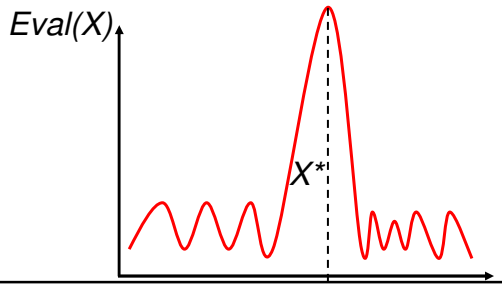
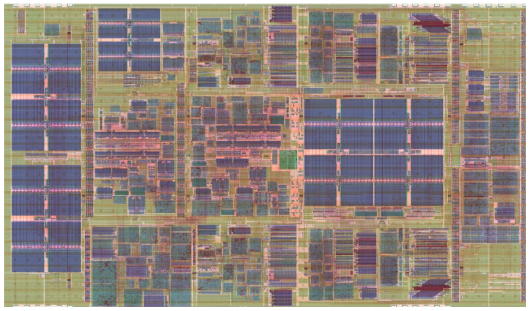
Local Search/Stochastic Search

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



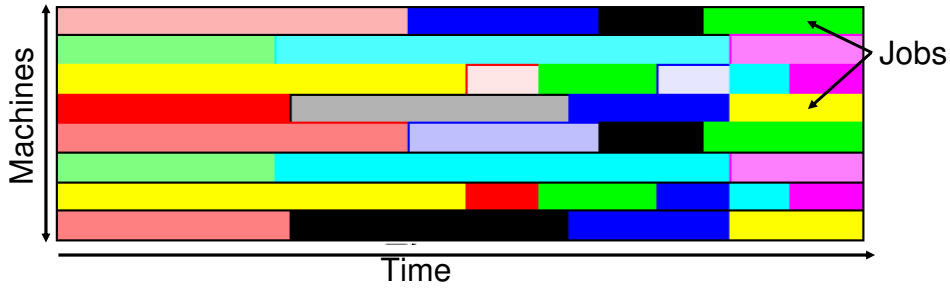
Real-World Examples



Placement
Floorplanning
Channel routing
Compaction

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

Real-World Examples



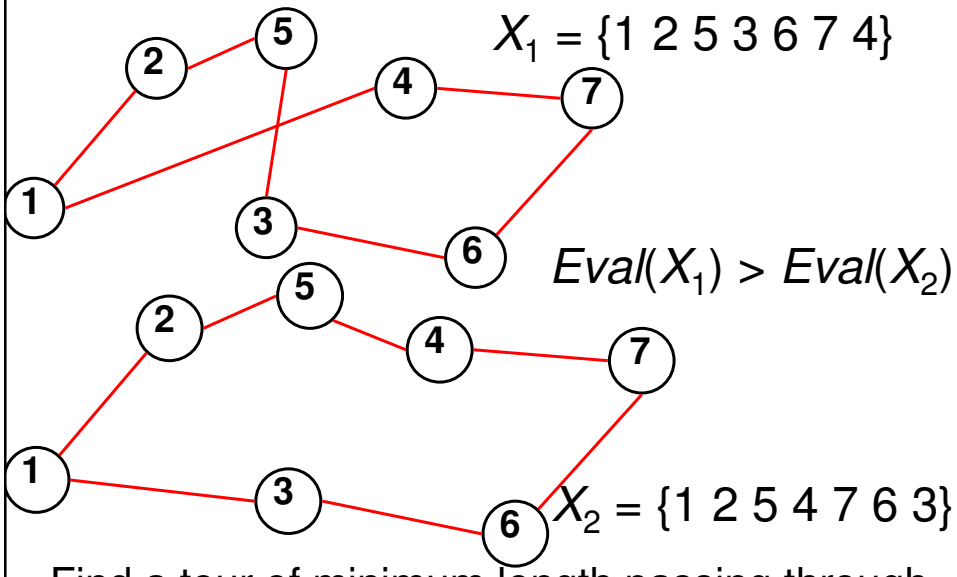
- Scheduling: Given *m* machines, *n* jobs
- *X* = assignment of jobs to machines
- *Eval* = completion time of the *n* jobs (minimize)

- Others: Vehicle routing, design, treatment sequencing, ……

What makes this challenging?

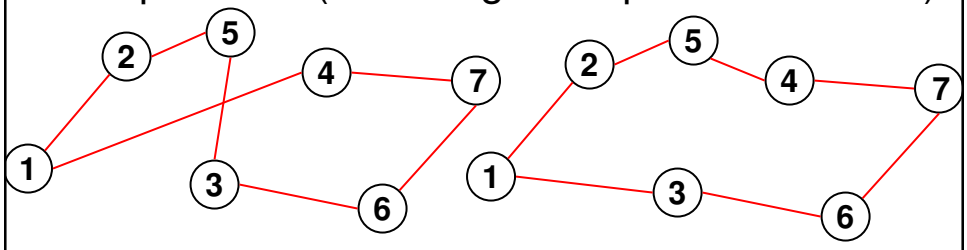
- Problems of particular interest:
  - Set of configurations too large to be enumerated explicitly
  - Computation of *Eval*(.) may be expensive
  - There is no algorithm for finding the maximum of *Eval*(.) efficiently
  - Solutions with similar values of *Eval*(.) are considered equivalent for the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

Example: TSP (Traveling Salesperson Problem)



- Find a tour of minimum length passing through each point once

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

Example: SAT (SATisfiability)

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

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

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

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

$$\neg\mathbf{A} \vee \neg\mathbf{C} \vee \mathbf{E} \quad \cdots\cdots\cdots$$

	A	**B**	**C**	**D**	**E**	*Eval*
X_1	*true*	*true*	*false*	*true*	*false*	**5**
X_2	*true*	*true*	*true*	*true*	*true*	**4**

Example: SAT (SATisfiability)

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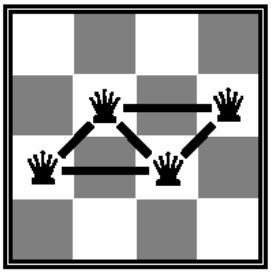
$\neg\mathbf{A} \vee \neg\mathbf{C} \vee \mathbf{E}$

.....

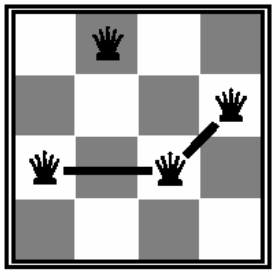
	A	**B**	**C**	**D**	**E**	*Eval*
X_1	*true*	*true*	*false*	*true*	*false*	**5**
X_2	*true*	*true*	*true*	*true*	*true*	**4**

- 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

Example: N-Queens

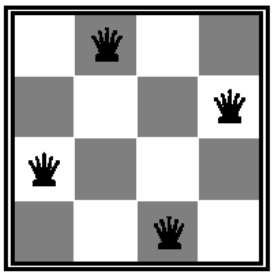


Eval(X) = 5



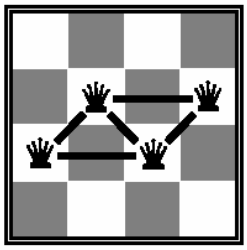
Eval(X) = 2

Find a configuration in which no queen can attack any other queen

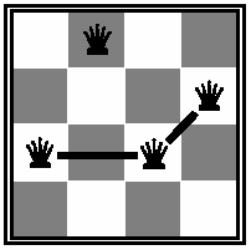


Eval(X) = 0

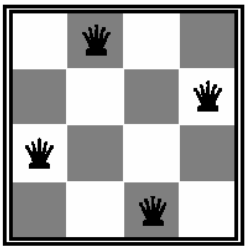
Example: N-Queens



Eval(*X*) = 5



Eval(*X*) = 2



Eval(*X*) = 0

- 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".

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

Local Search

The definition of the neighborhoods is not obvious or unique in general. The performance of the search algorithm depends critically on the definition of the neihborhood which is not straightforward in general.

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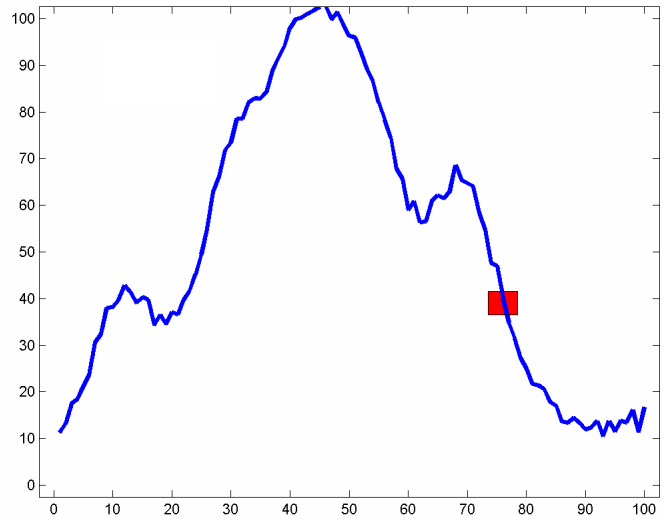
5. Move to X_{i+1}

Ingredient 1. Selection strategy: How to decide which neighbor to accept

Ingredient 2. Stopping condition

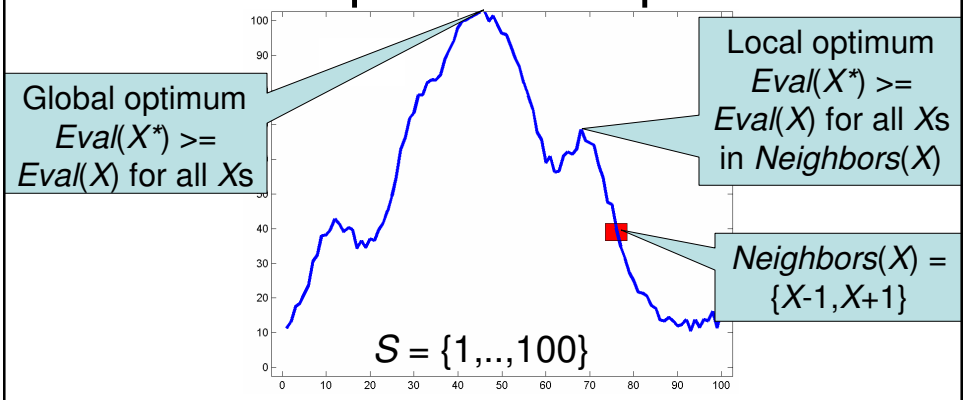
Simplest Example



$S = \{1,..,100\}$

Neighbors(X) = {X-1,X+1}

Simplest Example



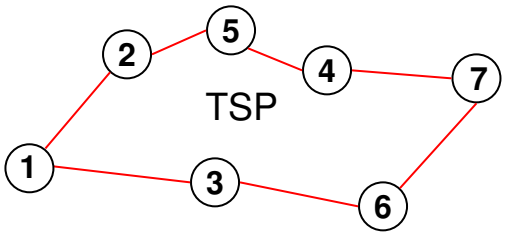
- We are interested in the *global* maximum, but we may have to be satisfied with a *local* maximum
- In fact, at each iteration, we can check only for *local* optimality
- The challenge: Try to achieve global optimality through a sequence of local moves

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

- X ← Initial configuration
- Iterate:
  1. $E \leftarrow Eval(X)$
  2. $\mathcal{N} \leftarrow Neighbors(X)$
  3. For each X_i in $\mathcal{N}$
     $E_i \leftarrow Eval(X_i)$
  4. If all E_i's are lower than E
     Return X
     Else
     $i^* = \text{argmax}_i (E_i)$ $X \leftarrow X_{i^*}$ $E \leftarrow E_{i^*}$

More Interesting Examples

- How can we define *Neighbors*(*X*)?



TSP

SAT

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

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

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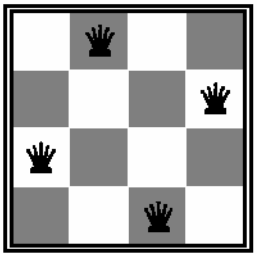
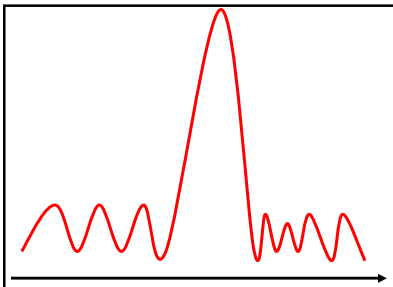
$\neg\mathbf{A} \vee \neg\mathbf{C} \vee \mathbf{E}$

……

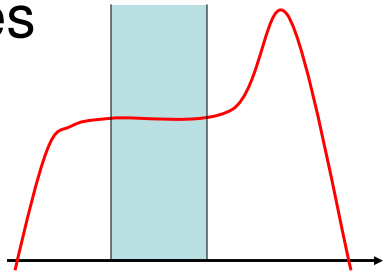
N-Queens



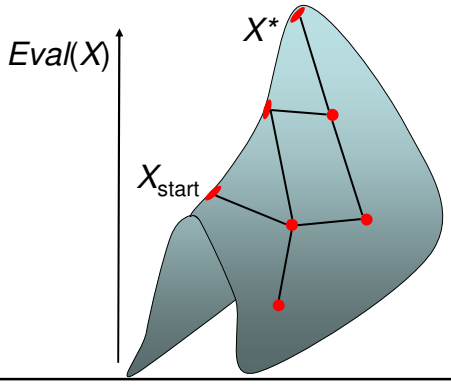
Issues



Multiple "poor" local maxima



Plateau = constant region of *Eval*(.)



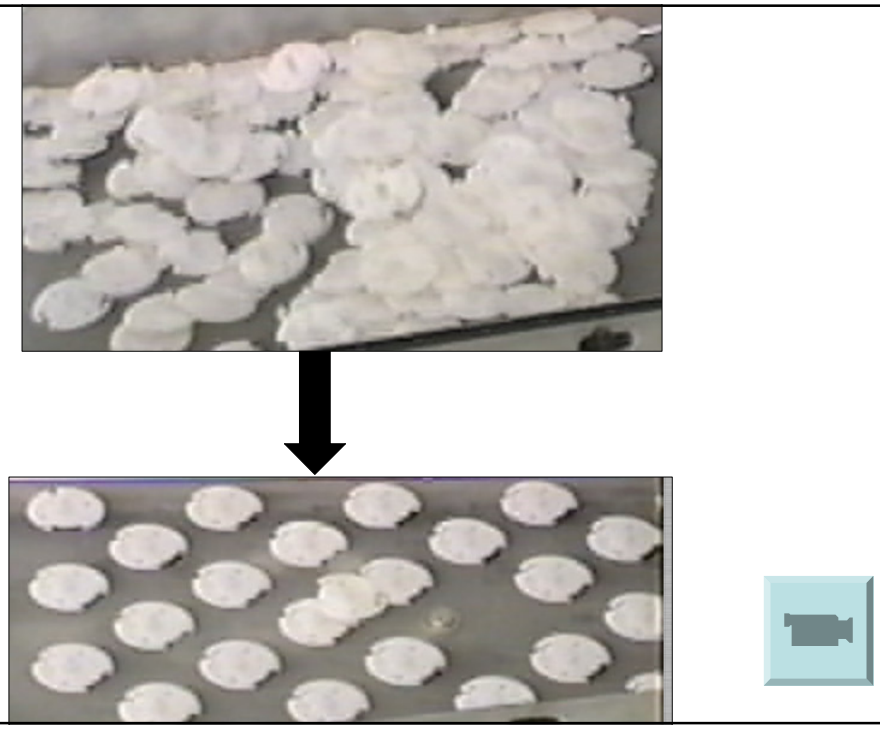
Ridge = Impossible to reach X^* from X_{start} using uphill moves only

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

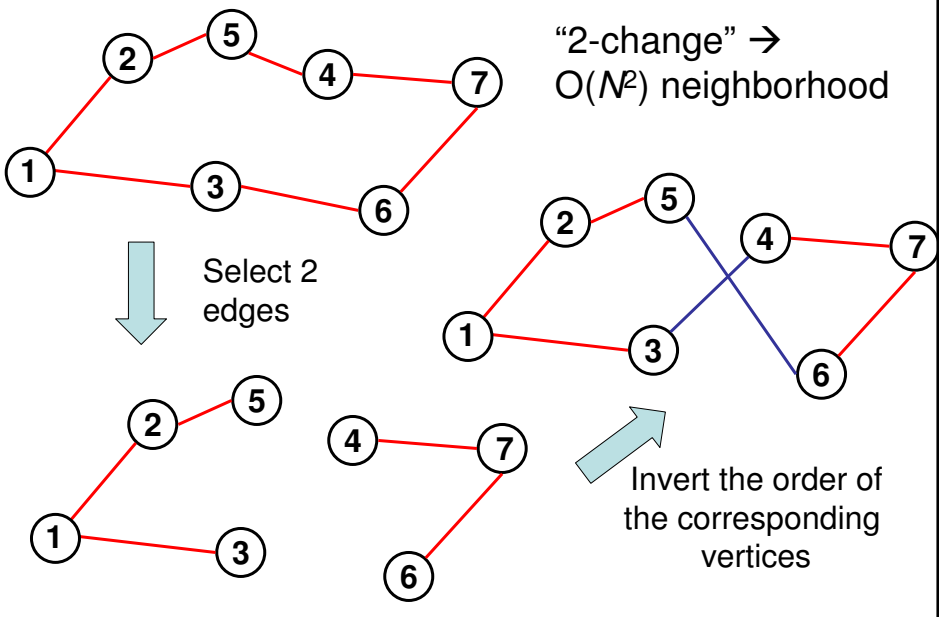
- $X \leftarrow$ Initial configuration
- Iterate:

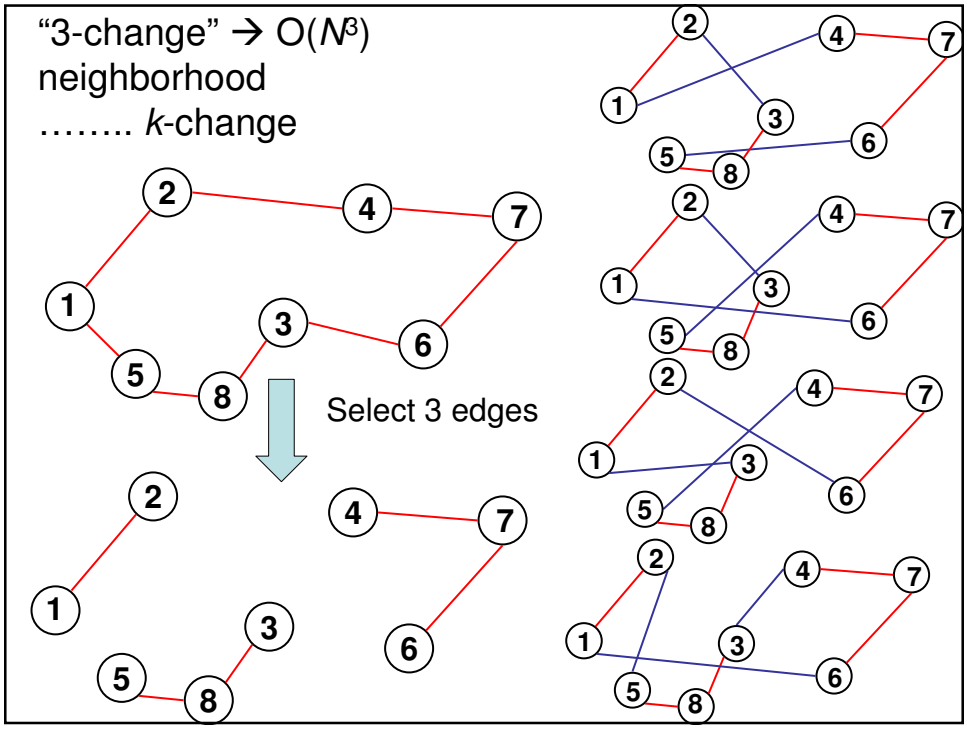
Until when?

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

Critical change: We no longer select the best move in the entire neighborhood

TSP Moves





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)
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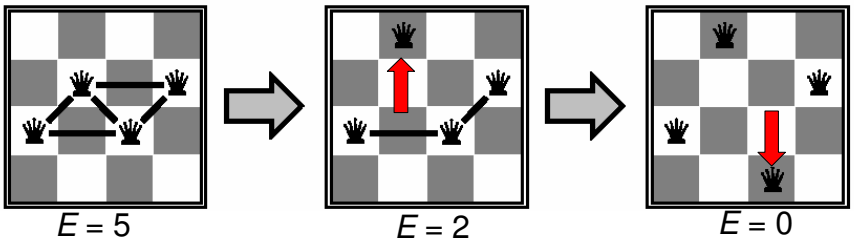
Hill-Climbing: N-Queens

- 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

$$\mathbf{A} \vee \neg\mathbf{B} \vee \mathbf{C} \qquad \neg\mathbf{C} \vee \neg\mathbf{D} \vee \neg\mathbf{E}$$
$$\neg\mathbf{A} \vee \mathbf{C} \vee \mathbf{D} \cdots\cdots\cdots \neg\mathbf{A} \vee \neg\mathbf{C} \vee \mathbf{E}$$

- State X = assignment of N boolean variables
- Initialize the variables (x_1,..,x_N) randomly to *true*/*false*
- Iterate until all clauses are satisfied or max iterations:
  1. Select an unsatisfied clause
  2. With probability *p*:
     Select a variable x_i at random
  3. With probability 1-*p*:
     Select the variable x_i such that changing x_i will unsatisfy the least number of clauses (Max of *Eval*(X))
  4. Change the assignment of the selected variable x_i

Random walk part

Greedy part

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/

Simulated Annealing

1. $E \leftarrow Eval(X)$
2. $X' \leftarrow$ 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*?

- $X \leftarrow$ Initial configuration
- Iterate:

1. $E \leftarrow Eval(X)$
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Else accept the move to X' with some probability *p*:
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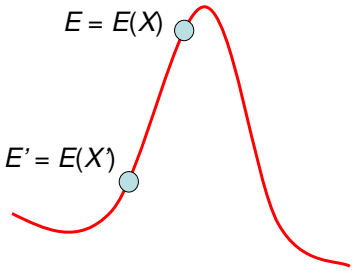
If *p* constant: We don't know how to set *p* → should depend on the shape of the *Eval* function

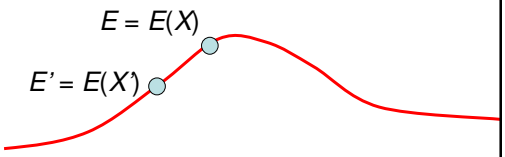
Decrease *p* as the iterations progress → We accept fewer downhill moves as we approach the global maximum

Decrease *p* as E-E' increases → Lower probability to move downhill if slope is high

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



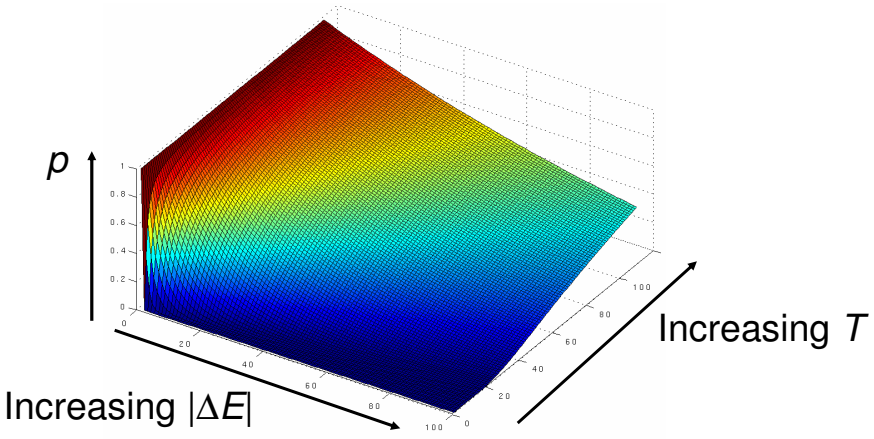
E – *E'* is small: It is likely that we are moving toward a shallow maximum that is likely to be a (uninteresting) local maximum, so we like to move downhill to explore other parts of the landscape

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")



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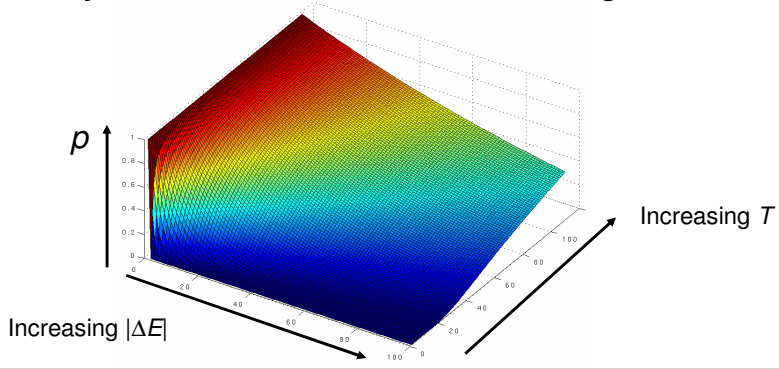


Simulated Annealing

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:

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 $E' >= E$

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

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

2. $T \leftarrow \alpha T$

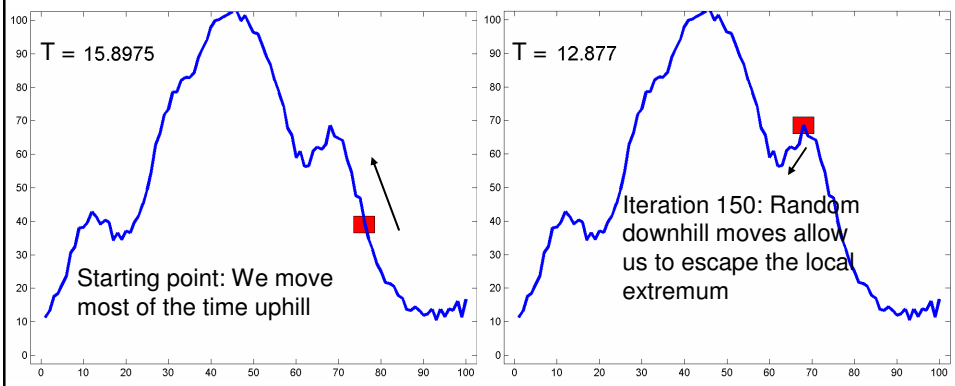
Iterate a number of times keeping the temperature fixed

Use the previous definition of the probability

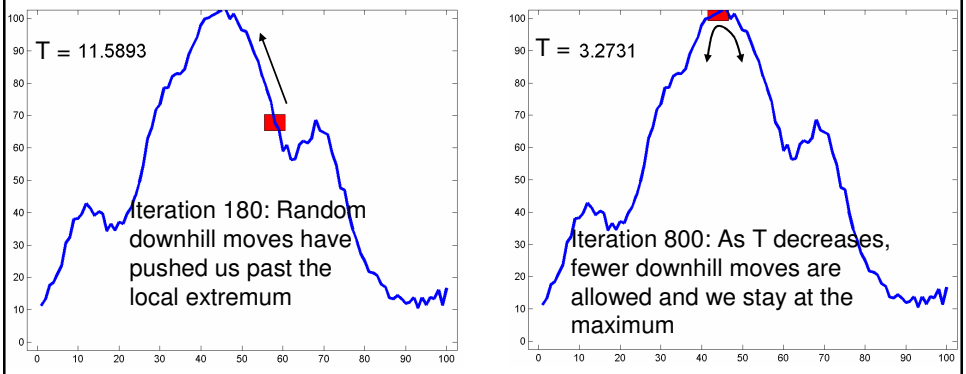
Progressively decrease the temperature using an exponential cooling schedule: $T(n) = \alpha^n T$ with $\alpha < 1$

$T = 0 \rightarrow$ Greedy hill climbing
$T = \infty \rightarrow$ Random walk

Basic Example



Basic Example



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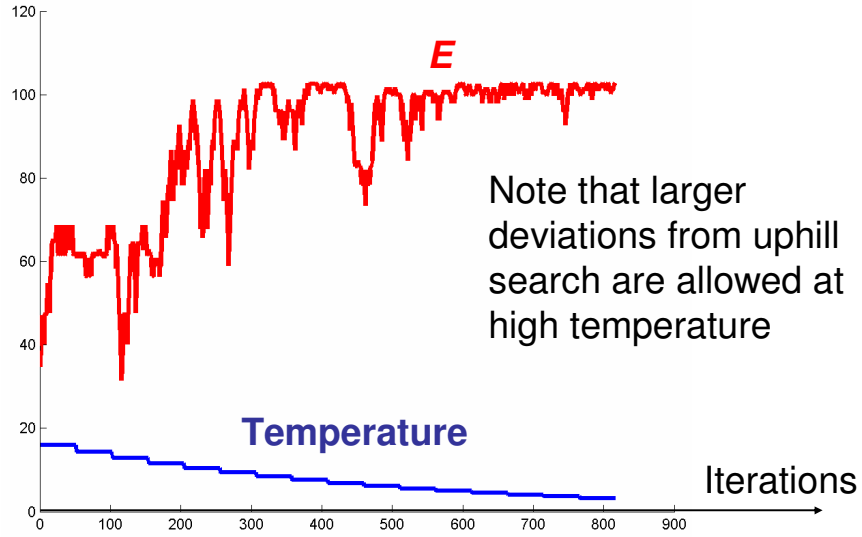


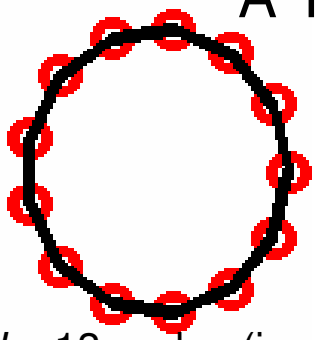
Where does this come from?

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

$$e^{-\Delta Energy/kT}$$

- 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 $e^{-Energy(State)/kT}$
- 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

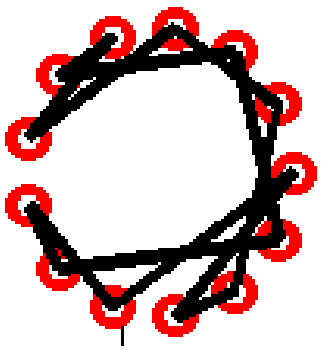
A TSP Example



$N = 13$ nodes (in a circle)

$K = 100N$

$E = 25$



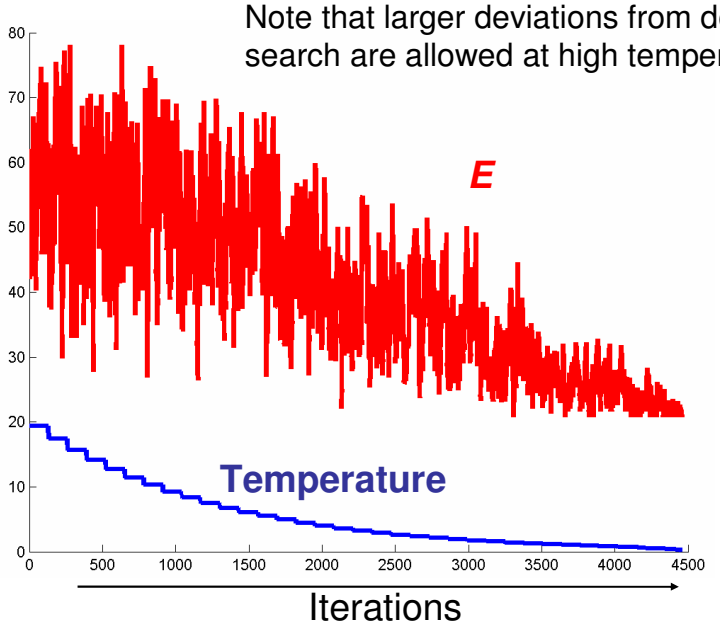
Starting configuration

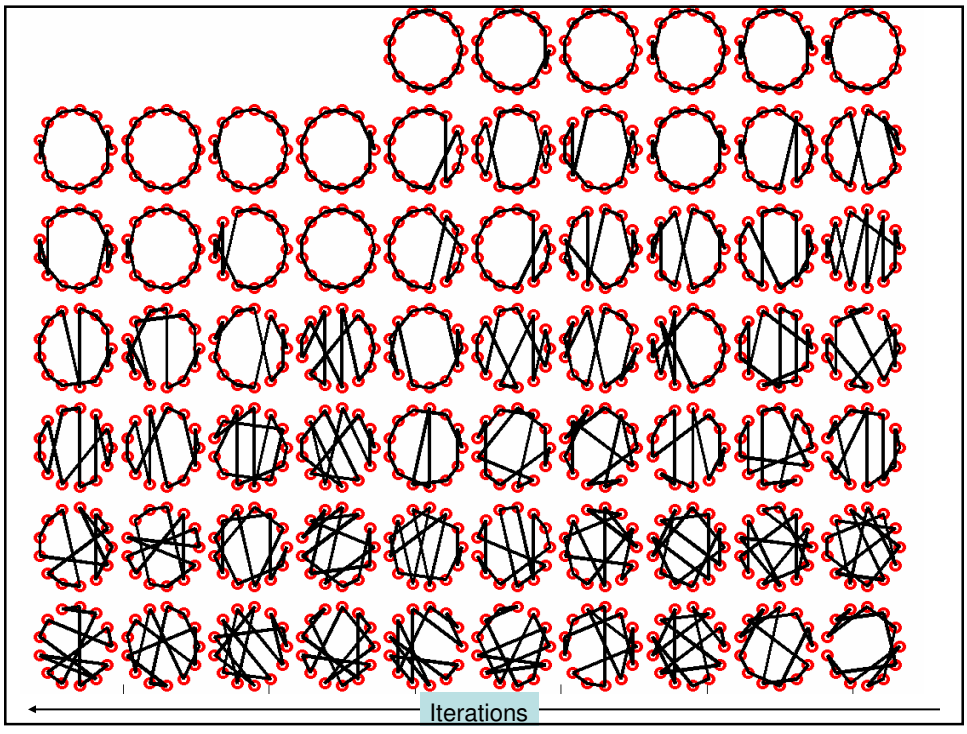
$E(X) = 55$

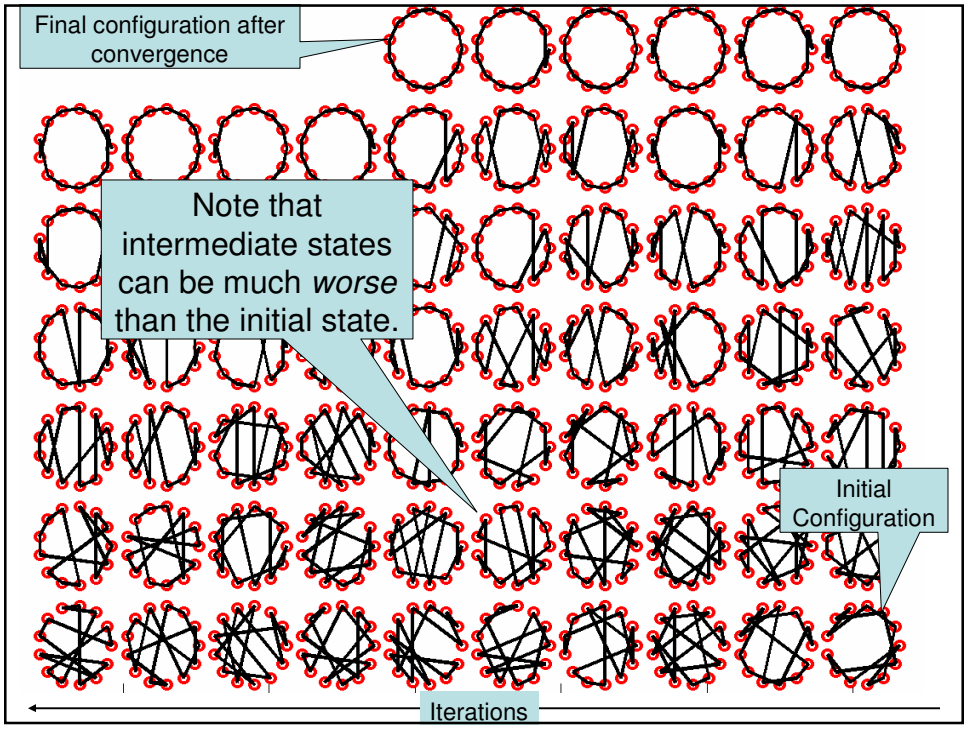
Note: Boring but it has an obvious solution

A TSP Example

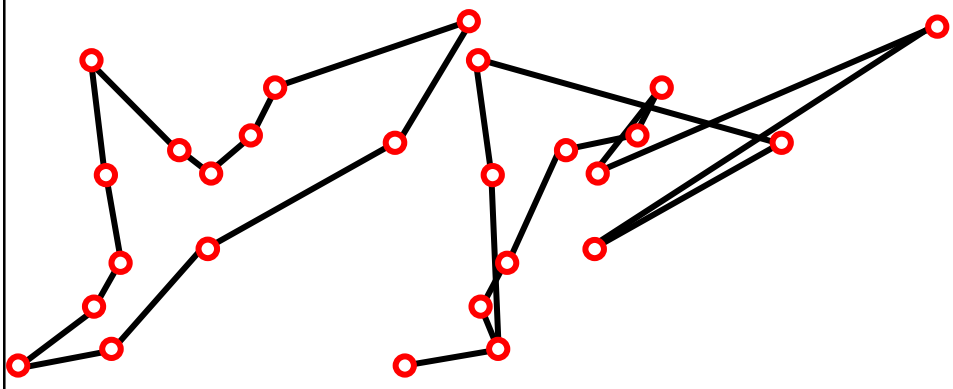
Note that larger deviations from downhill search are allowed at high temperature







Another Example

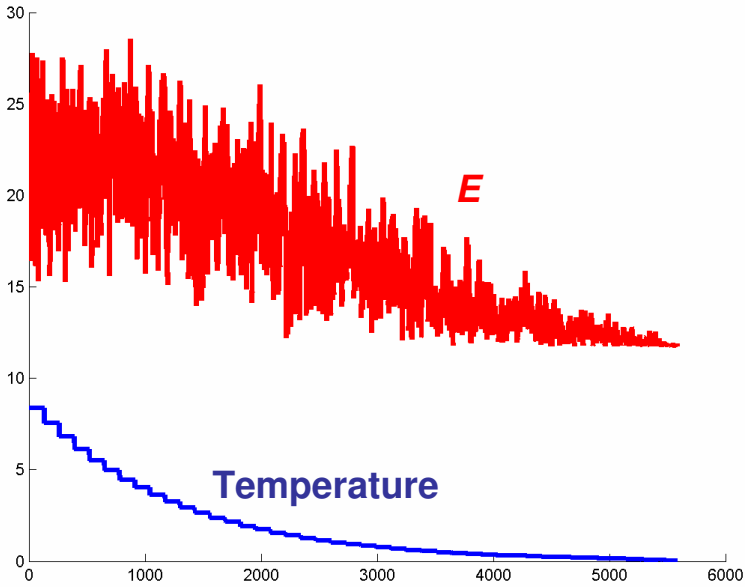


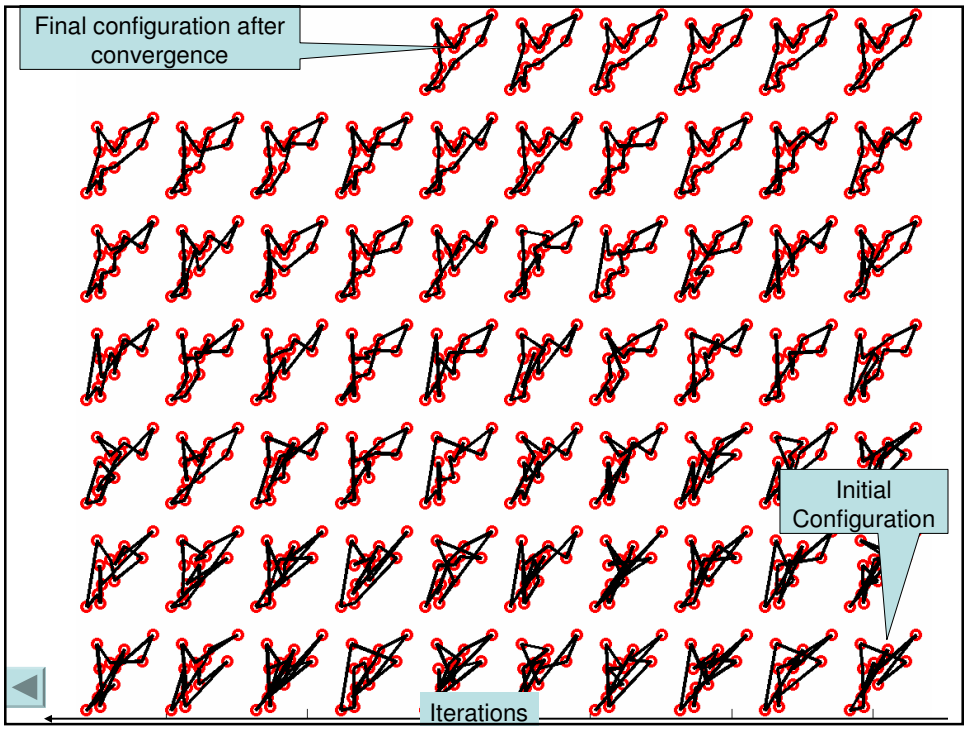
$N = 13$ nodes

Initial state

$K = 100N$

Another Example





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

- $X \leftarrow$ Initial configuration
- $T \leftarrow$ Initial high temperature
- Iterate:

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. $T \leftarrow \alpha T$

Many parameters need to be tweaked!!

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

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

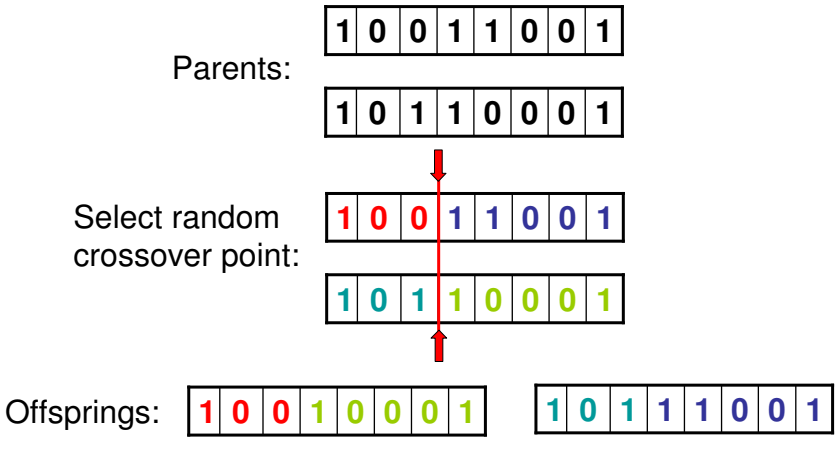
- Configurations represented by strings:

$X =$ | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 1 |

- 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

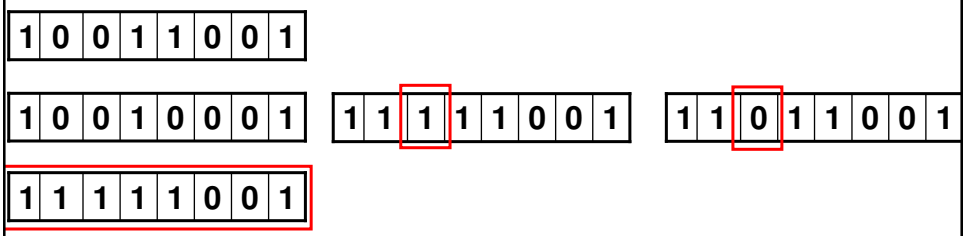
Genetic Algorithms: Reproduction



- An offspring receive part of the genes from each of the parents
- Implemented by crossover operation

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



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

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Stopping condition is not obvious?

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

Variation: Generate only one offspring

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

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

- 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)

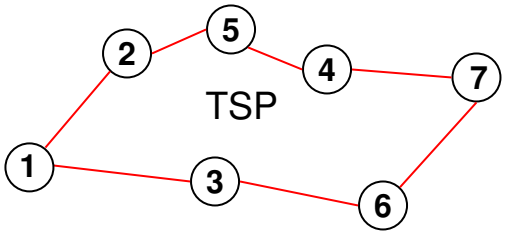
GA and Hill Climbing

- Create initial population $X = \{X_1,..,X_P\}$
- Iterate:
  1. Select K random
  2. For each pair of parents (X,X'):
     1.1 Generate offsprings (Y_1, Y_2) using crossover operation
     offspring Y_i:
     randomly selected element of the
     by Y_i
     With probability μ:
     Apply a random mutation to Y_i
- Return the best individual in the population

Hill-climbing component: Try to move uphill as much as possible

Random walk component: Move randomly to escape shallow local maxima

How would you set up these problems to use GA search?



TSP

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

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

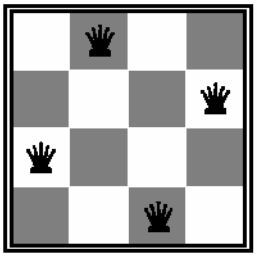
$\mathbf{B} \vee \mathbf{D} \vee \neg\mathbf{E}$

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

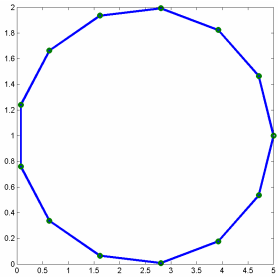
$\neg\mathbf{A} \vee \neg\mathbf{C} \vee \mathbf{E}$

……

N-Queens



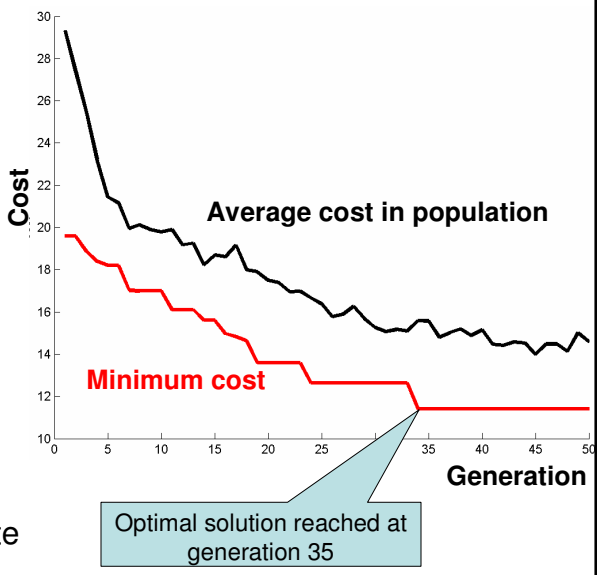
TSP Example

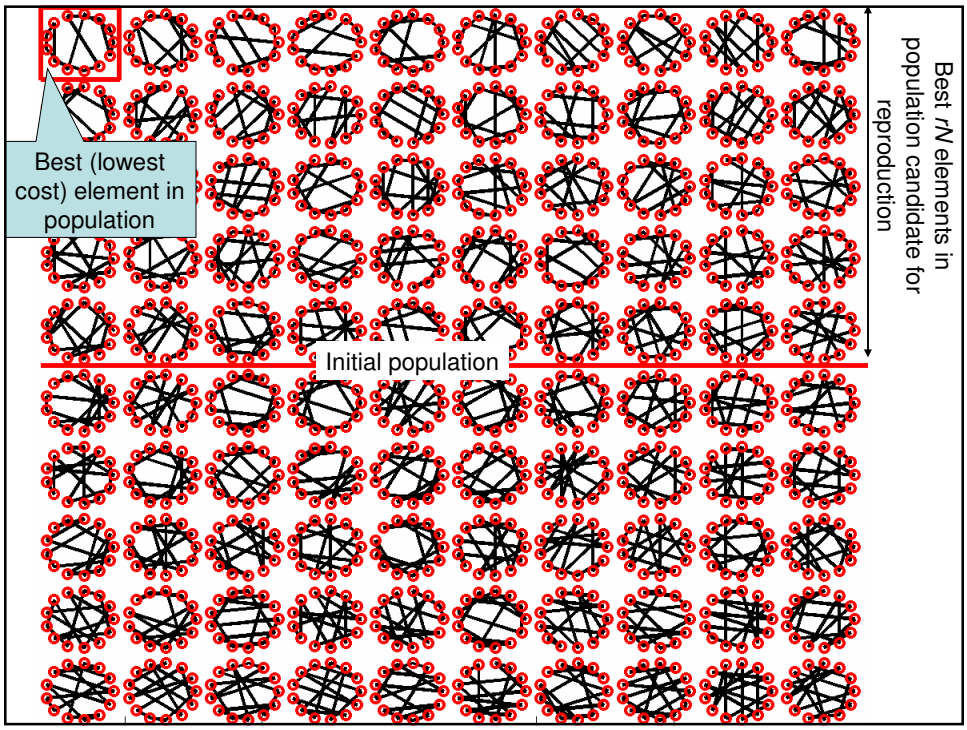


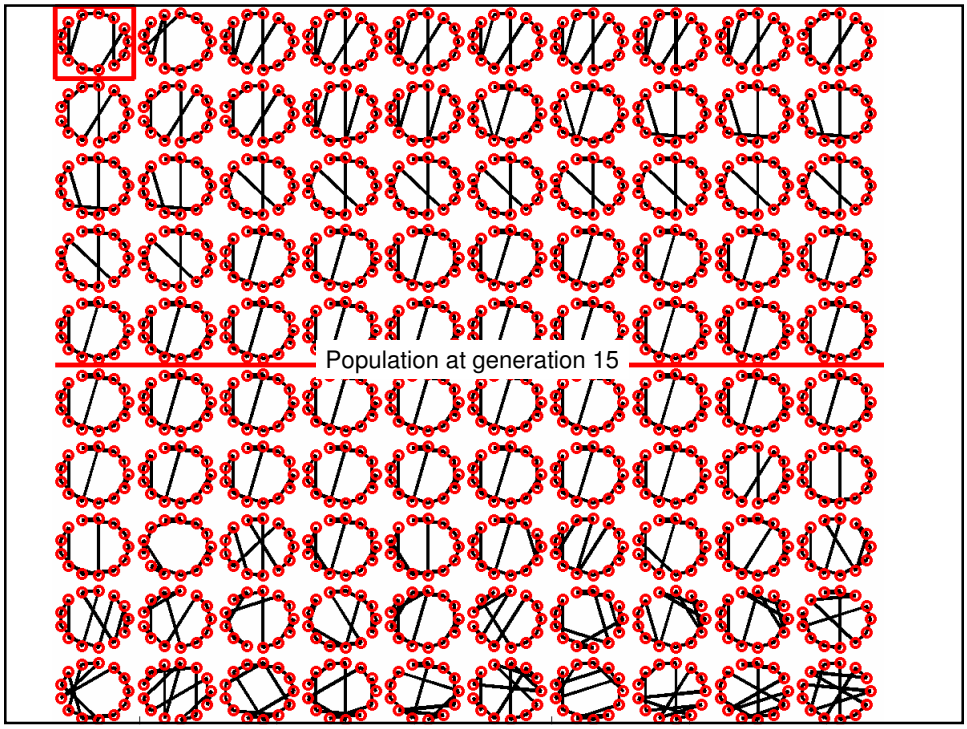
$N = 13$

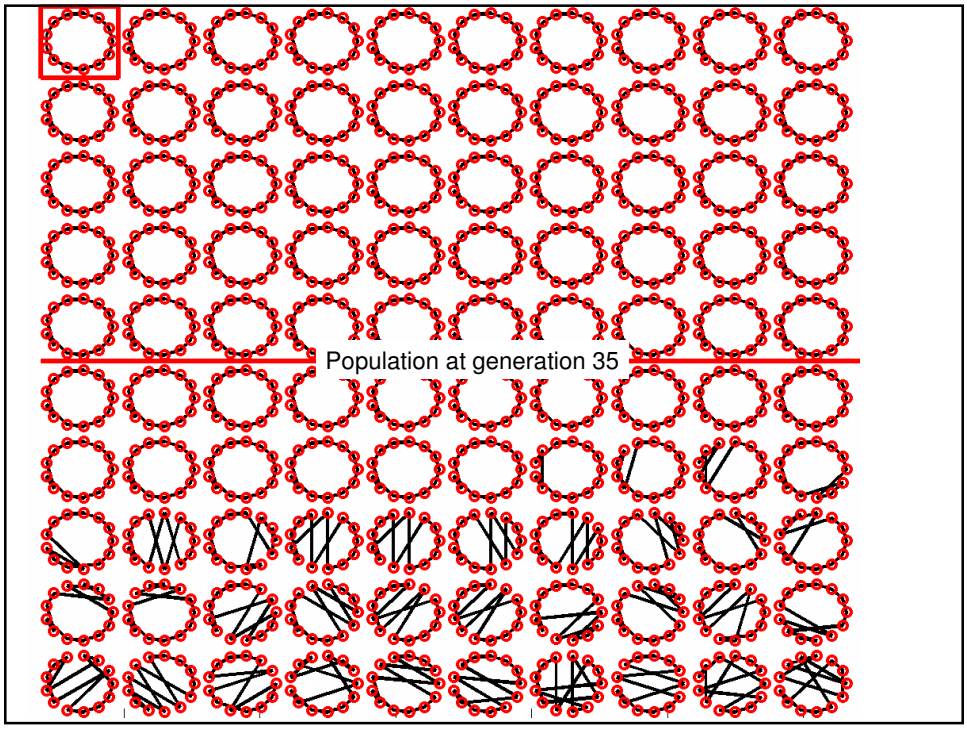
$P = 100$ elements in population

$\mu = 4\%$ mutation rate
$r = 50\%$ reproduction rate

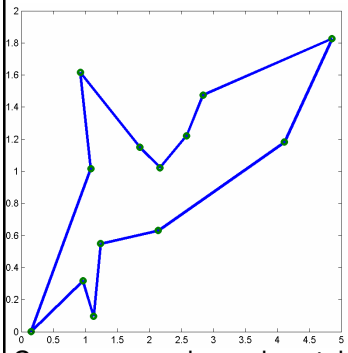


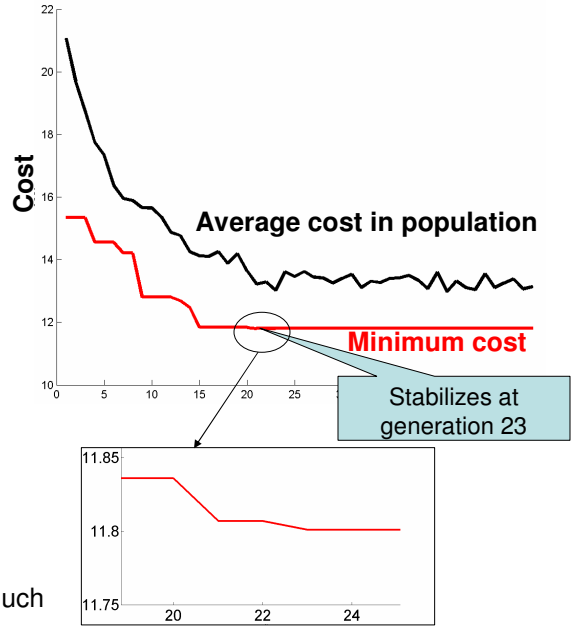



Population at generation 15


Population at generation 35

Another TSP Example





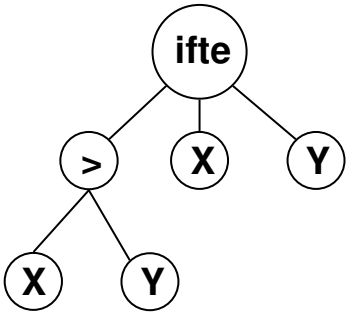
Converges and remains stable after generation 23

0.4% difference:
GA = 11.801
SA = 11.751

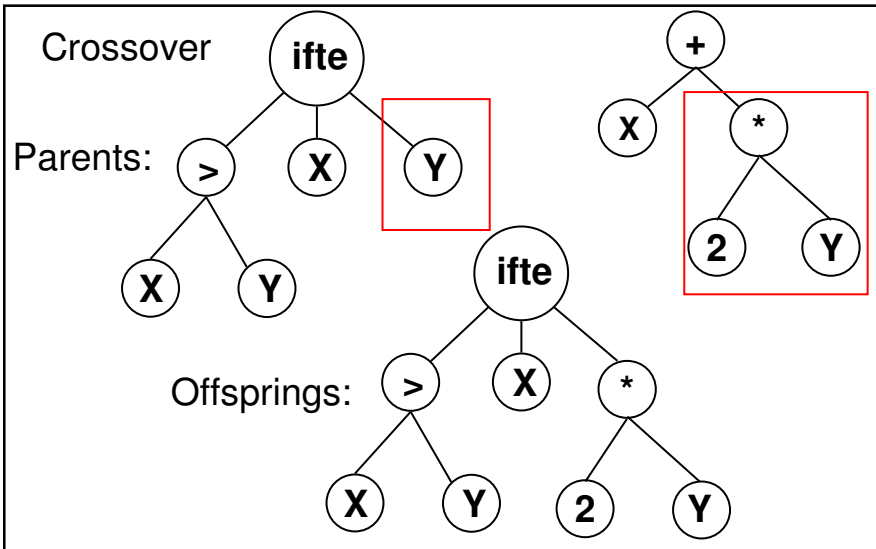
But: Number of operations (number of cost evaluations) much smaller (approx. 2500)

Even more radical ideas..

Individual = program
X = parse tree representing a program



(ifte (X > Y) X Y)



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 hill-climbing) → 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:

$$\text{Average of } \underset{X \text{ contains } s}{Eval(X)} \geq \text{Average of } \underset{Y \in \text{Population}}{Eval(Y)}$$

  - 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.

Summary

- Hill Climbing
- Stochastic Search
- Simulated Annealing
- Genetic Algorithms

- Class of algorithms applicable to many practical problems
- Not useful if more direct search methods can be used
- The algorithms are general black-boxes. What makes them work is the correct engineering of the problem representation
  - State representation
  - Neighborhoods
  - Evaluation function
  - Additional knowledge and heuristics

(Some) References

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