Lecture 5: Genetic algorithms. Constraint Satisfaction

- Global search algorithms
  - Genetic algorithms
- What is a constraint satisfaction problem (CSP)
- Applying search to CSP
- Applying iterative improvement to CSP

Recall from last time: Optimization problems

- There is a cost function we are trying to optimize (e.g. travelling salesman problem)
- There may be constraints that need to be satisfied
- The state space is the set of all possible solutions, which is usually combinatorial
- Local search methods start with some initial solution and try to improve it iteratively by moving to "neighbouring" solutions.
  - Hill-climbing (aka gradient descent)
  - Simulated annealing
- Today: *global search*
  - Can jump around arbitrarily between possible solutions
  - Example: genetic algorithms, ant colony optimization etc.

Evolutionary computation

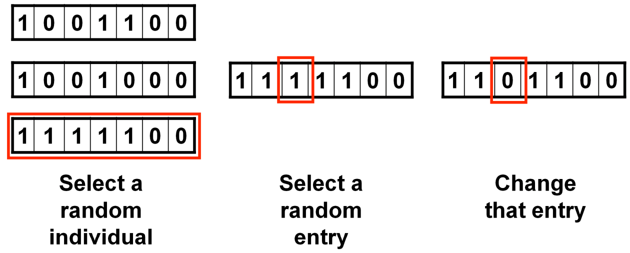
- Refers generally to computational procedures patterned after biological evolution
- Nature looks for the *best individual* (i.e. fittest)
- Many solutions (individuals) exist *in parallel*
- Evolutionary search procedures are also parallel, perturbing at random several potential solutions.

Genetic algorithms

- A candidate solution is called an *individual*
  - In a traveling salesman problem, an individual is a tour
- Each individual has a *fitness*: numerical value proportional to the evaluation function
- A set of individuals is called a *population*
- Populations change over *generations*, by applying *operations* to individuals: selection, mutation, crossover
- Individuals with higher fitness are more likely to survive, as well as to reproduce
- Individuals are typically represented by binary strings, to allow the evolutionary operations to be carried out easily

Mutation

- Mutation is a way of generating desirable features that are not present in the original population, by *injecting random changes*
- Typically mutation just means changing a 0 to a 1 (and vice versa)



- The mutation rate μ gives the probability that a mutation will occur in an individual
- We can allow mutation in all individuals, or just in "offspring"

Crossover

- Consists of *combining parts of individuals* to create new individuals
- Single-point crossover: choose a crossover point, cut the individuals there, swap the pieces. E.g.:

$$\begin{array}{ccc} 101|1100 & & 011|1110 \\ & \Longrightarrow \text{ crossover } \Longrightarrow & \\ 011|0101 & & 101|0101 \end{array}$$

- Implementation: use a crossover mask, m, which is a binary string. In our example, $m = 111000$.

  Given two parents i and j, the offspring are generated by: $(i \wedge m) \vee (j \wedge \neg m)$, and $(i \wedge \neg m) \vee (j \wedge m)$
- Multi-point crossover can simply be implemented using arbitrary (possibly random) masks
- In some applications, crossover has to be restricted, in order to produce "viable" offspring

Genetic algorithm generic code

GA(Fitness, threshold, p, μ, r)

1. Initialize population P with p random individuals
2. Repeat
   (a) For each $X_i \in P$, compute Fitness(X_i)
   (b) If $\max_i$ Fitness(X_i) $\geq$ threshold return the fittest individual;
   (c) Else generate a new generation P_s through the following operations:
      i. *Selection: Probabilistically* select $(1-r)*p$ members of P to "survive" and copy them to P_s
      ii. *Crossover:* Probabilistically select $r*p/2$ pairs of individuals from P. For each pair, produce two offspring by applying the *crossover operator* (see next slides). Include all offspring in P_s.
      iii. *Mutation:* Randomly select $\mu*p$ individuals and flip one randomly selected bit in each individual
      iv. $P \leftarrow P_s$

Selection: Survival of the fittest

- Like in natural evolution, we would like the *fittest individual to be more likely to survive*
- Several possible ways to implement this idea:
  – *Fitness proportionate selection:* $Pr(i) =$ Fitness$(i)/\sum_{j=1}^{p}$ Fitness(j) (assuming fitness is positive)
  – *Tournament selection:* pick i, j at random with uniform probability, then with probability p, select the fitter one
    Only requires comparing two individuals, which may be easier in some applications (e.g. games) than computing a fitness measure
  – *Rank selection:* sort all hypotheses by fitness; then probability of selection is proportional to rank
  – *Softmax (Boltzman) selection:*

$$Pr(i) = \frac{\exp(Fitness(i)/T)}{\left(\sum_{j=1}^{p}\exp(Fitness(j)/T)\right)}$$

Elitism

- The best solution can "die" during evolution
- In order to prevent this, the best solution ever encountered can always be "preserved" on the side
- If the "genes" from the best solution should always be present in the population, it can also be copied in the next generation automatically, bypassing the selection process.
- Note that the best solution ever encountered is typically saved in hill climbing and simulated annealing as well

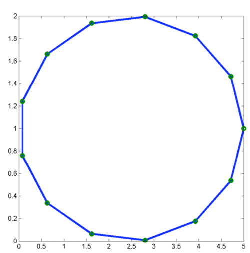
Genetic algorithms as search

- States: possible solutions
- Search operators: mutation, crossover, selection
- Parallel search, since several solutions are maintained in parallel
- An attempt at hill-climbing on the fitness function, but without following the gradient
- Mutation and crossover should allow getting out of local minima
- Very related to simulated annealing, but this is a global (not local) search method

TSP: Encoding as a GA

- Each individual is a tour (permutation of vertices)
- Mutation swaps a pair of edges (many other operations are possible, and have been tried in the literature)
- Crossover cuts the parents in two and swaps them *if this does not create an invalid offspring*
- Fitness is the length of the tour
- Note that the GA operations (crossover and mutation) are a lot fancier for this realistic problem than for simple binary examples!

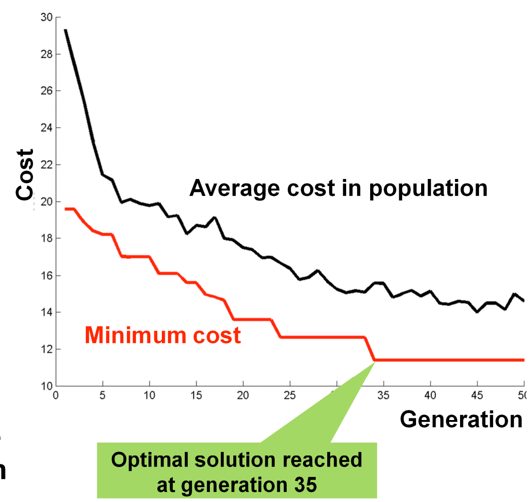
TSP example



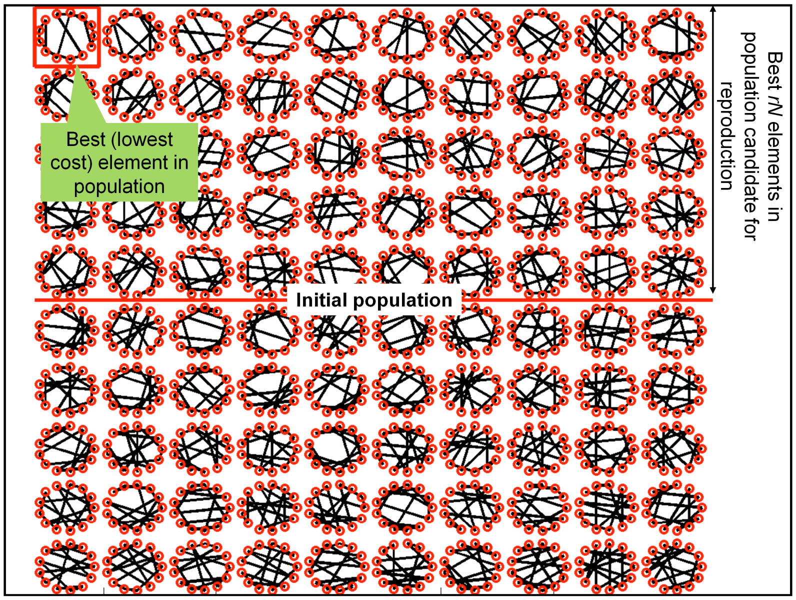
***N* = 13**

***P* = 100 elements in population**

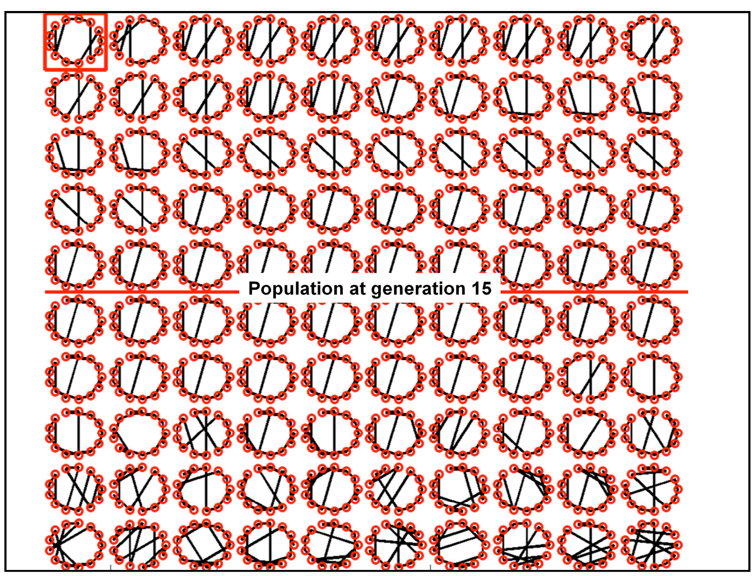
μ = 4% mutation rate
***r* = 50% reproduction rate**



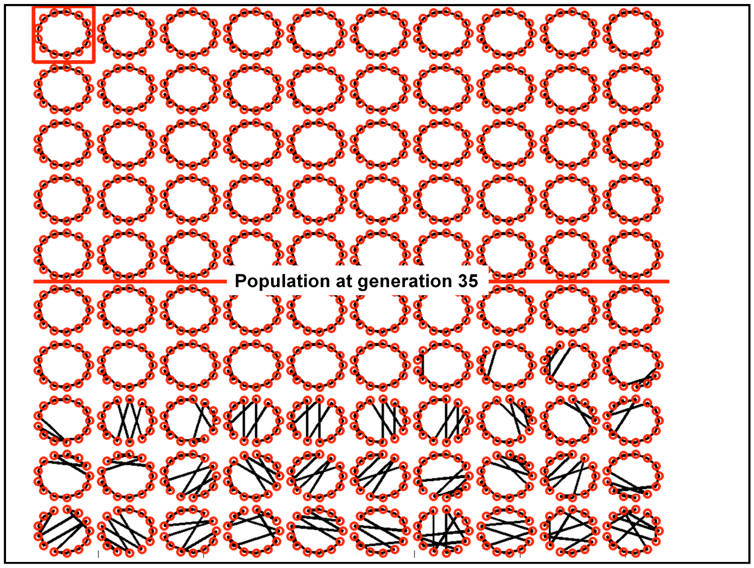
TSP example: Initial generation



TSP example: Generation 15



TSP example: Generation 30



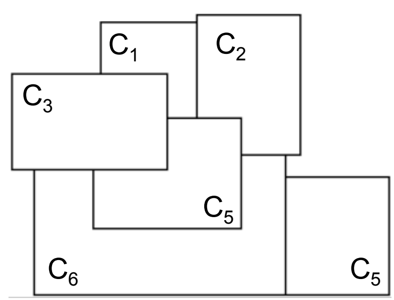
The good and bad of GAs

- Good things:
  - Aesthetically *pleasing*, due to evolution analogy
  - If tuned right, *can be very effective* (good solutions found with fewer calls to the evaluation function than for simulated annealing)
- Not-so-good things:
  - Performance depends crucially on the encoding of the problem for the GA, and *good encodings are difficult to find*
  - *Many parameters to tweak!* Bad parameter settings can result in very slow progress, or the algorithm becoming stuck
  - Some quirky phenomena, e.g *overcrowding:* too many individuals with the same genes are in the population, so genetic diversity is lost Overcrowding occurs especially if the mutation rate μ is too low, or if multiple copies of the same individual can be kept in the next generation

Constraint satisfaction problems

- We want to find a solution that satisfies a set of constraints
  Eg. Sudoku, crossword puzzles
- Typically, very few "legal" solutions exist
- One can think of this problem as a cost function with minimum value at the solution, maximum value elsewhere
- Hence, optimization algorithms may not be easy to apply directly

Canonical example: Graph coloring



- Color the nodes such that two adjacent vertices are not the same color
- *Variables*: V_i
- *Domains*: Red, Blue, Green
- *Constraints*: If there is an edge between V_i and V_j, their value (color) must be different)

Constraint satisfaction problems (CSPs)

- A CSP is defined defined by:
  - A set of *variables* V_i that can take *values* from *domain* D_i
  - A set of *constraints* specifying what combinations of values are allowed (for subsets of the variables)
  - Constraints can be represented:
    - Explicitly, as a list of allowable values (e.g., C_1 =red)
    - Implicitly, as a function testing for the satisfaction of the constraint (e.g. $C_1 \neq C_2$)
- A *CSP solution* is an assignment of values to variables such that all the constraints are true.
- We typically want to find *any solution* or find that there is *no solution*

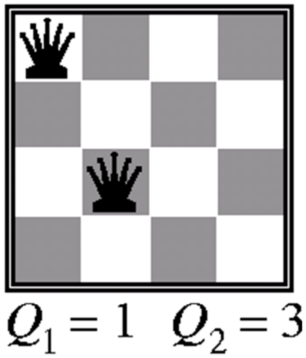
Example: 4-Queens as a CSP

Put one queen in each column. In which row does each one go?

Variables Q_1, Q_2, Q_3, Q_4

Domains $D_i = \{1, 2, 3, 4\}$

Constraints:
$Q_i \neq Q_j$ (cannot be in same row)
$|Q_i - Q_j| \neq |i - j|$ (or same diagonal)

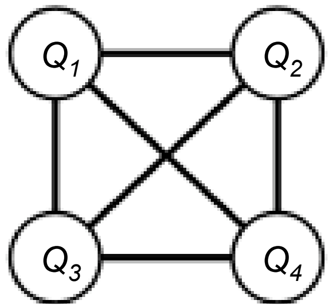


Translate each constraint into set of allowable values for its variables

E.g., values for (Q_1, Q_2) are $(1, 3)$ $(1, 4)$ $(2, 4)$ $(3, 1)$ $(4, 1)$ $(4, 2)$

Constraint graph

- *Binary CSP*: each constraint relates at most two variables
- *Constraint graph*: nodes are variables, arcs show constraints



- The structure of the graph can be exploited to provide problem solutions

Varieties of variables

- Boolean variables (e.g. satisfiability)
- Finite domain, discrete variables (e.g. colouring)
- Infinite domain, discrete variables (e.g. start/end of operation in scheduling)
- Continuous variables

Problems range from solvable in *poly-time* using linear programming to *NP-complete* to *undecidable*.

Varieties of constraints

- Unary: involve one variable and one value
- Binary
- Higher-order (involve 3 or more variables)
- *Preferences* (soft contraints): can be represented using costs, and lead to *constrained optimization problems*

Real-world CSPs

- Assignment problems (E.g., who teaches what class)
- Timetabling problems (E.g., which class is offered when and where?)
- Hardware configuration
- Transportation scheduling
- Factory scheduling
- Floor planning
- Puzzle solving (E.g. crosswords, Sudoku)

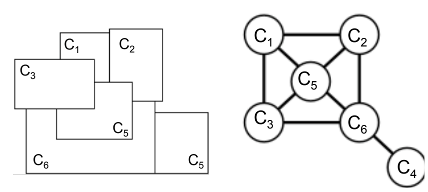
Applying standard search

- Assume a *constructive approach*:
  - States are defined by the values assigned so far
  - Initial state: all variables unassigned
  - Operators: assign a value to an unassigned variable
  - Goal test: all variables assigned, no constraints violated
- This is a general purpose algorithm, which works for all CSPs!

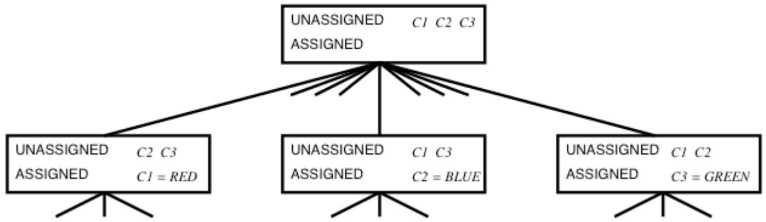
Example: Map coloring

Color a map so that no adjacent countries have the same color

Variables: Countries C_i
Domains: $\{Red, Blue, Green\}$
Constraints: $C_1 \neq C_2$, $C_1 \neq C_5$, etc.
Constraint graph:



Standard search applied to map coloring



Is this a practical approach? What is the complexity?

Analysis of the simple approach

- Maximum search depth = number of variables
  - All variables have to get some value
- Search algorithm to use: depth-first search
  - DFS is complete in this case because we know the maximum depth
- Branching factor $= \sum_i |D_i|$ (at the top of the tree, at least)
  - *This can be a big search!*

But: this can be improved dramatically by noting the following:

- The order in which variables are assigned is irrelevant, so many paths are equivalent
- Adding assignments cannot correct a violated constraint

Backtracking search

- Like depth-first search but:
  - Fix the order of assignment (branching factor becomes $|D_i|$)
- Algorithm:
  - Select the next unassigned variable X
  - For each value $x_i \in D_X$
    - If the value satisfies the constraint, assign $X = x_i$ and exit the loop
  - If an assignment was found, continue with the next variable
  - If no assignment was found, go back to the preceding variable and try a different value for it.
- This is the basic uninformed algorithm for CSPs

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

Forward checking

Main idea: Keep track of legal values for unassigned variables

- When assigning a value for variable X
  - Look at each unassigned variable Y connected to X by a constraint
  - Delete from Y's domain any value that is inconsistent with X's assignment

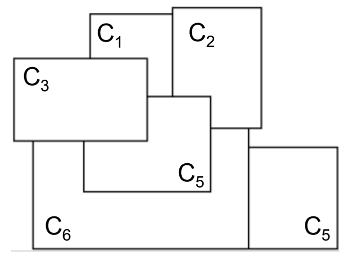
Can solve n-queens up to $n \approx 30$

Heuristics for CSPs

More intelligent decisions on:

- which value to choose for each variable
- which variable to assign next

Given C_1 = red, C_2 = green, choose C_3
Choose C_3 = green
least-constraining-value
Now what variable next? Choose C_5:
most-constrained-variable
For ties: *most constraining variable*



Taking advantage of problem structure

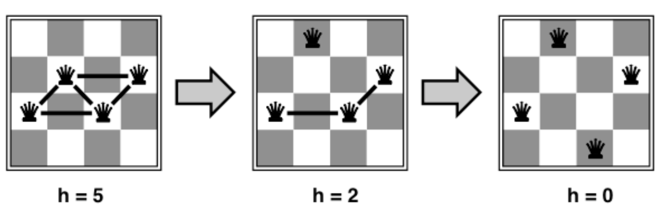
- Worst-case complexity is d^n (where d is the number of possible values and n is the number of variables)
- But a lot of problems are much easier!
- Disjoint components - can be solved independently
- Tree-structured constraint graphs - $O(nd^2)$
- Nearly-tree structured graphs - Complexity $O(d^c(n-c)d^2)$: Use *cutset conditioning*
  - Find a set of variables S which, when removed, turn the graph into a tree
  - Instantiate them all possible ways
  - Good if c, the size of the cutset S, is small

Iterative improvement algorithm for CSPs

- Start with a "broken" but complete assignment of values to variables
  - Allow states to have variable assignments that do not satisfy the constraints
- Randomly select conflicted variables
- Operators re-assign variable values
- This can be viewed as a relaxation of the cost function, which looks at the number of violated constraints as a cost to be minimized
  - *Min-conflicts heuristic*: choose value that violates the fewest constraints
  - I.e., approximate gradient descent on the total number of violated constraints
- Simulated annealing, genetic algorithms can be used here too.

Example: 4-Queens

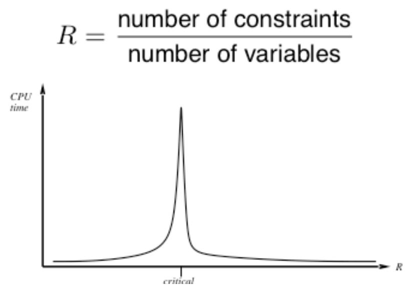
- States: 4 queens in 4 columns ($4^4 = 256$ states)
- Operators: move queen in column
- Goal test: no attacks
- Evaluation function: number of attacks



Performance of min-conflicts

- Given random initial state, can solve *n*-queens in almost constant time for arbitrary *n* with high probability (e.g., $n = 10^7$)
- The same appears to be true for any randomly-generated CSP *except* in a narrow range of the ratio

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



Summary

- CSPs are everywhere!
- Can be cast as search problems
- We can use either constructive methods or iterative improvement methods
- Iterative improvement methods using min-conflicts heuristic are very general, and often work better