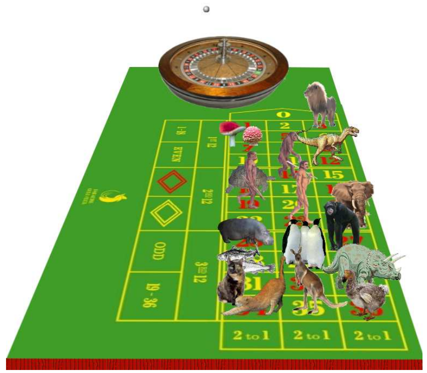
Algorithms and Analysis

Lesson 25: *Settle For Good Solutions*



neighbourhood search, heuristics, simulated annealing, GA

Outline

1. **Heuristic Search**
   - Constructive algorithms
   - Neighbourhood search
2. Simulated Annealing
3. Evolutionary Algorithms

Heuristic Algorithms

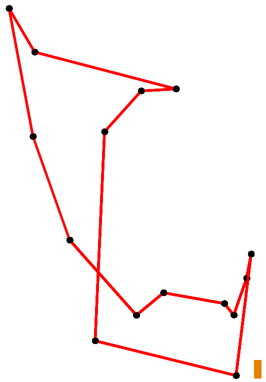
- Given that we know of no efficient algorithms for finding the optimal solution to NP-hard problems we must content ourselves with either
  - ⋆ Spending a very long time (e.g. using branch and bound)
  - ⋆ Accepting good solutions which aren't necessarily optimal
- Algorithms for finding good solutions are often called **approximation algorithms** or **heuristic algorithms**

Heuristics

- The idea behind heuristic algorithms is to use a rough guide or **heuristic** pointing you in reasonable direction
- If this heuristic is good you should find good solutions much faster than exhaustive search
- Two commonly used heuristics are
  - ⋆ A greedy heuristic (take the best move)
  - ⋆ Believe that good solutions are 'close' to each other

Constructive Algorithms

- Constructive algorithms build-up a solution
- They usually rely on a greedy heuristic
- They are very fast
- Once you have got a solution that's it
- They can give reasonable solutions quickly, but they are not usually very good



Neighbourhood search

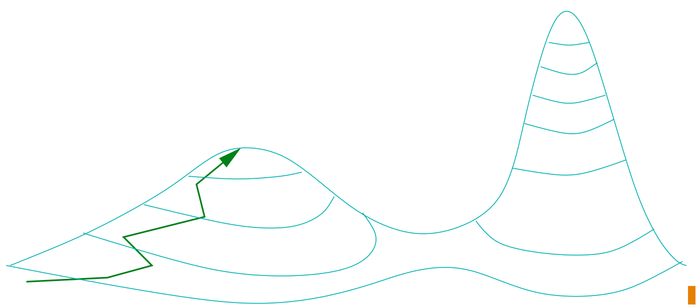
- An alternative to constructive algorithms are search algorithms relying on good solutions being close to each other
- In neighbourhood search we
  1. Start from some solution
  2. Examine the neighbouring solutions
  3. Move to a neighbour if it is better or, at least, not worse
  4. Repeat 2 until some stopping criteria
- If we are maximising this is often called a **hill-climber**
- If we are minimising it is often called **descent**

Iterative Improvement at its Best

- There are times when a neighbourhood algorithm will find the optimal solution
- The classic example of this is in **linear programming** where the simplex method leads to the optimal solution
- Other examples include
  - Maximum Flow
  - Maximum Matching in Bipartite Graphs
- Unfortunately, this doesn't always work

Local Optima

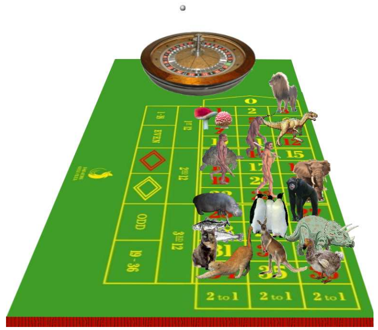
- Neighbourhood search is usually much slower than a constructive algorithm but tends to find better quality solutions
- However, it will often get stuck



Simple Fixes

- One simple fix is to restart from many different starting positions
- Or perturb the current solution and restart
- These give improvements over doing nothing, but aren't necessarily great strategies
- You can also increase the size of the neighbour to decrease the chance of getting stuck (e.g. in TSP swap more cites)

Outline

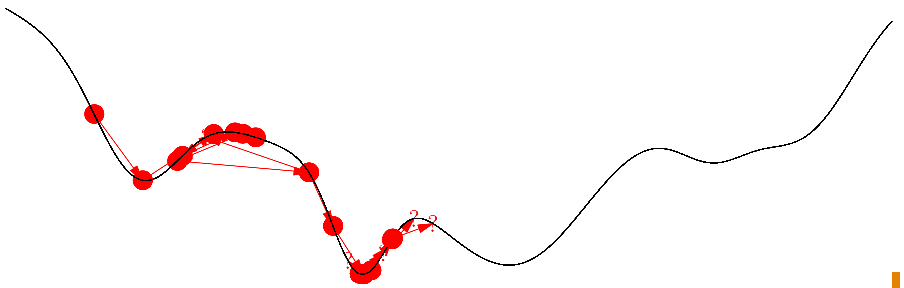


Simulated Annealing

- Simulated annealing is an example of a stochastic hill-climber
- Sometimes you go in the wrong direction (down-hill)
- Historically it is an idea from physics—where you tend to minimise energy
- Idea is to obtain a (low energy) crystalline material you very slowly let the material cool from a liquid state (opposite of quenching)

Stochastic Descent

- It is easier to fall down hill than to go back up



Simulated Annealing

- Algorithm to minimise energy $E(\boldsymbol{X})$ where $\boldsymbol{X} = (X_1, X_2, \ldots, X_N)$
- Starting from a random configuration $\boldsymbol{X}$
- Choose a neighbour $\boldsymbol{X}'$
- If the neighbour is better (lower energy) move to it
- Otherwise move to the neighbour with some probability
- The parameter β controls the probability of moving to a neighbour
- We increase β to reduce the probability of going uphill over time

Cooling Schedule

- The parameter β is known as the inverse temperature because of an analogy with physics
- Over time we have to increase β (decrease the temperature) so that the system will remain in the low energy state
- The way you reduce the temperature (increase β) is known as the cooling schedule
- Choosing a good cooling schedule can be critical
- Choosing a good cooling schedule is something of a black art

Convergence Theorem

- There is a theorem that says if you choose a slow enough cooling schedule you will end up in the global minimum eventually
- Unfortunately eventually is a very long time
- It is quicker to search all possible states
- Still people get very excited about convergence proofs

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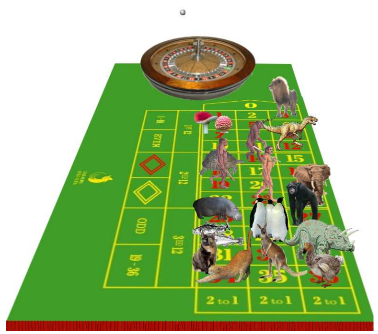
2. Simulated Annealing
3. **Evolutionary Algorithms**



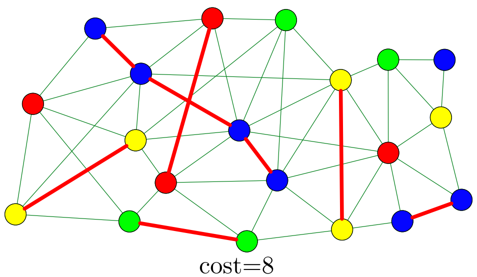
Genetic Algorithms

- Genetic algorithms are methods to evolve a population of potential candidates to find a good solution to an optimisation problem
- There are a whole set of related methods that go by the name of evolutionary algorithms, GAs are a subspecies of EAs
- They can be viewed as an engineering approach to solving hard problems
- I'm going to present my, highly prejudiced view of what's important in making a GA work

A Canonical GA

1. *Initialise population*
2. **for** $t = 1$ **to** T
   (a) *Evaluate fitness*
   (b) *Select* a new population based on fitness
   (c) *Mutate* members of the population
   (d) *Crossover* members of the population
3. Return best member of the population

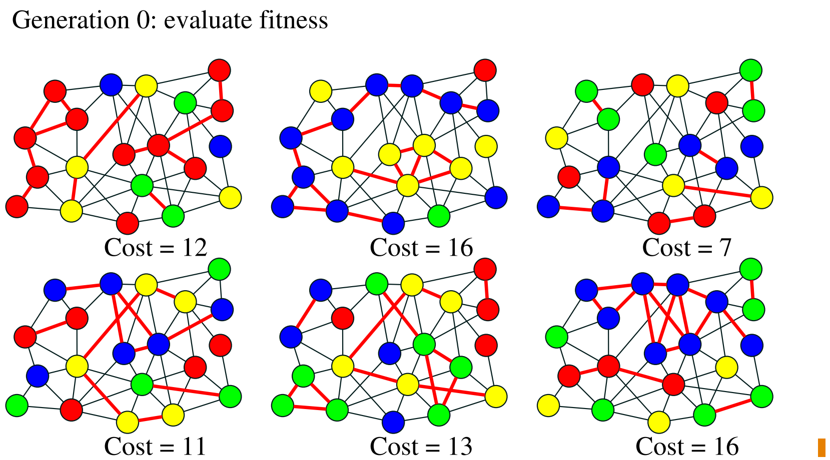
E.g. Graph Colouring



- Given a graph $G = (\mathcal{V}, \mathcal{E})$
- Assign colours, $c(v)$, to the vertices of the graph $v \in \mathcal{V}$
- Minimise the number of edges $e = (v, v') \in \mathcal{E}$ with the same coloured vertices $c(v) = c(v')$ (colour conflicts)

Initialise Population

Generate random colourings E.g.



Selection

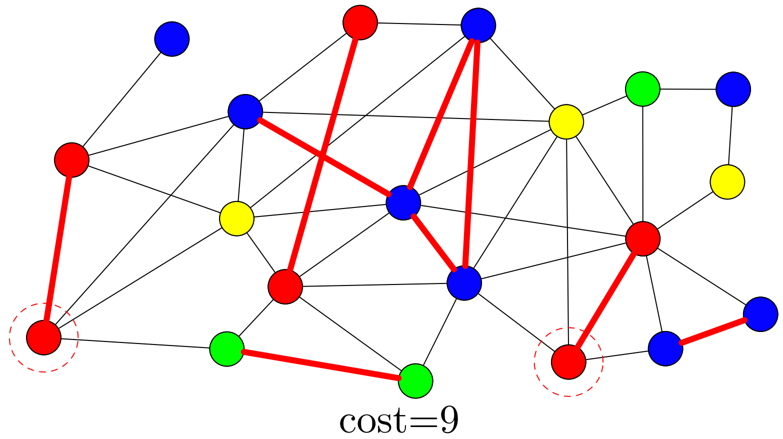
- Select a new population of P members preferentially choosing the fitter members
- Let w_α be a measure of the fitness of member α
- E.g. choose members α with a probability

$$p_\alpha = \frac{w_\alpha}{\sum_{\alpha'=1}^{P} w_{\alpha'}}$$

- Many different ways of doing this (some better than others)

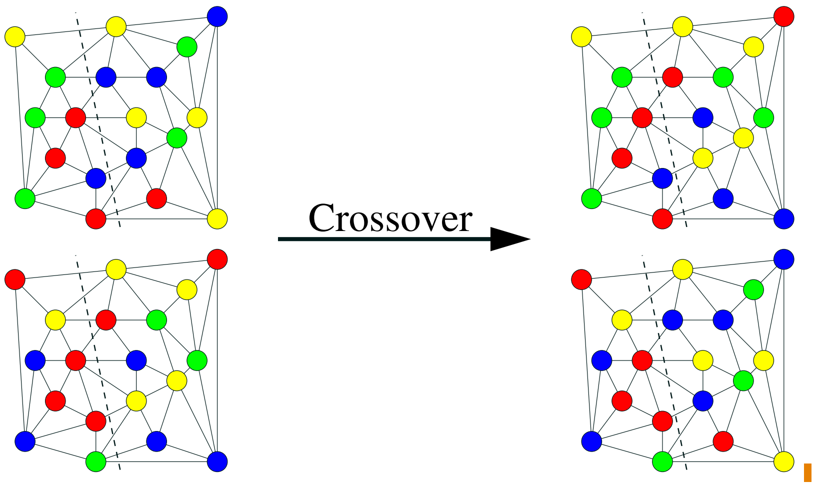
Mutation

Change the colour of one or more of the vertices E.g.



Crossover

Take two solutions and combine them to form a new solution E.g.



Crossover Operators

- Single-point crossover
  - Take two strings and cut them at some random site

$$\left.\begin{array}{l} (GRBGBR|BGGBGBG) \\ (RRBRGB|RGRBBGB) \end{array}\right\} \longrightarrow \left\{\begin{array}{l} (GRBGBR|RGRBBGB) \\ (RRBRGB|BGGBGBG) \end{array}\right.$$

- Multi-point crossover
  - Take two strings and cut them at several sites

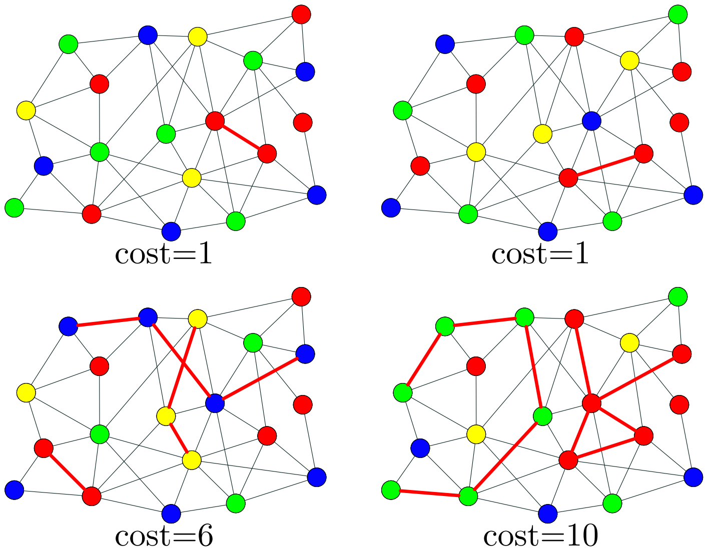
$$\left.\begin{array}{l} (GRBGBR|BGGB|GBG) \\ (RRBRGB|RGRB|BGB) \end{array}\right\} \longrightarrow \left\{\begin{array}{l} (GRBGBR|RGRB|GBG) \\ (RRBRGB|BGGB|BGB) \end{array}\right.$$

- Uniform Crossover
  - Take two strings and create children by a random shuffle

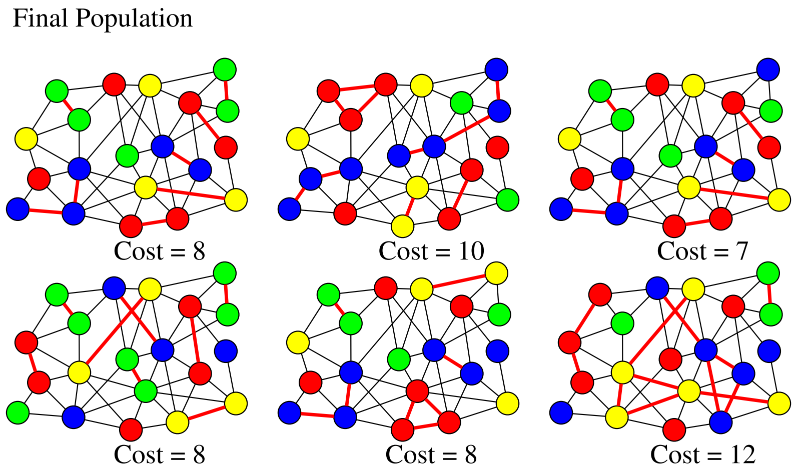
$$\left.\begin{array}{l} (GRBGBRBGGBGBG) \\ (RRBRGBRGRBBGB) \end{array}\right\} \longrightarrow \left\{\begin{array}{l} (GRBRGBRGRGGGB) \\ (RRBGBRBGGBBBG) \end{array}\right.$$

- Any of these crossover can be biased towards one parent

Cost of Crossover



GA



Bit Simulated Crossover

- Choose each variable independently with the probability proportional to the frequency of the allele in the population

$$\begin{array}{lll} (\cdots, B, \cdots) & (\cdots, R, \cdots) & (\cdots, G, \cdots) \\ (\cdots, R, \cdots) & (\cdots, B, \cdots) & (\cdots, G, \cdots) \\ (\cdots, B, \cdots) & (\cdots, G, \cdots) & (\cdots, B, \cdots) \\ (\cdots, B, \cdots) & & \end{array}$$

$$p_i(B) = 0.5, \quad p_i(G) = 0.3, \quad p_i(R) = 0.2$$

- New algorithms built on this idea, "Estimation of Distribution Algorithms" EDAs

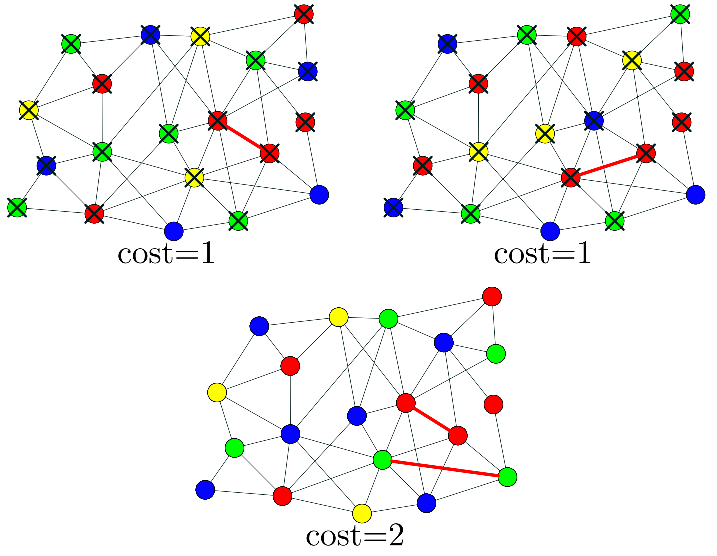
Galinier and Hao's Crossover Operator

- Choose two parents
- Sort nodes into colour-groups

	Parent 1	Parent 2
B	{1,3,4,8,. . . }	{3,5,7,10, . . . }
G	{2,6,7,10,. . . }	{1,11,12,13, . . . }
R	{5,9,11,12,. . . }	{2,3,6,8, . . . }
⋮	⋮	⋮

- Choose largest colour-group in parent 1
- Eliminate all nodes from that colour-group in parent 2
- Choose largest colour-group in parent 2
- etc.

Cost of Crossover



Other Heuristics

- There are many extensions to neighbourhood search, simulated annealing and genetic algorithms
- There are other techniques such as Tabu search
  - ⋆ Construct a list of place you cannot go to (usually the last few configurations)
  - ⋆ Make the best move you are allowed to make
  - ⋆ Rather a large number of *ad hoc* rules to make it work
  - ⋆ Often very fast but runs out of steam
- Many other EAs including particle swarm optimisations (PSO), ant colony optimisation (ACO), evolutionary strategies, . . .

Which Heuristic is Best?

- The best heuristic depends on the application
- Descent is very fast, but only finds local optima—good starting place
- Tabu search is often very fast, but sometimes fails to find really good solutions
- Simulated annealing and Genetic Algorithms are slow, but often find good solutions
- The best algorithms tend to be special purpose algorithms designed for the problem

Lessons

- For many problems the best strategy is to find a good solution, but not the best
- Iterative search usually give good quality solutions
- There are many variants of heuristic search
- Heuristic search algorithms aren't fast (don't use these techniques in an interactive program if you want to keep customers)
- For large combinatorial optimisation problems this is often the only choice