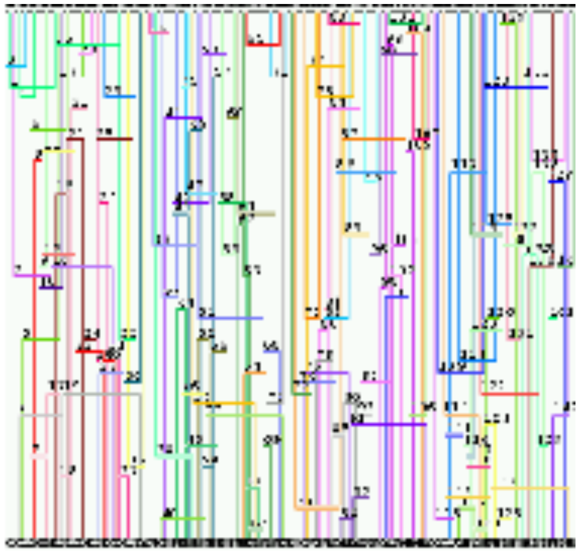
Iterative Improvement Search

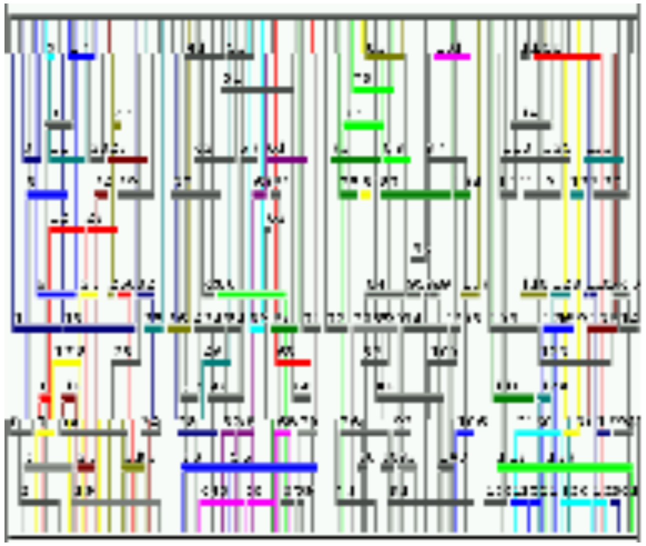
Hill Climbing, Simulated Annealing, WALKSAT, and Genetic Algorithms

Andrew W. Moore
Professor
School of Computer Science
Carnegie Mellon University
www.cs.cmu.edu/~awm
awm@cs.cmu.edu
412-268-7599

Example Problems

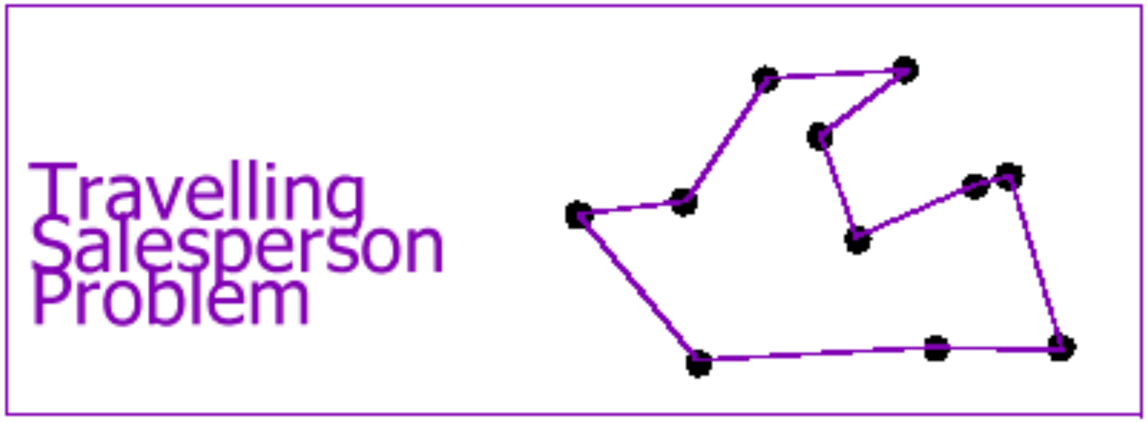


Channel Routing



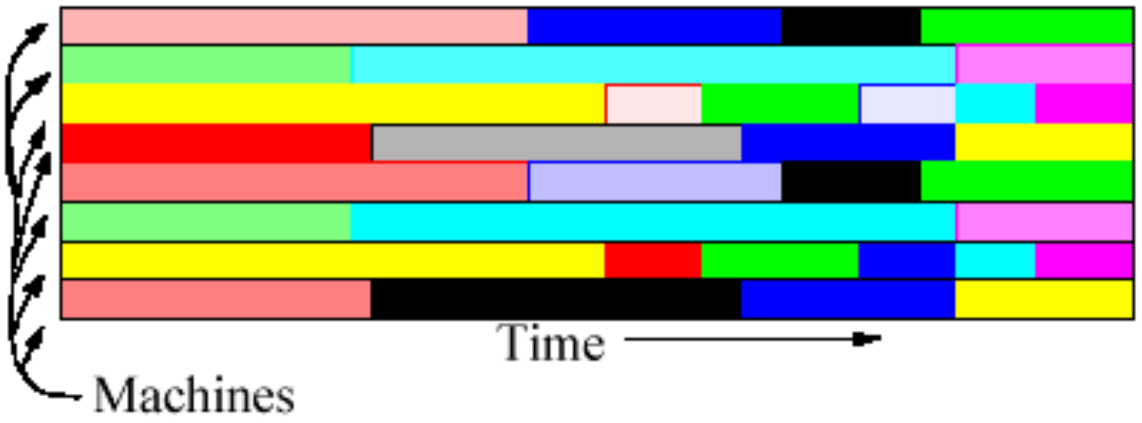
Lots of Chip Real-estate

Same connectivity, much less space



Example Problems

Least cost, constrained, schedule



Also:

parking lot layout, product design, aero-dynamic design, "Million Queens" problem, radiotherapy treatment planning, …

Boolean SATisfiability

$A \vee \neg B \vee C$

$\neg A \vee C \vee D$

$B \vee D \vee \neg E$

$\neg C \vee \neg D \vee \neg E$

$\neg A \vee \neg C \vee E$

(2000 variables, 8500 clauses)

Informal characterization

These are problems in which…

- There is some combinatorial structure being optimized.
- There is a cost function: Structure $\rightarrow$ Real, to be optimized, or at least a reasonable solution is to be found.
- (So basic CSP methods only solve part of the problem … they satisfy constraints but don't look for optimal constraint-satisfier.)
- Searching all possible structures is intractable.
- Depth first search approaches are too expensive.
- There's no known algorithm for finding the optimal solution efficiently.
- Very informally, similar solutions have similar costs.

Iterative Improvement

Intuition: consider the configurations to be laid out on the surface of a landscape. We want to find the highest point.

(Unlike other AI search problems like 8-puzzle, we don’t care how we get there.)

“Iterative Improvement” methods:

Start at a random configuration; repeatedly consider various moves; accept some & reject some. When you’re stuck, restart.

We must invent a **moveset** that describes what moves we will consider from any configuration. Let’s invent movesets for out four sample problems.

Hill-climbing

Hill-climbing: Attempt to maximize Eval(X) by moving to the highest configuration in our moveset. If they're all lower, we are stuck at a "local optimum."

```
1. Let X := initial config
2. Let E := Eval(X)
3. Let N = moveset_size(X)
4. For ( i = 0 ; i<N ; i := i+1)
Let $E_i$ := Eval(move(X,i))
5. If all $E_i$'s are $\leq$ E, terminate, return X
6. Else let i* = $\mathrm{argmax}_i\, E_i$
7. X := move(X,i*)
8. E := $E_{i*}$
9. Goto 3
```

(Not the most sophisticated algorithm in the world.)

Hill-climbing Issues

- Trivial to program
- Requires no memory (since no backtracking)
- MoveSet design is critical. This is the real ingenuity – not the decision to use hill-climbing.
- Evaluation function design often critical.
  - Problems: dense local optima or plateaux
- If the number of moves is enormous, the algorithm may be inefficient. What to do?
- If the number of moves is tiny, the algorithm can get stuck easily. What to do?
- It's often cheaper to evaluate an incremental change of a previously evaluated object than to evaluate from scratch. Does hill-climbing permit that?
- What if approximate evaluation is cheaper than accurate evaluation?
- Inner-loop optimization often possible.

Randomized Hill-climbing

```
1. Let X := initial config
2. Let E := Eval(X)
3. Let i = random move from the moveset
4. Let $E_i$ := Eval(move(X,i))
5. If E < $E_i$ then
X := move(X,i)                    E := $E_i$
6. Goto 3 unless bored.
```

What stopping criterion should we use?

Any obvious pros or cons compared with our previous hill climber?

Hill-climbing example: GSAT

$A \vee \neg B \vee C$	1
$\neg A \vee C \vee D$	1
$B \vee D \vee \neg E$	0
$\neg C \vee \neg D \vee \neg E$	1
$\neg A \vee \neg C \vee E$	1

Maximize:
Eval(config) = # of satisfied clauses

Moveset:
flip any 1 variable

Example Configuration:
(1,0,1,0,1)

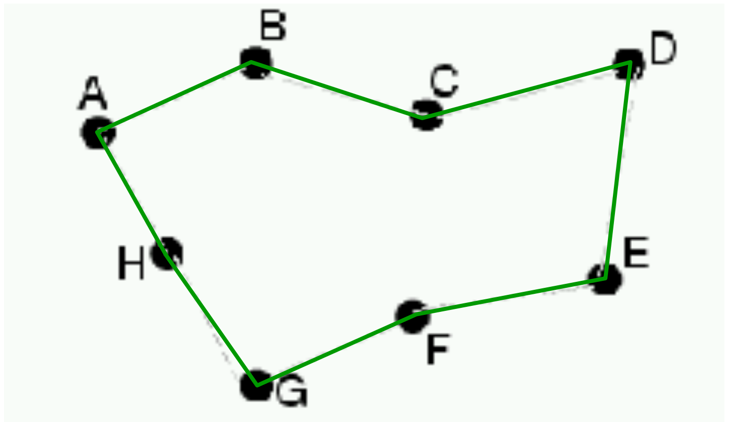
WALKSAT (randomized GSAT):

Pick a random unsatisfied clause;
Consider 3 moves: flipping each variable.
If any improve Eval, accept the best.
If none improve Eval, then 50% of the time, pick the move that is the least bad; 50% of the time, pick a random one.

This is the best known algorithm for satisfying Boolean formulae! [Selman]

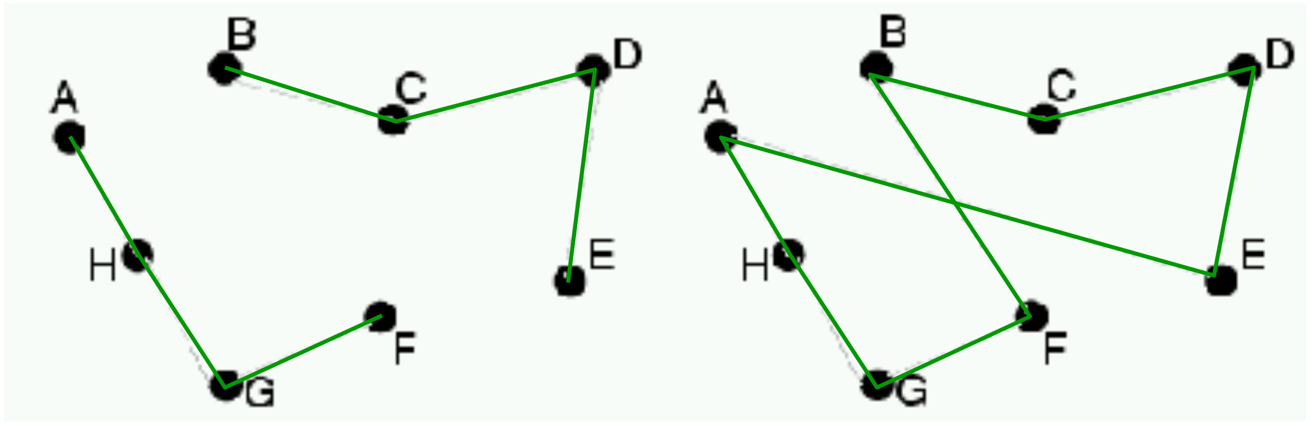
Hill-climbing Example: TSP

Minimize: Eval(Config) = length of tour

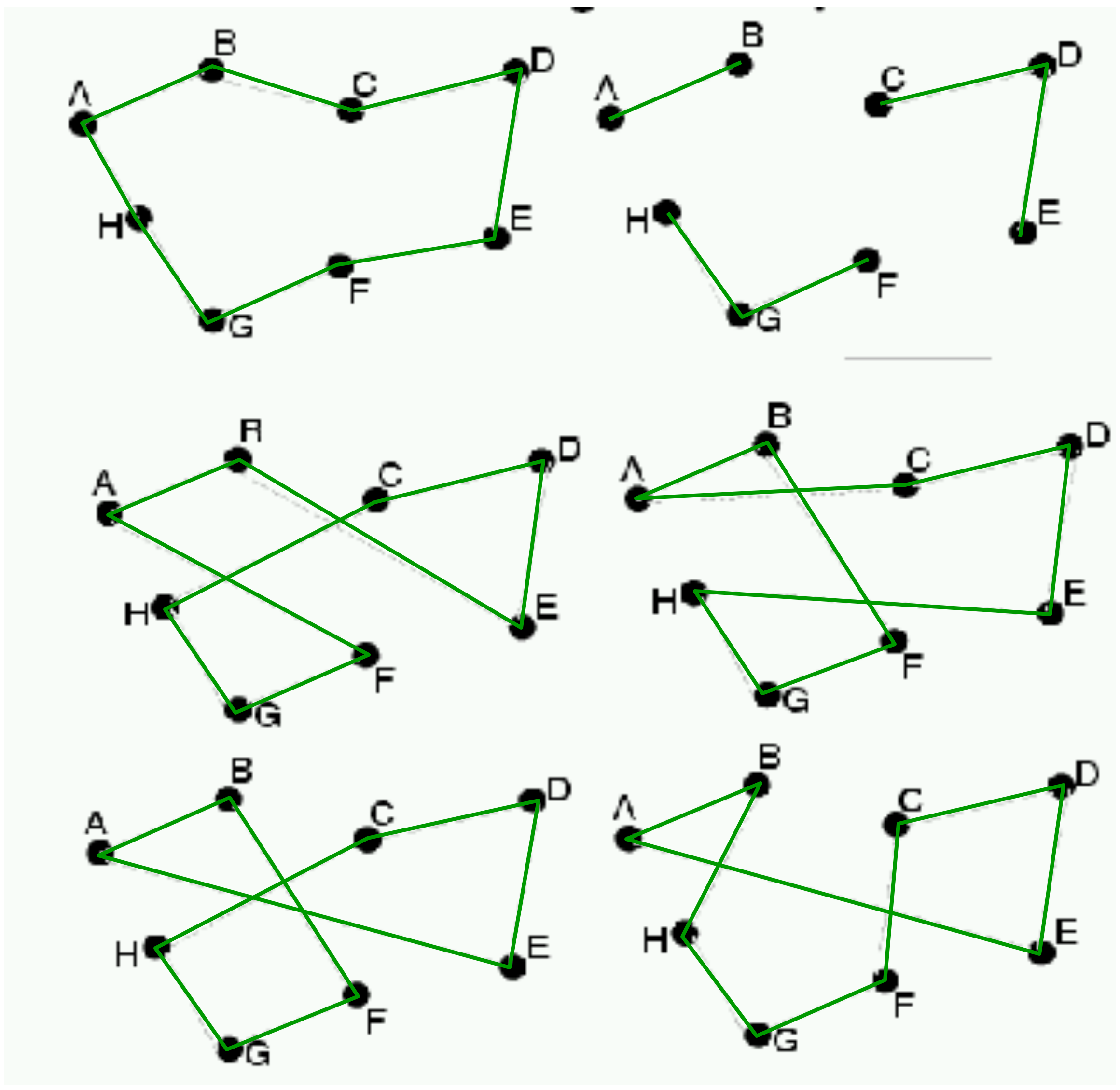


MoveSet: 2-change … k-change

Example: 2-change



3-change Example



Hill-climbing Example: TSP

This class of algorithms for the TSP is usually referred to as k-opt

(MoveSet: 2-change, … *k*-change) for some constant *k*.

Lin showed empirically:

- 3-opt solutions are much better than 2-opt
- 4-opt solutions are not sufficiently better than 3-opt to justify the extra compute time
- A 3-opt tour for the 48-city problem of Held and Karp has about a probability of 0.05 of being optimal (100 random restarts will yield the optimal solution with probability 0.99)
- Further for his particular class of TSP, a 3-opt tour is optimal with probability $2^{-n/10}$ where *n* is a number of cities.

There is no theoretical justification for any of these results.

Simulated Annealing

```
1. Let X := initial config
2. Let E := Eval(X)
3. Let i = random move from the moveset
4. Let $E_i$ := Eval(move(X,i))
5. If E < $E_i$ then
       X := move(X,i)
       E := $E_i$
   Else
       with some probability, accept the move even though things get worse:
       X := move(X,i)
       E := $E_i$
6. Goto 3 unless bored.
```

Simulated Annealing

```
1. Let X := initial config
2. Let E := Eval(X)
3. Let i = random move from the moveset
4. Let $E_i$ := Eval(move(X,i))
5. If E < $E_i$ then
       X := move(X,i)
       E := $E_i$
   Else with some probability, accept the move even though things get worse:
       X := move(X,i)
       E := $E_i$
6. Goto 3 unless bored.
```

This may make the search fall out of mediocre local minima and into better local maxima.

How should we choose the probability of accepting a worsening move?

1. *Idea One.* Probability = 0.1
2. *Idea Two.* Probability decreases with time
3. *Idea Three.* Probability decreases with time, and also as $E – E_i$ increases.

Simulated Annealing

If $E_i >= E$ then definitely accept the change.

If $E_i < E$ then accept the change with probability

$$\mathbf{exp}\,(-(E - E_i)/\mathbf{T}_{\boldsymbol{i}})$$

(called the Boltzman distribution)

…where $\mathbf{T}_{\boldsymbol{i}}$ is a "temperature" parameter that gradually decreases. Typical cooling schedule: $\mathbf{T}_{\boldsymbol{i}} = \mathbf{T}_0 \cdot \boldsymbol{r}^{\boldsymbol{i}}$

High temp: accept all moves (Random Walk)
Low temp: Stochastic Hill-Climbing

When enough iterations have passed without improvement, terminate.

This idea was introduced by Metropolis in 1953. It is "based" on "similarities" and "analogies" with the way that alloys manage to find a nearly global minimum energy level when they are cooled slowly.

Aside: Analogy-based algorithms

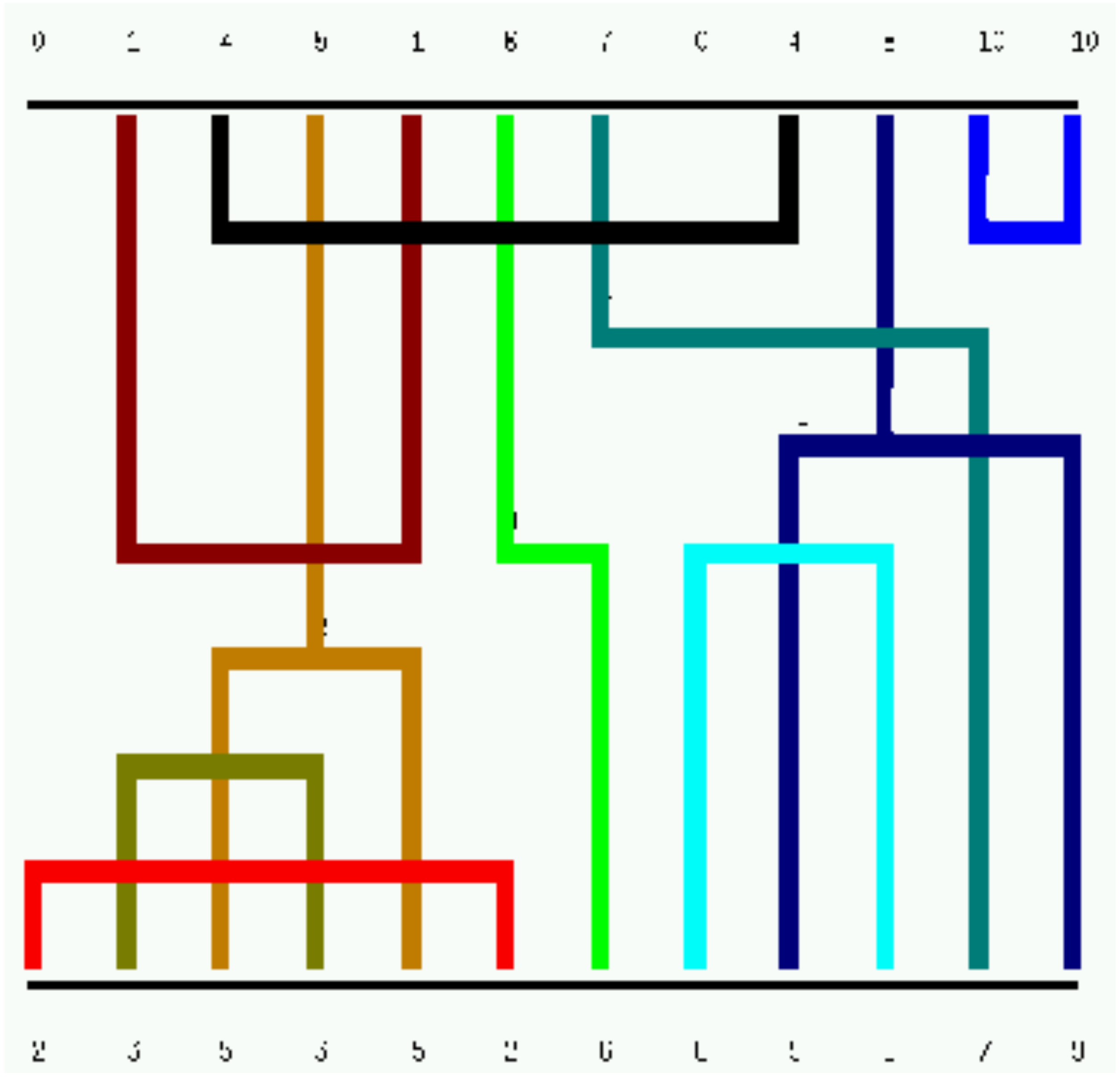
Your lecturer predicts that for any natural phenomenon you can think of, there will be at least one AI research group that will have a combinatorial optimization algorithm “based” on “analogies” and “similarities” with the phenomenon. Here’s the beginning of the list…

- Metal cooling annealing
- Evolution / Co-evolution / Sexual Reproduction
- Thermodynamics
- Societal Markets
- Management Hierarchies
- Ant/Insect Colonies
- Immune System
- Animal Behavior Conditioning
- Neuron / Brain Models
- Hill-climbing (okay, that’s a stretch…)
- Particle Physics
- Inability of Elephants to Play Chess

Simulated Annealing Issues

- MoveSet design is critical. This is the real ingenuity – not the decision to use simulated annealing.
- Evaluation function design often critical.
- Annealing schedule often critical.
- It's often cheaper to evaluate an incremental change of a previously evaluated object than to evaluate from scratch. Does simulated annealing permit that?
- What if approximate evaluation is cheaper than accurate evaluation?
- Inner-loop optimization often possible.

Manhattan Channel Routing

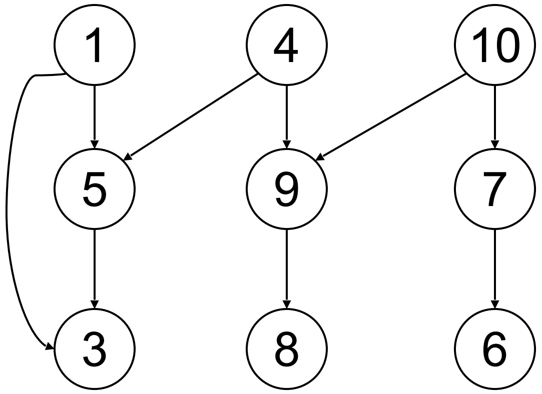


Channel Routing: Moveset

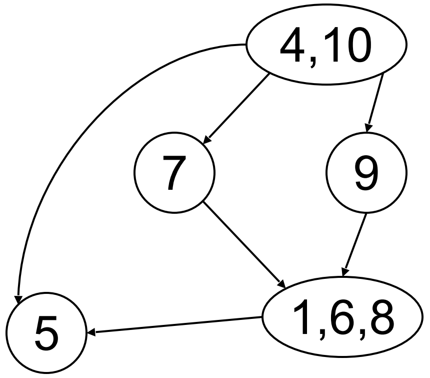
Simple moveset: pick up a wire and move it to another track at random. (Problem: almost all such moves are illegal!)

Fancy moveset: makes search more efficient

Draw vertical constraints in a graph (arrow means “must lie above”)



Packing wires onto the same track = = merging nodes. (The graph must remain acyclic, and you must check horizontal constraints too.)



Channel Routing: Cost Function

“Clearly, the objective function to be minimized is the channel width **w**. However, **w** is too crude a measure of the quality of intermediate solutions. Instead, … the following cost function is used:”

$$\boldsymbol{c} = \boldsymbol{w}^2 + \lambda_{\boldsymbol{p}} \cdot \boldsymbol{p}^2 + \lambda_{\boldsymbol{u}} \cdot \boldsymbol{u}$$

where

p is a lower bound on the size of the constraint graph after future merge operations,

u measures the variance of how tightly the horizontal tracks are packed,

and $\lambda_{\boldsymbol{p}}$ and $\lambda_{\boldsymbol{u}}$ are hand-tweaked constants.

--- Wong, *Simulated Annealing for VLSI Design*

“Modified Lam” schedule

(This is just to give you and idea of how wacky these things can be.)

Idea: dynamically lower and raise temp to meet a target accept rate over time.

Advantages: few parameters to tweak; you know in advance how long the algorithm will run; works well empirically.

SA Discussion

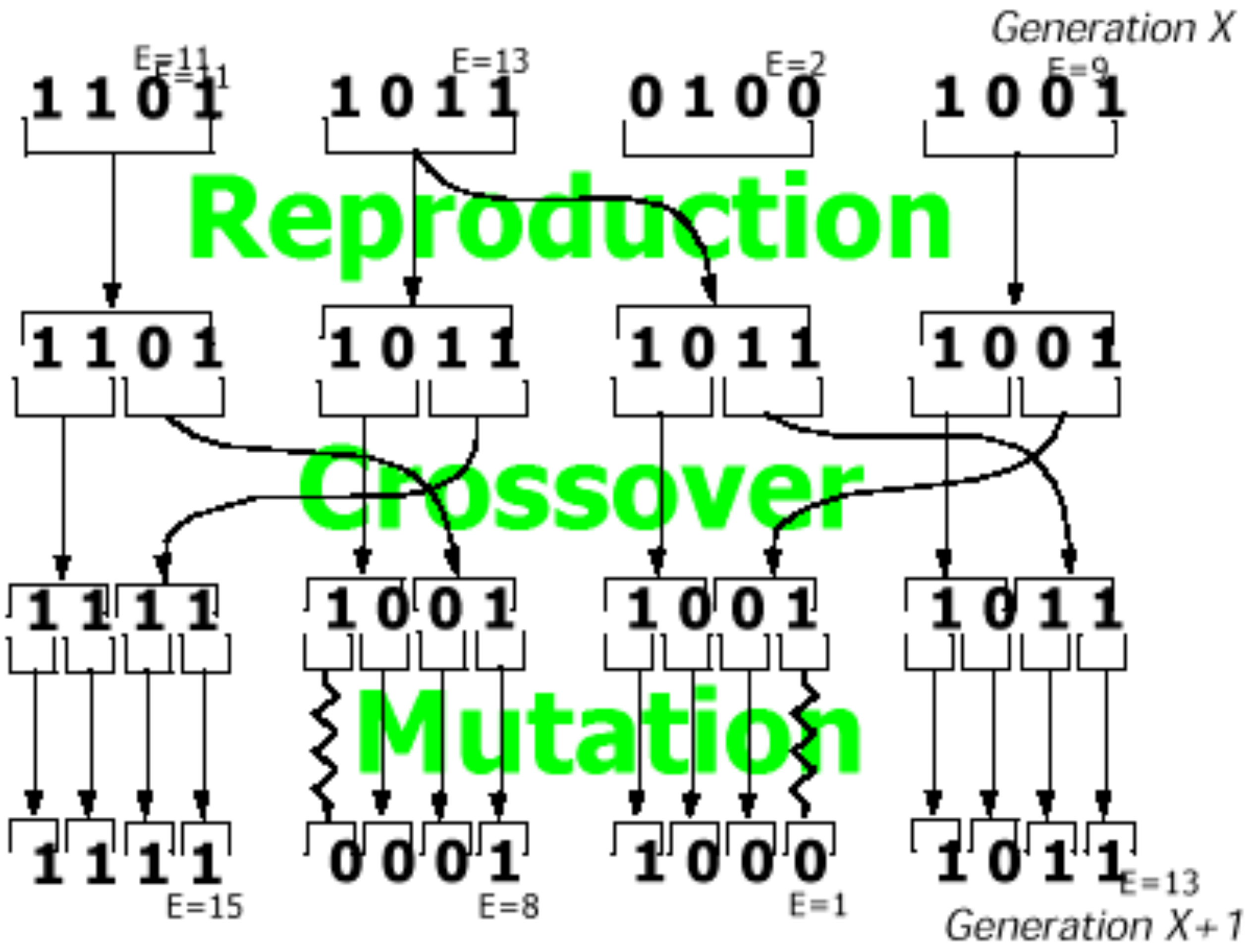
Simulated annealing is sometimes empirically much better at avoiding local minima than hill-climbing. It is a successful, frequently-used, algorithm. Worth putting in your algorithmic toolbox.

Sadly, not much opportunity to say anything formal about it (though there is a proof that with an infinitely slow cooling rate, you'll find the global optimum).

There are mountains of practical, and problem-specific, papers on improvements.

Genetic Algorithms

In the basic GA, objects are coded up (carefully) as binary strings. Goal is to optimize some function of the bit-strings.



(Diagram shamelessly copied from "Dean et al: AI: Theory and Practice".)

Genetic Algorithm

A set of bitstrings. This set is called a Generation. the algorithm produces a new generation from an old generation thusly:

- Let *G* be the current generation of *N* bitstrings.
- For each bitstring (call them b_0, b_1, … b_{N-1}) define

$p_i = \text{Eval}(b_i) / \Sigma_j \text{Eval}(b_j)$.

- Let *G'* be the next generation. Begin with it empty.
- For $k = 0$; $k < N/2$; $k = k+1$
    - Choose two parents each with probability $Prob(Parent = b_i) = p_i$
    - Randomly swap bits in the two parents to obtain two new bitstrings
    - For each bit in turn in the new bitstring, randomly invert it with some low probability
    - Add the two new bitstrings to *G'*

Let your first generation consist of random bitstrings.

GA Issues

- Bitstring representation is critical. This is the real ingenuity – not the decision to use genetic algorithms. *(How to encode TSP?)*
- Evaluation function design often critical. In-laws always critical.
- It's often cheaper to evaluate an incremental change of a previously evaluated object than to evaluate from scratch. Do Genetic Algorithms permit that?
- What if approximate evaluation is cheaper than accurate evaluation?
- Inner-loop optimization often possible.

Numerous twiddles:

- Use rankings not evaluations in creating your p_i parent selection probabilities.
- Cross over contiguous chunks of the string instead of random bits?
- Needn't be bit strings .. could use strings over other finite alphabets.
- Optimize over sentences from a grammar representing functions or programs. Called Genetic Programming.

General Discussion

- Often, the “second best way” to solve a problem.
- But relatively easy to implement. Can save a great deal of programming effort.
- But great care is needed in designing representations and movesets. If someone tells you that SA/Hillclimbing solved their problem, that person is probably not giving enough credit to their own problem-formulation-ability.
- DON’T solve a problem with these methods that could be solved by Linear Programming, A-Star search or Constraint Propagation!
- What if evaluating the objective function is really expensive?

What you should know about Iterative Improvement algs.

- Hill-climbing
- Simulated Annealing
- SAT and Channel Routing domains
- Given a simple problem (e.g. graph coloring from the CSP lectures) be able to give sensible suggestions as to how to code it up for the above algorithms.

References:

Simulated Annealing: See *Numerical Recipes in C*, or for practical details of Modified Lam schedule etc.: Ochotta 1994 Ph.D. thesis, CMU ECE.
Hillclimbing: Discussion in Russell and Norvig.
GSAT, WALKSAT: papers by Bart Selman and Henry Kautz (www.research.att.com)
Channel Routing: Wong et al., *Simulated Annealing for VLSI Design*, Kluwer 1988.