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ARTIFICIAL INTELLIGENCE

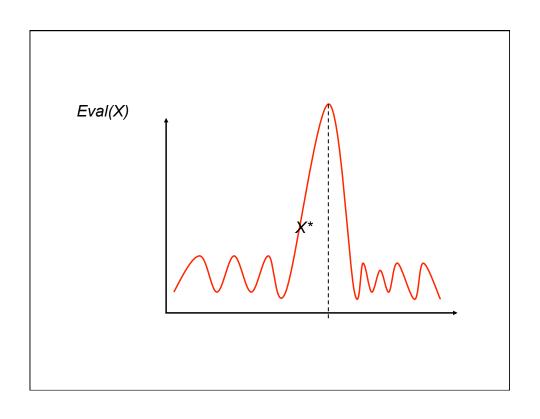
Administration

- Quiz results: very informative!
- Reading: Expected to read in advance of lecture
- Homework: Can use 8 late days, at most 2 per homework
- No laptops or cell phones
 - We expect total participation in class
- Extra credit: Participation through
 - Clickers/question response
 - in-class question/answer
 - Will ask students randomly by name

 please help me with pronounciation!!!

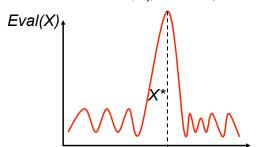
Optimization: Local Search & Stochastic Search

Drew Bagnell
(With thanks to Andrew Moore,
Martial Hebert, Illah Nourbakhsh,
Alexandre Bayen, Matt Zucker,
and many more for slides...)

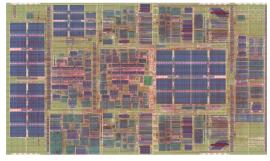


Today's Class of Search Problems

- · Given:
 - A set of states (or configurations) $S = \{X_1..X_M\}$
 - A function that evaluates each configuration:Eval(X)
- · Solve:
 - Find global extremum: Find X^* such that $Eval(X^*)$ is greater than all $Eval(X_i)$ for all possible values of X_i

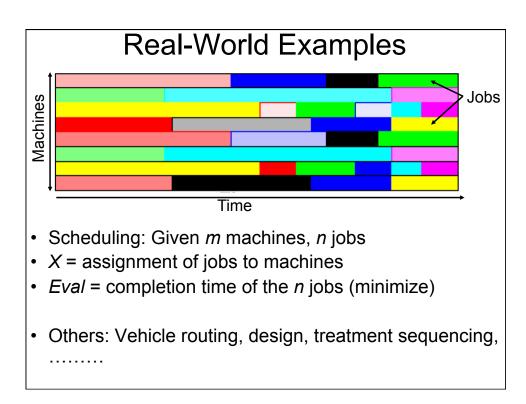


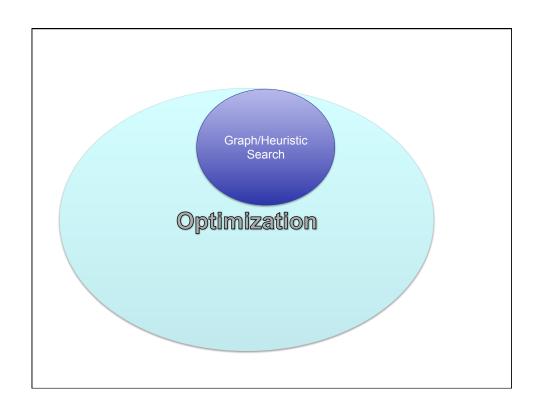
Real-World Examples



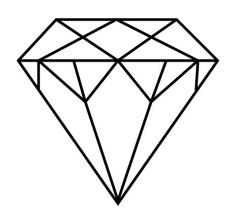
Placement Floorplanning Channel routing Compaction

- VLSI layout:
 - X = placement of components + routing of interconnections
 - Eval = Distance between components + % unused + routing length

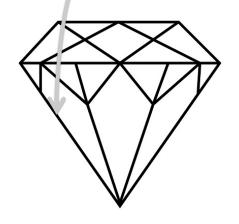






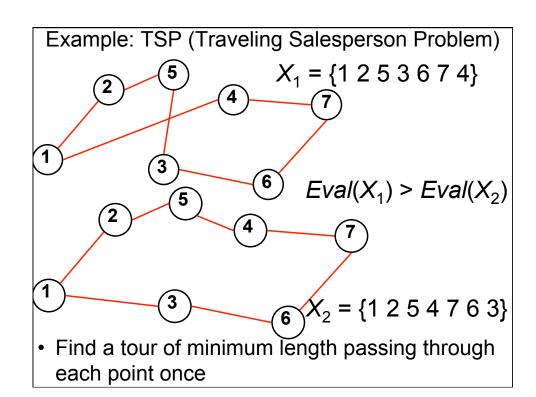


A.I. = Optimization

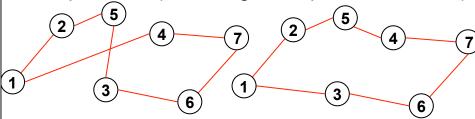


What makes this challenging?

- Problems of particular interest:
 - Set of configurations too large to be enumerated explicitly
 - Computation of Eval(.) may be expensive
 - There is no (known) algorithm for finding the maximum of Eval(.) efficiently
 - Solutions with similar values of Eval(.) are considered equivalent for the problem at hand
 - We do not care how we get to X*, we care only about the description of the configuration X*



Example: TSP (Traveling Salesperson Problem)



$$X_1 = \{1 \ 2 \ 5 \ 3 \ 6 \ 7 \ 4\}$$
 $X_2 = \{1 \ 2 \ 5 \ 4 \ 7 \ 6 \ 3\}$
 $Eval(X_1) > Eval(X_2)$

- Configuration X = tour through nodes {1,..,N}
- Eval = Length of path defined by a permutation of {1,..,N}
- Find X* that realizes the minimum of Eval(X)
- Size of search space = order (N-1)!/2
- Note: Solutions for *N* = hundreds of thousands

$$\neg A \lor C \lor D$$

$$\mathbf{B} \vee \mathbf{D} \vee \neg \mathbf{E}$$

$$\neg C \lor \neg D \lor \neg E$$

$$\neg \mathbf{A} \lor \neg \mathbf{C} \lor \mathbf{E} \cdots \cdots$$

	Α	В	С	D	E	Eval
X_1	true	true	false	true	false	5
X_2	true	true	true	true	true	4

Example: SAT (SATisfiability)

 $\neg A \lor C \lor D$

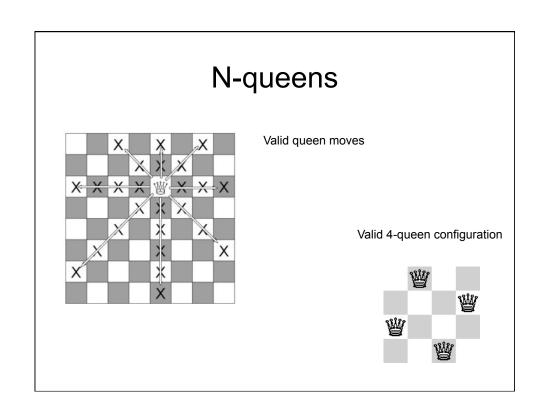
 $\mathbf{B} \vee \mathbf{D} \vee \neg \mathbf{E}$

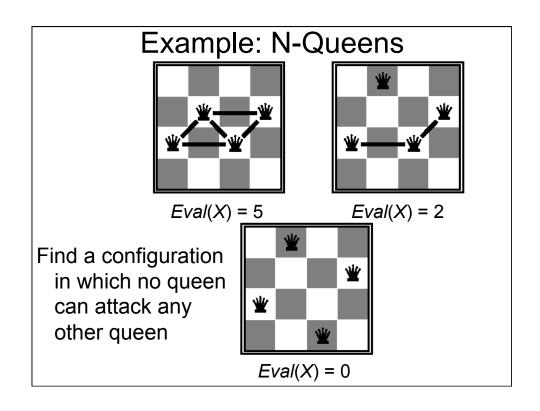
 $\neg C \lor \neg D \lor \neg E$

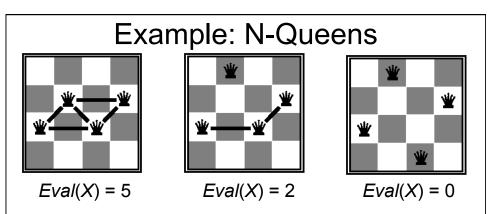
 $\neg A \lor \neg C \lor E$

	Α	В	С	D	E	Eval
<i>X</i> ₁	true	true	false	true	false	5
X_2	true	true	true	true	true	4

- Configuration X = Vector of assignments of N Boolean variables
- Eval(X) = Number of clauses that are satisfied given the assignments in X
- Find X* that realizes the maximum of Eval(X)
- Size of search space = 2^N
- Note: Solutions for 1000s of variables and clauses







- Configuration X = Position of the N queens in N columns
- Eval(X) = Number of pairs of queens that are attacking each other
- Find X^* that realizes the minimum: $Eval(X^*) = 0$
- Size of search space: order N^N
- Note: Solutions for N = millions

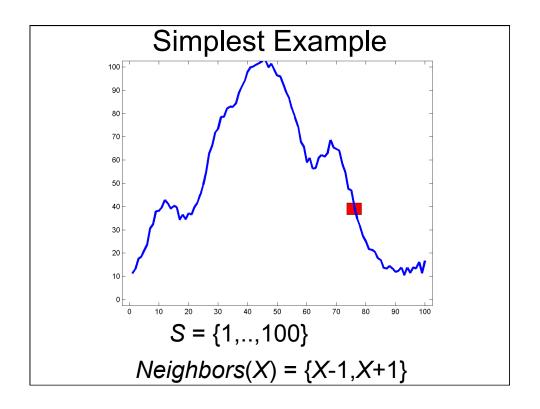
Local Search

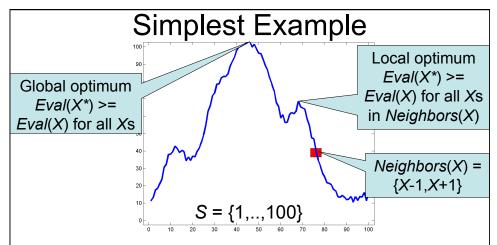
 Assume that for each configuration X, we define a neighborhood (or "moveset") Neighbors(X) that contains the set of configurations that can be reached from X in one "move".

$X_o \leftarrow$ Initial state

- 1. Repeat until we are "satisfied" with the current configuration:
- 2. Evaluate some of the neighbors in Neighbors(X_i)
- 3. Select one of the neighbors X_{i+1}
- 4. Move to X_{i+1}

₋ocal Search The definition of the neighborhoods is not obvious or unique in general. The performance ial state of the search algorithm depends critically on the htil we are "satisfied" with the definition of the neihborhood which is not straightforward in general. Infiguration: 3. Evalue e some of the ne hbors in Neighbors(X_i) 4. Select one of the neighbol 5. Move to Ingredient 2. Stopping Ingredient 1. Selection condition strategy: How to decide which neighbor to accept





- We are interested in the *global* maximum, but we may have to be satisfied with a *local* maximum
- In fact, at each iteration, we can check only for local optimality
- The challenge: Try to achieve global optimality through a sequence of local moves

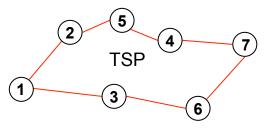
Most Basic Algorithm: Hill-Climbing (Greedy Local Search)

- X ← Initial configuration
- Iterate:
 - 1. $E \leftarrow Eval(X)$
 - 2. $N \leftarrow Neighbors(X)$
 - 3. For each X_i in N $E_i \leftarrow Eval(X_i)$
 - 4. If all E_i 's are lower than EReturn XElse

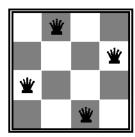
 $i^* = \operatorname{argmax}_i(E_i) \quad X \leftarrow X_{i^*} \quad E \leftarrow E_{i^*}$

More Interesting Examples

• How can we define *Neighbors*(*X*)?



N-Queens



 $\mathbf{A} \vee \neg \mathbf{B} \vee \mathbf{C}$

 $\neg A \lor C \lor D$

SAT $\mathbf{B} \vee \mathbf{D} \vee \neg \mathbf{E}$

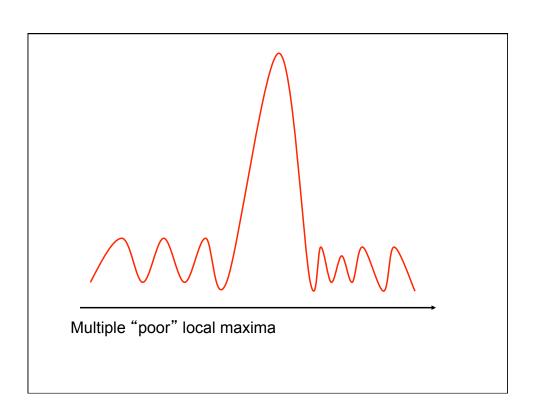
 $\neg C \lor \neg D \lor \neg E$

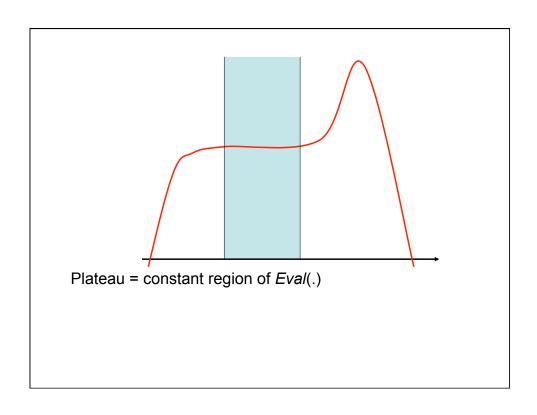
 $\neg A \lor \neg C \lor E$

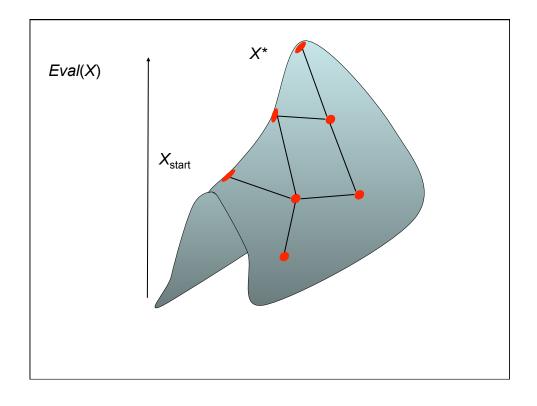
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Issues

- Trade-off on size of neighborhood
- → larger neighborhood = better chance of finding a good maximum but may require evaluating an enormous number of moves
- → smaller neighborhood = smaller number of evaluations but may get stuck in poor local maxima







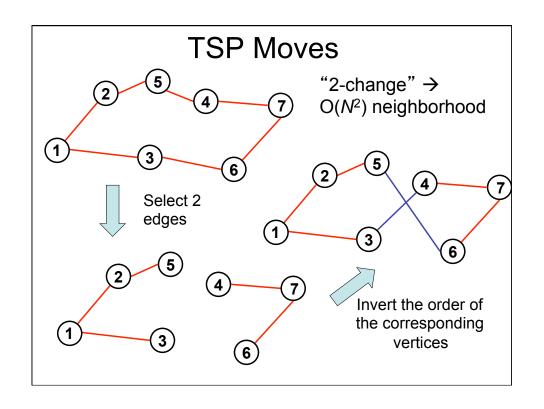
Issues

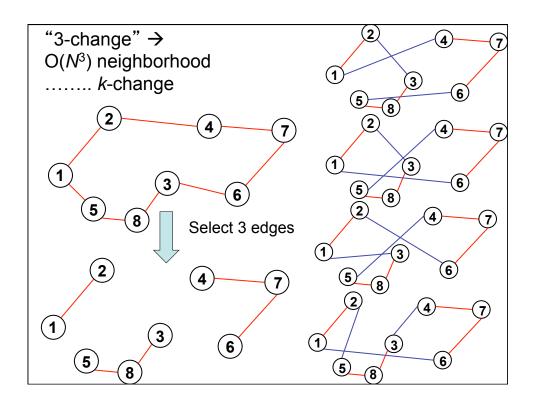
- Constant memory usage
- All we can hope is to find the local maximum "closest" to the initial configuration → Can we do better than that?
- Ridges and plateaux will plague all local search algorithms

Issues

- Constant memory usage
- All we can hope is to find the local maximum "closest" to the initial configuration → Can we do better than that?
- Ridges and plateaux will plague all local search algorithms
- Design of neighborhood is critical (as important as design of search algorithm)
- · Trade-off on size of neighborhood
- → larger neighborhood = better chance of finding a good maximum but may require evaluating an enormous number of moves
- → smaller neighborhood = smaller number of evaluation but may get stuck in poor local maxima

Stochastic Search: Randomized Hill-Climbing • *X* ← Initial configuration • Iterate:-Until when? 1. $E \leftarrow Eval(X)$ 2. $X' \leftarrow$ one configuration randomly selected in *Neighbors (X)* 3. $E' \leftarrow Eval(X')$ Critical change: We no longer select the best 4. If E' > Emove in the entire $X \leftarrow X'$ neighborhood $E \leftarrow E'$





Hill-Climbing: TSP Example							
	% error from min cost (N=100)	% error from min cost (N=1000)	Running time (N=100)	Running time (N=1000)			
2-Opt	4.5%	4.9%	1	11			
2-Opt (Best of 1000)	1.9%	3.6%					
3-Opt	2.5%	3.1%	1.2	13.7			
3-Opt (Best of 1000)	1.0%	2.1%					
Data from: Aarts & Lenstra, "Local Search in Combinatorial Optimization", Wiley Interscience Publisher							

Hill-Climbing: TSP Example • k-opt = Hill-climbing with k-change neighborhood

- Some results:
 - 3-opt better than 2-opt
 - 4-opt not substantially better given increase in computation time
 - Use random restart to increase probability of success

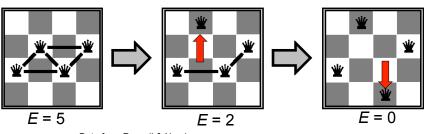
- Better measure: % away from (estimated) minimum cost

	% error from min cost (N=100)	% error from min cost (N=1000)	Running time (N=100)	Running time (N=1000)
2-Opt	4.5%	4.9%	1	11
2-Opt (Best of 1000)	1.9%	3.6%		
3-Opt	2.5%	3.1%	1.2	13.7
3-Opt (Best of 1000)	1.0%	2.1%	Data from: Aarts & Lenstra, "Local Search in Combinatorial Optimization", Wiley Interscience Publisher	

Hill-Climbing: N-Queens

- · Basic hill-climbing is not very effective
- · Exhibits plateau problem because many configurations have the same cost
- · Multiple random restarts is standard solution to boost performance

N = 8	% Success	Average number of moves
Direct hill climbing	14%	4
With sideways moves	94%	21 (success)/64 (failure)



Data from Russell & Norvig

Hill-Climbing: SAT

- State X = assignment of N boolean variables
- Initialize the variables (x₁,..,x_N) randomly to true/false

- Iterate until all clauses are satisfied or max iterations:
 - 1.Select an unsatisfied clause

Random walk part

2. With probability p:—

Select a variable x_i at random

3. With probability 1-p:

Select the variable x_i such that cha unsatisfy the least number of clauses (Max of Eval(X))

4. Change the assignment of the selected variable x_i

Hill-Climbing: SAT

- WALKSAT algorithm still one of the most effective for SAT
- Combines the two ingredients: random walk and greedy hill-climbing
- Incomplete search: Can never find out if the clauses are not satisfiable

For more details and useful examples/code: http://www.cs.washington.edu/homes/kautz/walksat/

Optimization Method For Emergency Use Only



Simulated Annealing

- 1. $E \leftarrow Eval(X)$
- 2. X' ← one configuration randomly selected in Neighbors (X)
- 3. $E' \leftarrow Eval(X')$
- 4. If E' >= E

 $X \leftarrow X'$

 $E \leftarrow E'$

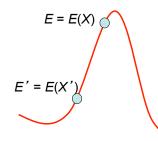
Critical change: We no longer move always uphill. Next question: How to choose *p*?

Else accept the move to X' with some probability p:

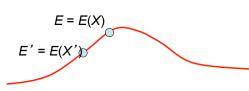
$$X \leftarrow X'$$

 $E \leftarrow E'$

How to set p? Intuition



E – E' is large: It is more likely that we are moving toward a (promising) sharp maximum so we don't want to move downhill too much



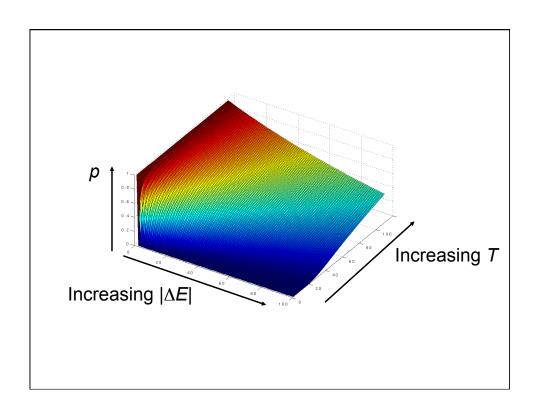
E-E' is small: It is likely that we are moving toward a shallow maximum that is likely to be a (uninteresting) local maximum, so we like to move downhill to explore other parts of the landscape

Choosing p: Simulated Annealing

- If E' >= E accept the move
- Else accept the move with probability:

$$p = e^{-(E - E')/T}$$

 Start with high temperature T and decrease T gradually as iterations increase ("cooling schedule")



Simulated Annealing

- 1. Do *K* times:
 - $1.1 E \leftarrow Eval(X)$
 - 1.2 $X' \leftarrow$ one configuration randomly selected in *Neighbors* (X)
 - $1.3 E' \leftarrow Eval(X')$
 - 1.4 If E' >= E

$$X \leftarrow X'; E \leftarrow E';$$

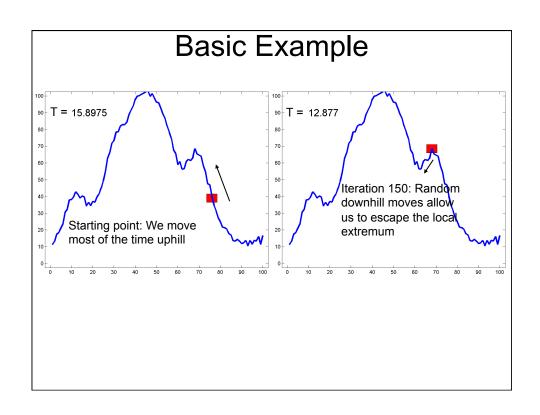
Else accept the move with probability

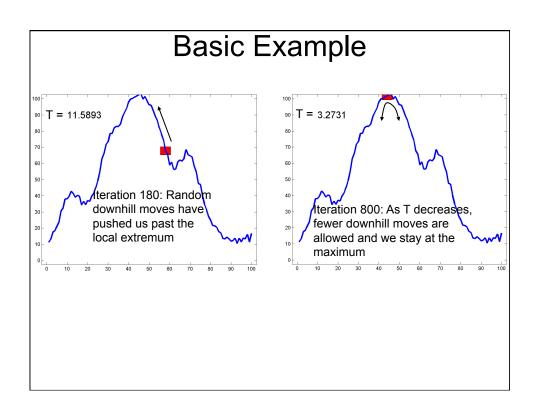
$$p = e^{-(E - E')/T}$$
:

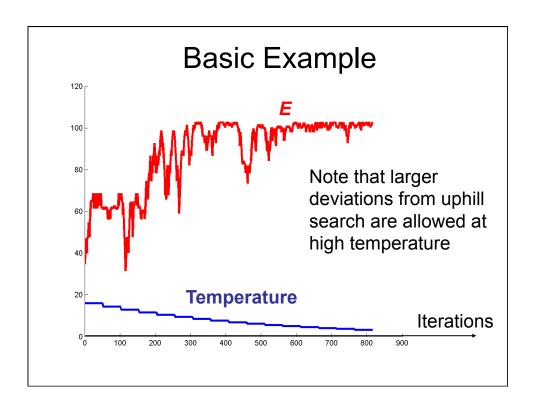
$$X \leftarrow X'; E \leftarrow E';$$

2. $T \leftarrow \alpha T$

Simulated Annealing $X \leftarrow$ Initial configuration $T \leftarrow$ Initial high temperature Iterate a number of times keeping Iterate: the temperature fixed 1. Do K times: $1.1 E \leftarrow Eval(X)$ 1.2 $X' \leftarrow$ one configuration randomly selected in Neighbors (X) Use the previous definition of $1.3 E' \leftarrow Eval(X)$ the probability 1 / If F' >= F Progressively decrease the temperature using an exponential cooling schedule: $T(n) = \alpha^n T$ with $\alpha < 1$ bility $p = e^{-(E - E')/T}$ $X': E \leftarrow E':$ $T = 0 \rightarrow$ Greedy hill climbing 2. $T \leftarrow \alpha T$ $T = \infty \rightarrow \text{Random walk}$



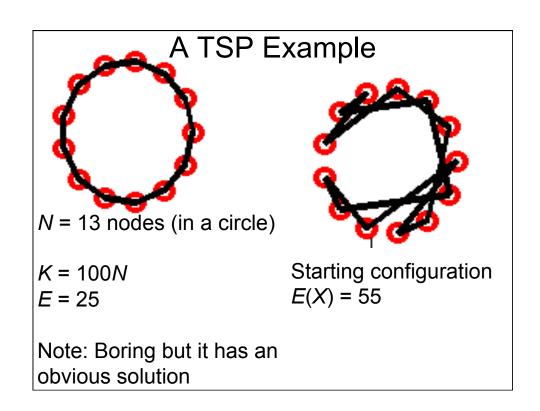


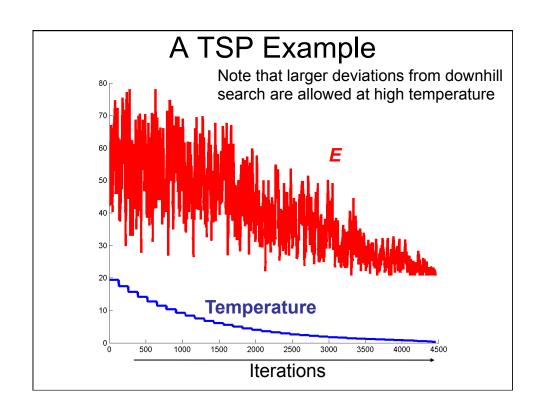


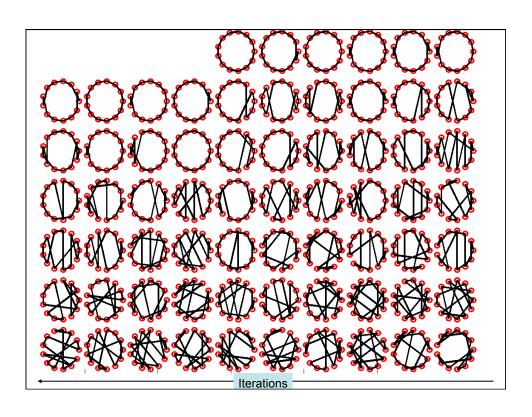
Where does this come from?

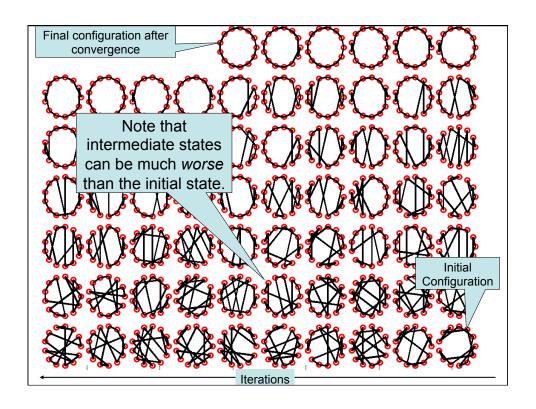
• If the temperature of a solid is *T*, the probability of moving between two states of energy is:

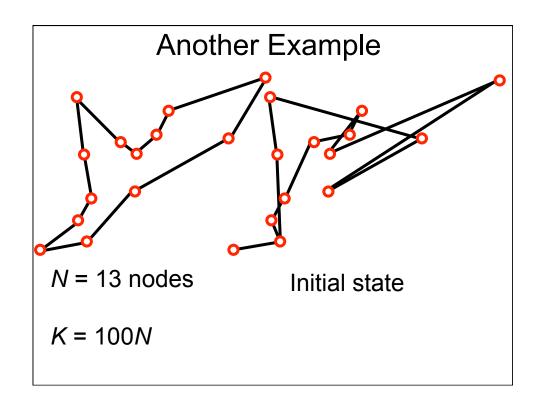
- If the temperature *T* of a solid is decreased slowly, it will reach an equilibrium at which the probability of the solid being in a particular state is:
- Probability (State) proportional to € -Energy(State)/kT
- Boltzmann distribution → States of low energy relative to T are more likely
- Analogy:
 - State of solid ←→ Configurations X
 - Energy ←→ Evaluation function Eval(.)
- N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth. A.H. Teller and E. Teller, *Journal Chem. Phys.* 21 (1953) 1087-1092

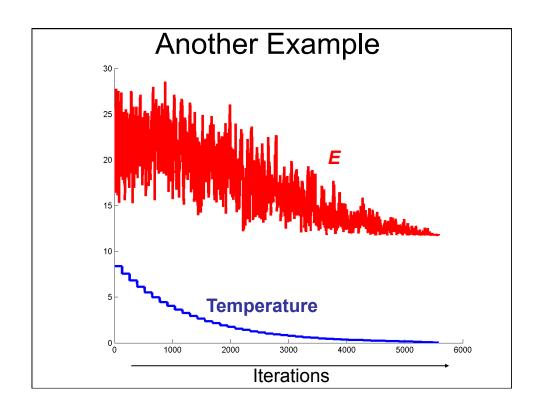


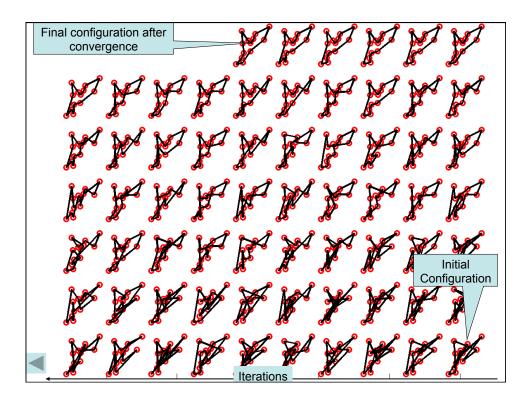












What can we say about convergence?

• In theory:

$$\lim_{T\to 0}\lim_{K\to\infty}\Pr(X(T,K)\in S^*)=1$$

In words: Probability that the state reached after K iterations at temperature T is a global optimum

- · In practice:
 - Perform a large enough number of iterations (K "large enough")
 - Decrease temperature slowly enough (α "close enough" to 1)
 - But, if not careful, we may have to perform an enormous number of evaluations

Simulated Annealing

- X ← Initial configuration
- T ← Initial high temperature
- Iterate:
- 1. Do K times:

Many parameters need to be tweaked!!

1.1 $E \leftarrow Eval(X)$

1.2 X' ← one configuration randomly selected in Neighbors (X)

 $1.3 E' \leftarrow Eval(X')$

1.4 If E' >= E

 $X \leftarrow X'; E \leftarrow E';$

Else accept the move with probability $p = e^{-(E - E')/T}$ $X \leftarrow X'$; $E \leftarrow E'$;

2. $T \leftarrow \alpha T$

SA Discussion

- Design of neighborhood is critical
- How to choose K? Typically related to size of neighborhood
- How to choose α ? Critical to avoid large number of useless evaluations. Especially a problem close to convergence (empirically, most of the time spent close to the optimum)

SA Discussion

- How to choose starting temperature? Typically related to the distribution of anticipated values of ΔE (e.g., T_{start} = max{ΔE over a large sample of pairs of neighbors})
- What if we choose a really bad starting X? Multiple random restart.
- How to avoid repeated evaluation? Use a bit more memory by remembering the previous moves that were tried ("Tabu search")
- Use (faster) approximate evaluation if possible (How?)

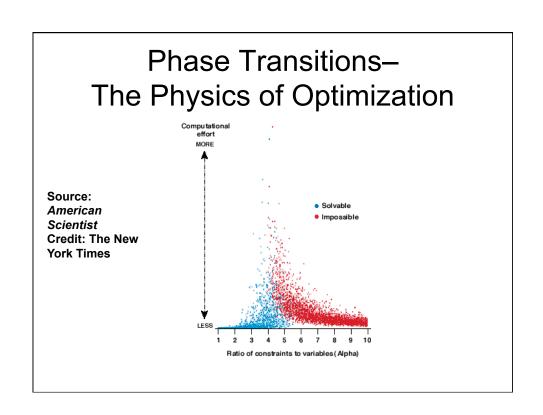
SA Discussion

- Often better than hill-climbing. Successful algorithm in many applications
- Many parameters to tweak. If not careful, may require very large number of evaluations
- Semi-infinite number of variations for improving performance depending on applications

Phase Transitions— The Physics of Optimization

- Over the last 20 years, physicists and computer scientists working in AI have discovered close connections between
 - the statistical behavior of matter
 - Computational hardness
- Consider the 3-SAT problem, and particularly the behavior in terms of
 - Alpha: ratio of constraints to variables
- What do you expect to happen?

http://www.nytimes.com/library/national/science/071399sci-satisfiability-problems.html



Reminder Example: SAT (SATisfiability) A v ¬B v C

$$\mathbf{A} \vee \neg \mathbf{B} \vee \mathbf{C}$$

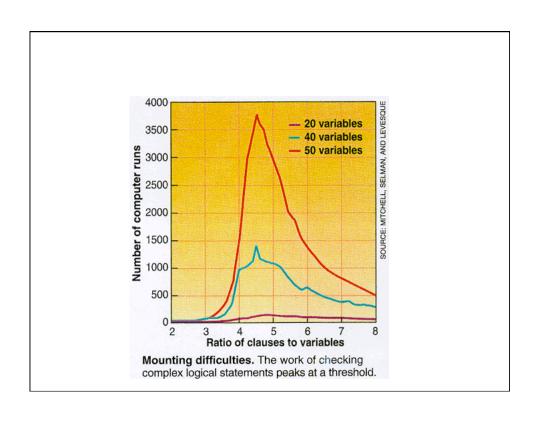
$$\neg A \lor C \lor D$$

$$\mathbf{B} \vee \mathbf{D} \vee \neg \mathbf{E}$$

$$\neg C \lor \neg D \lor \neg E$$

$$\neg A \lor \neg C \lor E \cdots$$

	Α	В	С	D	E	Eval
X_1	true	true	false	true	false	5
X_2	true	true	true	true	true	4



Genetic/Evolutionary Algorithms

Genetic Algorithms

- View optimization by analogy with evolutionary theory → Simulation of natural selection
- View configurations as individuals in a population
- View Eval as a measure of fitness
- Let the least-fit individuals die off without reproducing
- Allow individuals to reproduce with the best-fit ones selected more often
- Each generation should be overall better fit (higher value of Eval) than the previous one
- If we wait long enough the population should evolve so toward individuals with high fitness (i.e., maximum of *Eval*)

Genetic Algorithms: Implementation

· Configurations represented by strings:

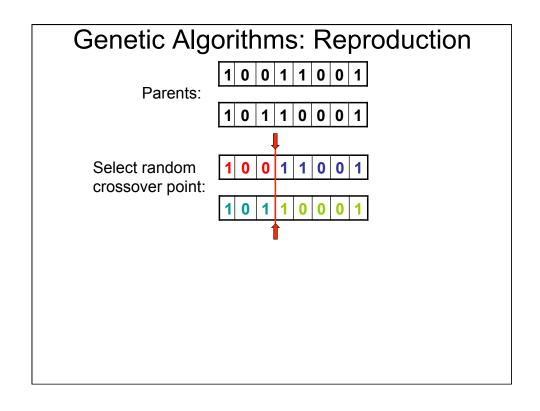
- Analogy:
 - The string is the chromosome representing the individual
 - String made up of genes
 - Configuration of genes are passed on to offsprings
 - Configurations of genes that contribute to high fitness tend to survive in the population
- Start with a random population of P configurations and apply two operations
 - Reproduction: Choose 2 "parents" and produce 2 "offsprings"
 - Mutation: Choose a random entry in one (randomly selected) configuration and change it

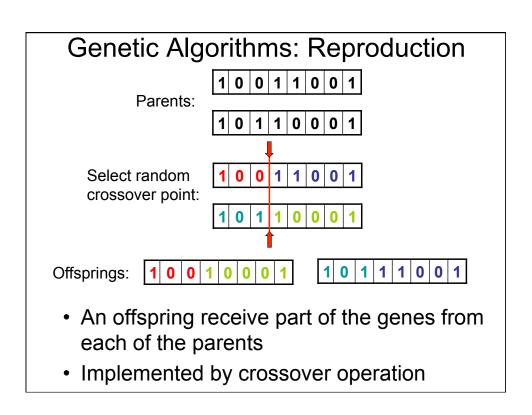
Genetic Algorithms: Reproduction

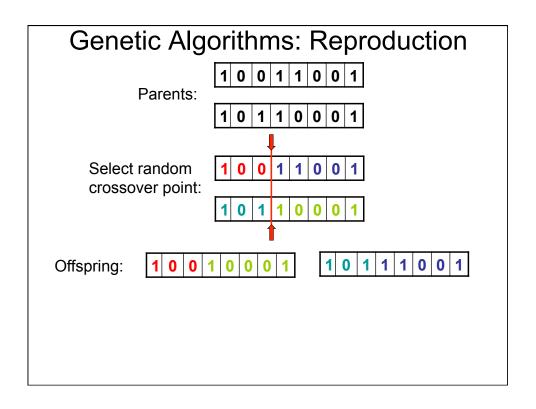
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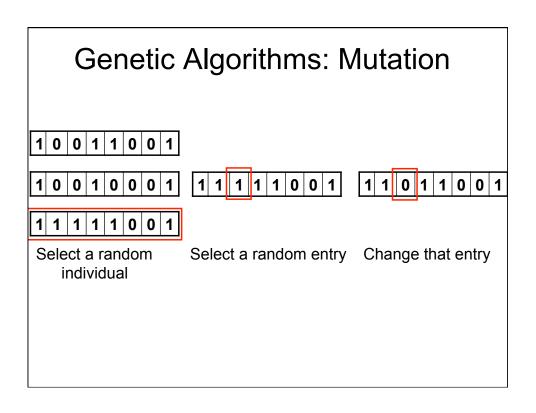
Parents:

1 0 1 1 0 0 0 1









Genetic Algorithms: Mutation

- Random change of one element in one configuration
 - →Implements random deviations from inherited traits
 - → Corresponds loosely to "random walk": Introduce random moves to avoid small local extrema

1 0 0 1 1 0 0 1

1 0 0 1 0 0 0 1

1 1 1 1 0 0 1 1 1 0 1 1 0 0 1

1 1 1 1 1 0 0 1

Select a random individual

Select a random entry Change that entry

Basic GA Outline

- Create initial population $X = \{X_1,...,X_P\}$
- Iterate:
 - 1. Select K random pairs of parents (X,X')
 - 2. For each pair of parents (X,X'):
 - 1.1 Generate offsprings (Y_1, Y_2) using crossover operation
 - 1.2 For each offspring Y_i:

Replace randomly selected element of the population by Y_i

With probability μ :

Apply a random mutation to Y_i

Return the best individual in the population

Basic GA Outline

- Create initial population $X = \{X_1,...,X_p\}$
- Iterate: Stopping condition is not obvious?
 - 1. Select K random pairs of pa
 - 2. For each pair of parents
 - 1.1 Generate offsprings_(Y₁

Variation:

Generate only one offspring Y_i :

Possible strategy:
Select the best *rP*individuals (*r* < 1) for
reproduction and
discard the rest →
Implements selection of
the fittest

 κ eplace randomly selected element of the population by γ

With probability μ :

Apply a random mutation to Y_i

Return the best individual in the population

Genetic Algorithms: Selection

- Discard the least-fit individuals through threshold on *Eval* or fixed percentage of population
- Select best-fit (larger Eval) parents in priority
- Example: Random selection of individual based on the probability distribution

$$Pr(individual X selected) = \frac{Eval(X)}{\sum_{Y \in nonulation} Eval(Y)}$$

- Example (tournament): Select a random small subset of the population and select the best-fit individual as a parent
- · Implements "survival of the fittest"
- Corresponds loosely to the greedy part of hill climbing (we try to move uphill)

GA and Hill Climbing

- Create initial population $X = \{X_1,...,X_P\}$
- · Iterate:
 - 1. Select *K* random Hill-climbing component: Try to move uphill as much as possible
 - 2. For each pair of parents (X,X'):
 - 1.1 Generate offsprings (Y_1, Y_2) using crossover operation

Random walk component: Move randomly to escape shallow local maxima

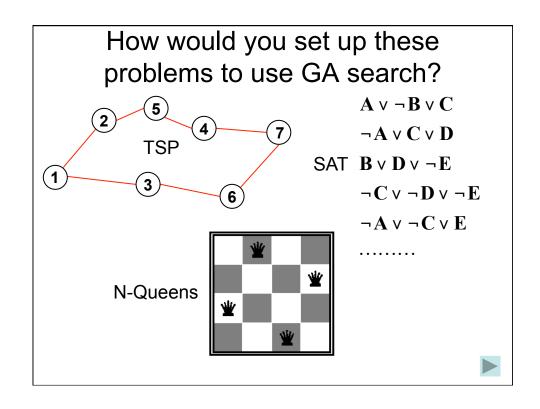
offspring Y_i:

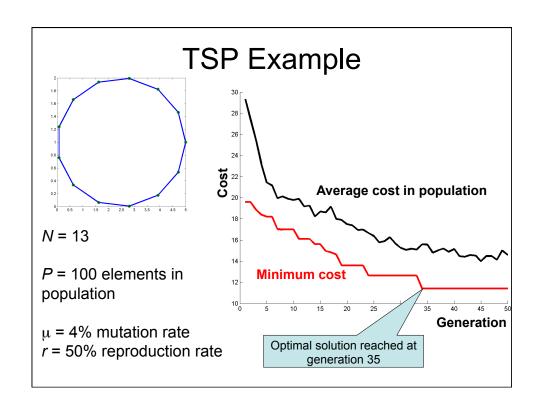
randomly selected element of the by Y_i

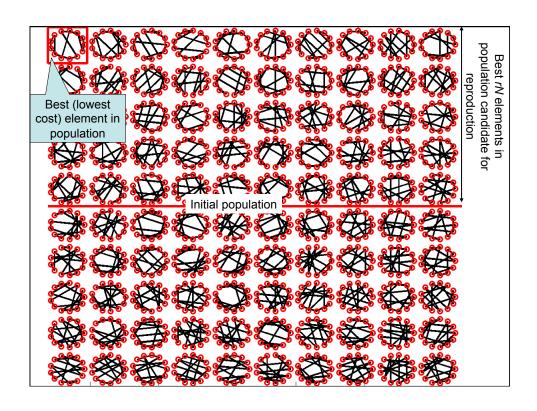
With probability u:

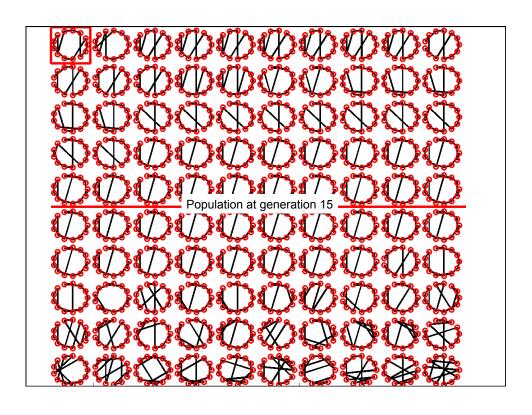
Apply a random mutation to Y_i

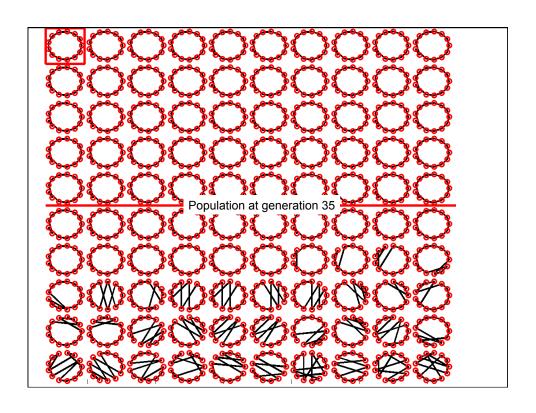
Return the best individual in the population

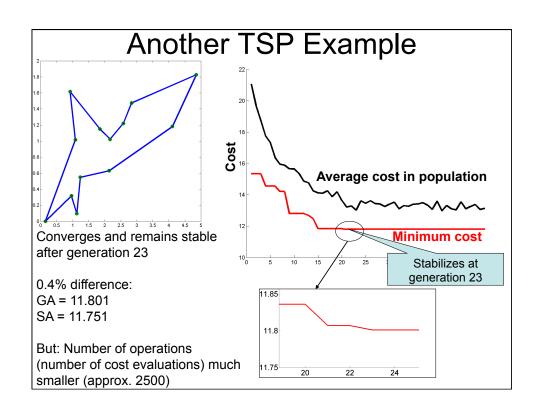


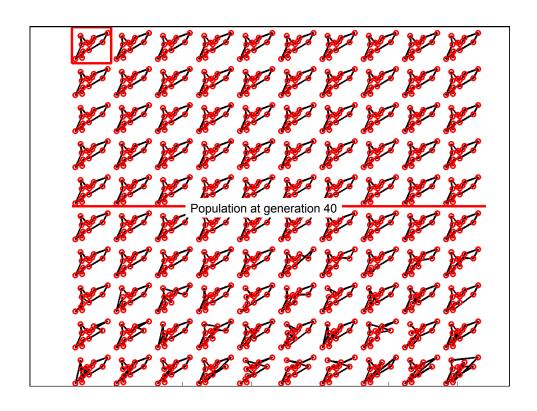








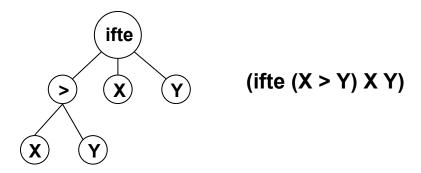


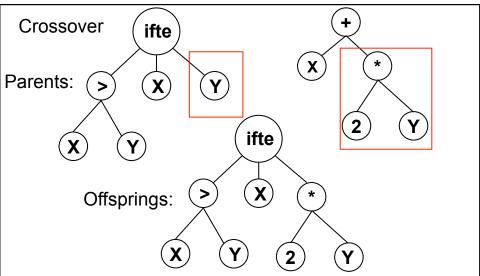


Even more radical ideas..

Individual = program

X = parse tree representing a program





Use genetic algorithms as before with this definition of crossover Example applications: robot controller, signal processing, circuit design Intriguing, but alternative solutions exist for most of these applications; this is not the first approach to consider!!!

Koza. Genetic programming: On the programming of computers by means of natural selection. MIT Press. 1992 http://www.genetic-programming.org/

GA Discussion

- Many parameters to tweak: μ, P, r
- Many variations on basic scheme. Examples:
 - Multiple-point crossover
 - Dynamic encoding
 - Selection based on rank or relative fitness to least fit individual
 - Multiple fitness functions
 - Combine with a local optimizer (for example, local hillclimbing) → Deviates from "pure" evolutionary view
- In many problems, assuming correct choice of parameters, can be surprisingly effective

GA Discussion

- Why does it work at all?
- Limited theoretical results (informally!):
 - Suppose that there exists a partial assignment of genes s such that:

Average of
$$Eval(X) \ge Average$$
 of $Eval(Y)$
 $X = X \text{ contains } S$

- Then the number of individuals containing s will increase in the next generation
- Key consequence: The design of the representation (the chromosomes) is critical to the performance the GA. It is probably more important than the choice of parameters of selection strategy, etc.