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

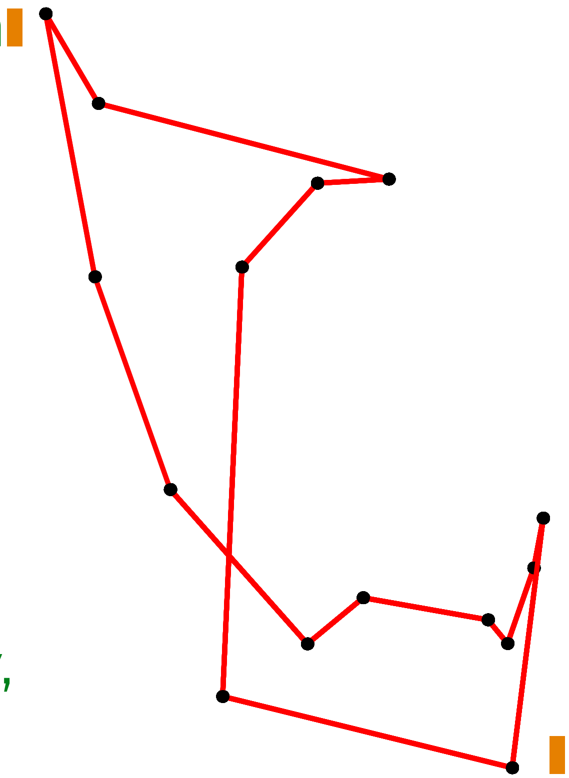
- Given that we know of no efficient algorithms for finding the optimal solution to NP-hard problems we must content ourselves with either
  - ⋆ Spending a very long time (e.g. using branch and bound)
  - ⋆ Accepting good solutions which aren't necessarily optimal
- Algorithms for finding good solutions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

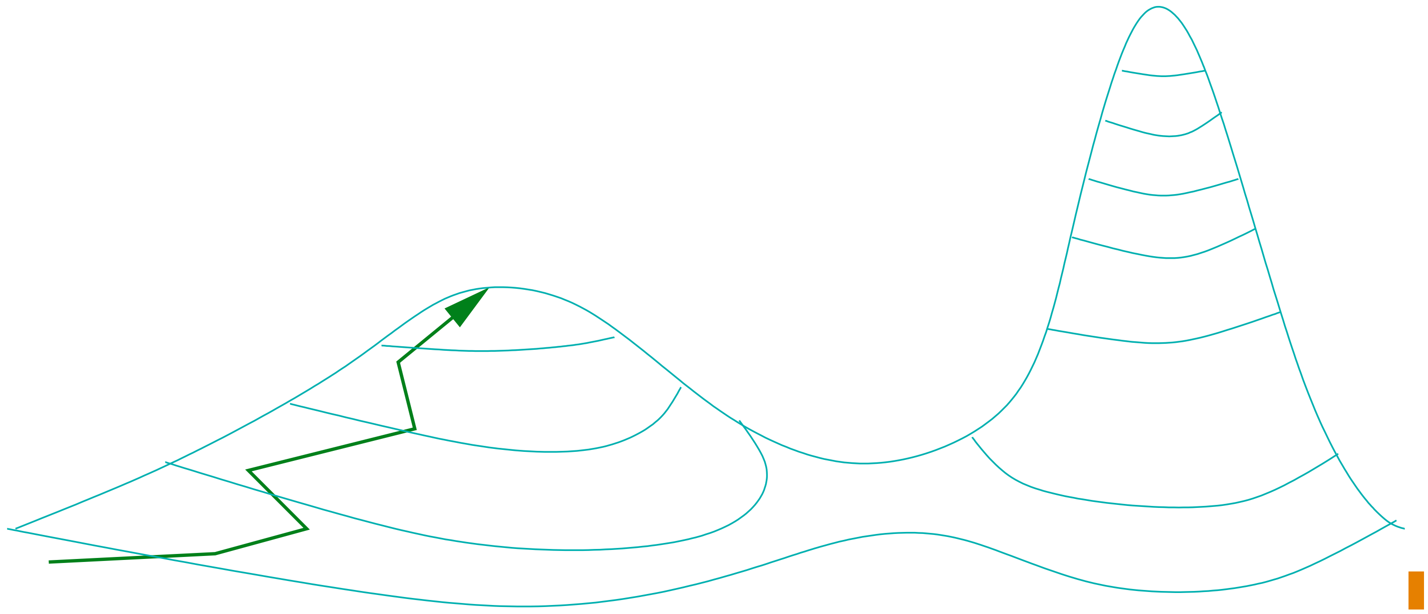
- An alternative to constructive algorithms are search algorithms relying on good solutions being close to each other
- In neighbourhood search we
  1. Start from some solution
  2. Examine the neighbouring solutions
  3. Move to a neighbour if it is better or, at least, not worse
  4. Repeat 2 until 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

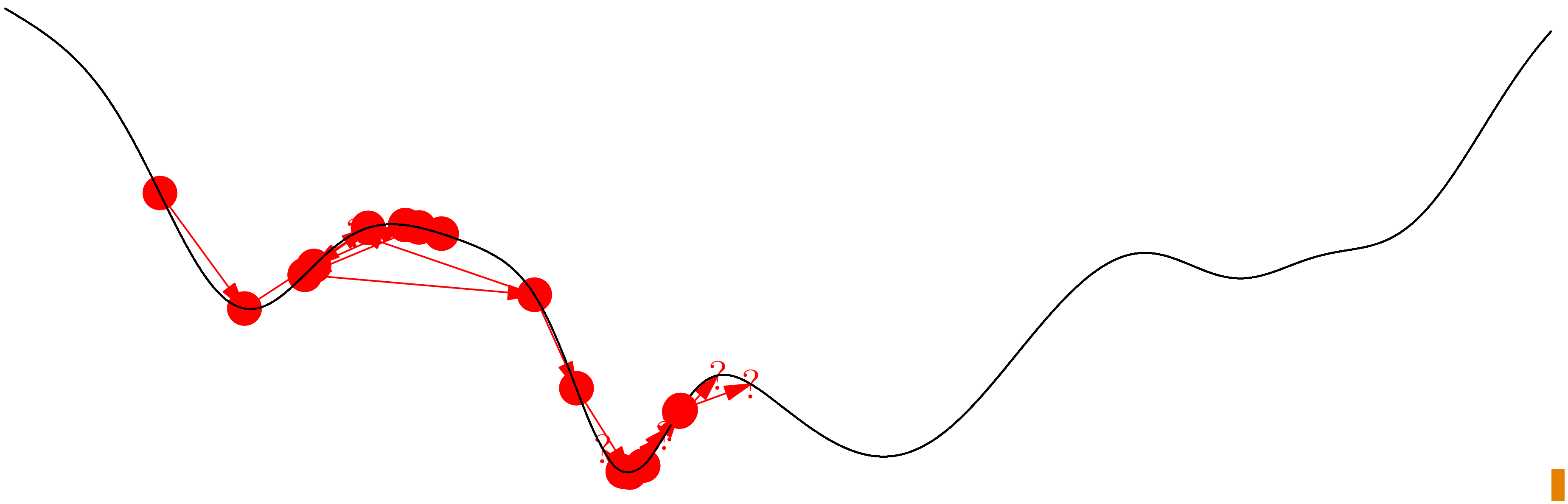
1. Heuristic Search
   - Constructive algorithms
   - Neighbourhood search
2. **Simulated Annealing**
3. Evolutionary Algorithms

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

Outline

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

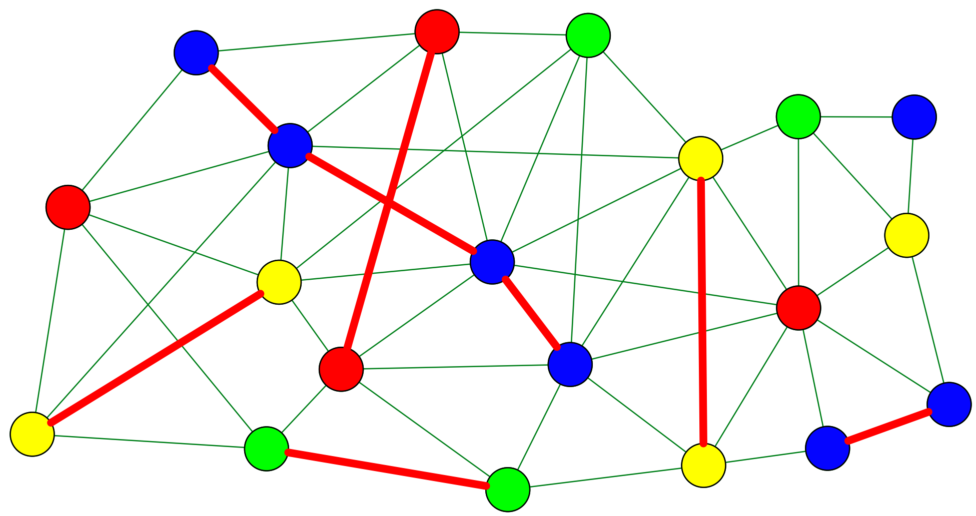
Genetic Algorithms

- 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



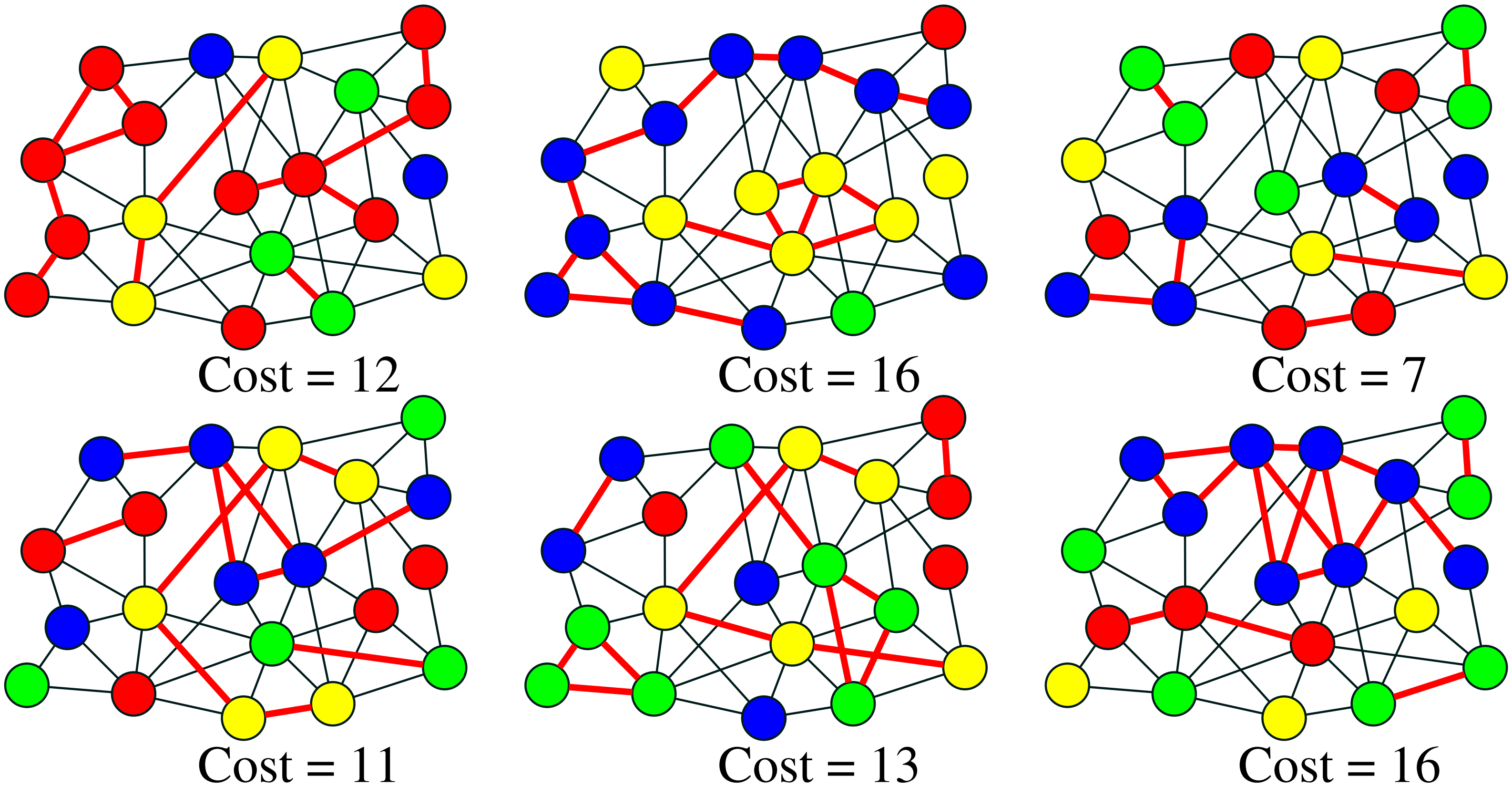
cost=8

- 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.

Generation 0: evaluate fitness



Selection

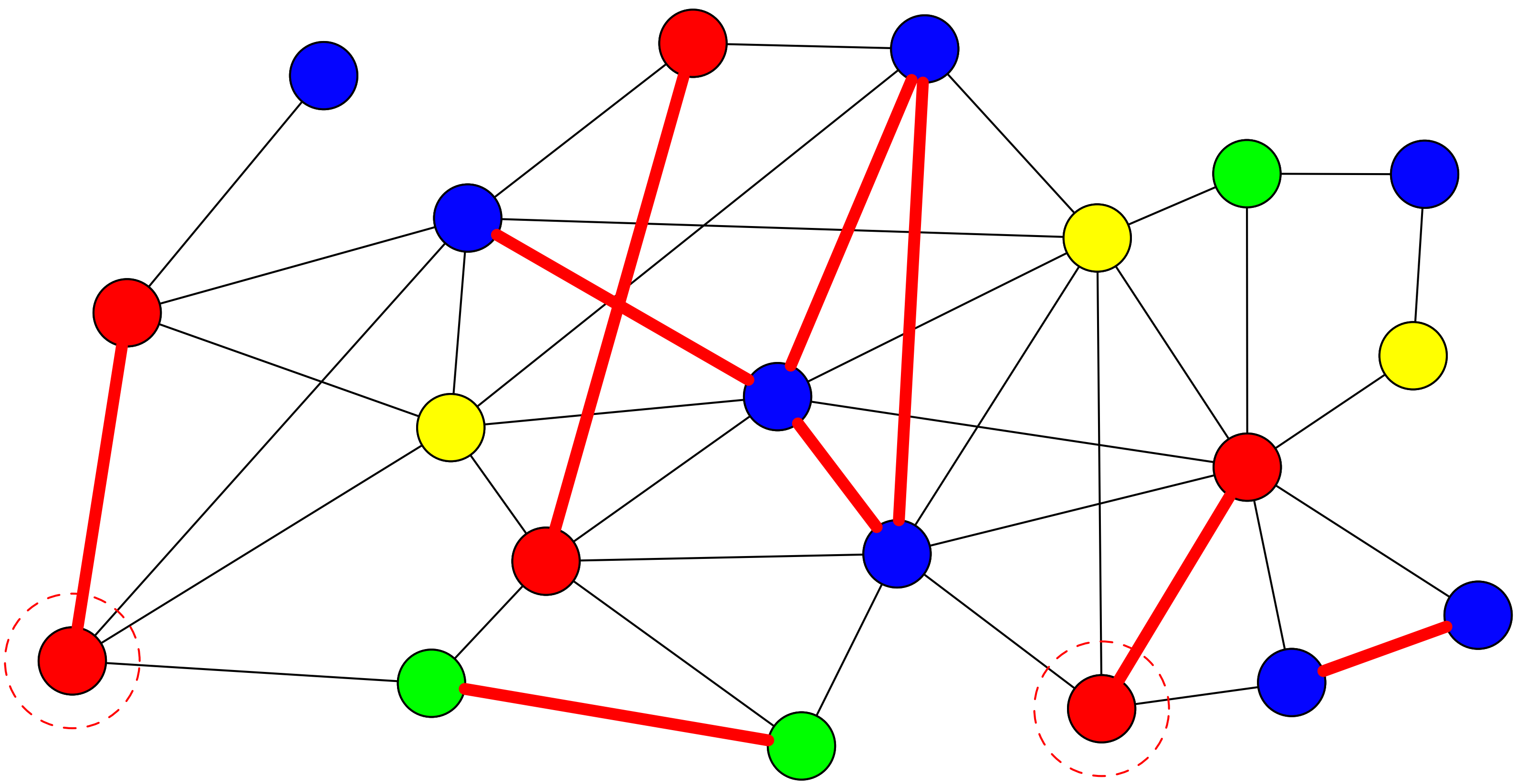
- Select a new population of P members preferentially choosing the fitter members
- Let w_α be a measure of the fitness of member α
- E.g. choose members α with a probability

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

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

Mutation

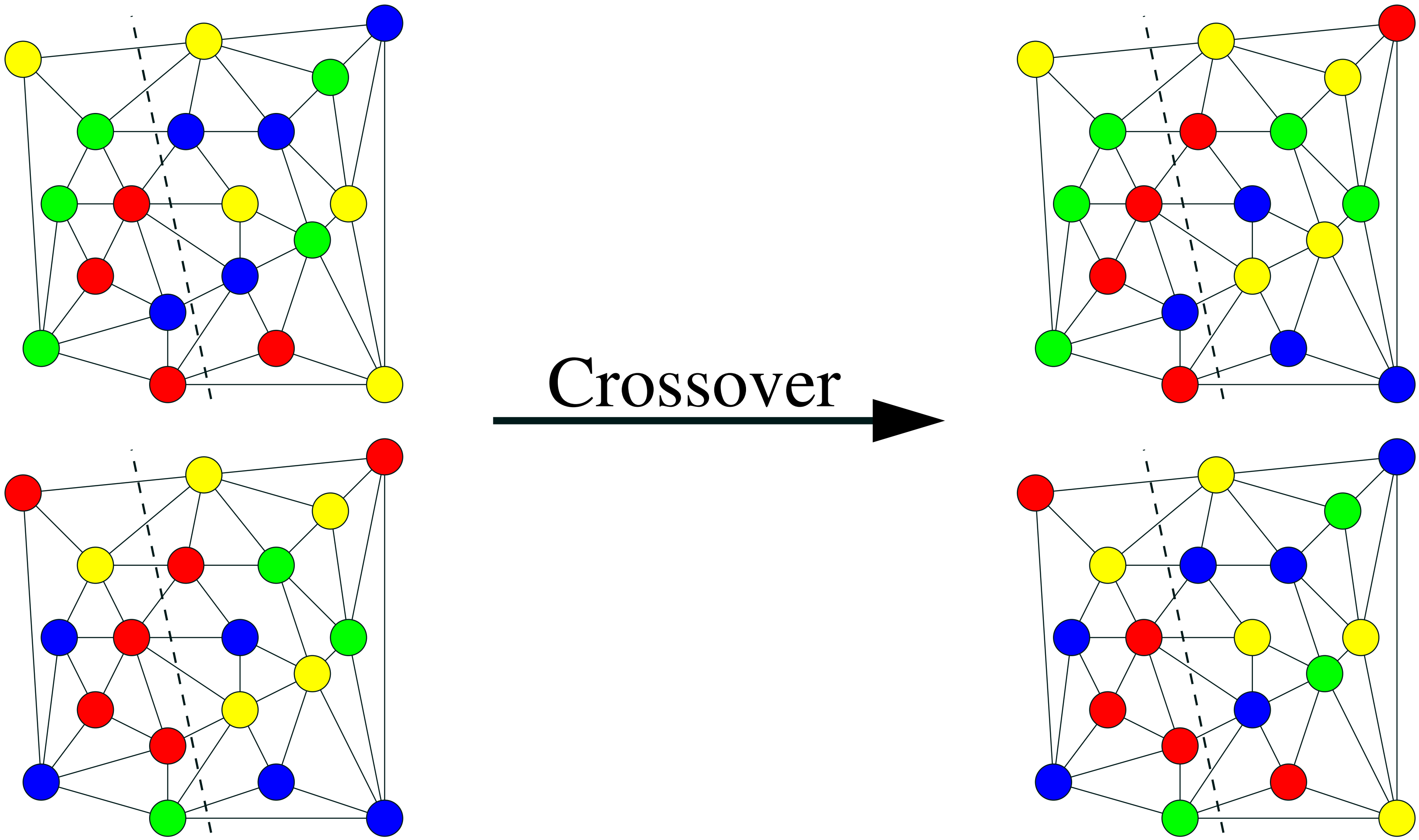
Change the colour of one or more of the vertices. E.g.



$\mathrm{cost}=9$

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

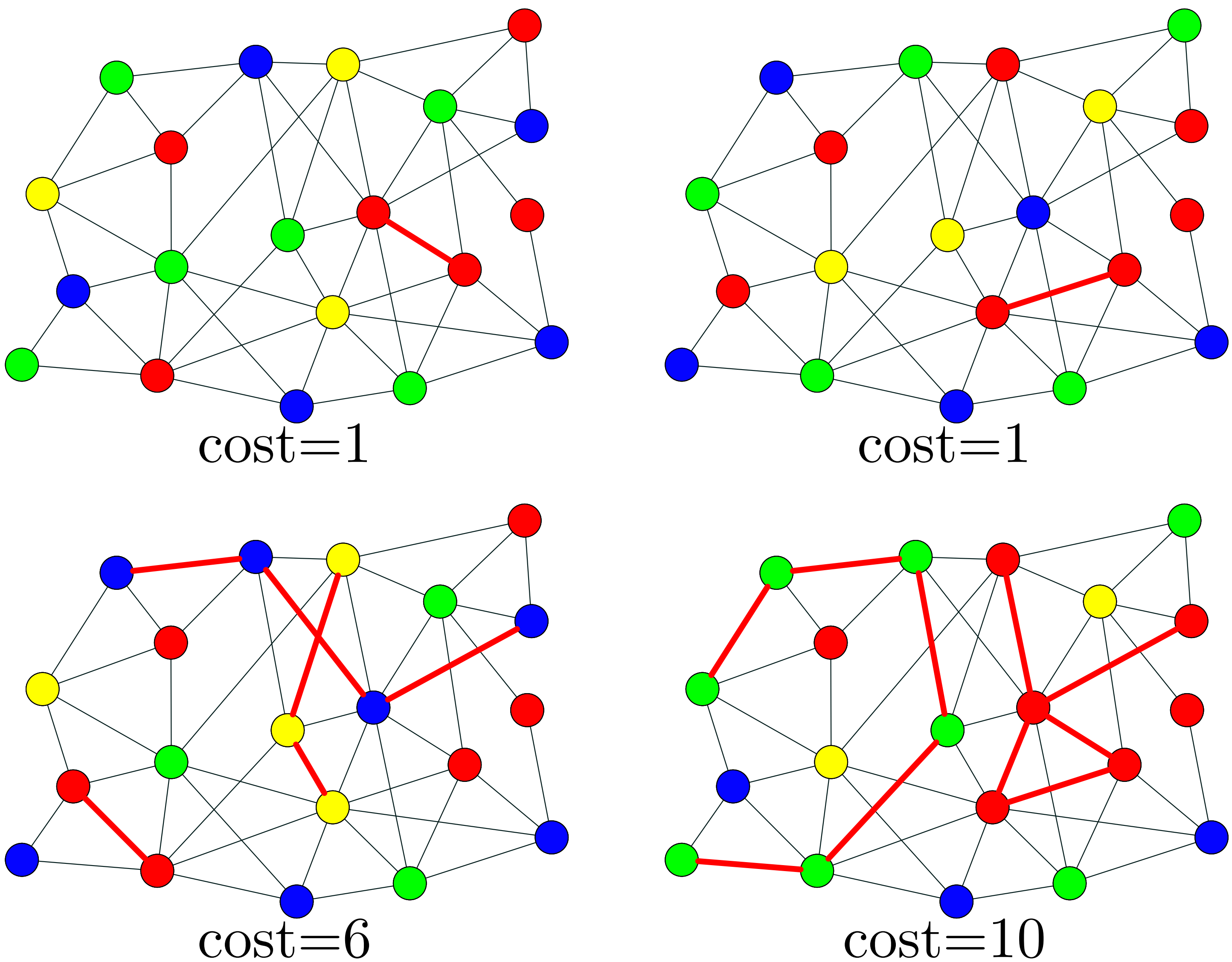
$$\left.\begin{array}{l}(GRBGBR|BGGB|GBG)\\(RRBRGB|RGRB|BGB)\end{array}\right\} \longrightarrow \left\{\begin{array}{l}(GRBGBR|RGRB|GBG)\\(RRBRGB|BGGB|BGB)\end{array}\right.$$

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

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

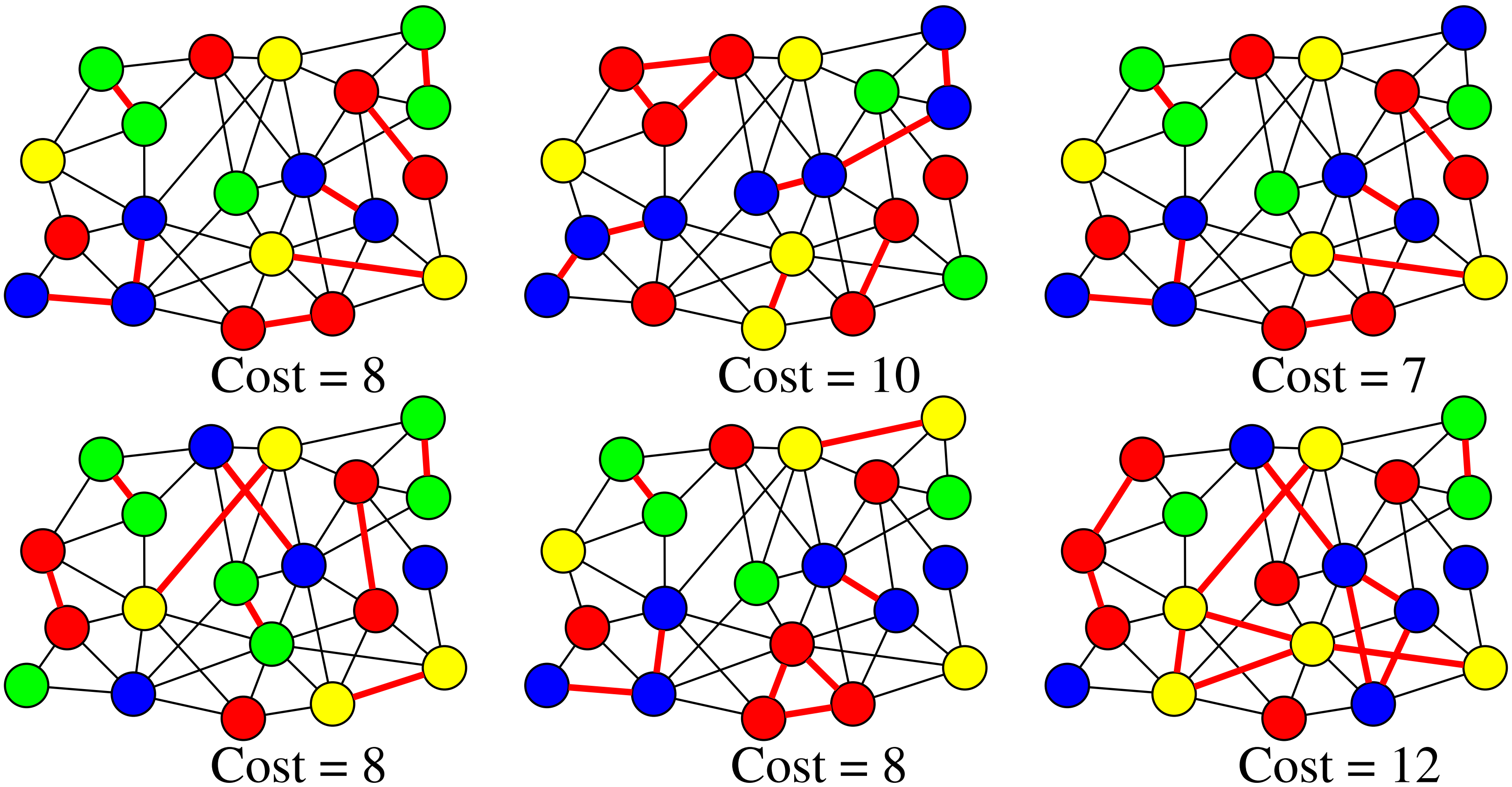
- Any of these crossover can be biased towards one parent

Cost of Crossover



GA

Final Population



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

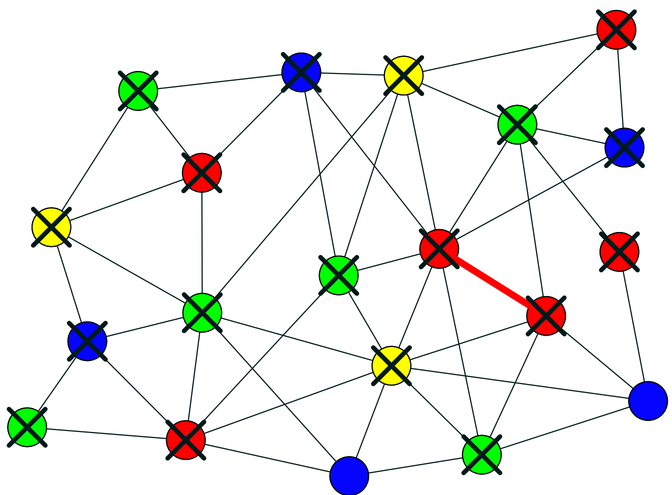
Galinier and Hao's Crossover Operator

- Choose two parents
- Sort nodes into colour-groups

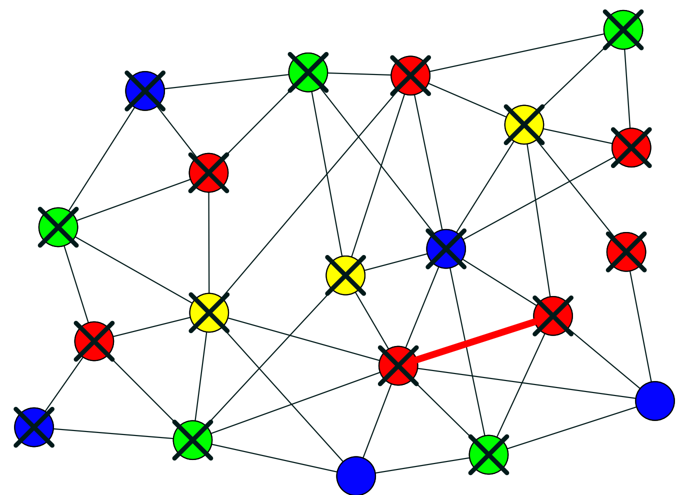
	Parent 1	Parent 2
B	{1,3,4,8,. . . }	{3,5,7,10, . . . }
G	{2,6,7,10,. . . }	{1,11,12,13, . . . }
R	{5,9,11,12,. . . }	{2,3,6,8, . . . }
⋮	⋮	⋮

- 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.

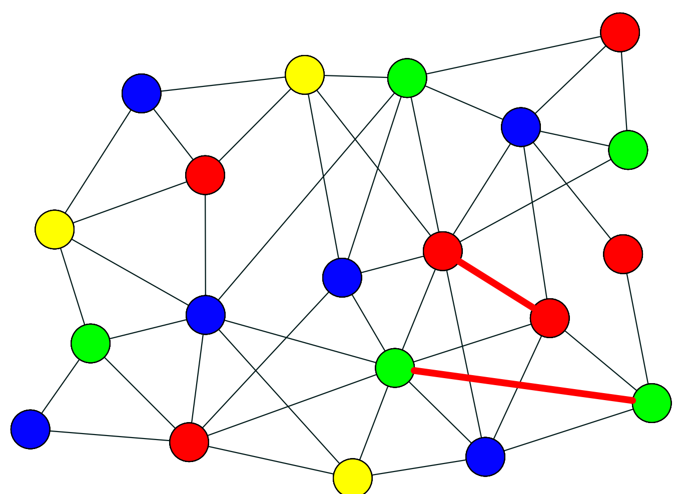
Cost of Crossover



cost=1



cost=1



cost=2

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