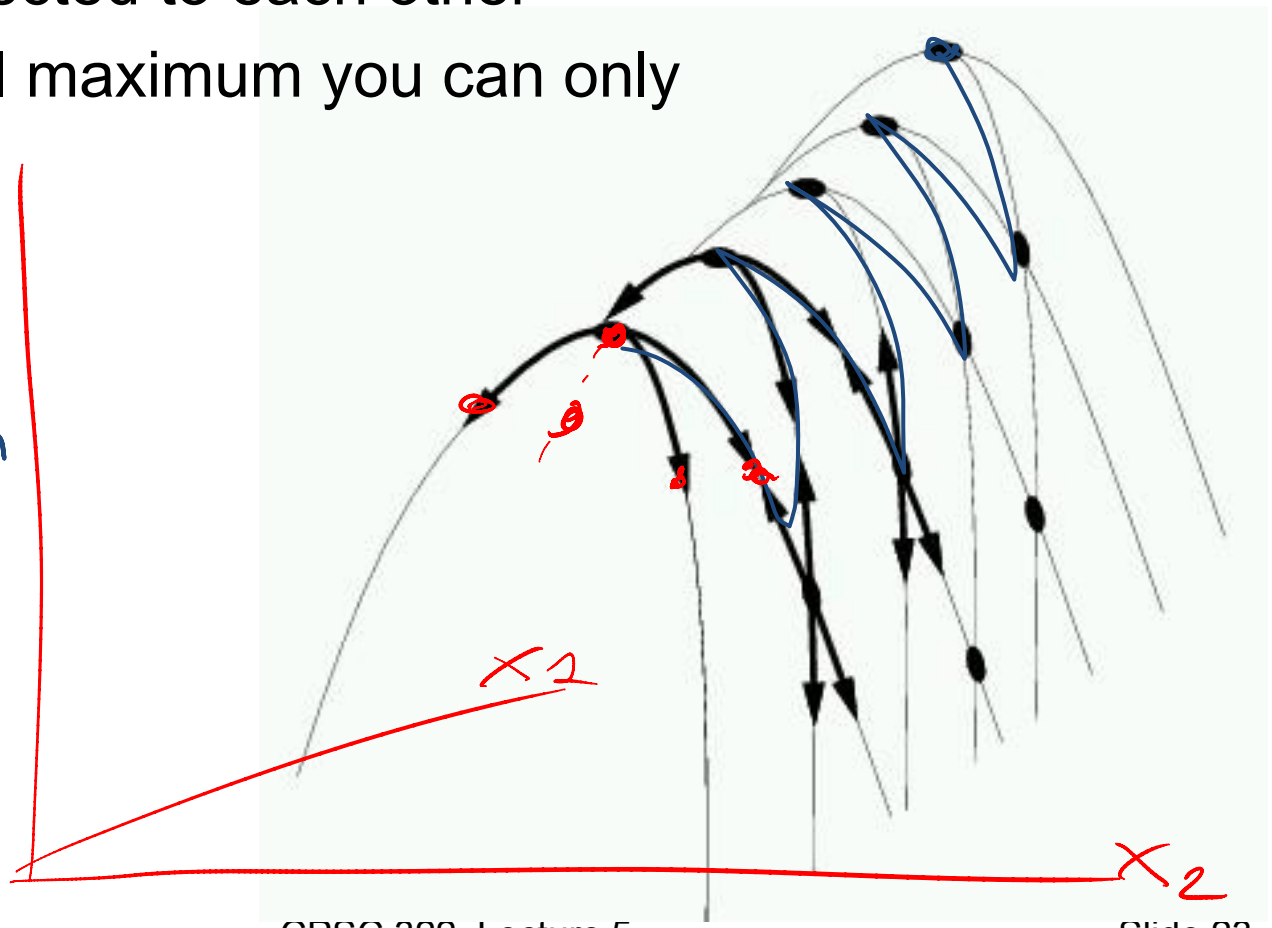
A local minimum with $h = 1$

$h = 0$ for solution

Even more Problems in higher dimensions

E.g., Ridges – sequence of local maxima not directly connected to each other

From each local maximum you can only go downhill



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Local Search: Summary

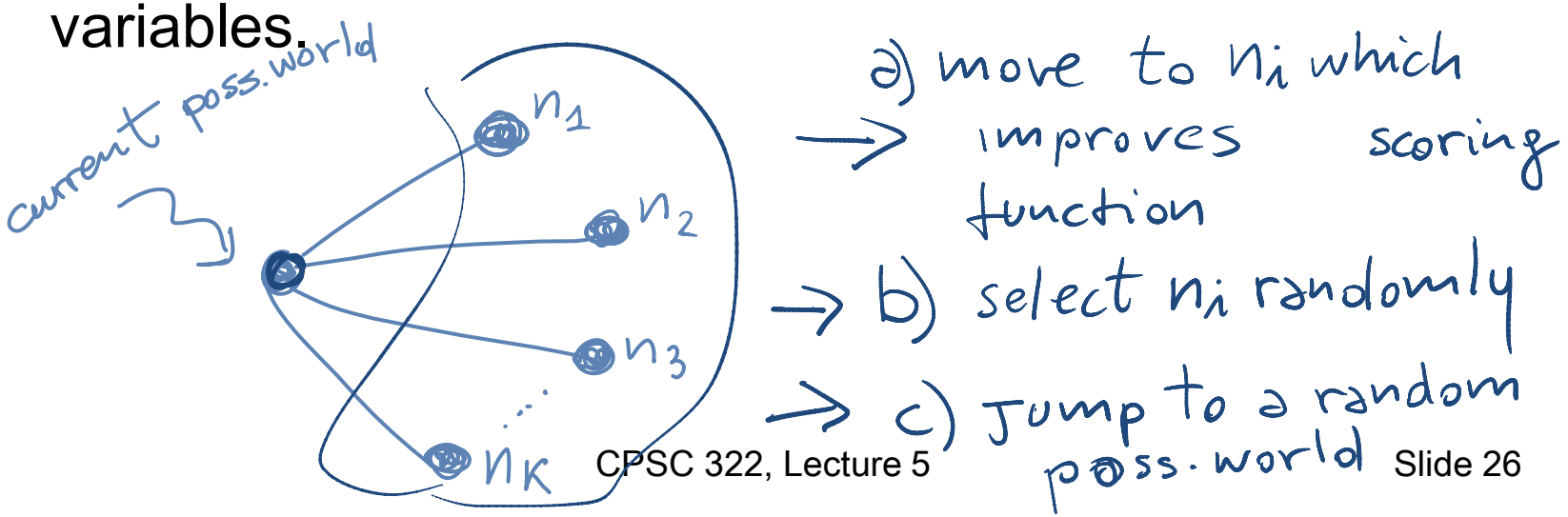
- A useful method in practice for large CSPs
  - Start from a possible world (randomly chosen)
  - Generate some neighbors ("similar" possible worlds)
    e.g. differ from current poss. world only by one variable's value
  - Move from current node to a neighbor, selected to minimize/maximize a scoring function which combines:
    - ✓ Info about how many constraints are violated
    - ✓ Information about the cost/quality of the solution (you want the best solution, not just a solution)

Stochastic Local Search

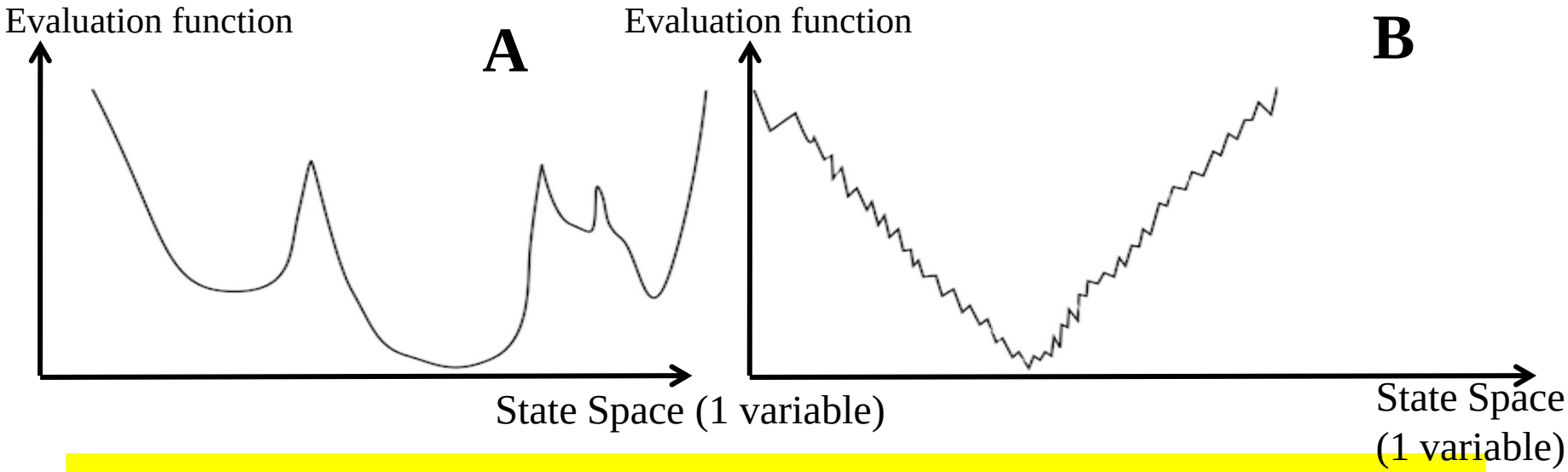
GOAL: We want our local search

- to be guided by the scoring function
- Not to get stuck in local maxima/minima, plateaus etc.

- **SOLUTION:** We can alternate
  a) Hill-climbing steps
  b) Random steps: move to a random neighbor.
  c) Random restart: reassign random values to all variables.



Which randomized method would work best in each of these two search spaces?



Greedy descent with random steps best on A

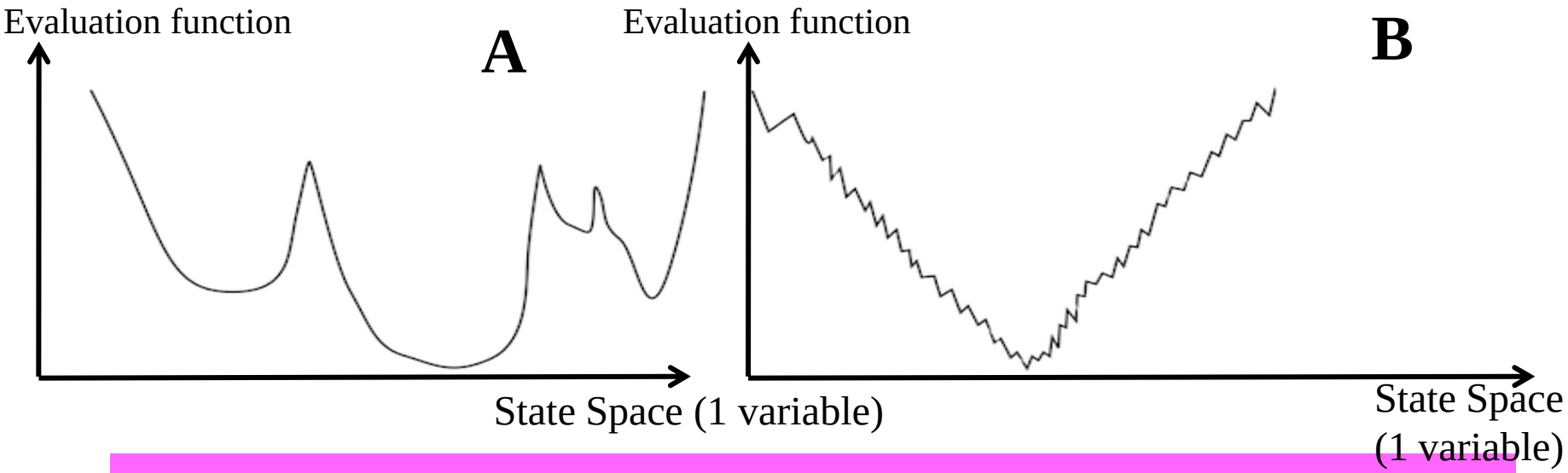
Greedy descent with random restart best on B

Greedy descent with random steps best on B

Greedy descent with random restart best on A

equivalent

Which randomized method would work best in each of the these two search spaces?



Greedy descent with random steps best on B

Greedy descent with random restart best on A

- But these examples are simplified extreme cases for illustration
  - in practice, you don't know what your search space looks like

- Usually integrating both kinds of randomization works best

Random Steps (Walk)

Let's assume that neighbors are generated as

- assignments that differ in one variable's value

How many neighbors there are given n variables with domains with d values?

$n(d-1)$

One strategy to add randomness to the selection variable-value pair. Sometimes choose the pair

1. According to the scoring function
2. A random one

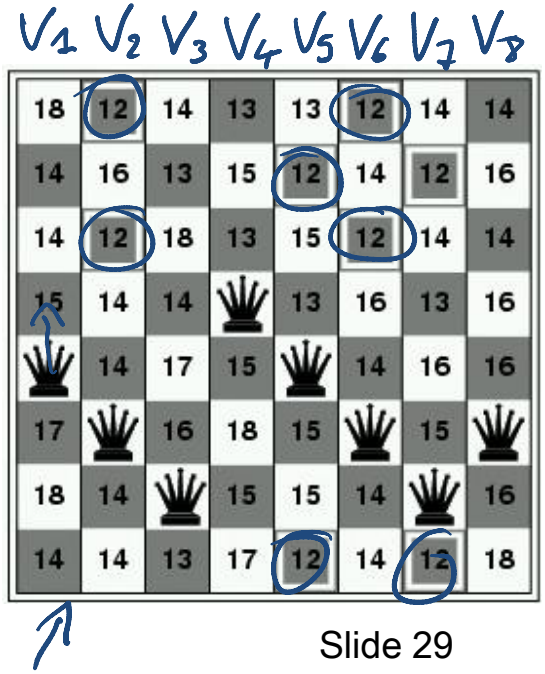
E.G in 8-queen

- How many neighbors?
- 1. choose one of the circled ones

  2 choose randomly one of the 56

$8 \cdot 7 = 56$ (8 values, 8 variables)

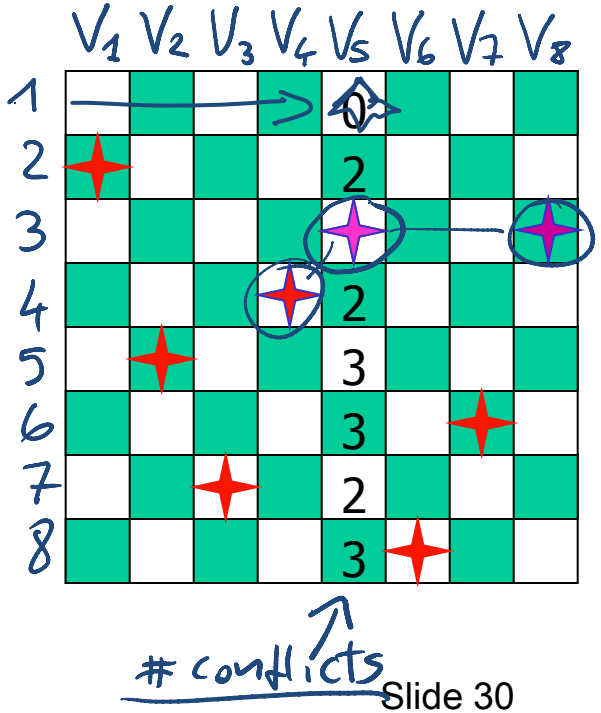
# of conflicts



Random Steps (Walk): two-step

Another strategy: select a variable first, then a value:

- Sometimes select variable:
  1. that participates in the largest number of conflicts.
  2. at random, any variable that participates in some conflict.
  3. at random
- Sometimes choose value
  a) That minimizes # of conflicts
  b) at random



Aispace

2 a: Greedy Descent with Min-Conflict Heuristic

Successful application of SLS

- **Scheduling of Hubble Space Telescope**: **reducing time** to schedule 3 weeks of observations:

from one week to around 10 sec.

Example: SLS for RNA secondary structure design

RNA strand made up of four bases: cytosine (C), guanine (G), adenine (A), and uracil (U)

2D/3D structure RNA strand folds into is important for its function

Predicting structure for a strand is "easy": $O(n^3)$

But what if we want a strand that folds into a certain structure?

- Local search over strands
  - ✓ Search for one that folds into the right structure
- Evaluation function for a strand
  - ✓ Run $O(n^3)$ prediction algorithm
  - ✓ Evaluate how different the result is from our target structure
  - ✓ Only defined implicitly, but can be evaluated by running the prediction algorithm

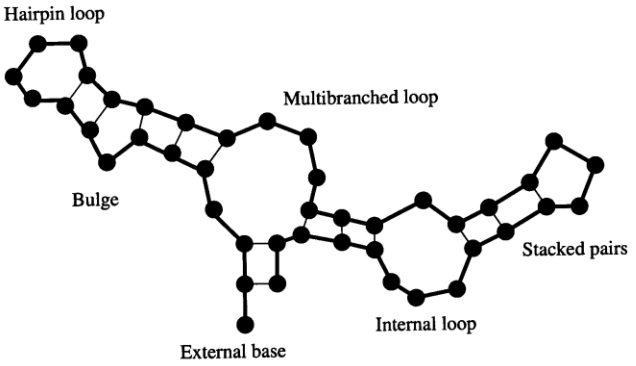
RNA strand

GUCCCAUAGGAUGUCCCAUAGGA

Easy

Hard

Secondary structure



Best algorithm to date: Local search algorithm RNA-SSD developed at UBC [Andronescu, Fejes, Hutter, Condon, and Hoos, Journal of Molecular Biology, 2004]

CSP/logic: formal verification

Hardware verification
(e.g., IBM)

Software verification
(small to medium programs)

Most progress in the last 10 years based on:
Encodings into propositional satisfiability (SAT)

(Stochastic) Local search advantage: Online setting

- **When the problem can change** (particularly important in scheduling)
- **E.g., schedule for airline:** thousands of flights and thousands of personnel assignment
  - Storm can render the schedule infeasible
- **Goal:** Repair with minimum number of changes
- This can be easily done with a local search starting form the current schedule
- Other techniques usually:
  - require more time
  - might find solution requiring many more changes

SLS limitations

- **Typically no guarantee to find a solution even if one exists**
  - SLS algorithms can sometimes stagnate
    - ✓ Get caught in one region of the search space and never terminate
  - Very hard to analyze theoretically

- **Not able to show that no solution exists**
  - SLS simply won't terminate
  - You don't know whether the problem is infeasible or the algorithm has stagnated

SLS Advantage: anytime algorithms

- When should the algorithm be stopped ?
  - When a solution is found
    (e.g. no constraint violations)
  - Or when we are out of time: you have to act NOW
  - Anytime algorithm:
    - ✓ maintain the node with best h found so far (the “incumbent”)
    - ✓ given more time, can improve its incumbent

Learning Goals for today's class – part1

You can:

- Implement local search for a CSP.
  - Implement different ways to generate neighbors
  - Implement scoring functions to solve a CSP by local search through either greedy descent or hill-climbing.
- Implement SLS with
  - random steps (1-step, 2-step versions)
  - random restart

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- Local search
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  - **Comparing SLS algorithms**
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30 MINS BREAK (projector off)

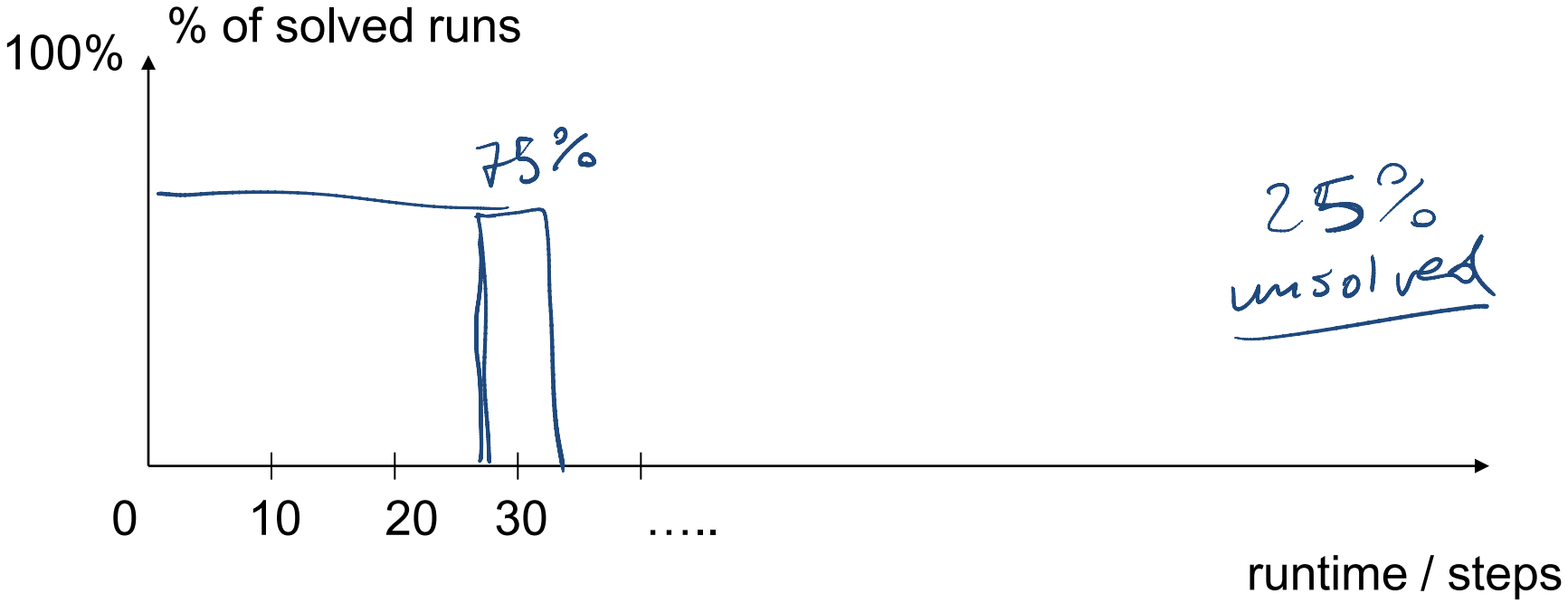
Evaluating SLS algorithms

- SLS algorithms are randomized
  - The time taken until they solve a problem is a random variable
  - It is entirely normal to have runtime variations of 2 orders of magnitude in repeated runs!
    - ✓ E.g. 0.1 seconds in one run, 10 seconds in the next one
    - ✓ On the same problem instance (only difference: random seed)
    - ✓ Sometimes SLS algorithm doesn't even terminate at all: stagnation

- If an SLS algorithm sometimes stagnates, what is its mean runtime (across many runs)?
  - Infinity!
  - In practice, one often counts timeouts as some fixed large value X
  - Still, summary statistics, such as **mean** run time or **median** run time, don't tell the whole story
    - ✓ E.g. would penalize an algorithm that often finds a solution quickly but sometime stagnates

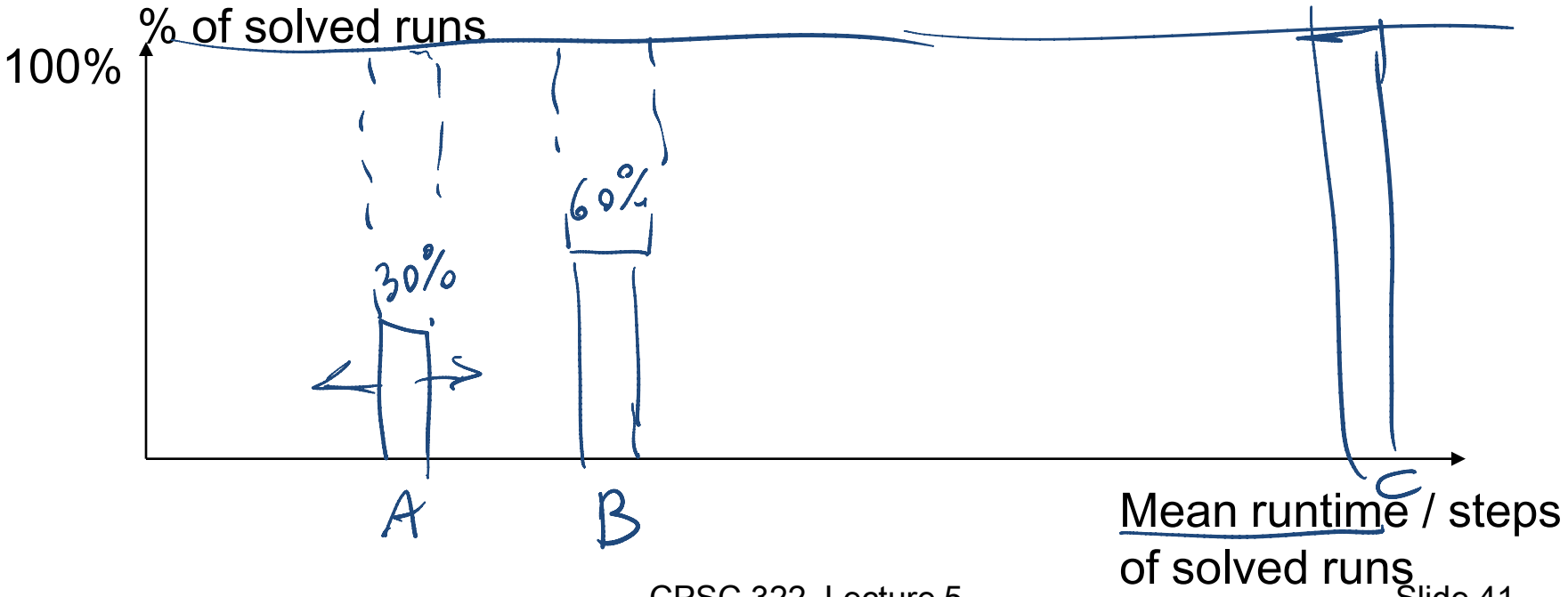
Comparing Stochastic Algorithms: Challenge

- Summary statistics, such as **mean** run time, **median** run time, and **mode** run time don't tell the whole story
  - What is the running time for the runs for which an algorithm ***never*** finishes (infinite? stopping time?)



First attempt….

- How can you compare three algorithms when
  - A. one solves the problem 30% of the time very quickly but doesn't halt for the other 70% of the cases
  - B. one solves 60% of the cases reasonably quickly but doesn't solve the rest
  - C. one solves the problem in 100% of the cases, but slowly?



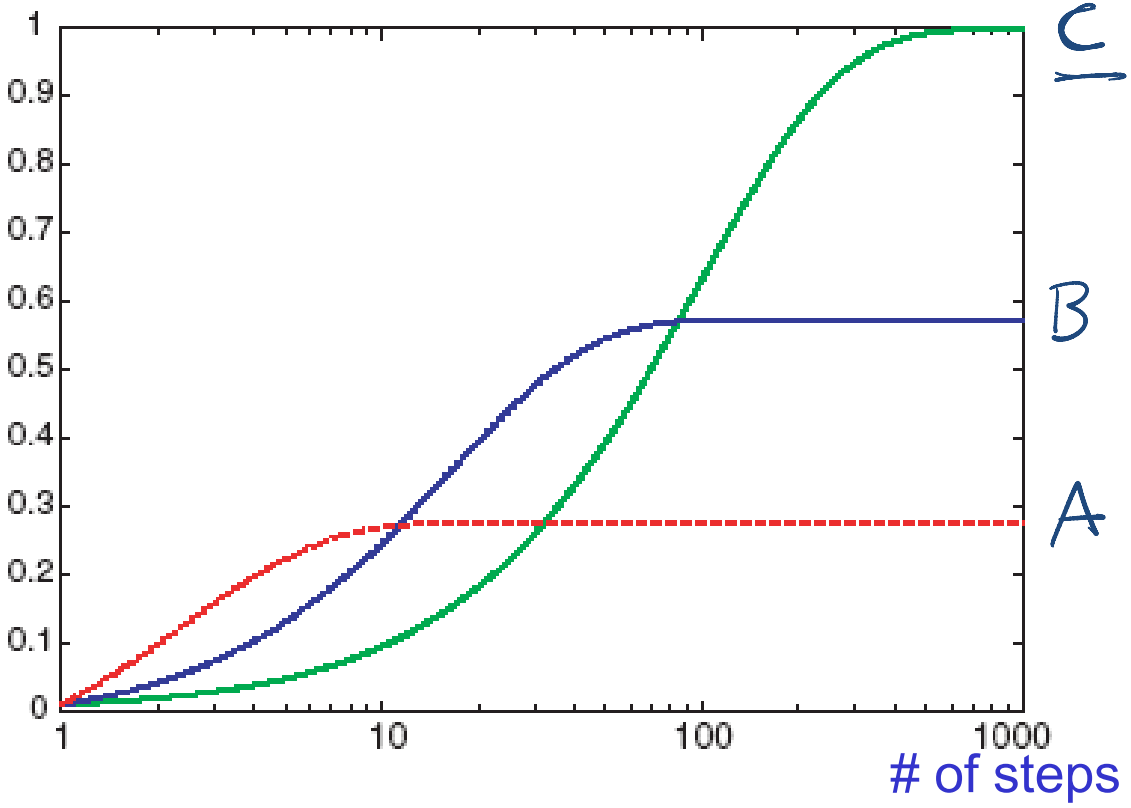
Runtime Distributions are even more effective

Plots runtime (or number of steps) and the proportion (or number) of the runs that are solved within that runtime.

- log scale on the *x* axis is commonly used

Fraction of solved runs, i.e.

P(solved by this # of steps/time)



Comparing runtime distributions

x axis: runtime (or number of steps)
y axis: proportion (or number) of runs solved in that runtime

- Typically use a log scale on the x axis

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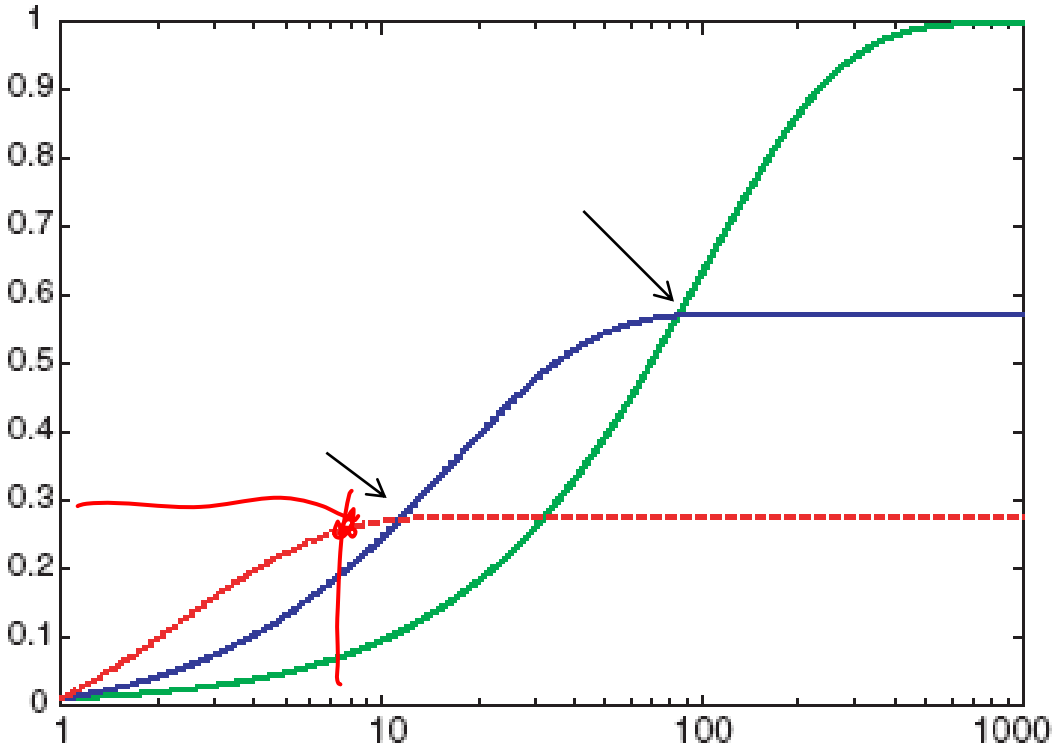

Which algorithm is most likely to solve the problem within 7 steps?

blue red green

Comparing runtime distributions

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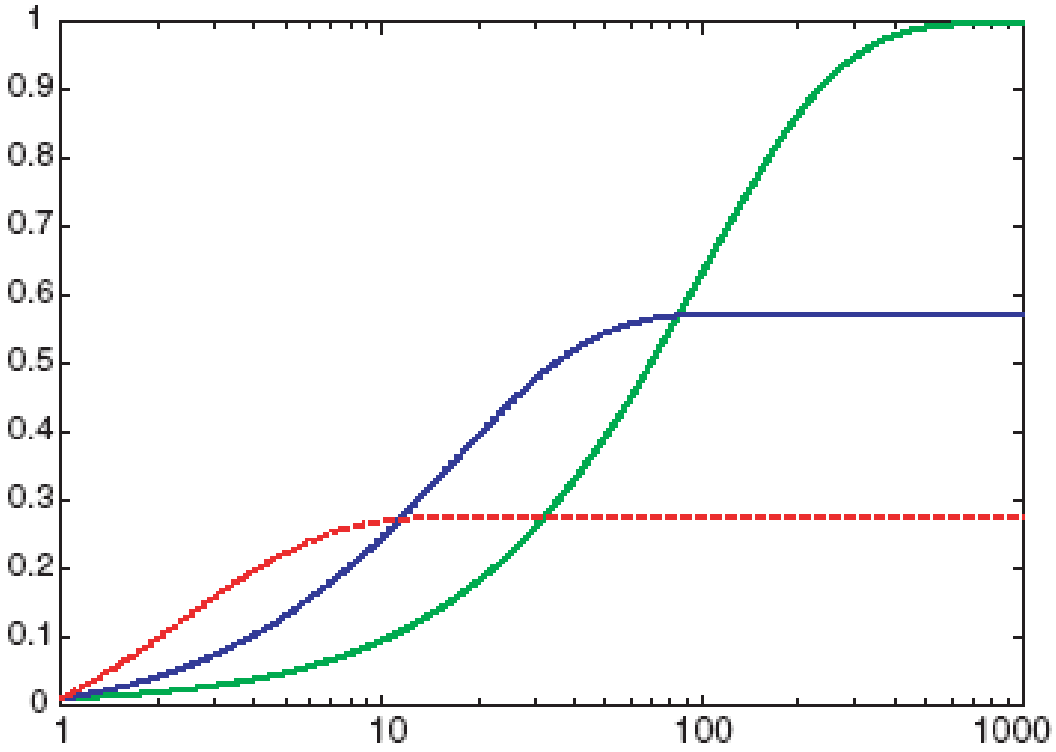


Which algorithm is most likely to solve the problem within 7 steps?

red

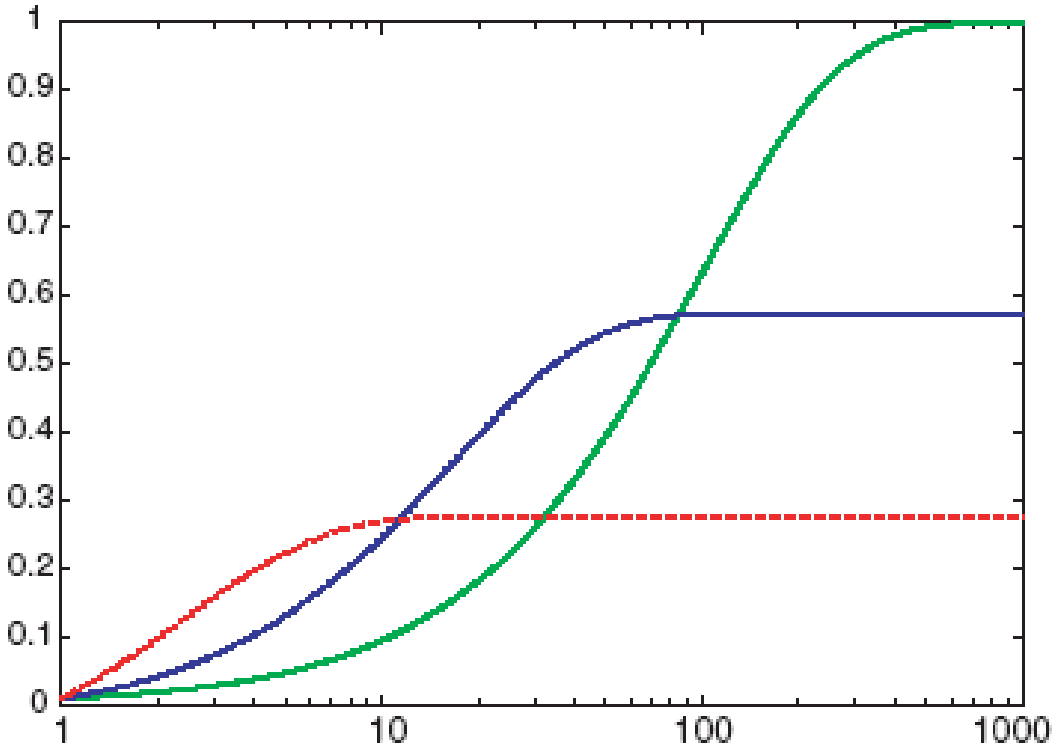
Comparing runtime distributions

- Which algorithm has the best median performance?
  - I.e., which algorithm takes the fewest number of steps to be successful in 50% of the cases?

blue

Fraction of solved runs, i.e.

P(solved by this # of steps/time)



Comparing runtime distributions

- Which algorithm has the best median performance?
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blue red green

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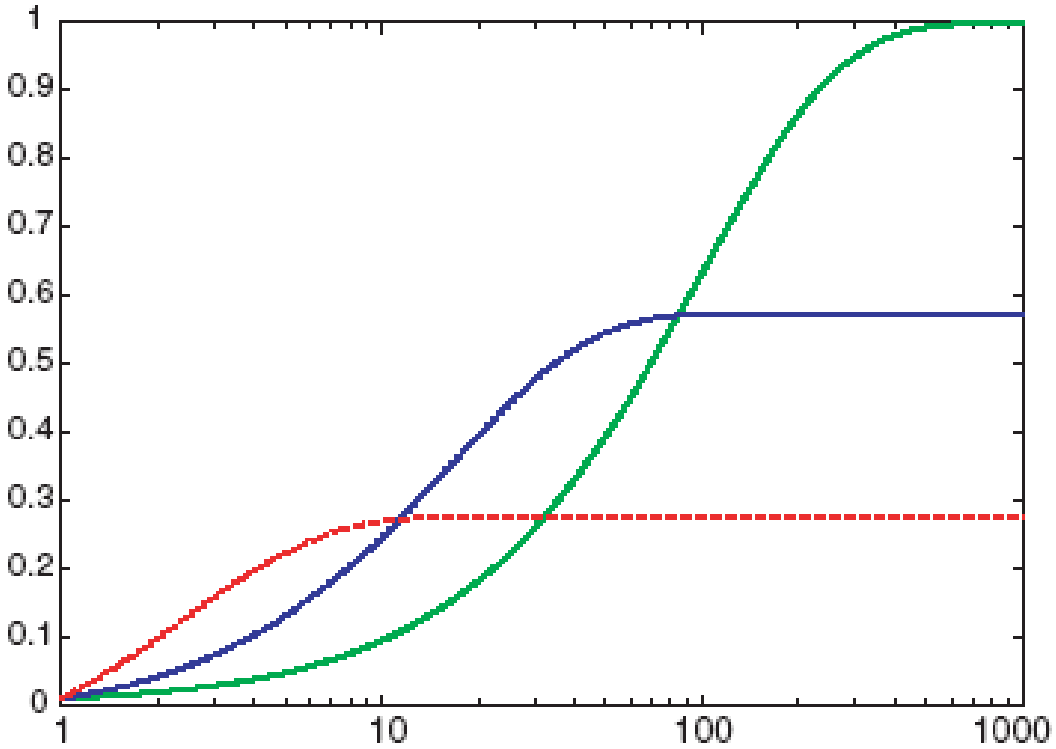

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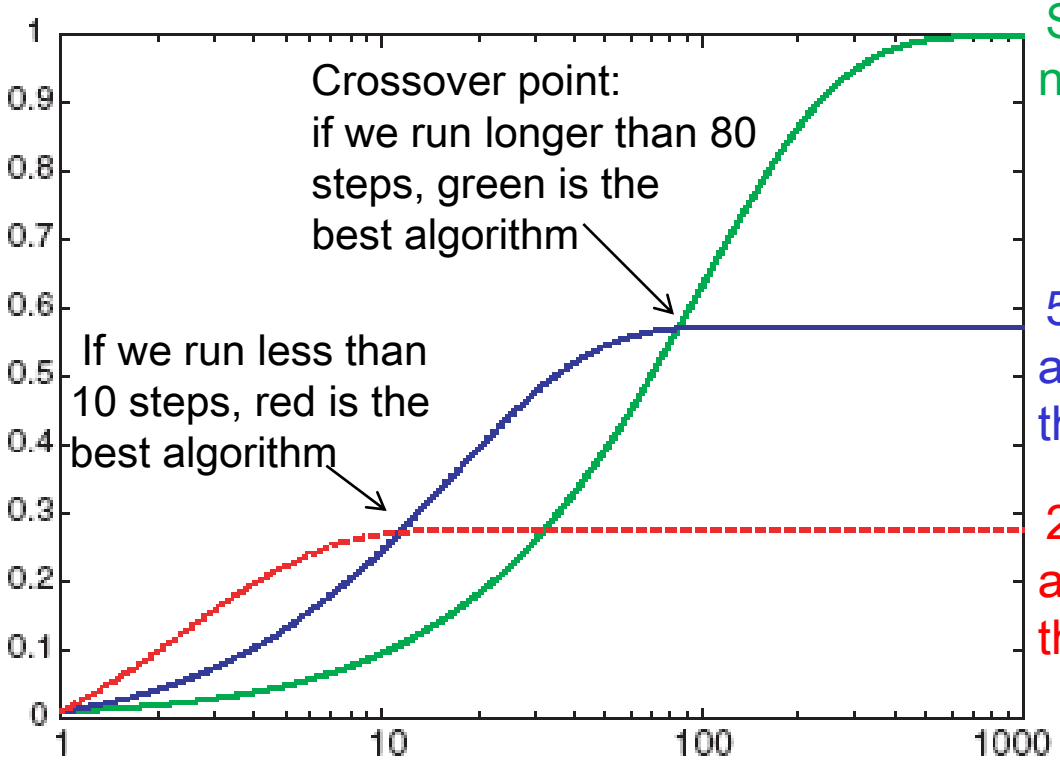


Slow, but does not stagnate

57% solved after 80 steps, then stagnate

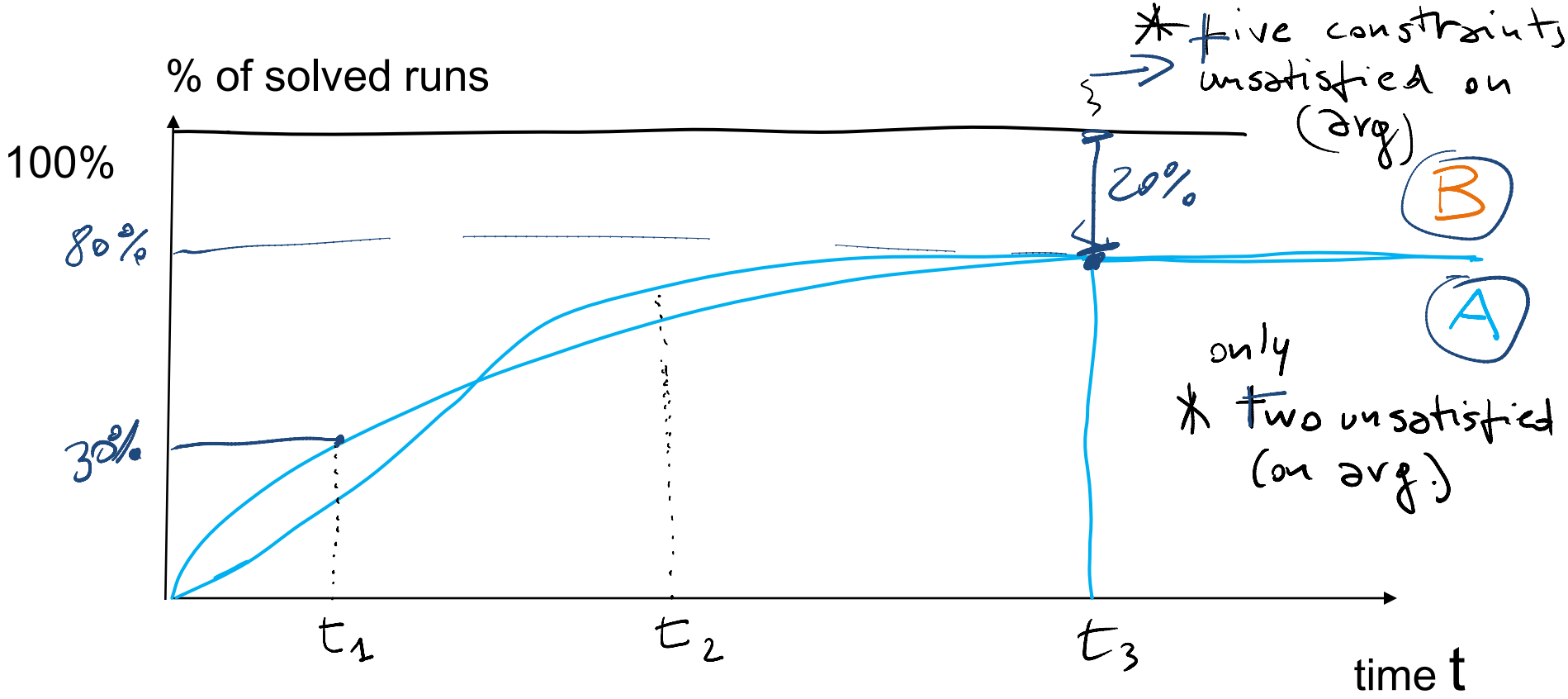
28% solved after 10 steps, then stagnate

Runtime distributions in AIspace

- Let's look at some algorithms and their runtime distributions:
  1. Greedy Descent
  2. Random Sampling
  3. Random Walk
  4. Greedy Descent with random walk

- Simple scheduling problem 2 in AIspace:

Runtime Distributions



Which one would you use if you could wait

- t = t_1 ? A
- t = t_2 ? B
- t = t_3 ? A (because of the quality of the answers on unsolved problems see *)

What are we going to look at in AIspace

When selecting a variable first followed by a value:

- Sometimes select variable:
  1. that participates in the largest number of conflicts.
  2. at random, any variable that participates in some conflict.
  3. at random
- Sometimes choose value
  a) That minimizes # of conflicts
  b) at random

…..

AIspace terminology

Random sampling (keeps restarting) restart

Random walk 3b

Greedy Descent 1a

Greedy Descent Min conflict 2a

Greedy Descent with random walk 2ab

Greedy Descent with random restart

Stochastic Local Search

- **Key Idea:** combine greedily improving moves with randomization
  - As well as improving steps we can allow a "small probability" of:
    - Random steps: move to a random neighbor.
    - Random restart: reassign random values to all variables.
  - Always keep best solution found so far
  - Stop when
    - Solution is found (in vanilla CSP ……)
    - Run out of time (return best solution so far)

Lecture Overview

- Local search
  - Constrained Optimization
  - Greedy Descent / Hill Climbing: Problems
- Stochastic Local Search (SLS)
  - Comparing SLS algorithms
  - SLS variants
    - ✓Tabu lists
    - ✓Simulated Annealing
  - Population Based
    - ✓Beam search
    - ✓Genetic Algorithms

Tabu lists

- To avoid search to
  - Immediately going back to previously visited candidate
  - To prevent cycling

- Maintain a tabu list of the k last nodes visited.
  - Don't visit a poss. world that is already on the **tabu list**.

- Cost of this method depends on…. k

Simulated Annealing

- **Key idea:** Change the degree of randomness….

- Annealing: a metallurgical process where metals are hardened by being slowly cooled.
  - Analogy: start with a high ``temperature'': a high tendency to take random steps
  - Over time, cool down: more likely to follow the scoring function
- Temperature reduces over time, according to an annealing schedule

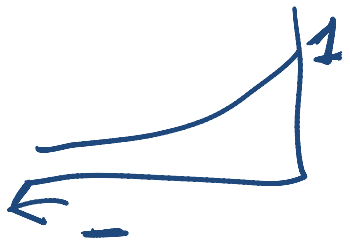
Simulated Annealing: algorithm

Here's how it works (for maximizing):

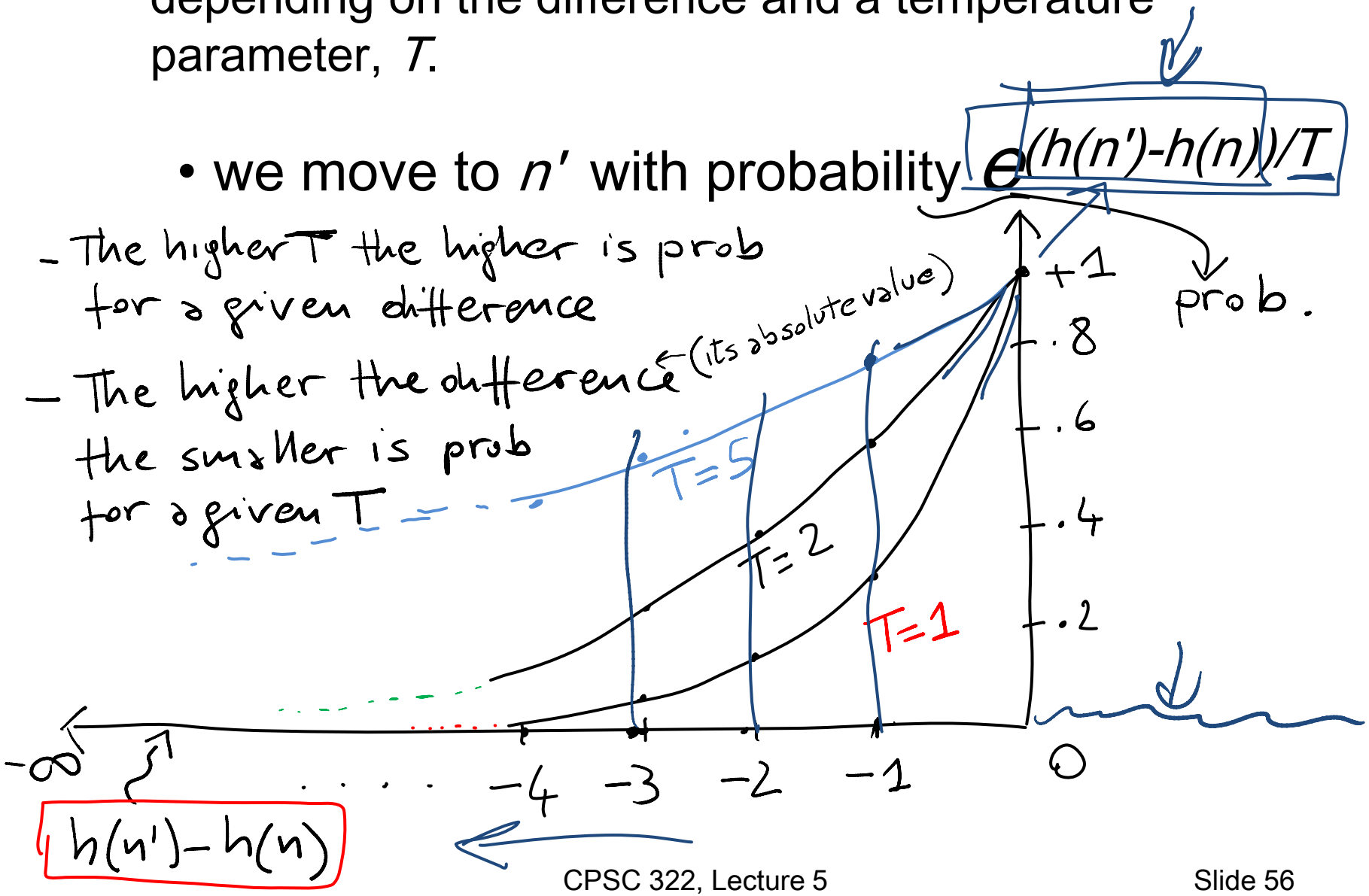
- You are in node n. Pick a variable at random and a new value at random. You generate n'
- If it is an improvement i.e., $h(n') \geq h(n)$, adopt it.
- If it isn't an improvement, adopt it probabilistically depending on the difference and a temperature parameter, T.
  - we move to n' with probability $e^{(h(n')-h(n))/T}$

$h(n') < h(n)$; $h(n') - h(n) < 0$

see next slide



- If it isn't an improvement, adopt it probabilistically depending on the difference and a temperature parameter, *T*.
  - we move to *n'* with probability $e^{(h(n')-h(n))/T}$



Properties of simulated annealing search

One can prove: If T decreases slowly enough, then simulated annealing search will find a global optimum with probability approaching 1

Widely used in VLSI layout, airline scheduling, etc.

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  - Comparing SLS algorithms
  - SLS variants
    - ✓Tabu lists
    - ✓Simulated Annealing
  - **Population Based**
    - ✓Beam search
    - ✓Genetic Algorithms

Population Based SLS

Often we have more memory than the one required for current node (+ best so far + tabu list)

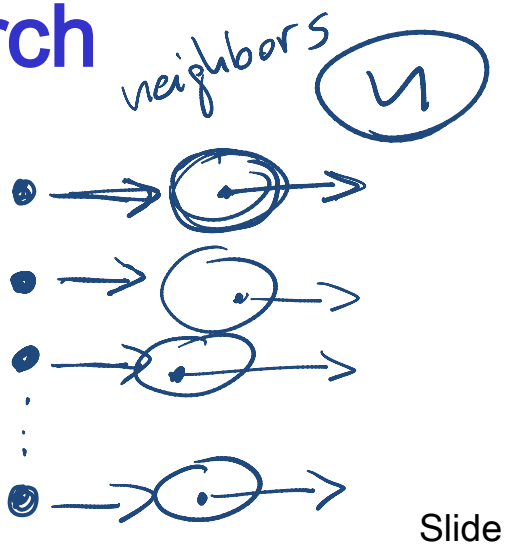
Key Idea: maintain a population of k individuals

- At every stage, update your population.
- Whenever one individual is a solution, report it.

Simplest strategy: Parallel Search

- All searches are independent
- Like k restarts

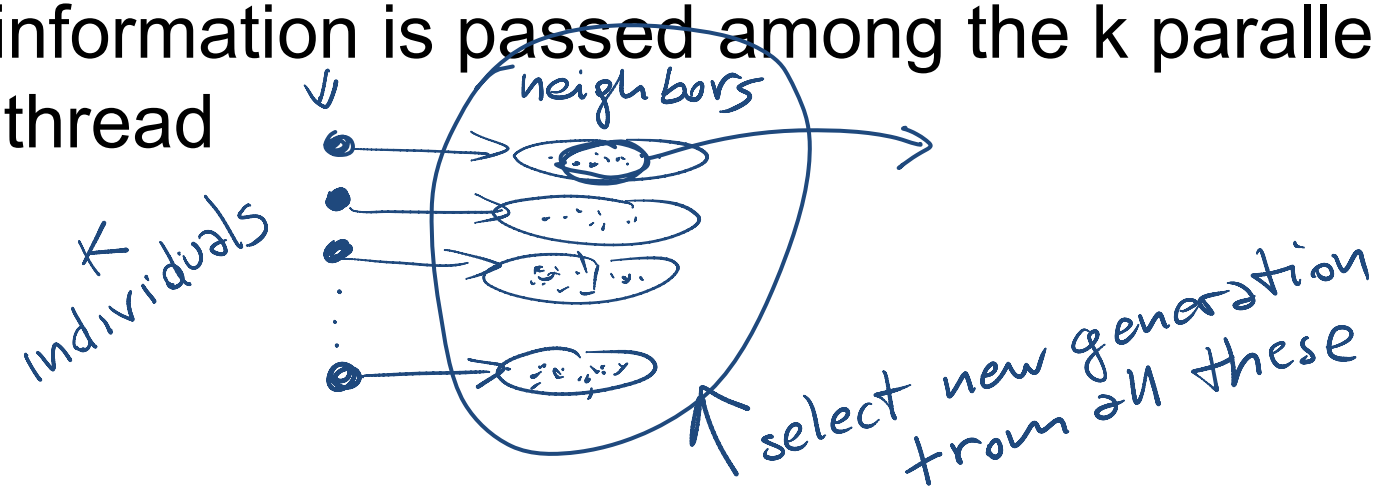
but more memory :(
no reasons to use it!



Population Based SLS: Beam Search

Non Stochastic

- Like parallel search, with *k* individuals, but you choose the *k* best out of all of the neighbors.
- Useful information is passed among the k parallel search thread



- **Troublesome case:** If one individual generates several good neighbors and the other k-1 all generate bad successors…. the next generation will comprise very similar individuals :(

Population Based SLS: Stochastic Beam Search

- **Non Stochastic** Beam Search may suffer from lack of diversity among the k individual (just a more expensive hill climbing)
- **Stochastic** version alleviates this problem:
  - Selects the k individuals at random
  - But probability of selection proportional to their value (according to scoring function)

m neighbors $\{n_1 \dots n_m\}$

h: scoring function

$$\text{Probability of selecting } (n_J) = \frac{h(n_J)}{\sum_i h(n_i)}$$

Stochastic Beam Search: Advantages

- It **maintains diversity** in the population.
- **Biological metaphor** (asexual reproduction):
  - ✓each individual generates "mutated" copies of itself (its neighbors)
  - ✓The scoring function value reflects the fitness of the individual
  - ✓the higher the fitness the more likely the individual will survive (i.e., the neighbor will be in the next generation)

Population Based SLS: Genetic Algorithms

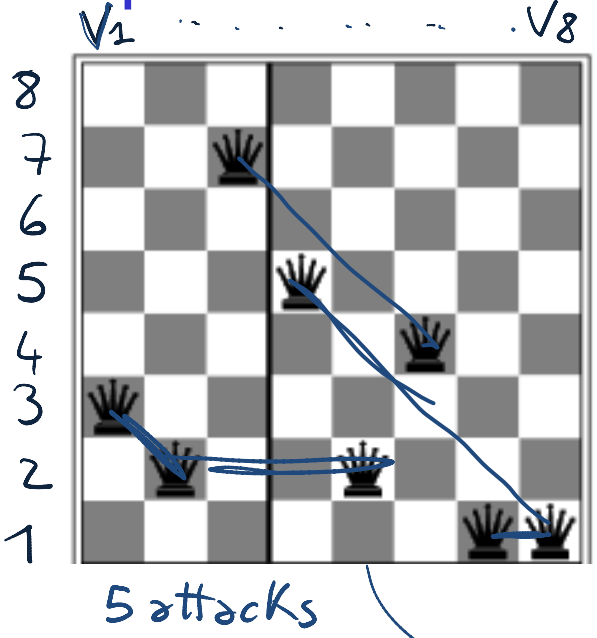
- Start with *k* randomly generated individuals (population)
- An individual is represented as a string over a finite alphabet (often a string of 0s and 1s)
- A successor is generated by combining two parent individuals (loosely analogous to how DNA is spliced in sexual reproduction)
- Evaluation/Scoring function (fitness function). Higher values for better individuals.
- Produce the next generation of individuals by selection, crossover, and mutation

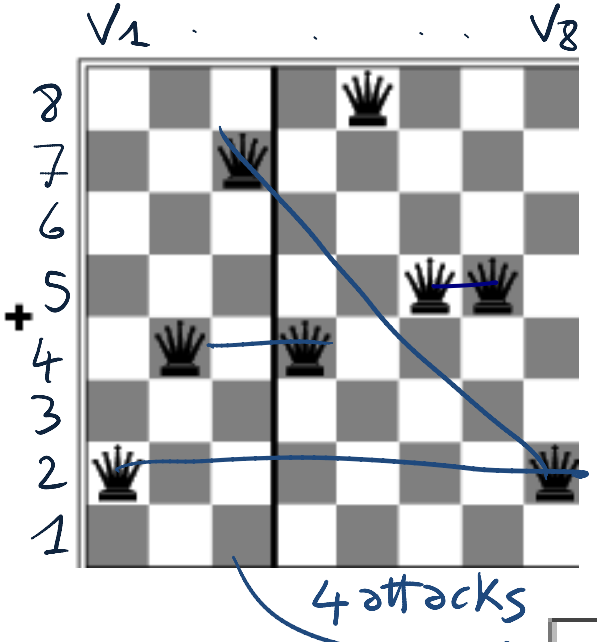
Genetic algorithms: Example 8-queen

Representation and fitness function

of queen pairs possibly attacking each other

$\frac{8 \cdot 7}{2} = 28$





State: string over finite alphabet

24748552

32752411

Fitness function: higher value better states.

queen pairs not attacking each other

28 - 4

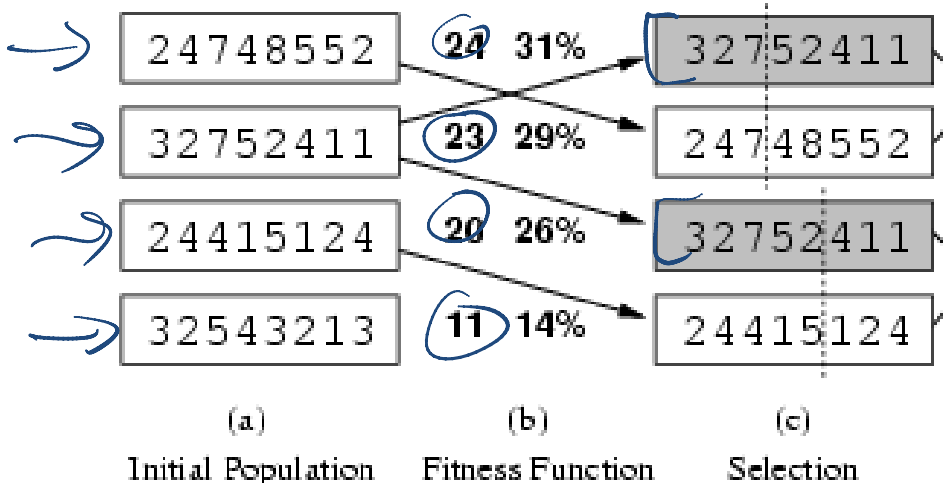
24

23

(28 - 5)

Genetic algorithms: Example

Selection: common strategy, probability of being chosen for reproduction is directly proportional to fitness score



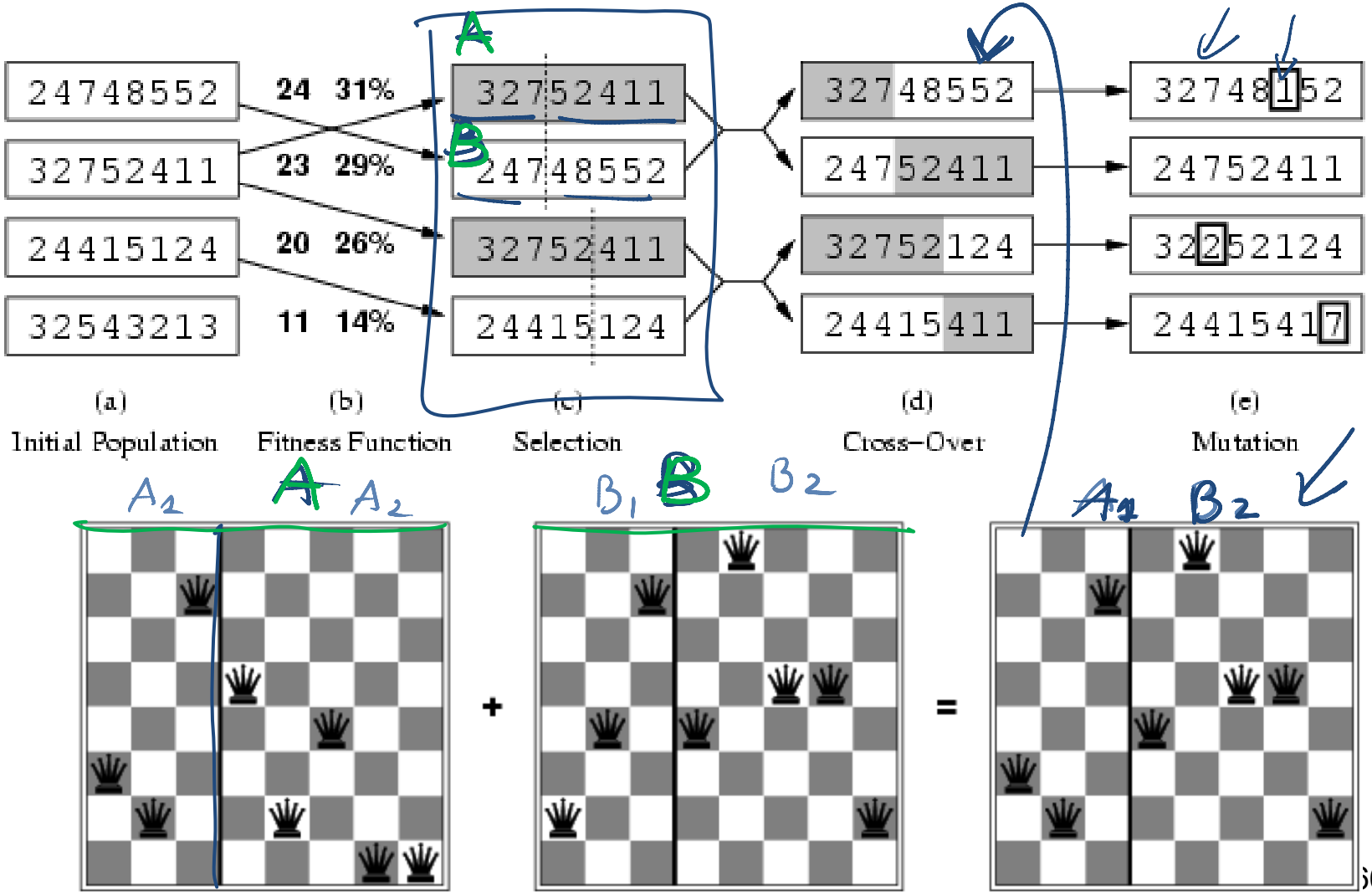
24/(24+23+20+11) = 31%

23/(24+23+20+11) = 29% etc

same as Beam Search

Genetic algorithms: Example

Reproduction: cross-over and mutation



Genetic Algorithms: Conclusions

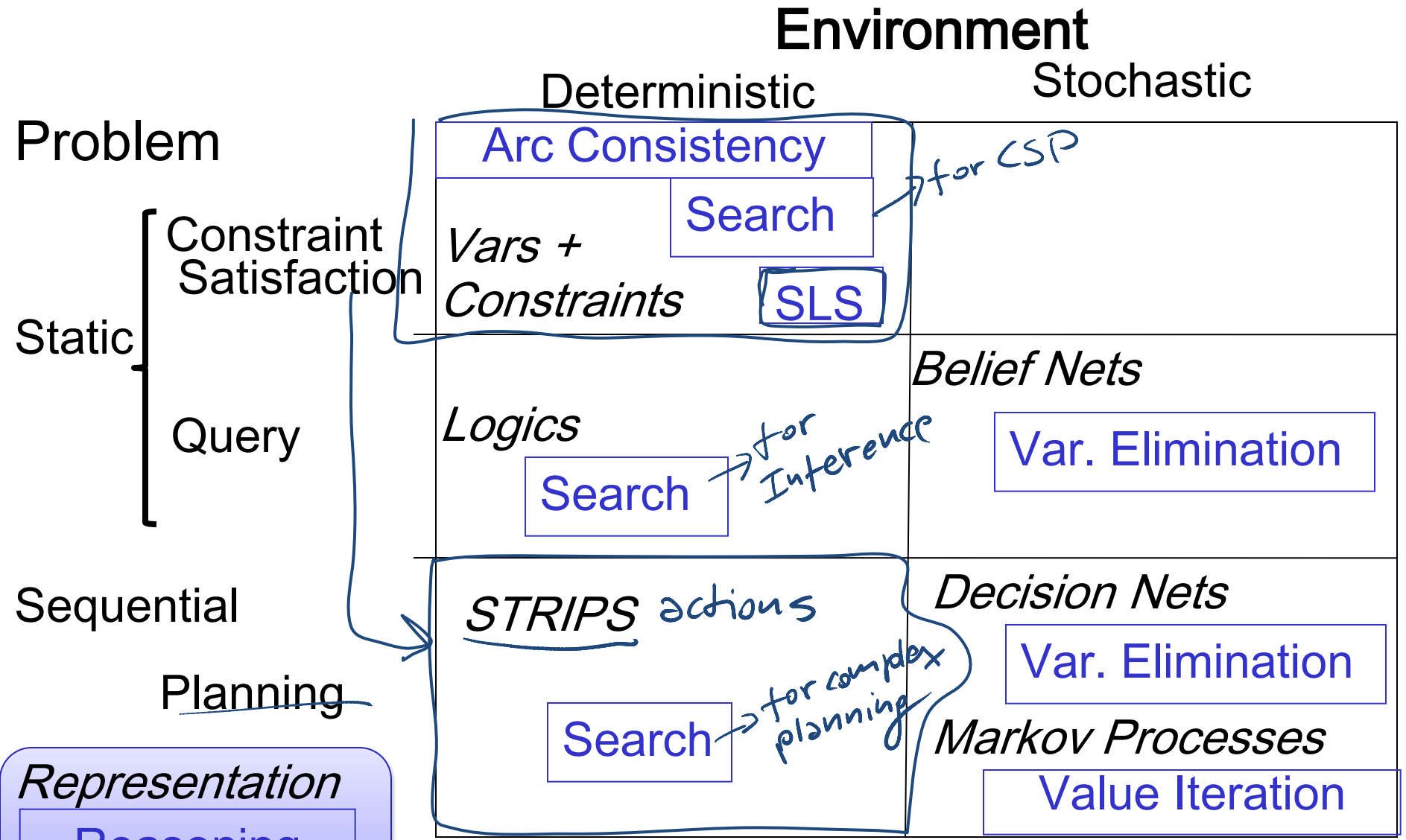
- Their performance is very sensitive to the choice of state representation and fitness function
- **Extremely slow** (not surprising as they are inspired by evolution!)

Learning Goals for today's class part-2

You can:

- Compare SLS algorithms with runtime distributions
- Implement a tabu-list.
- Implement the simulated annealing algorithm
- Implement population based SLS algorithms:
  - Beam Search
  - Genetic Algorithms.
- Explain pros and cons of different SLS algorithms .

Modules we'll cover in this course: R&Rsys



Next class

Posted on WebCT

- Assignment2 on CSPs (due on Thurs!)

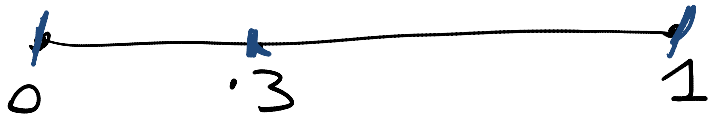
- **Planning** (Chp 8.1-8.2, 8.4): How to select and organize a sequence of actions to achieve a given goal…
- **Start Logics** (Chp 5-1-5.3)

Sampling a discrete probability distribution

e.g. Sim. Annealing. Select n' with probability P

P = .3

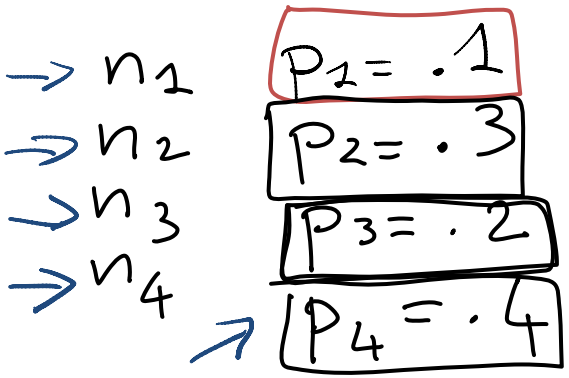
generate random number in [0,1]

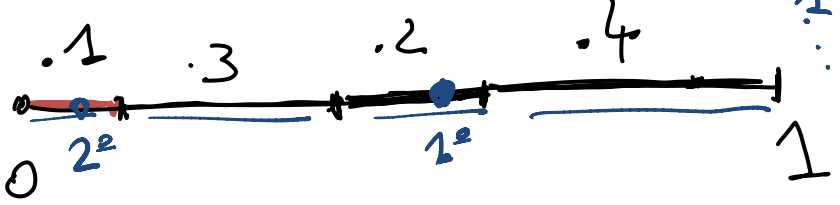


If < .3 accept n'

e.g. Beam Search: Select K individuals. Probability of selection proportional to their value

SAME HERE





n_3 first sample

n_1 second sample

Systematically solving CSPs: Summary

- Build Constraint Network
- Apply Arc Consistency
  - One domain is empty → no solution
  - Each domain has a single value → unique solution
  - Some domains have more than one value → may or may not be a solution
- Apply Depth-First Search with Pruning
- Split the problem in a number of disjoint cases
  - Apply Arc Consistency to each case

CSPs summary

Find a single variable assignment that satisfies all of our constraints (atemporal)

- Systematic Search approach (search space …..?)
  - Constraint network support
    - ✓ inference e.g., Arc Consistency (can tell you if solution does not exist)
    - ✓ Decomposition
  - Heuristic Search (degree, min-remaining)
- (Stochastic) Local Search (search space …..?)
  - Huge search spaces and highly connected constraint network but solutions densely distributed
  - No guarantee to find a solution (if one exists).
  - Unable to show that no solution exists

Local Search: Motivation

- Solving CSPs is NP-hard
  - Search space for many CSPs is huge
  - Exponential in the number of variables
  - Even arc consistency with domain splitting is often not enough

- Alternative: local search
  - use algorithms that search the space locally, rather than systematically
  - Often finds a solution quickly, but are not guaranteed to find a solution if one exists (thus, cannot prove that there is no solution)

Local Search Problem: Definition

Definition: A local search problem consists of a:

CSP: a set of variables, domains for these variables, and constraints on their joint values.

A node in the search space will be a complete assignment to all of the variables.

Neighbour relation: an edge in the search space will exist when the neighbour relation holds between a pair of nodes.

Scoring function: h(n), judges cost of a node (want to minimize)

- E.g. the number of constraints violated in node n.
- E.g. the cost of a state in an optimization context.

Example

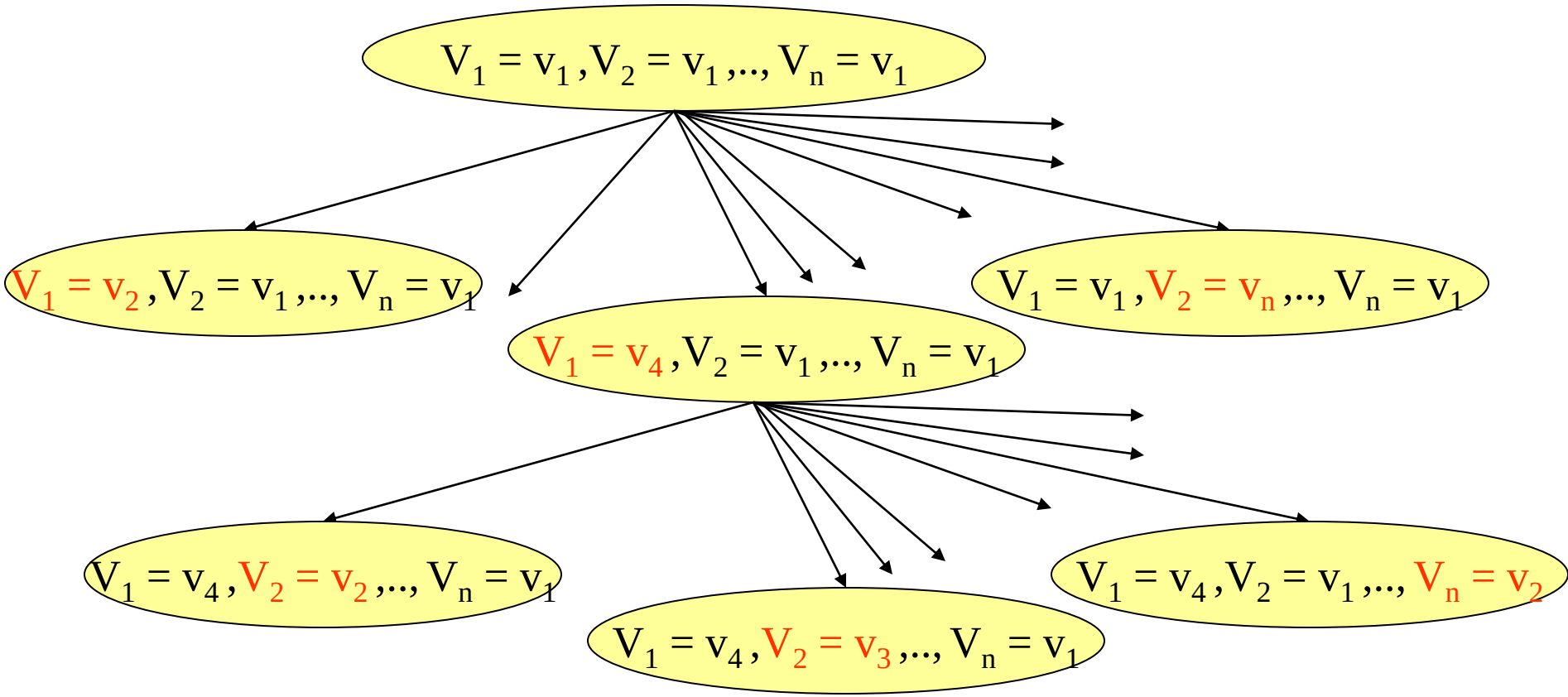
- Given the set of variables $\{V_1 \ldots, V_n\}$, each with domain Dom(V_i)
- The start node is any assignment $\{V_1 / v_1, \ldots, V_n / v_n\}$.

- The neighbors of node with assignment

  $A = \{V_1 / v_1, \ldots, V_n / v_n\}$

  are nodes with assignments that differ from A for one value only

Search Space



- Only the current node is kept in memory at each step.
- Very different from the systematic tree search approaches we have seen so far!
- Local search does NOT backtrack!