

Algorithms and Analysis

Lesson 26: *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**

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- 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)
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- 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

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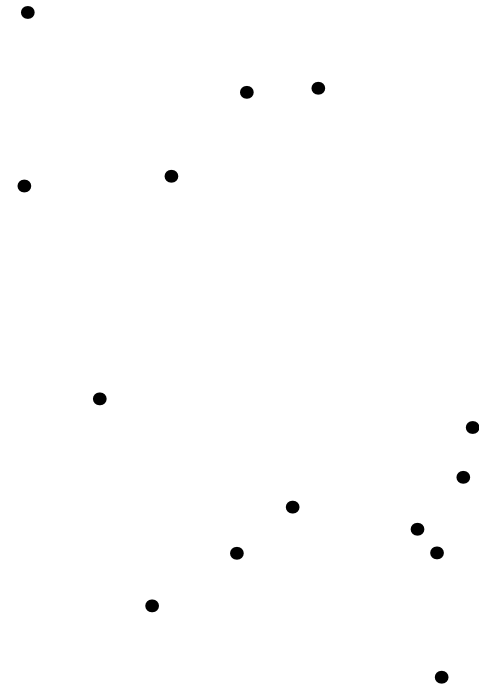
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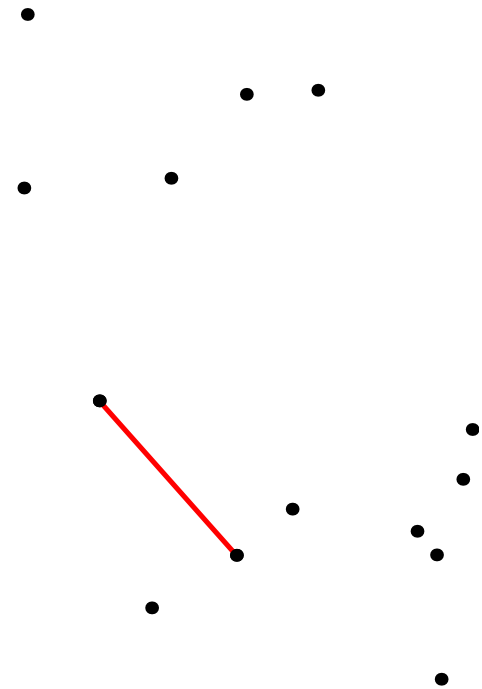
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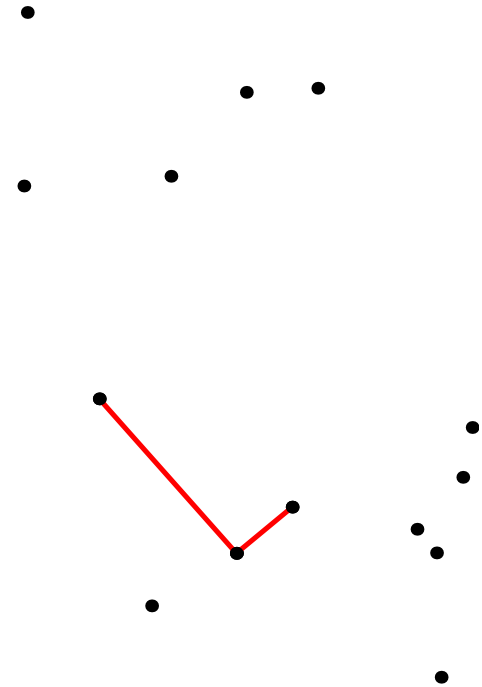
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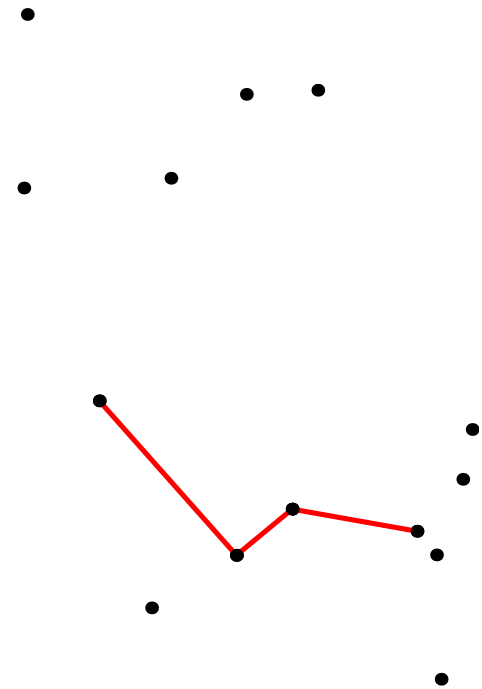
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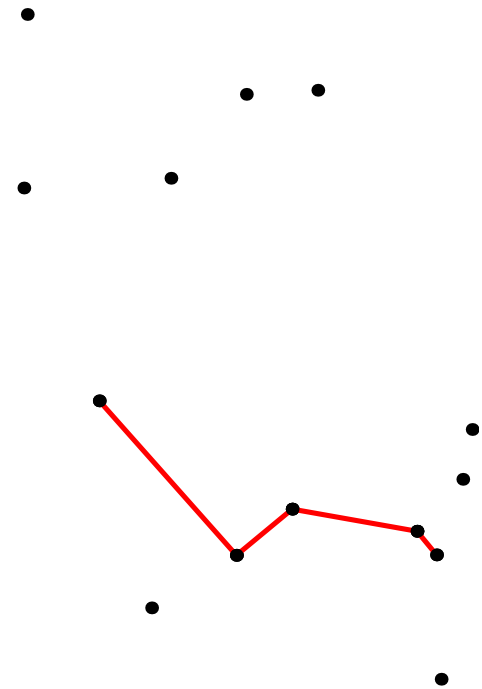
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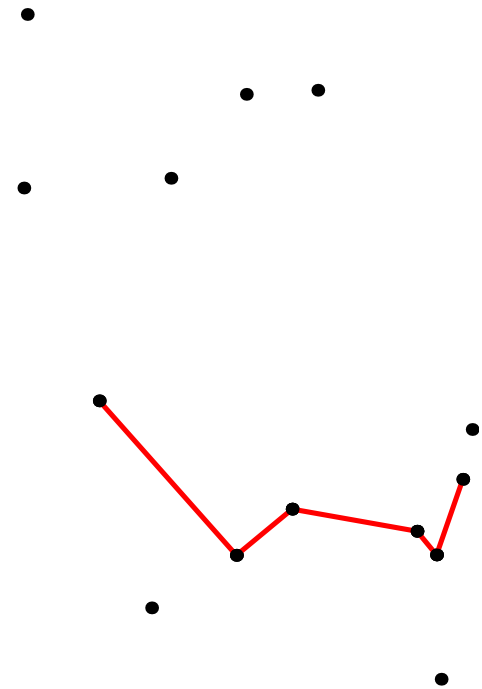
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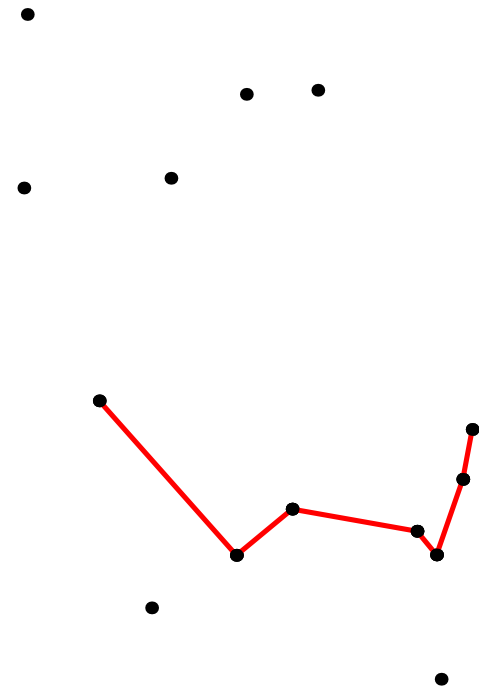
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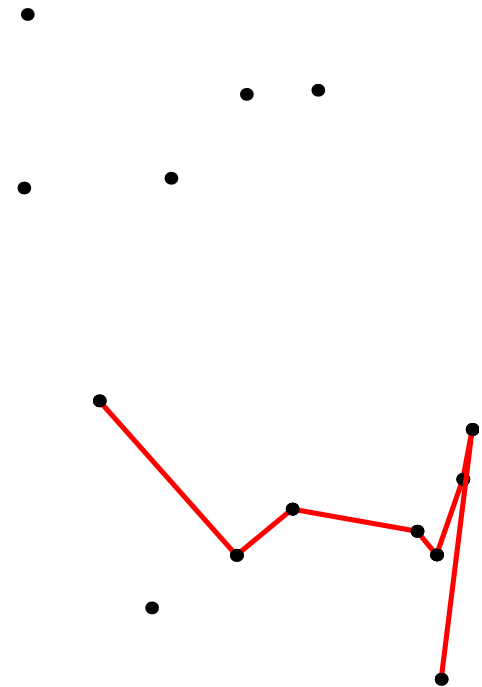
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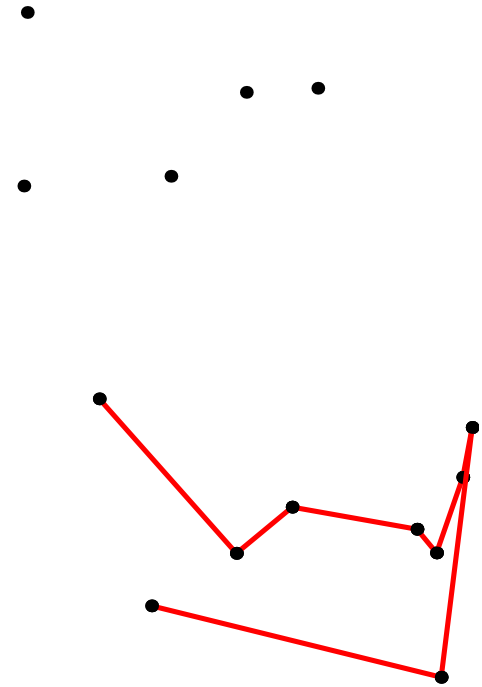
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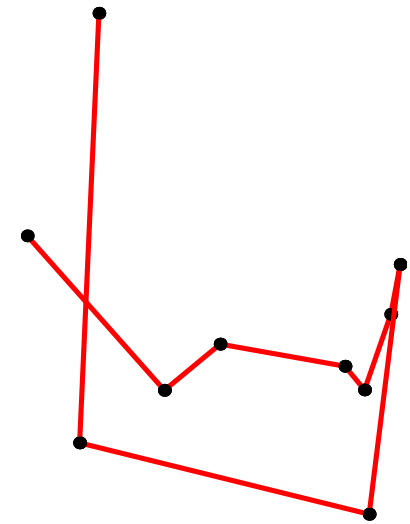
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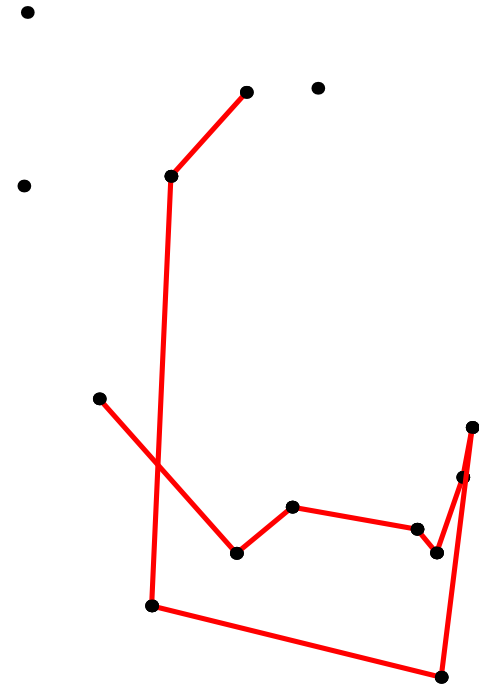
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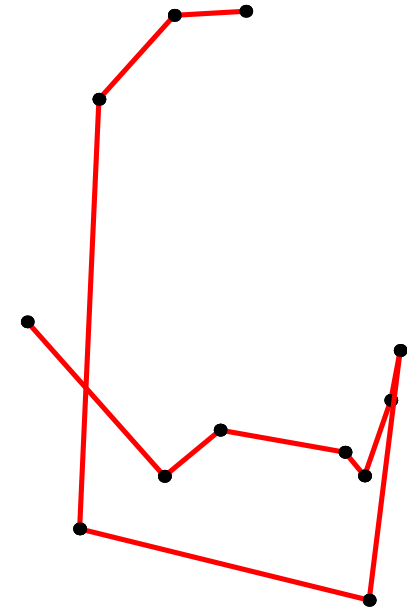
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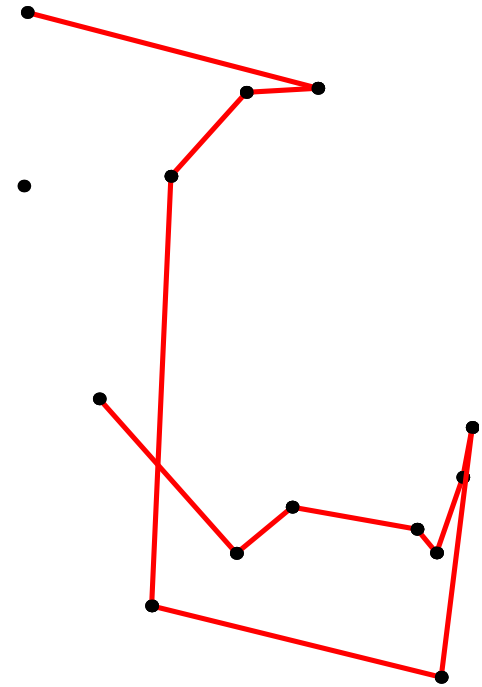
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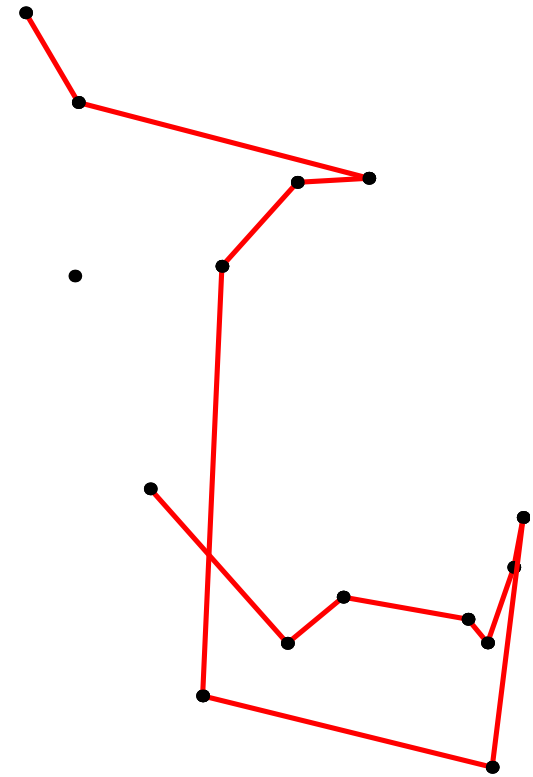
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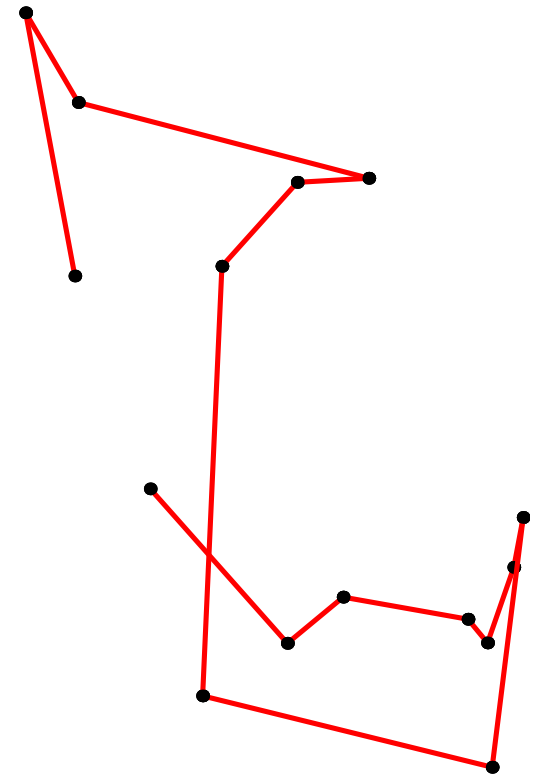
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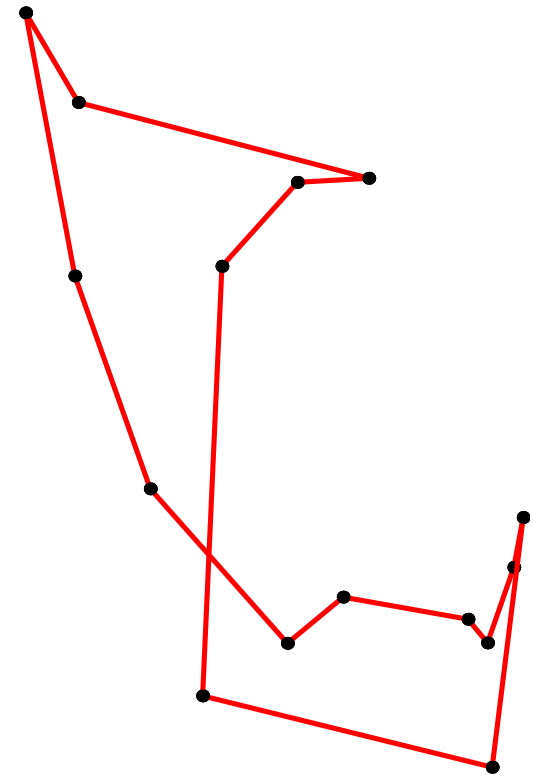
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Neighbourhood search

- 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**

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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

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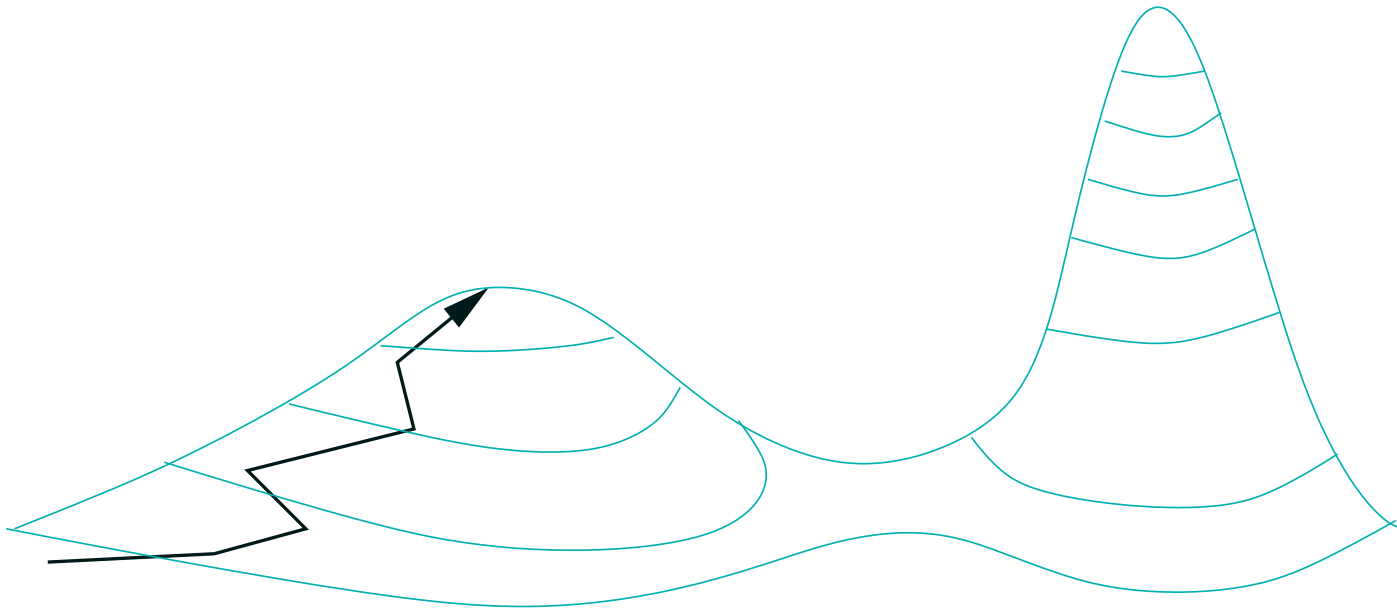
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- Unfortunately, this doesn't always work

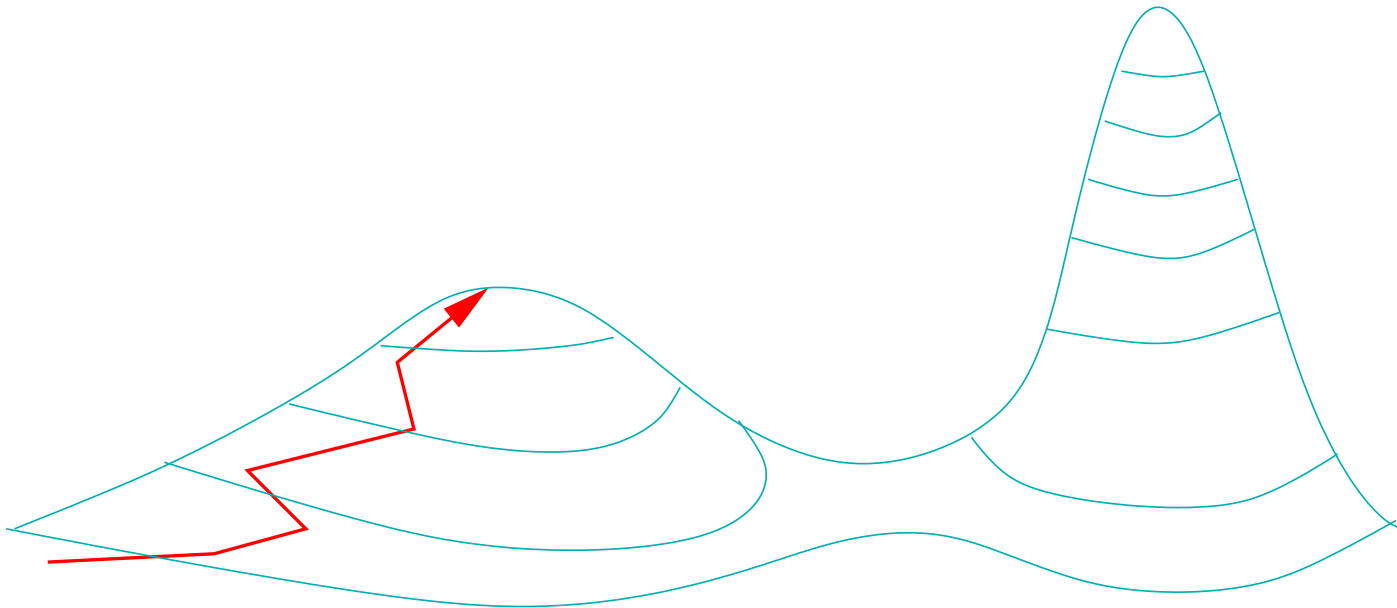
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Simple Fixes

- 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 cities)

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- 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)

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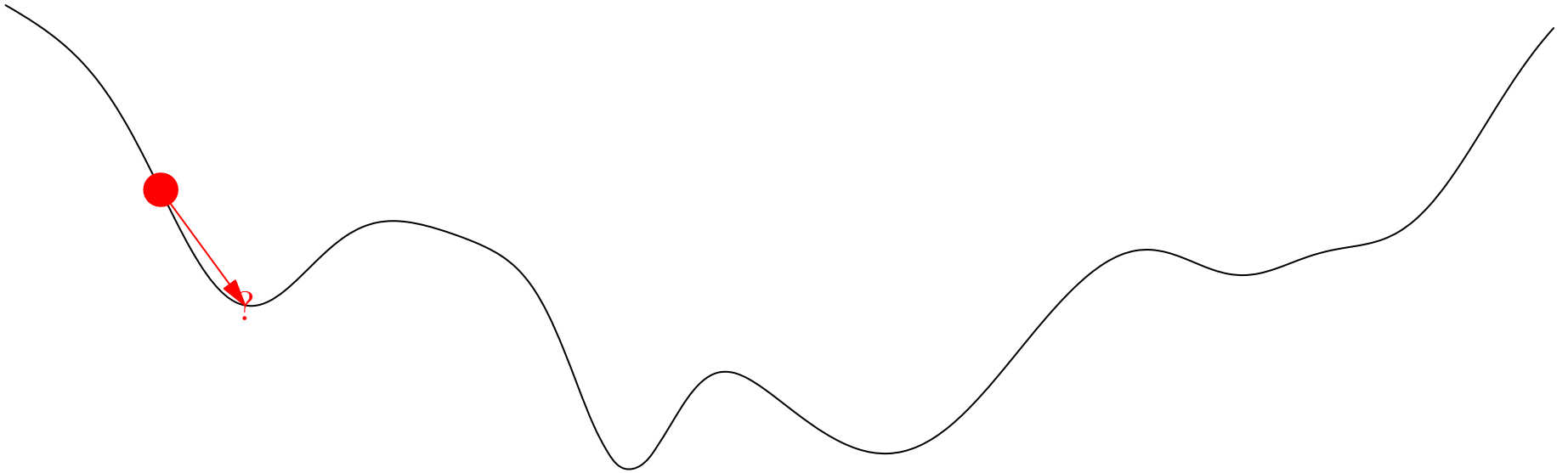
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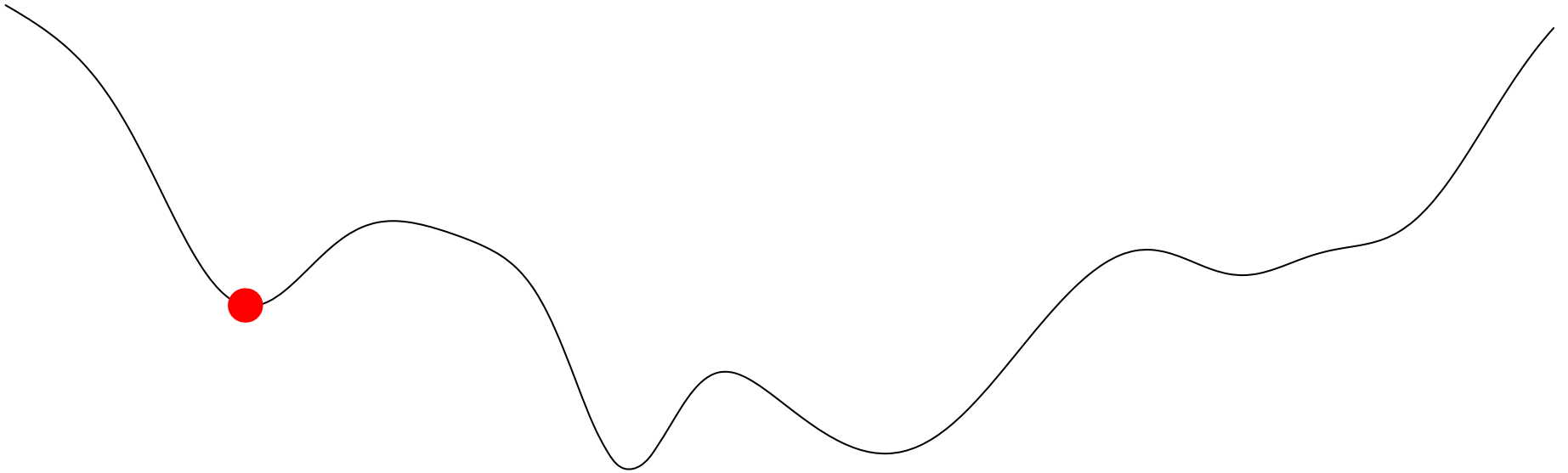
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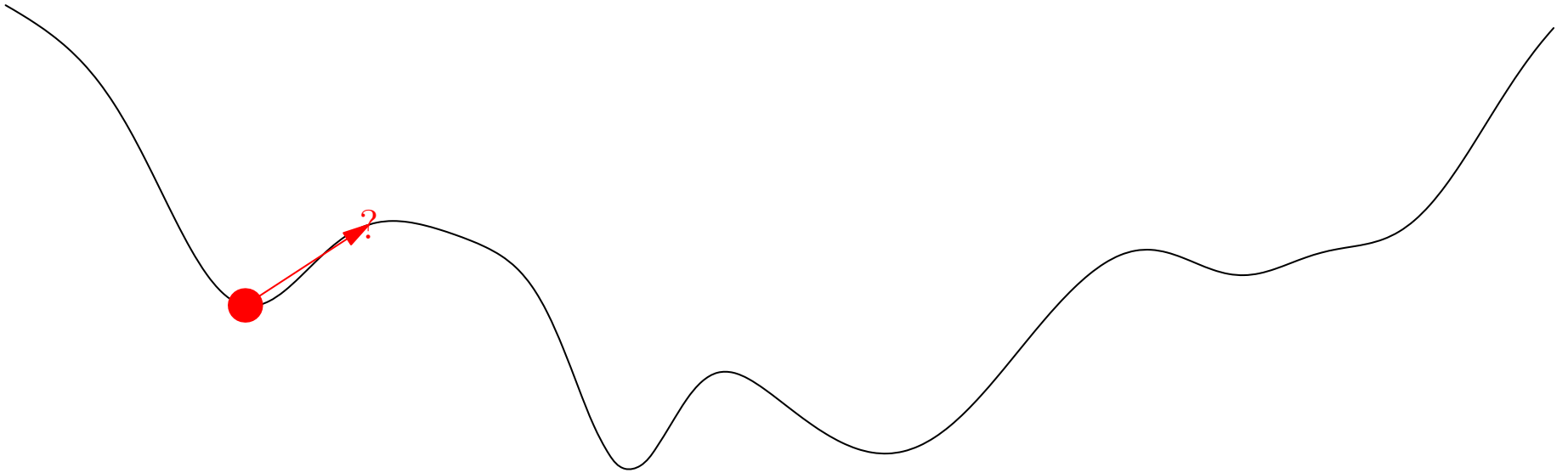
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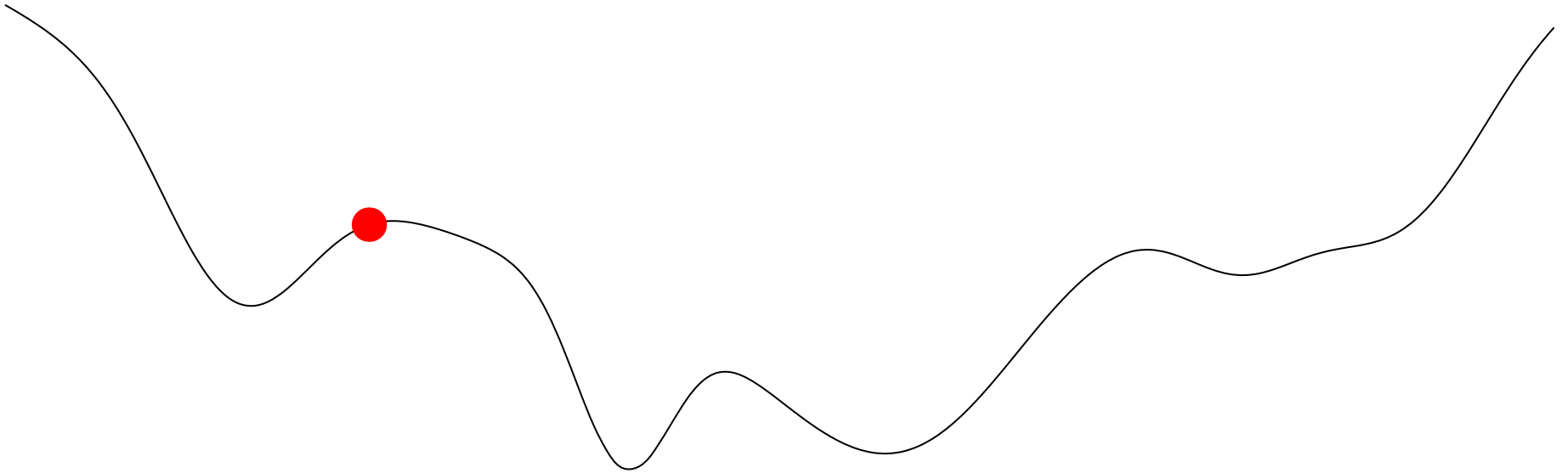
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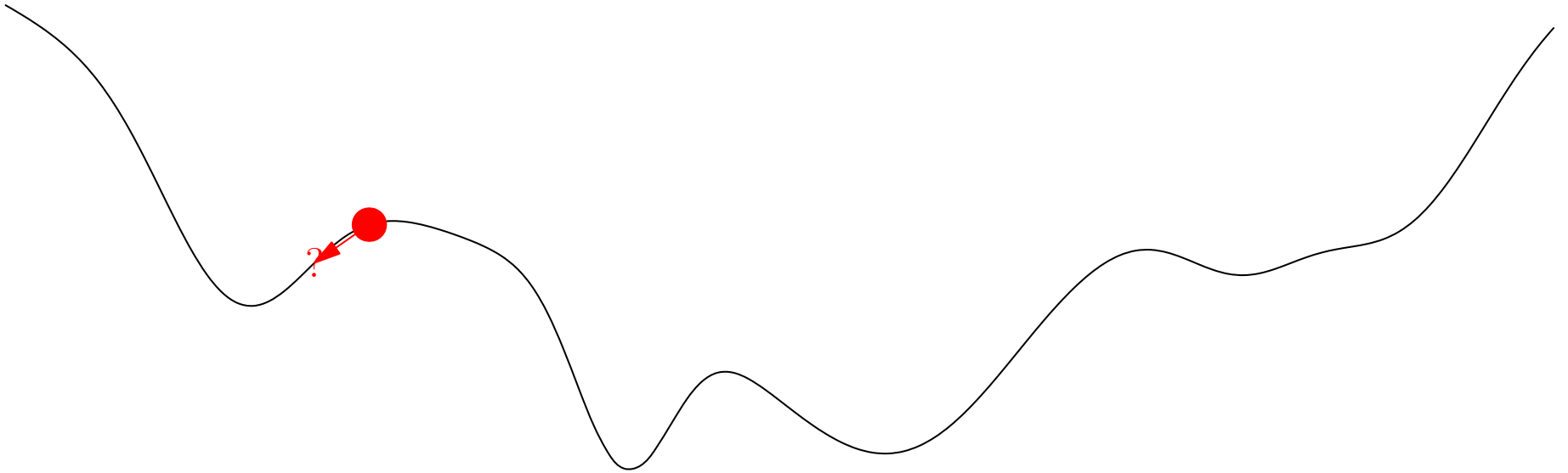
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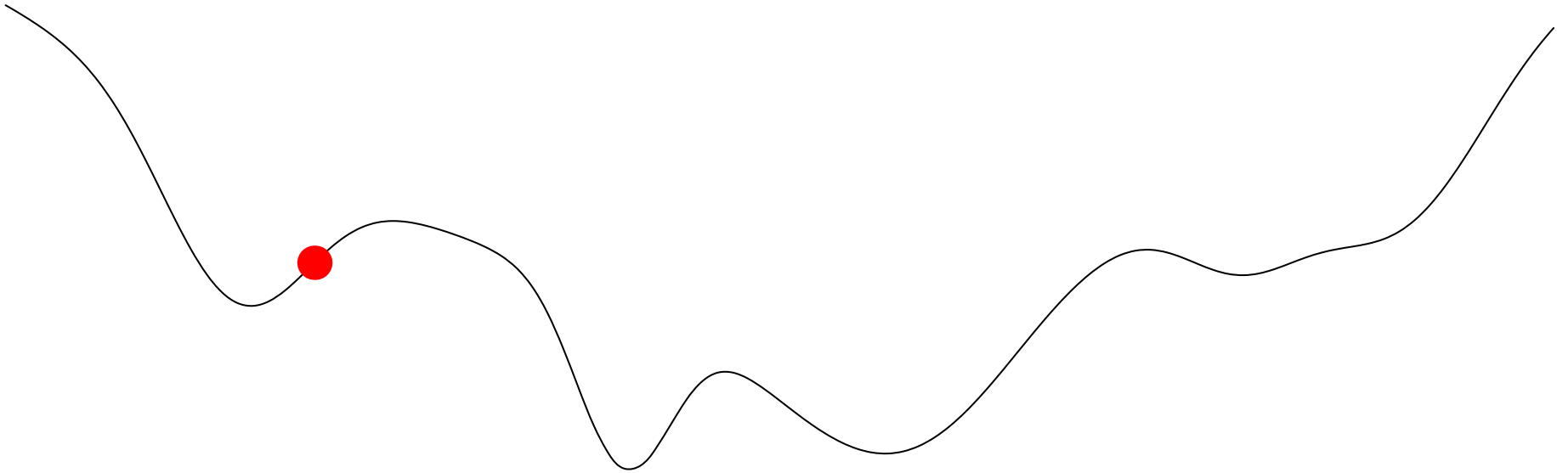
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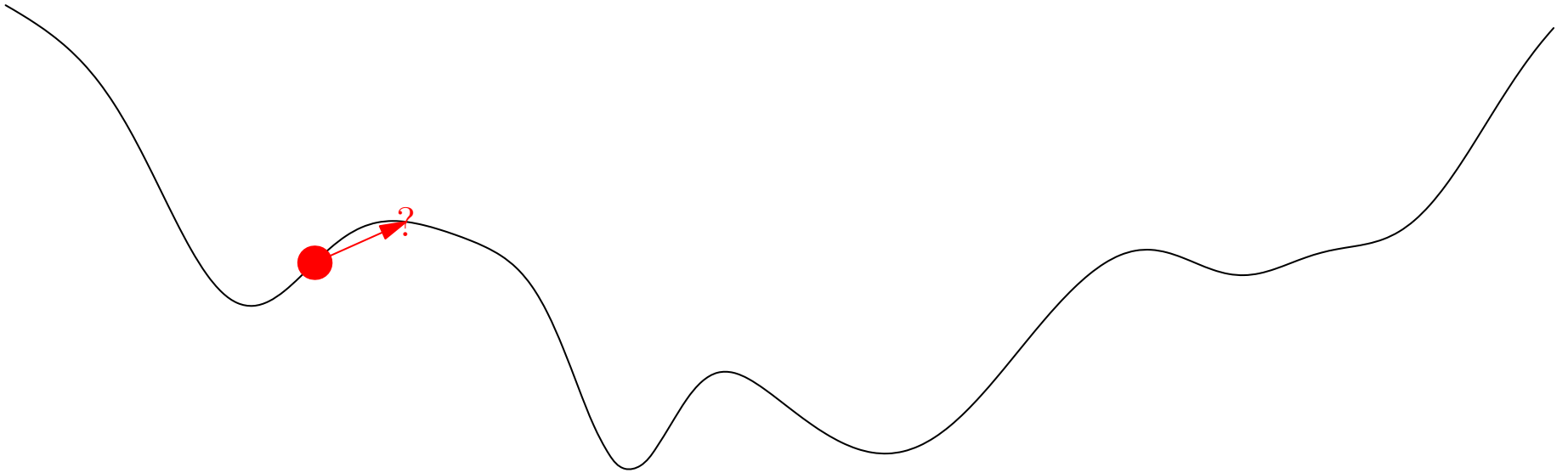
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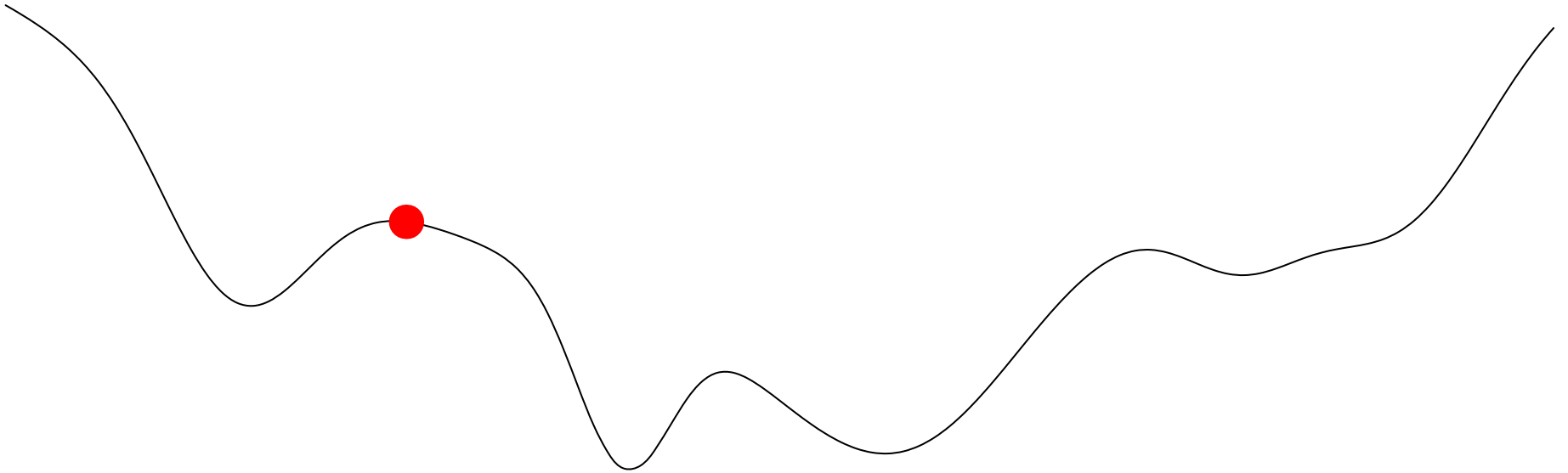
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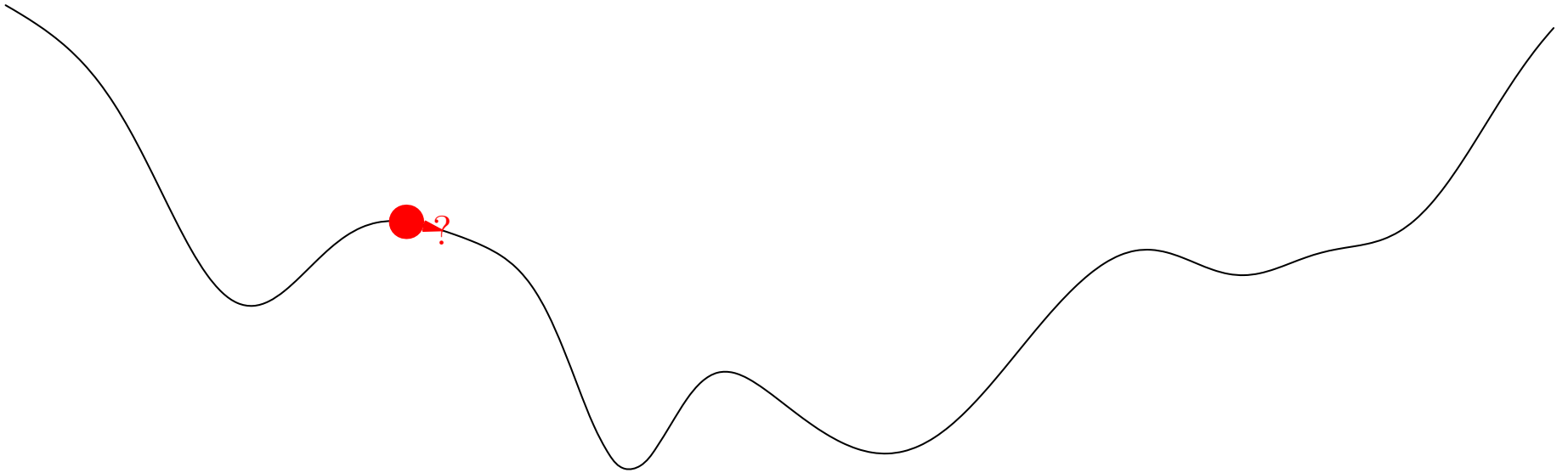
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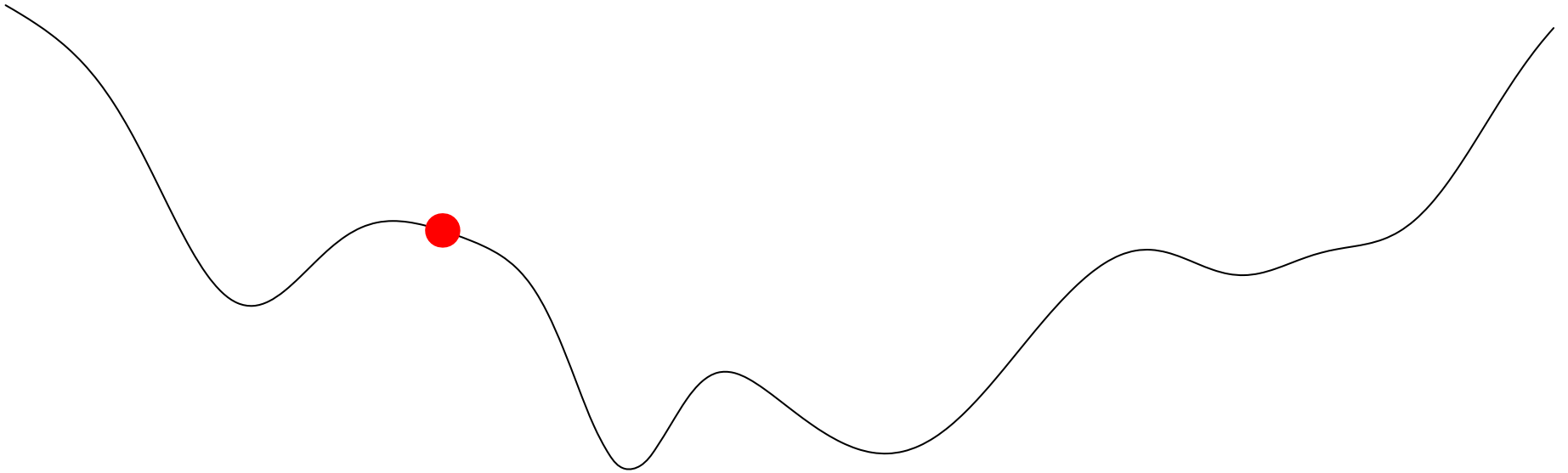
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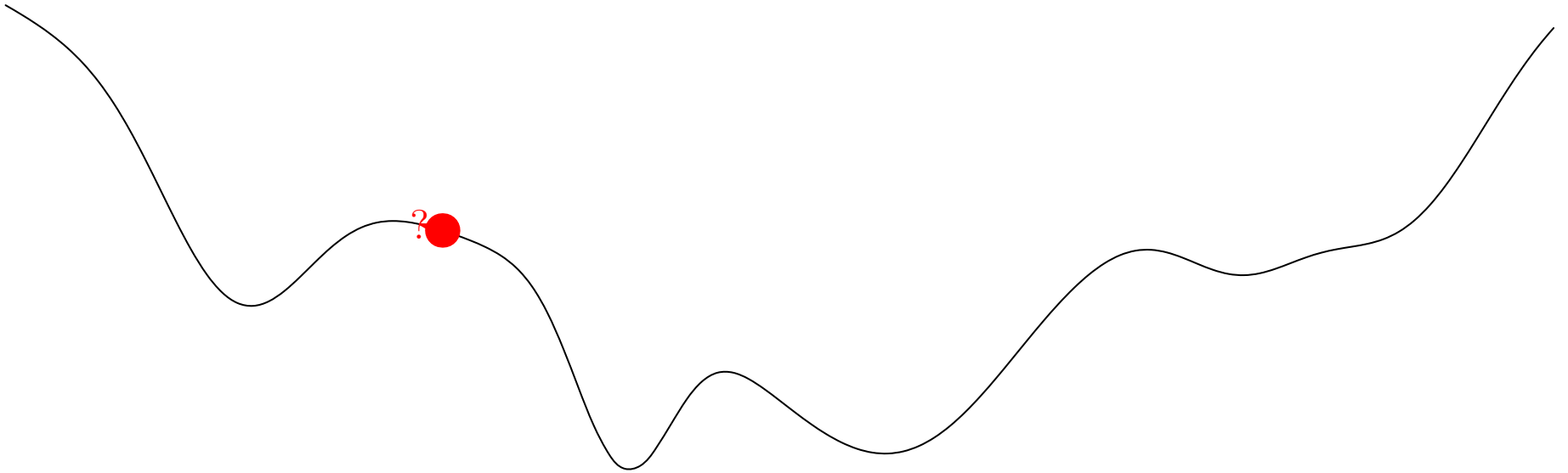
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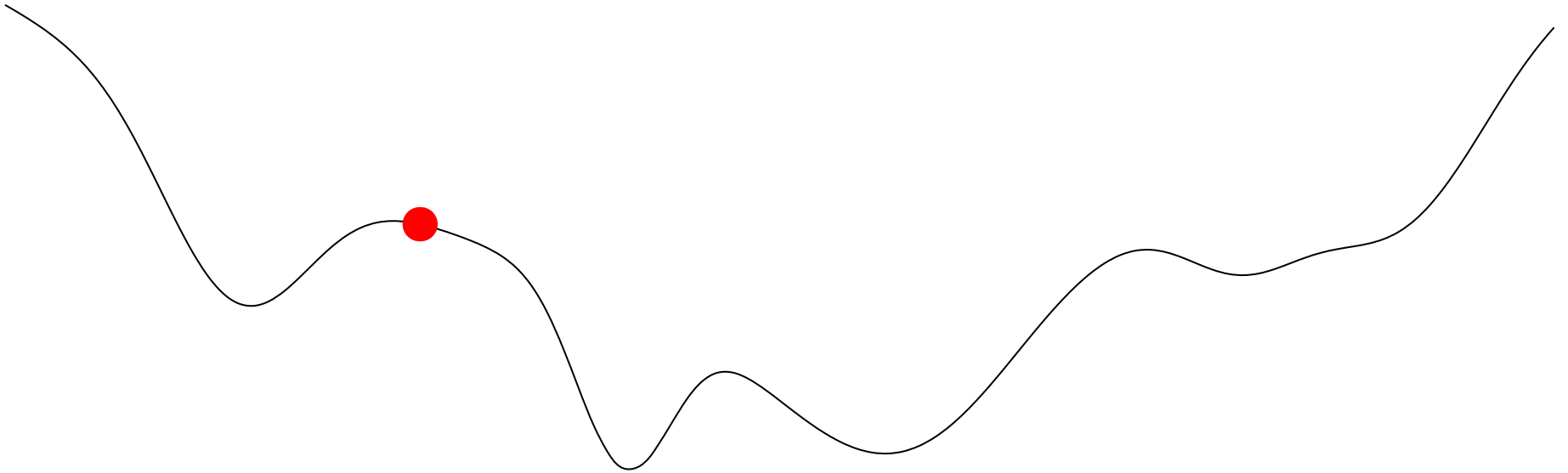
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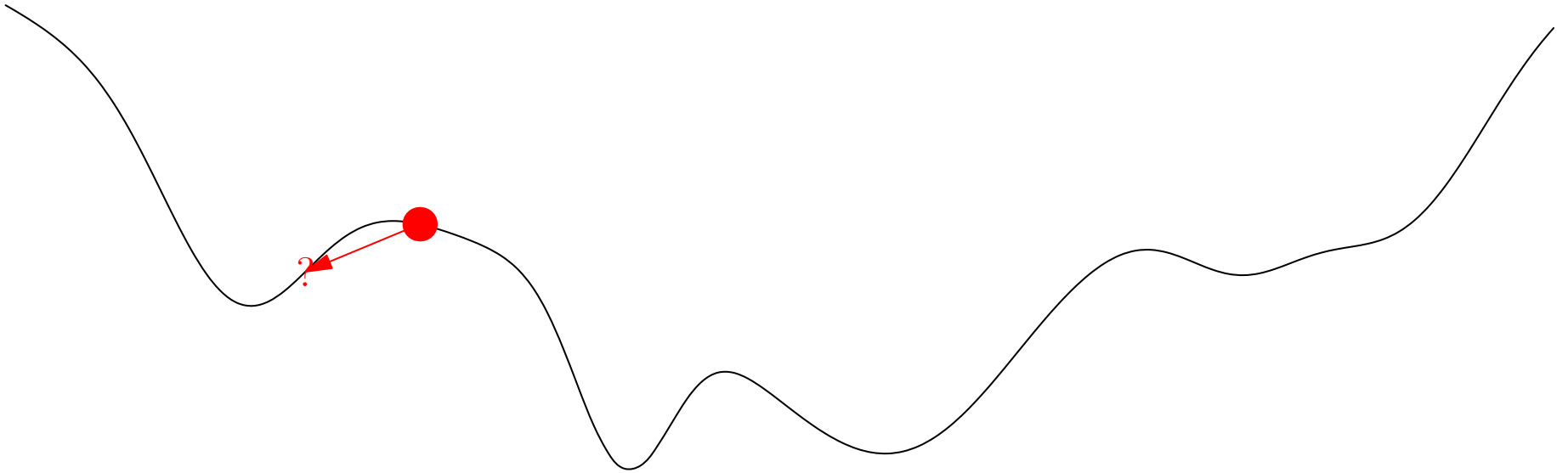
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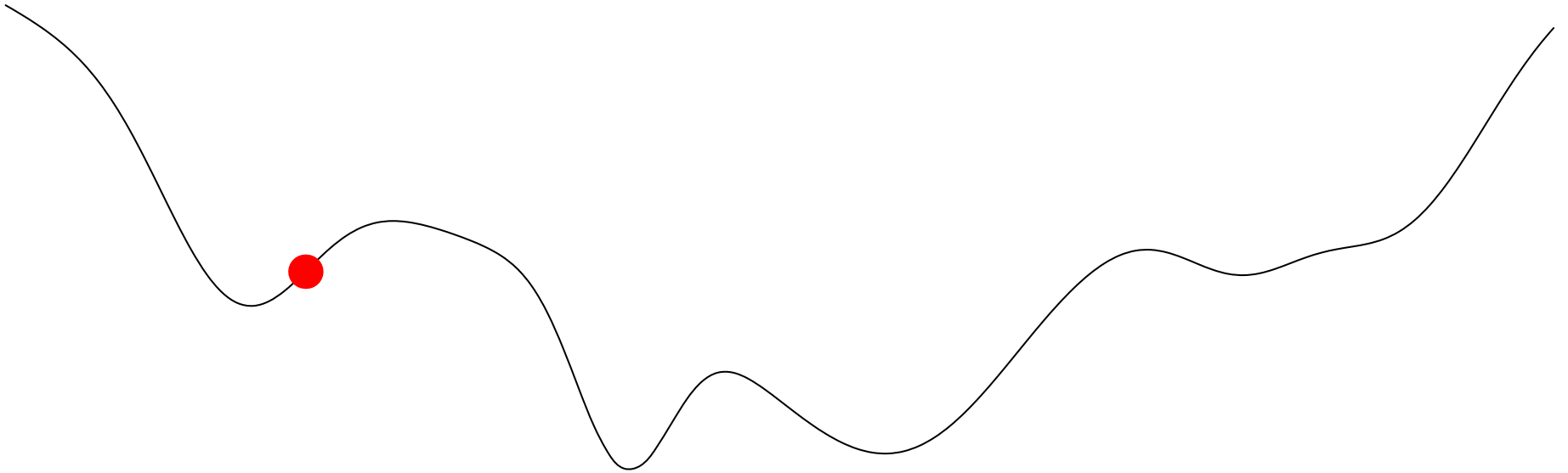
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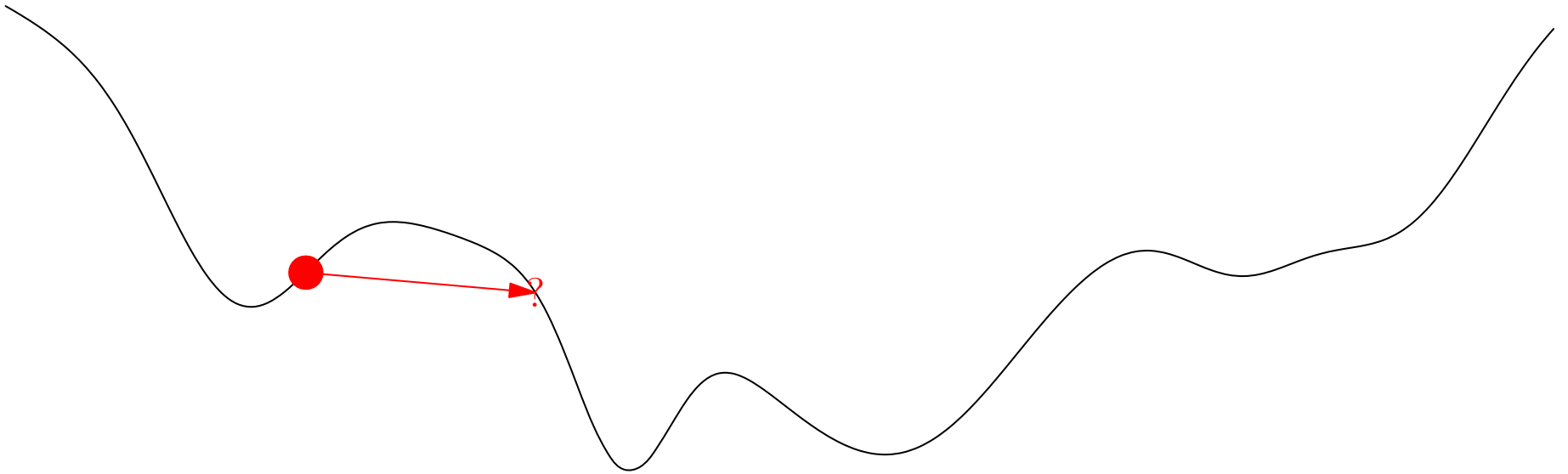
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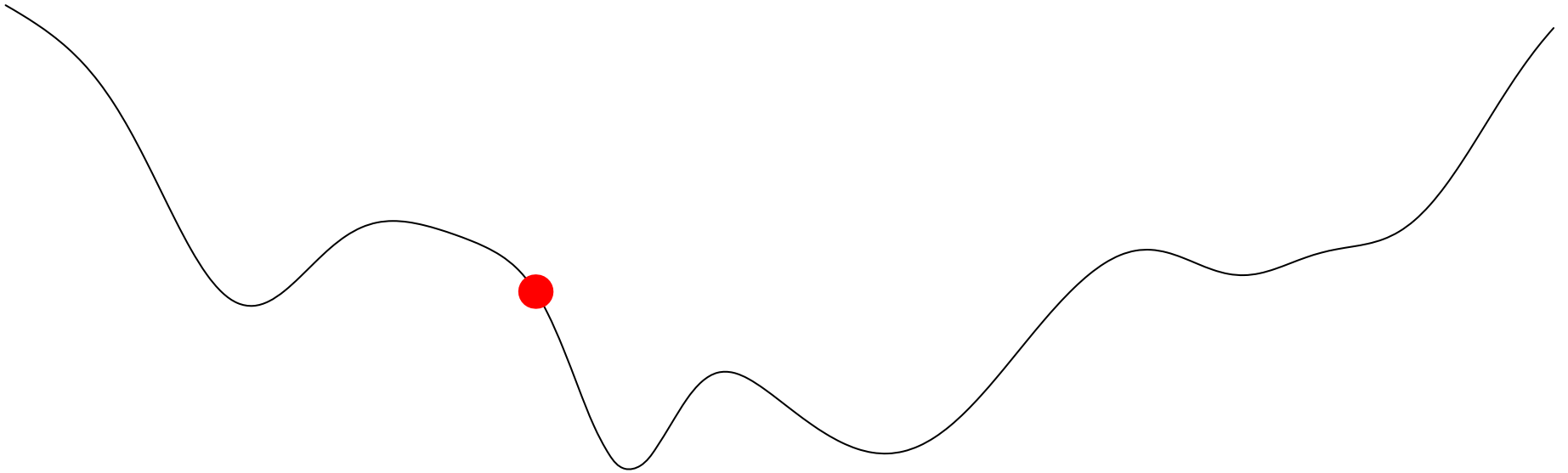
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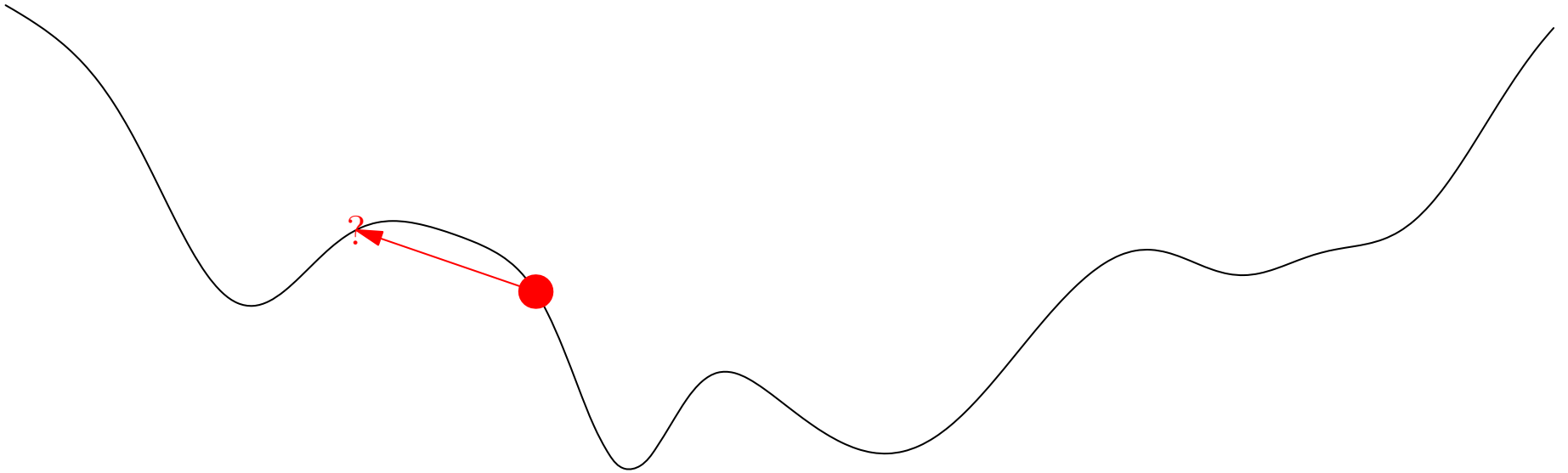
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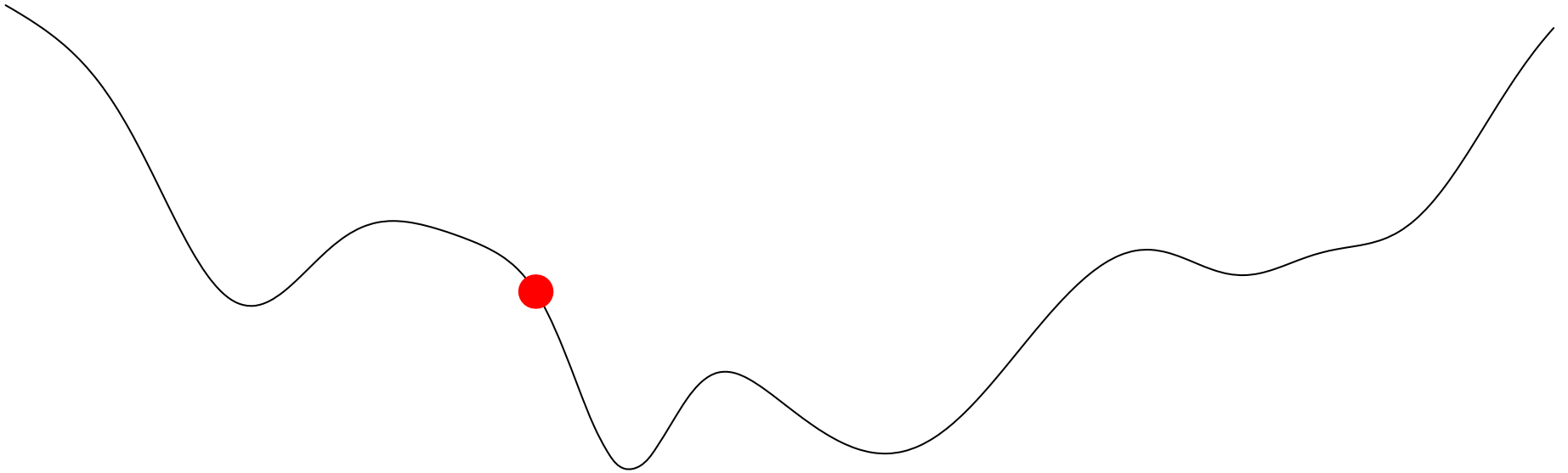
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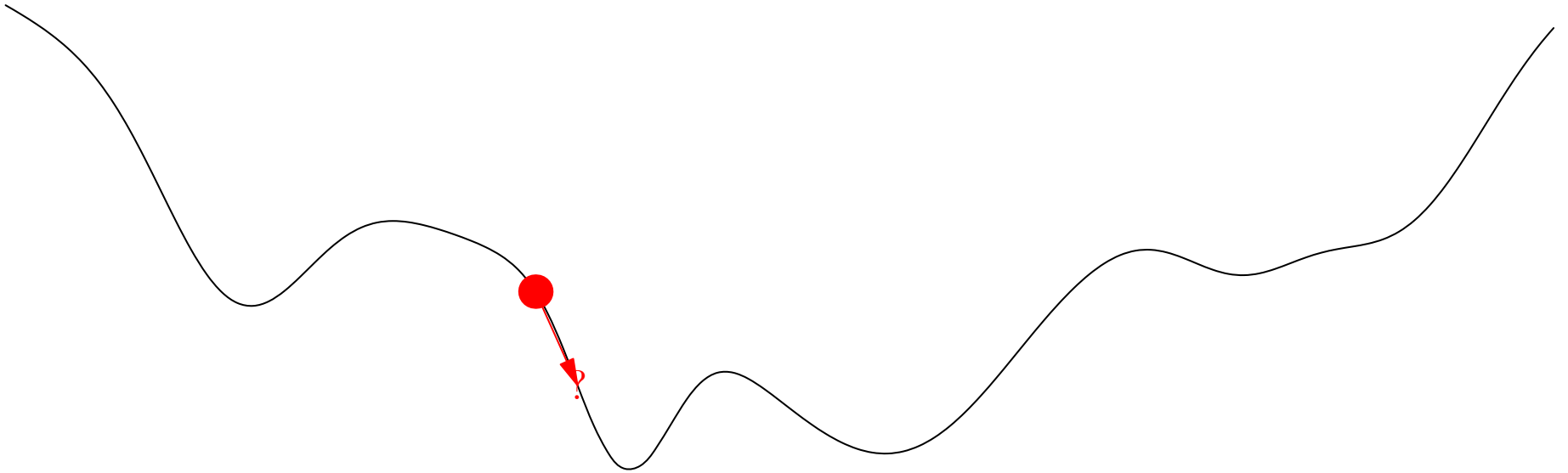
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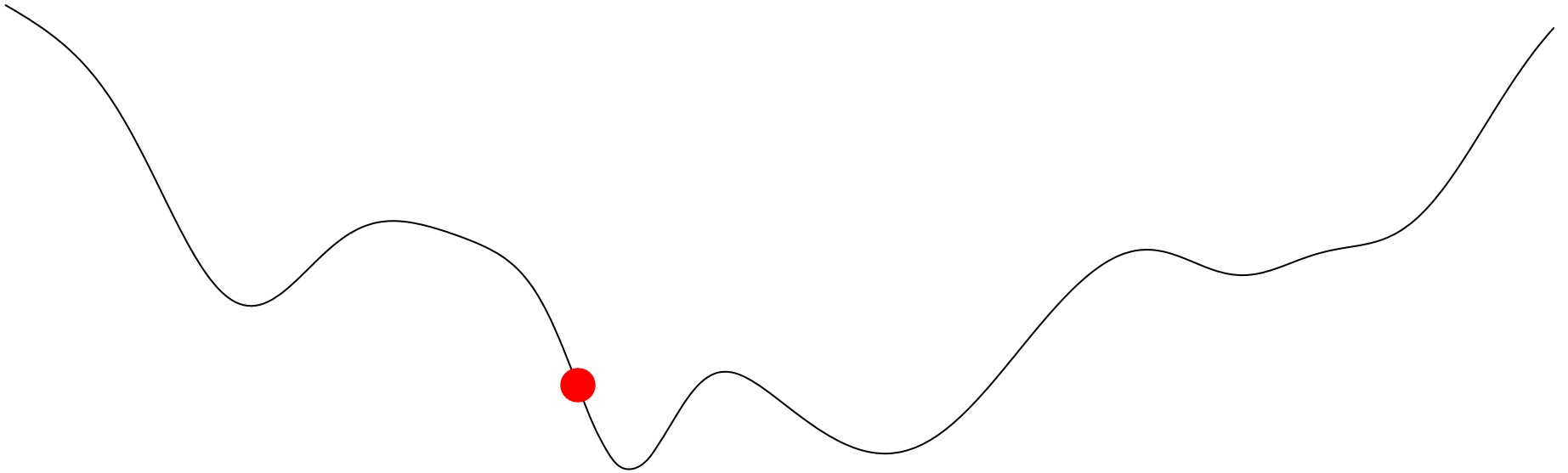
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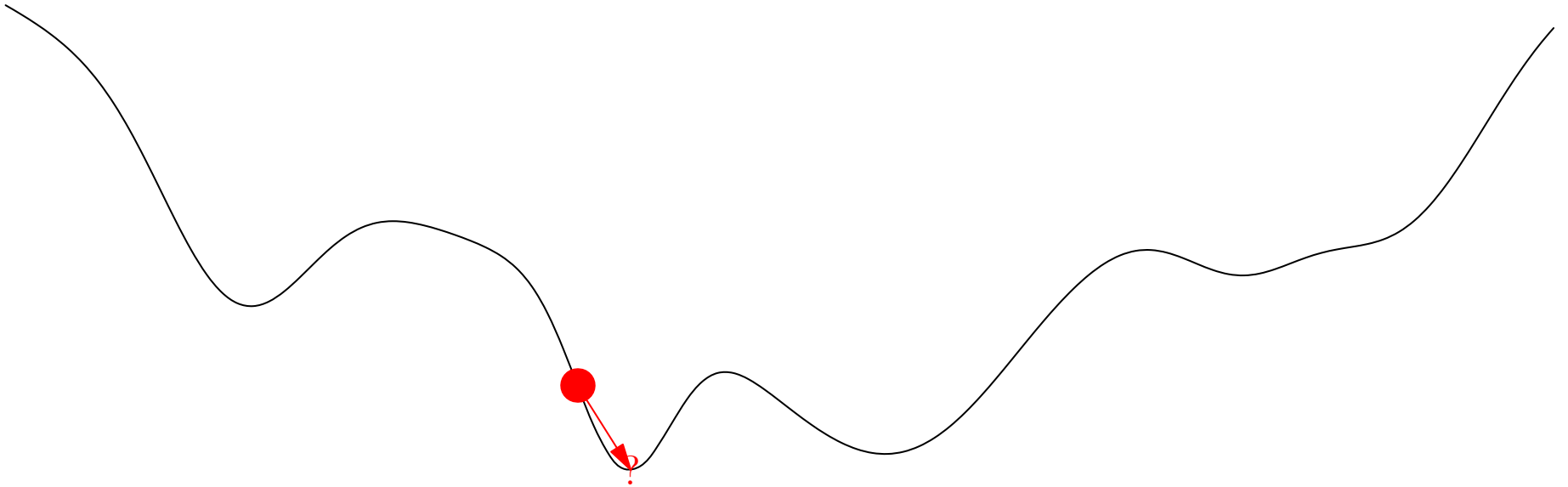
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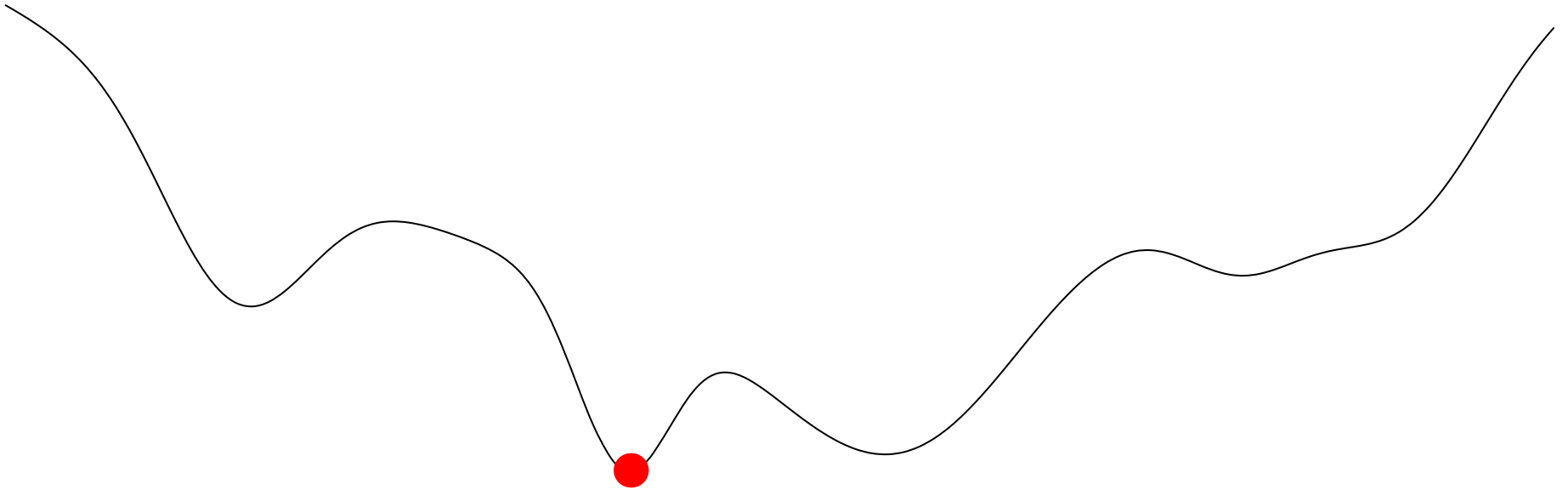
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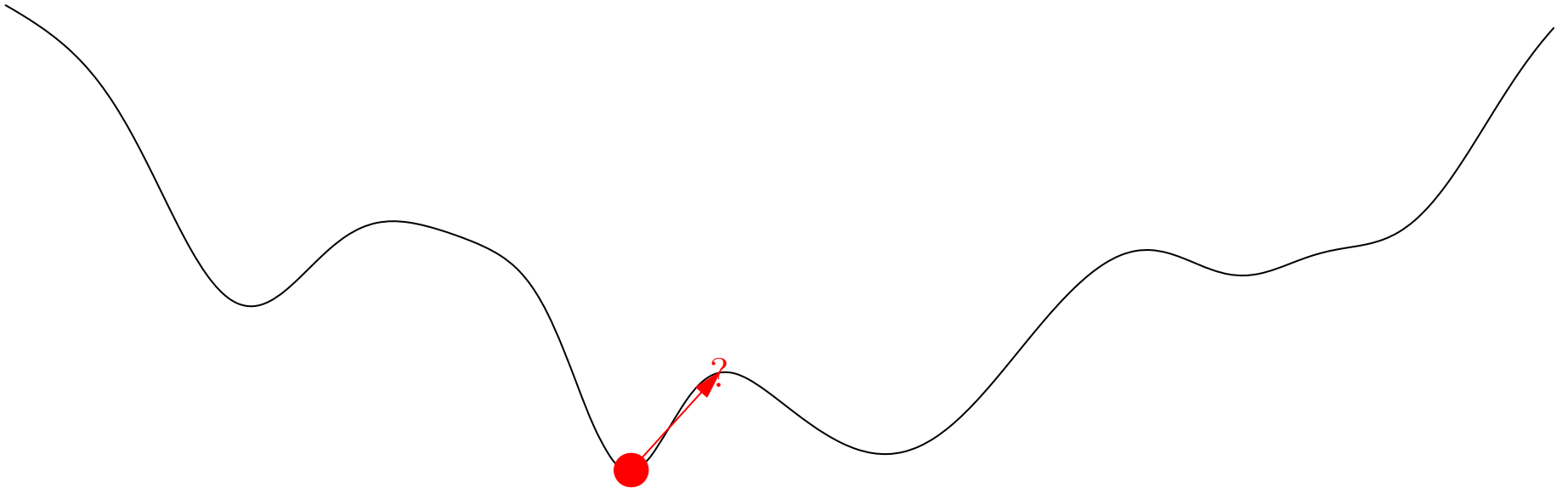
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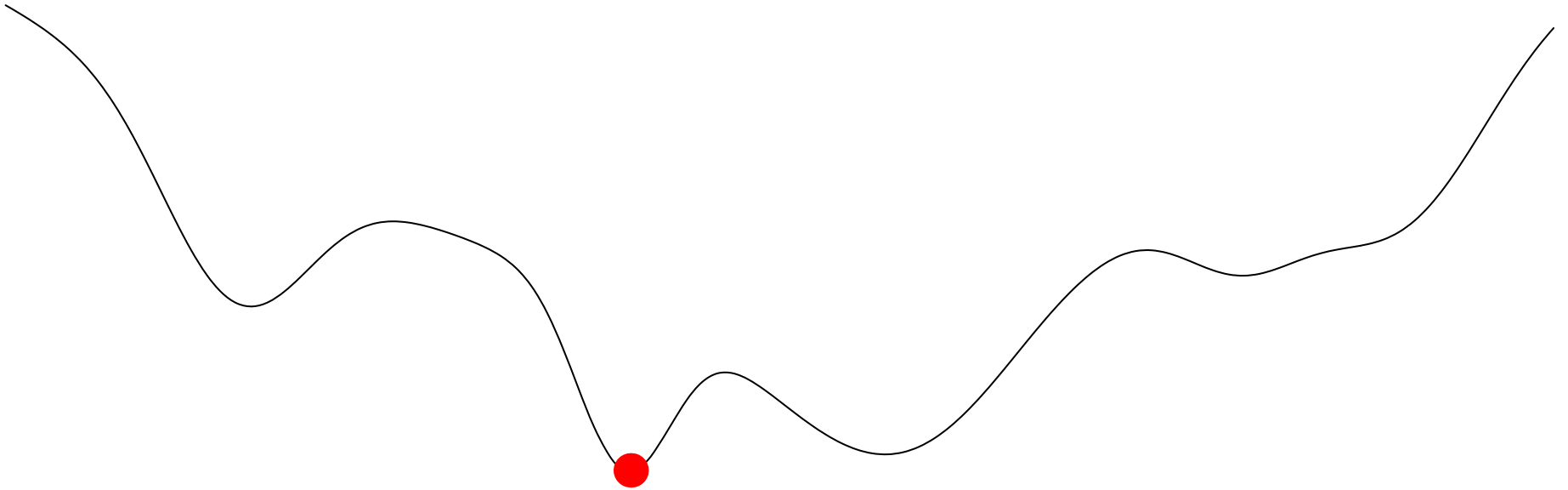
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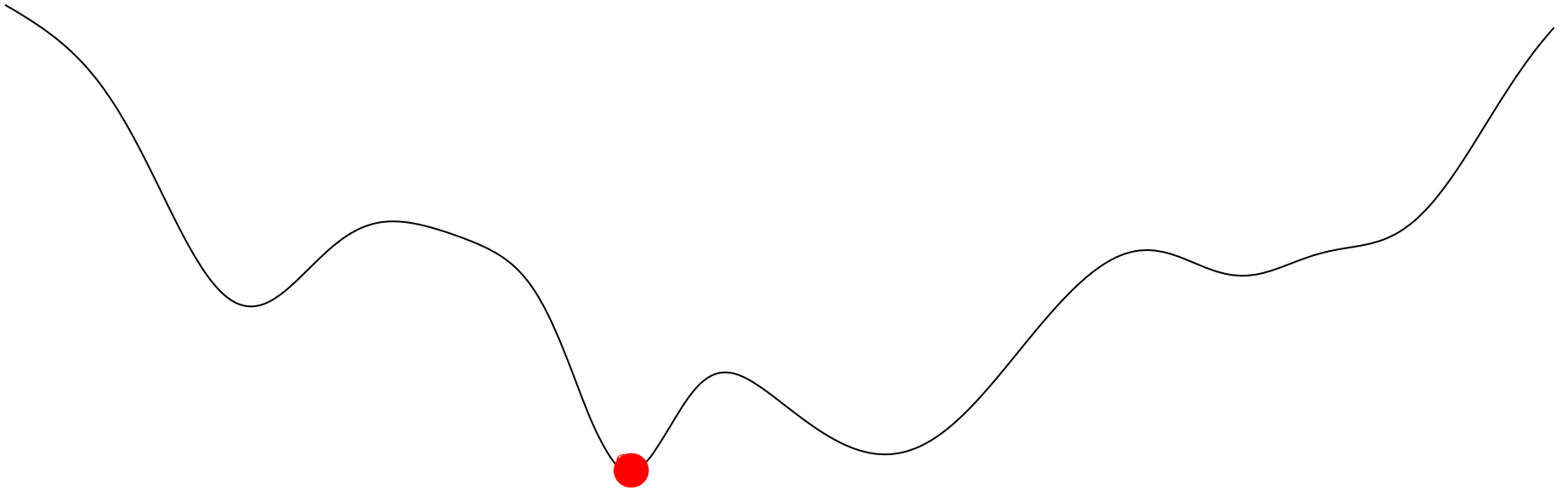
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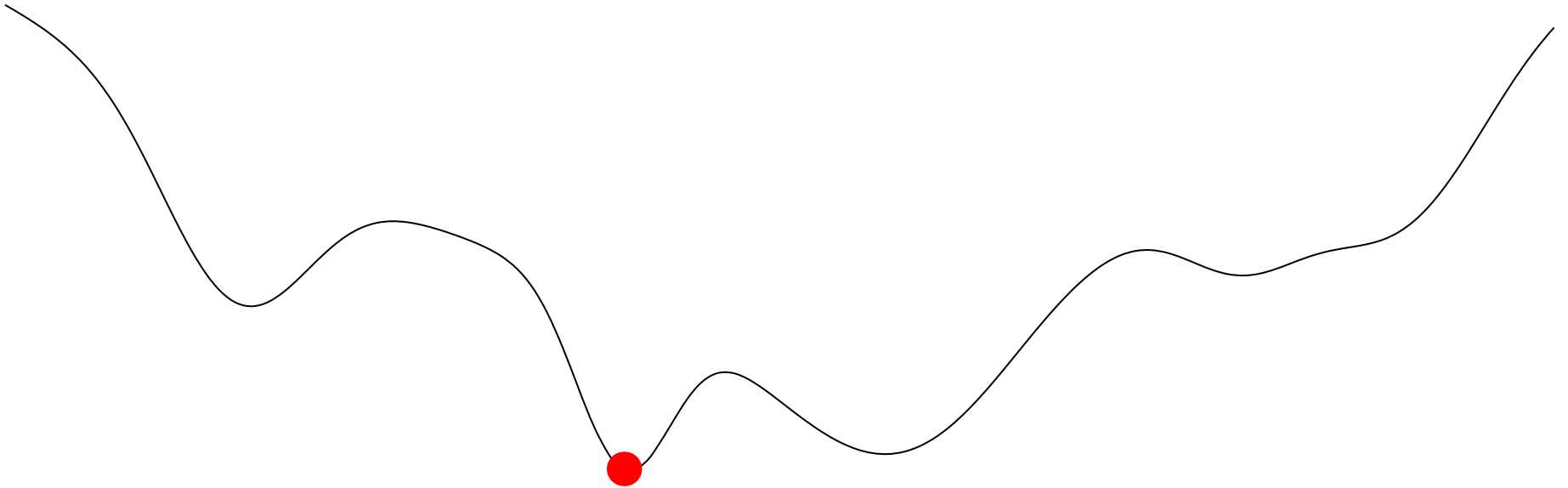
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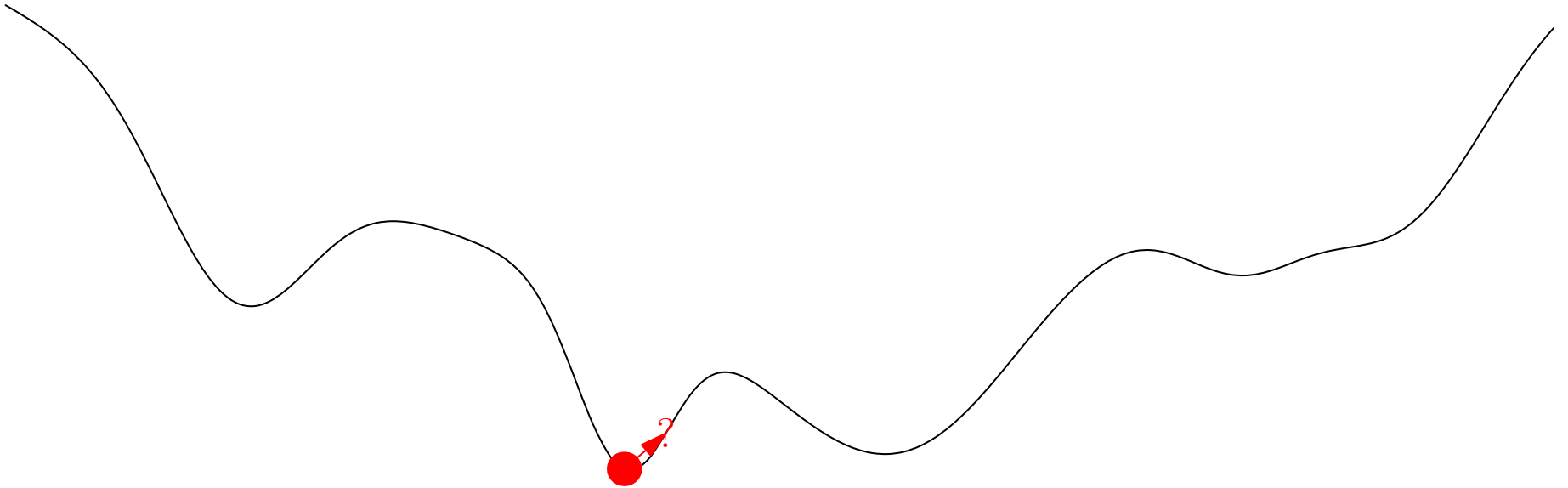
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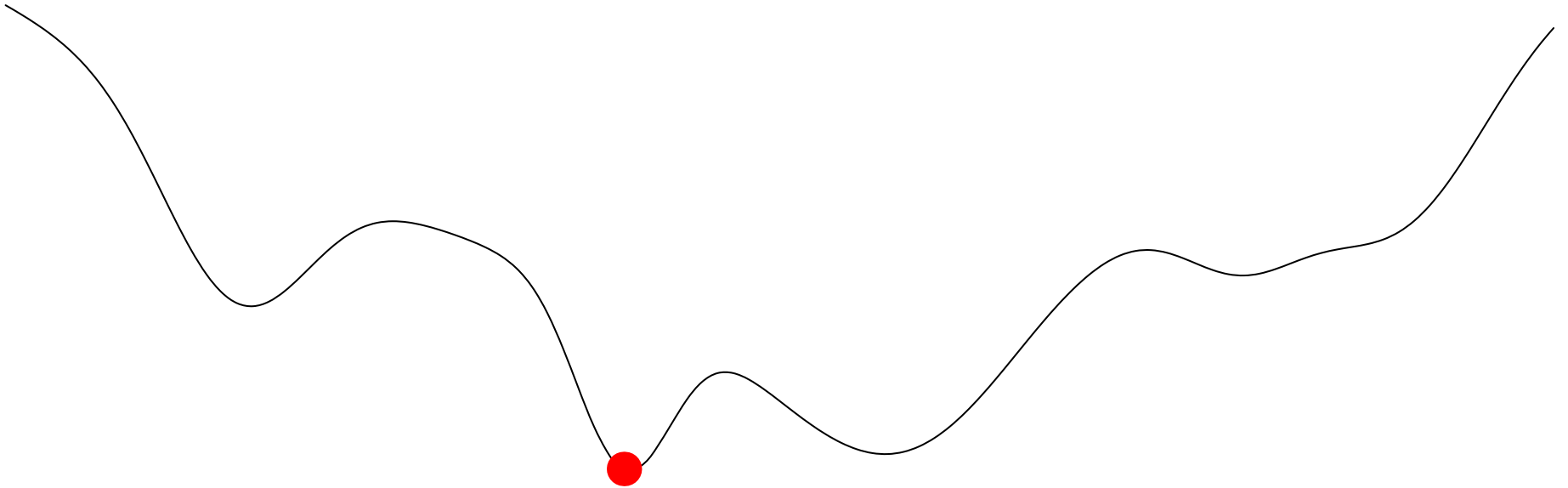
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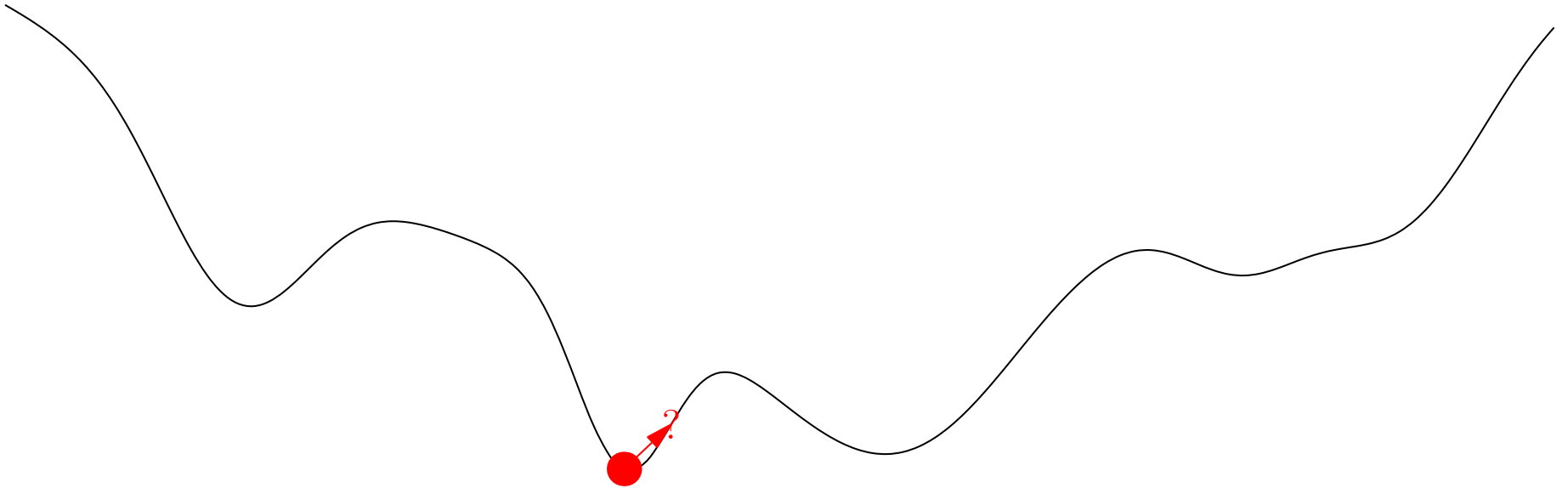
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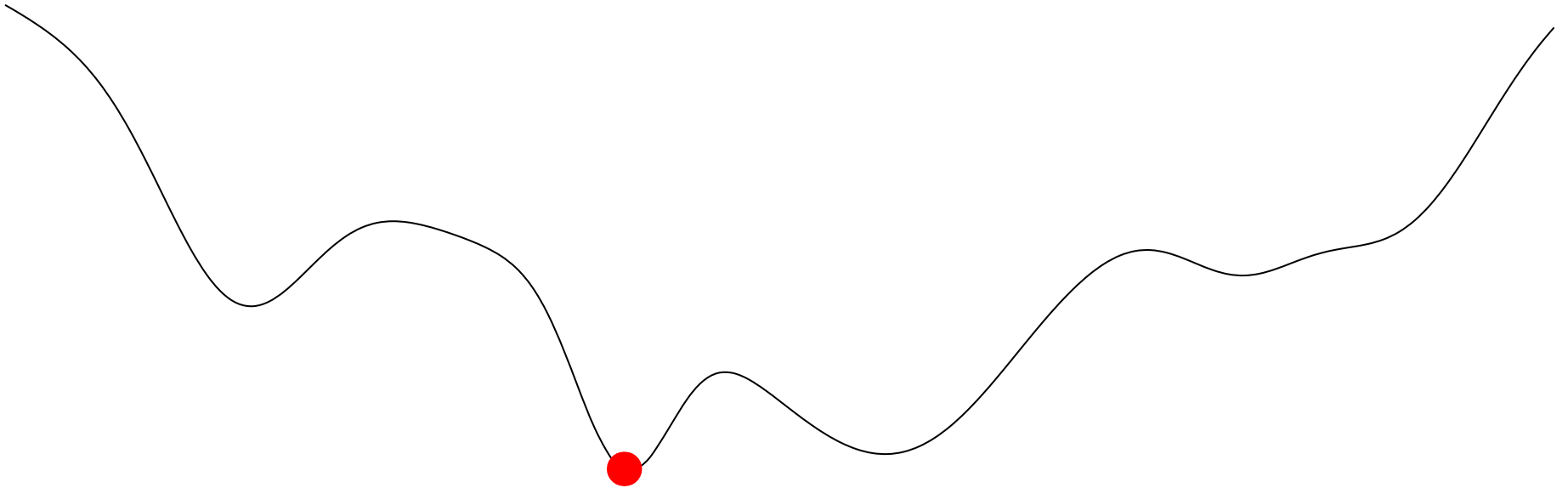
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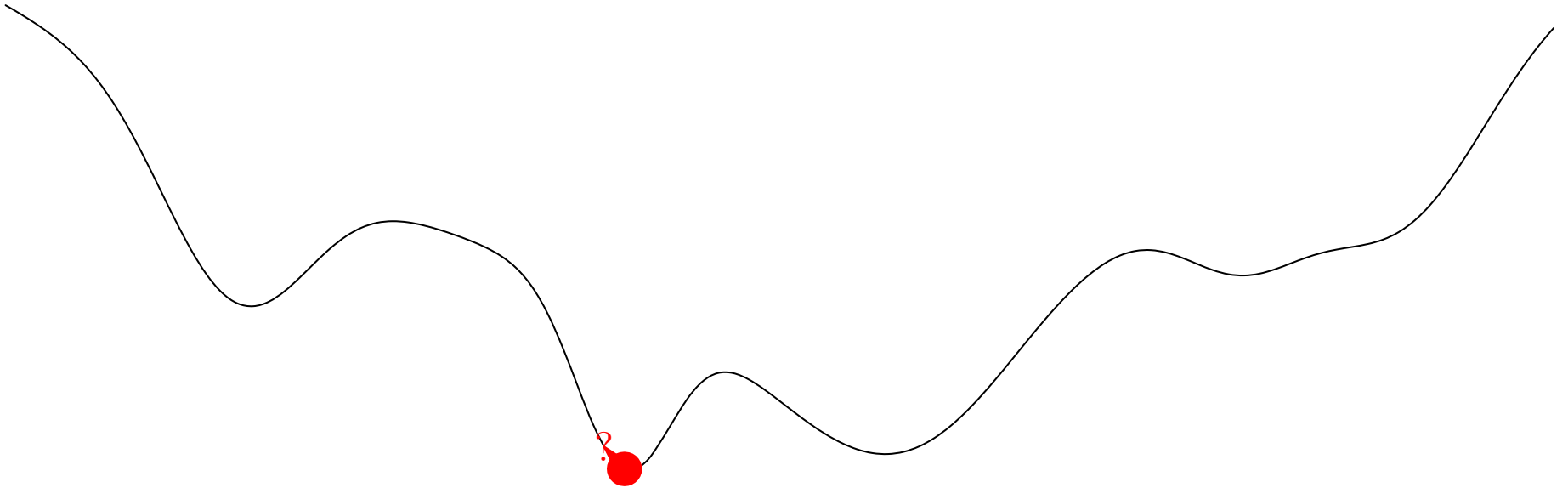
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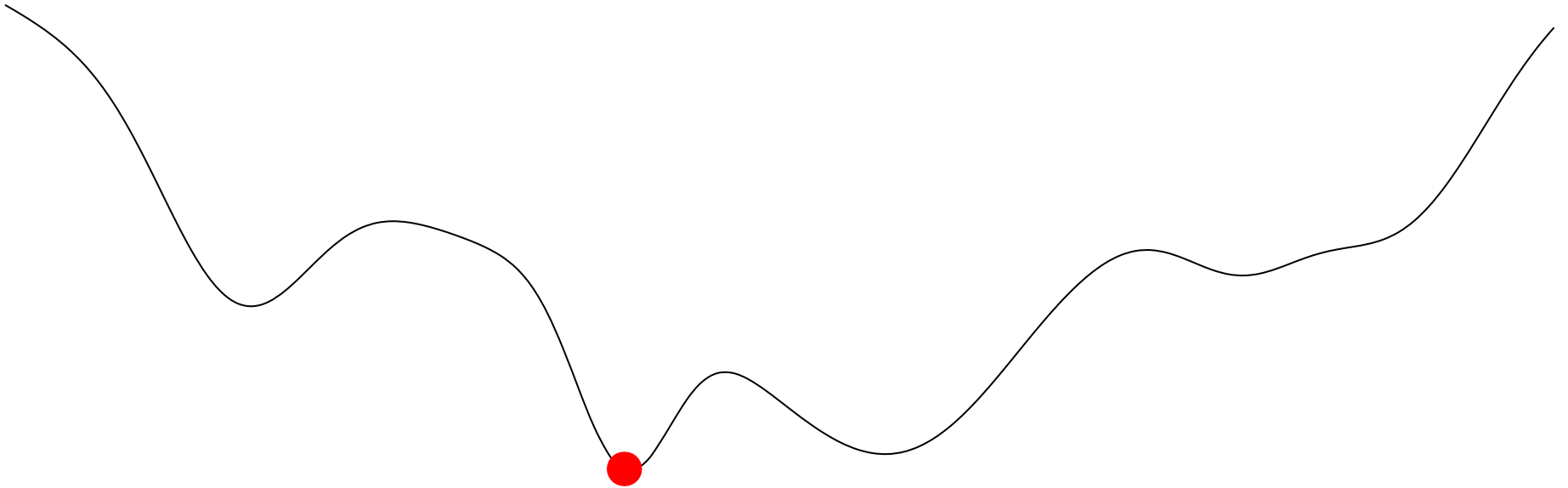
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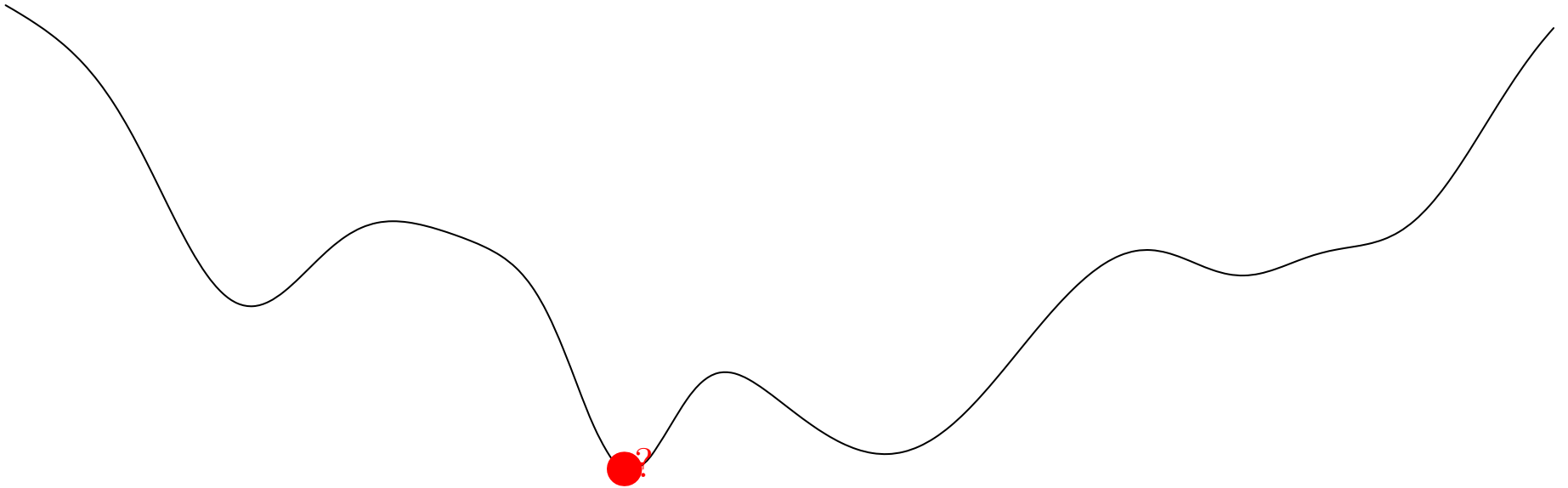
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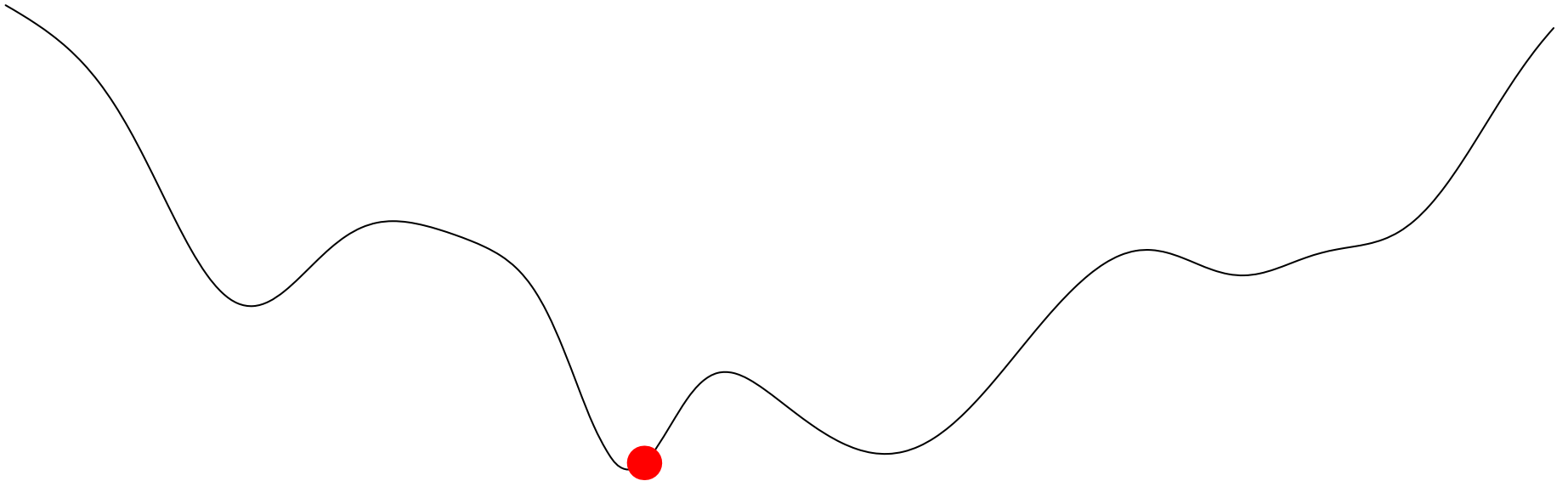
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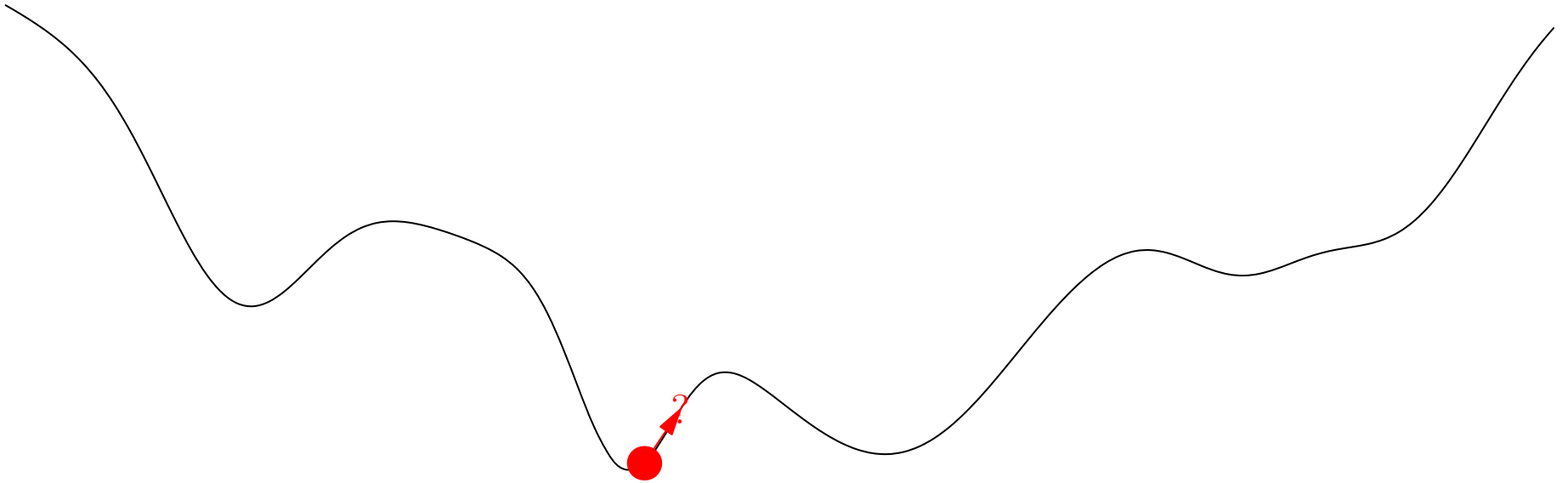
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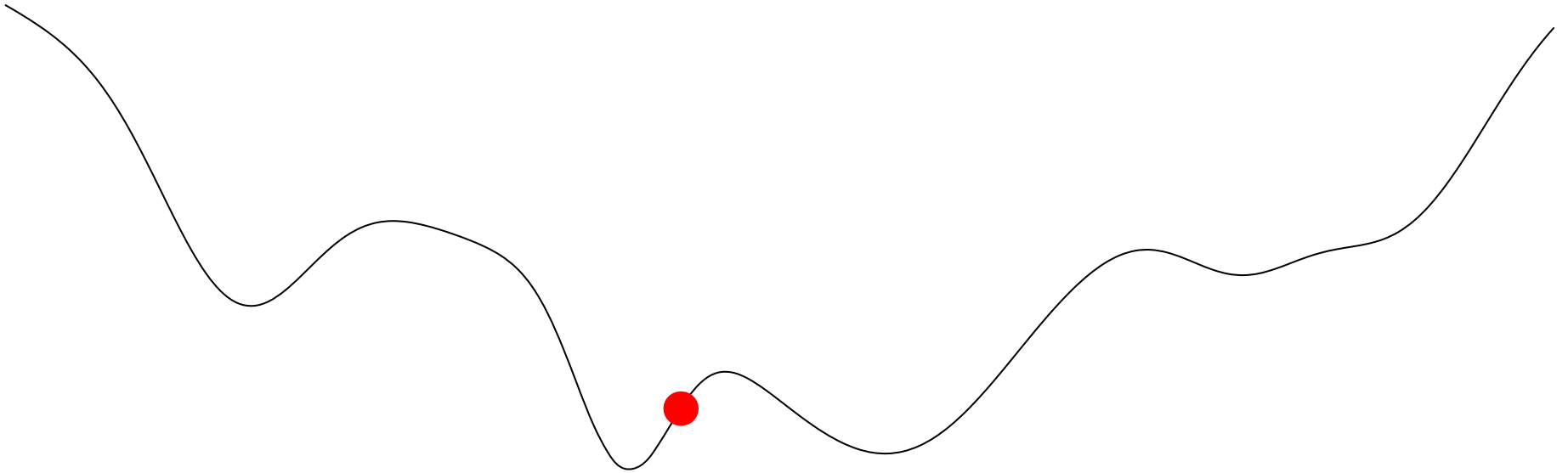
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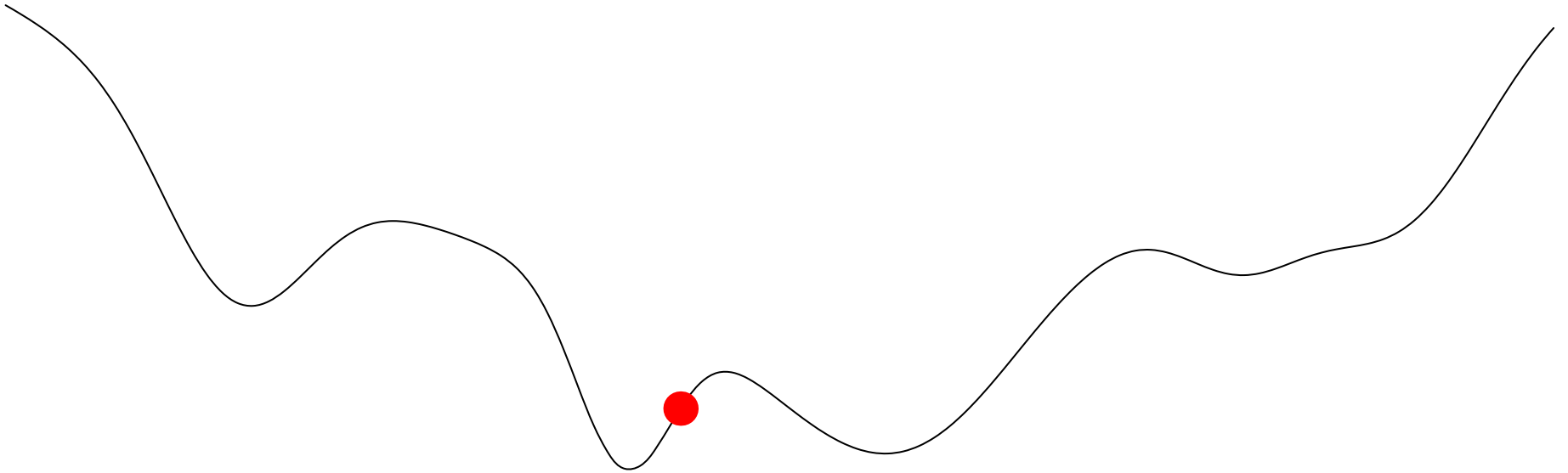
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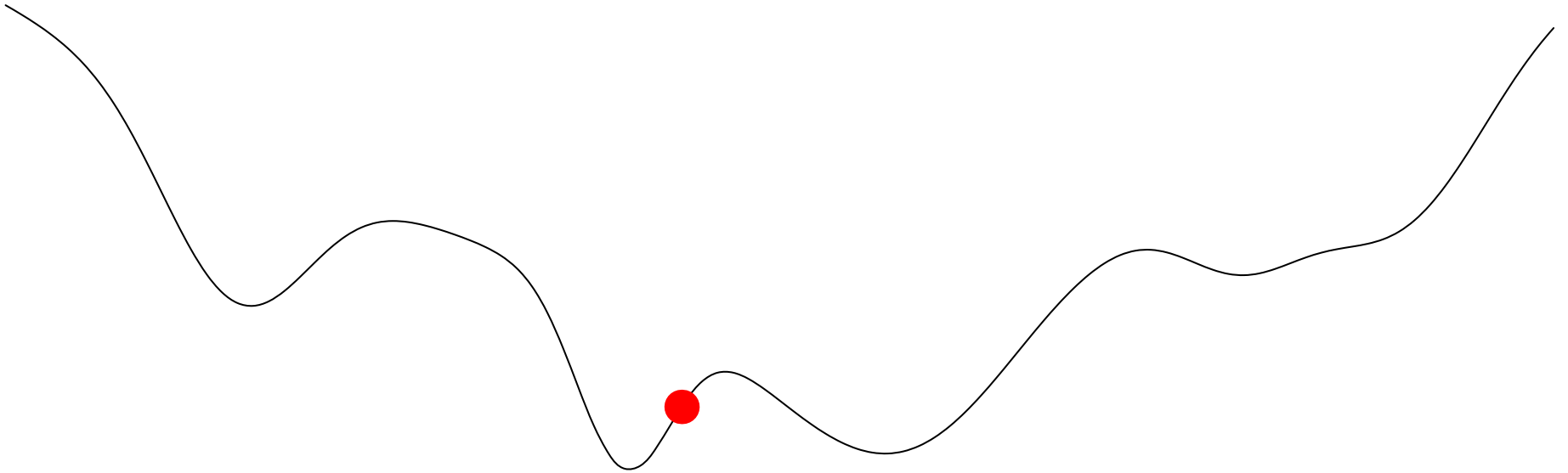
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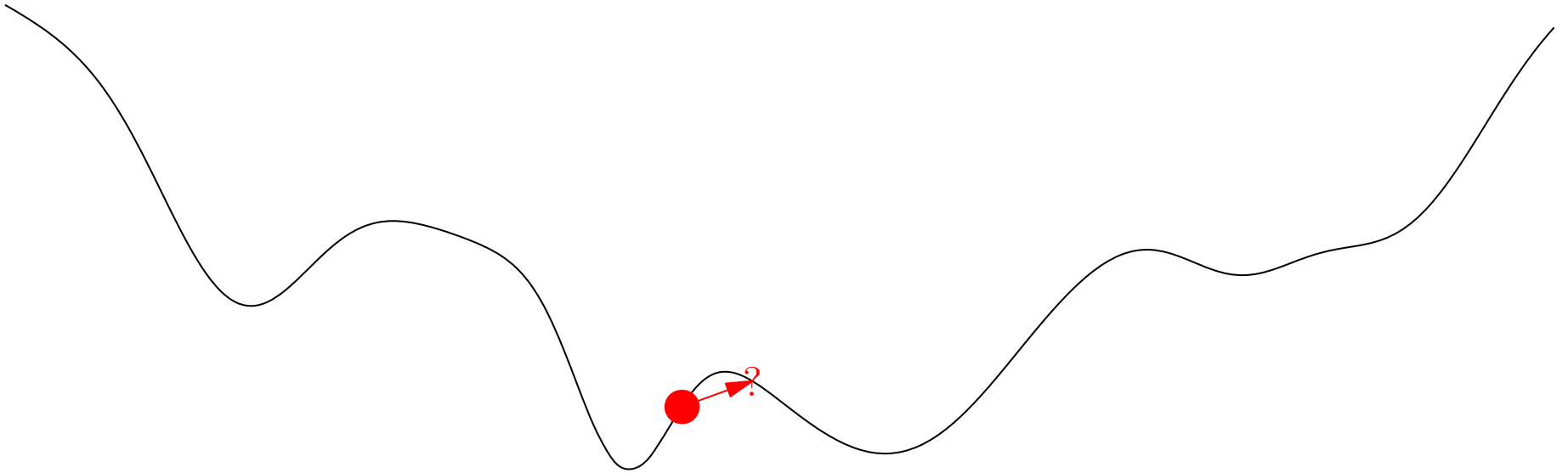
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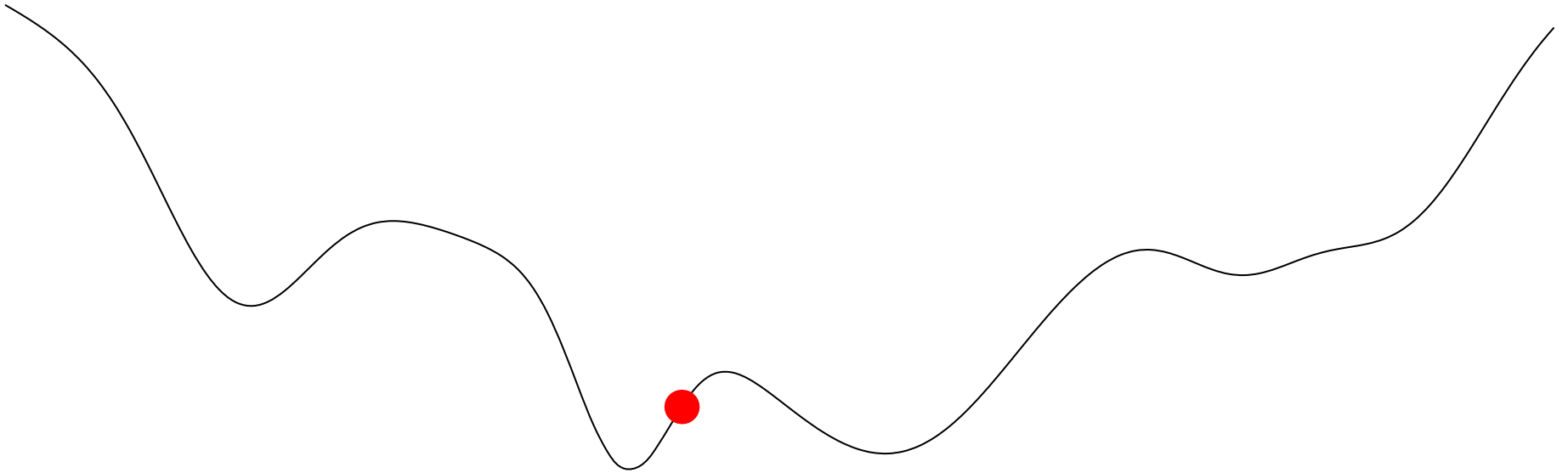
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Simulated Annealing

- Algorithm to minimise energy $E(\mathbf{X})$ where $\mathbf{X} = (X_1, X_2, \dots, X_N)$
- Starting from a random configuration \mathbf{X}
- Choose a neighbour \mathbf{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
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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
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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
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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
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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

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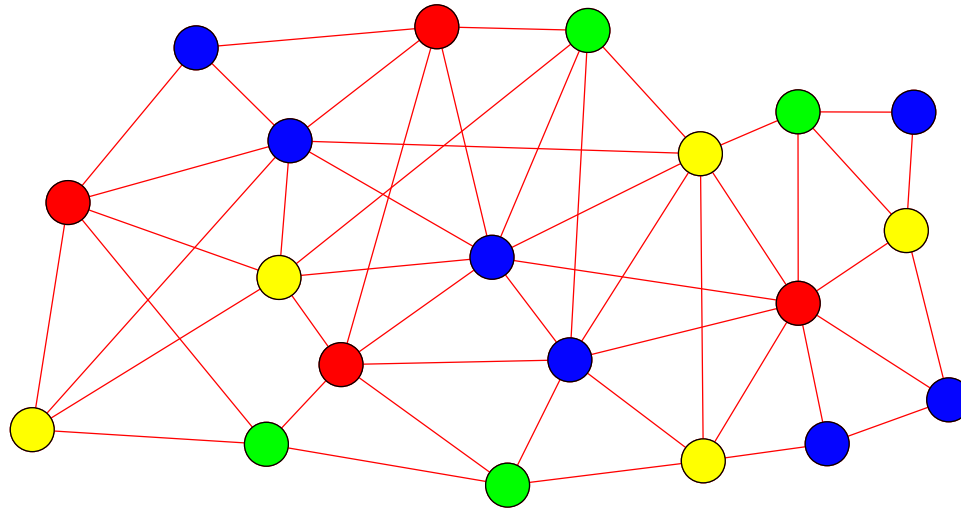
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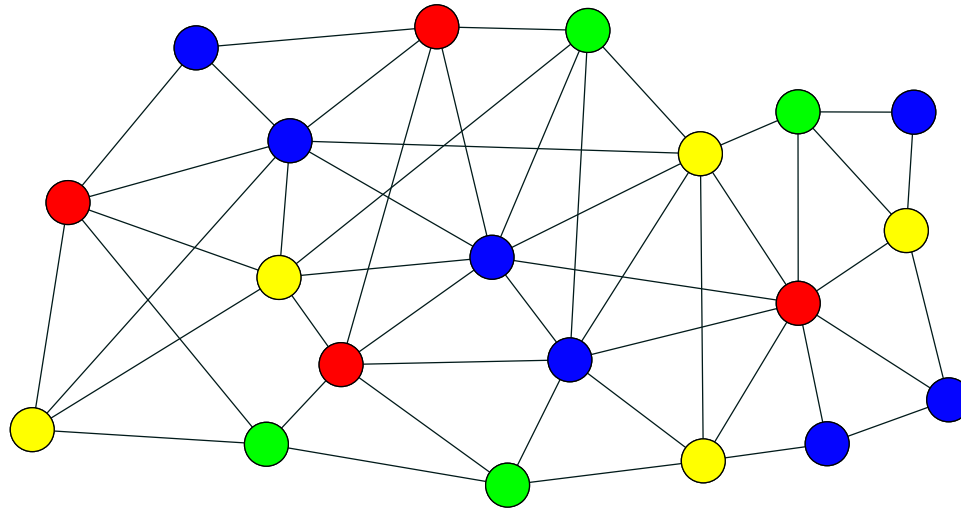
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E.g. Graph Colouring



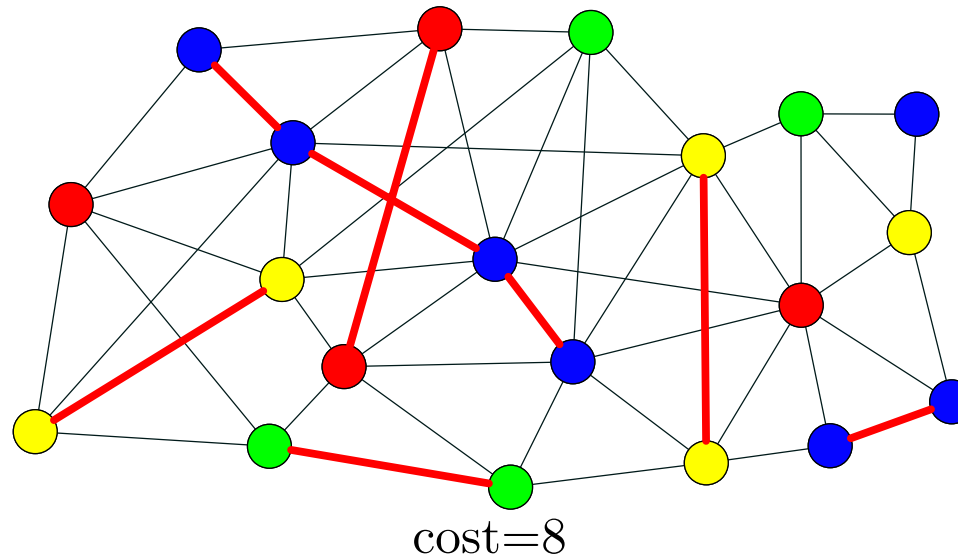
- Given a graph $G = (\mathcal{V}, \mathcal{E})$
- Assign colours, $c(v)$, to the vertices of the graph $v \in \mathcal{V}$
- Minimise the number of edges $e = (v, v') \in \mathcal{E}$ with the same coloured vertices $c(v) = c(v')$ (colour conflicts)

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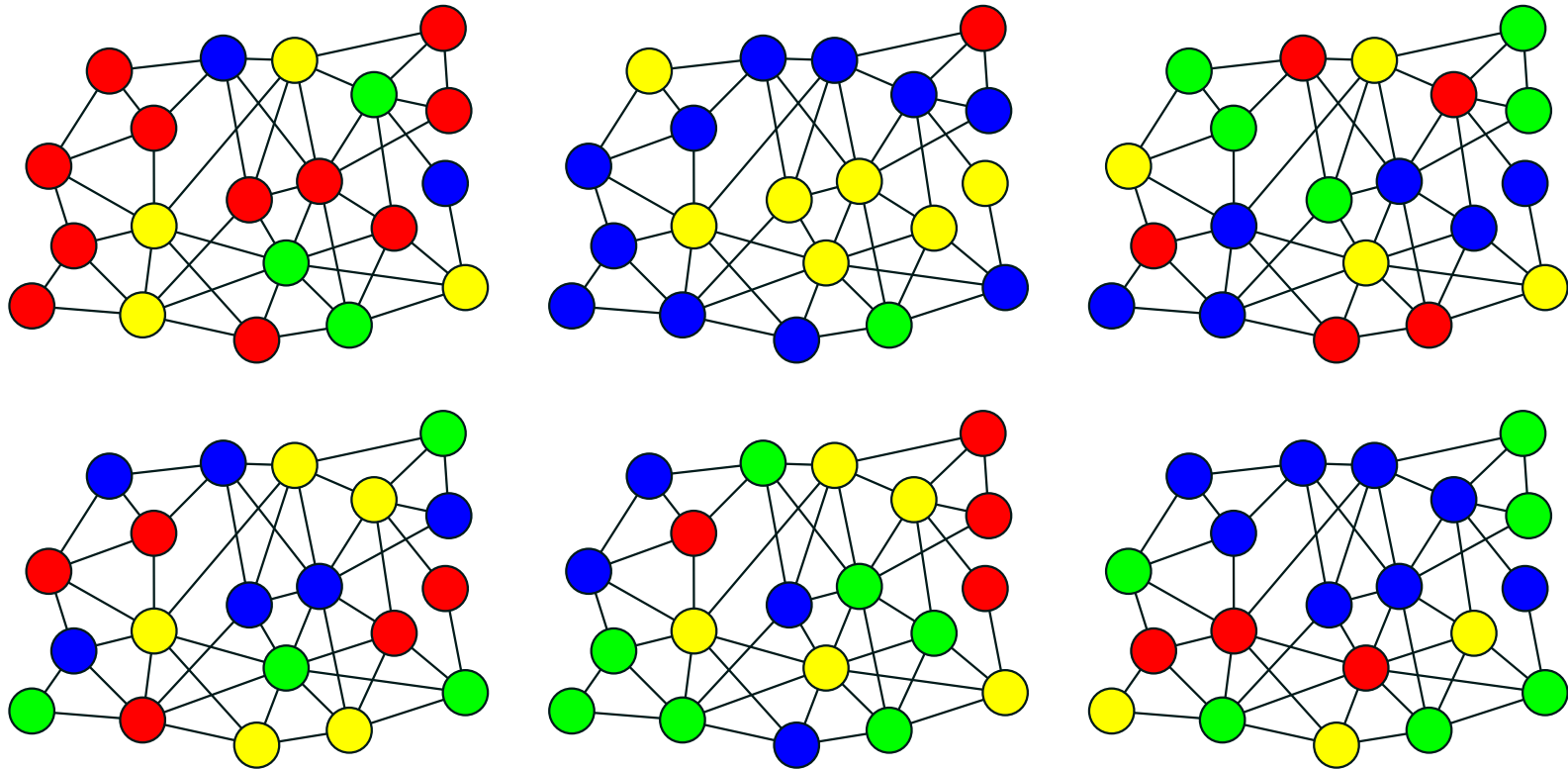
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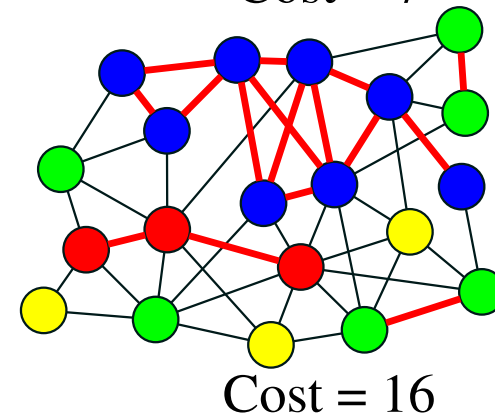
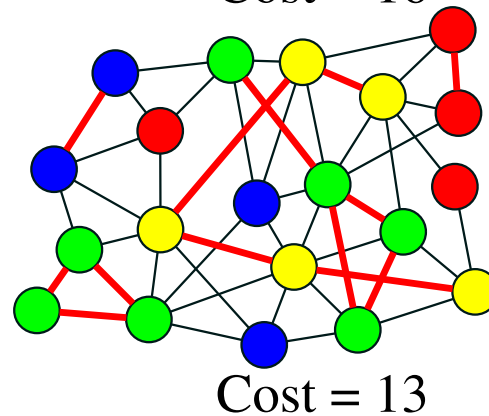
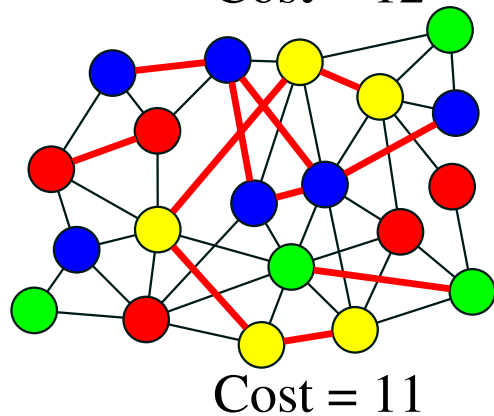
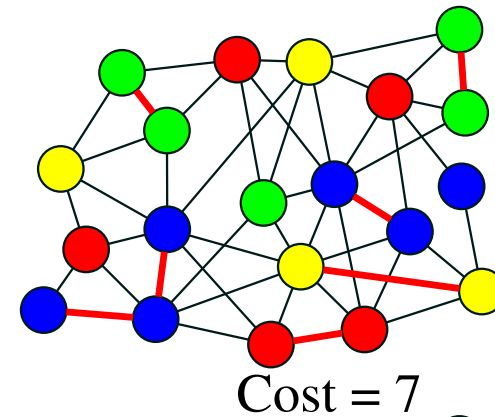
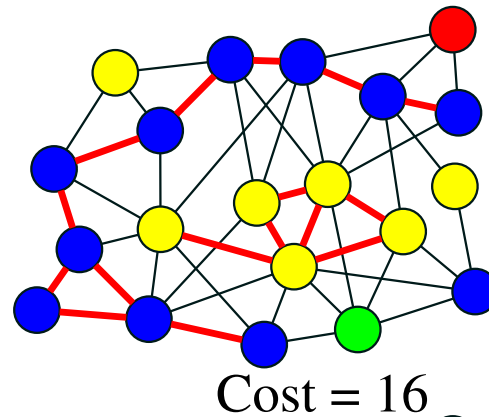
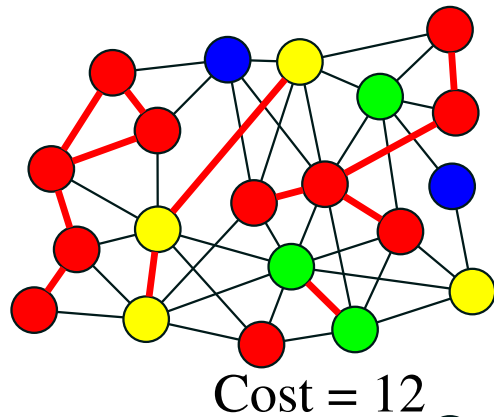
Generation 0



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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

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

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

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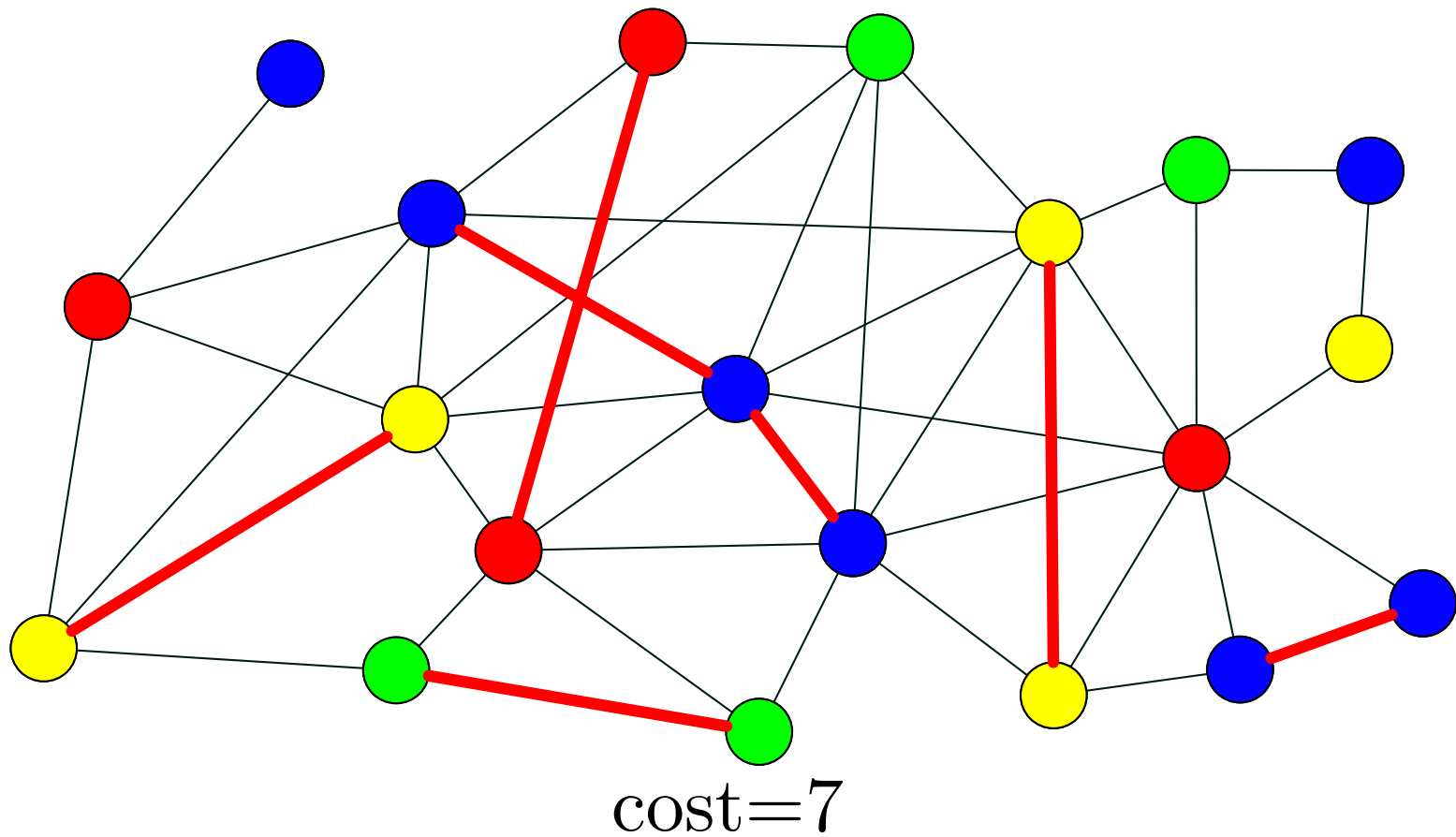
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Change the colour of one or more of the vertices

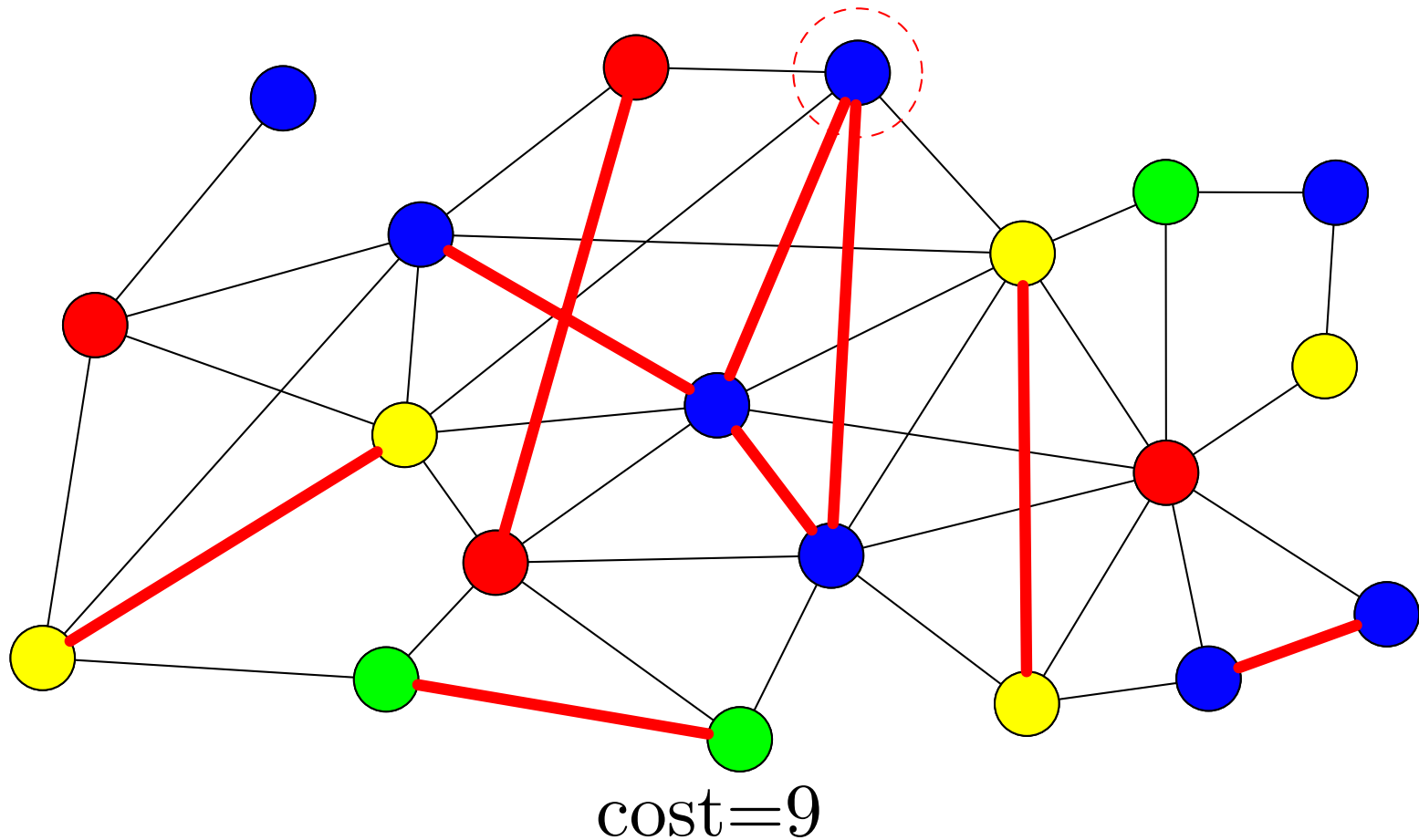
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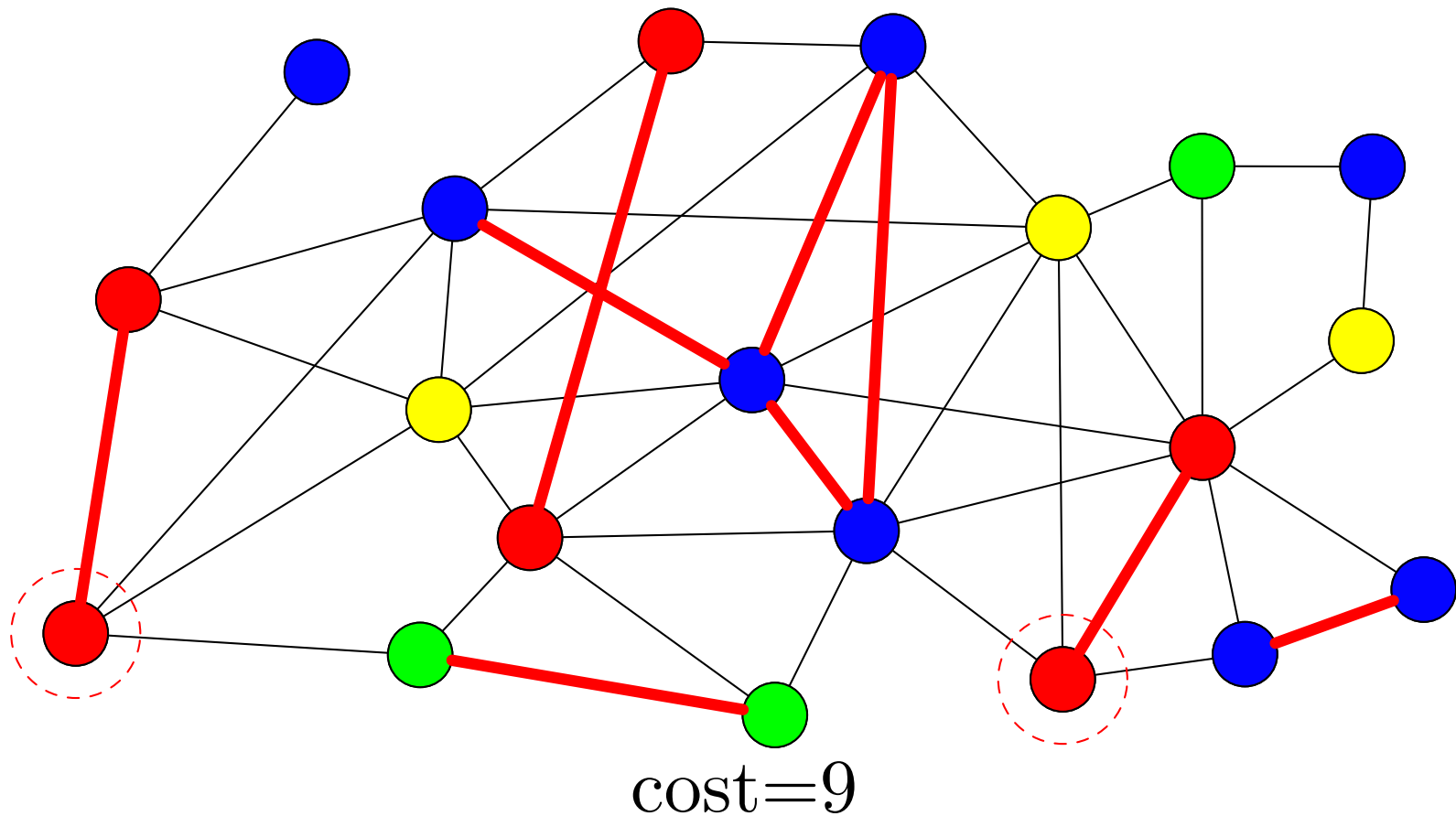
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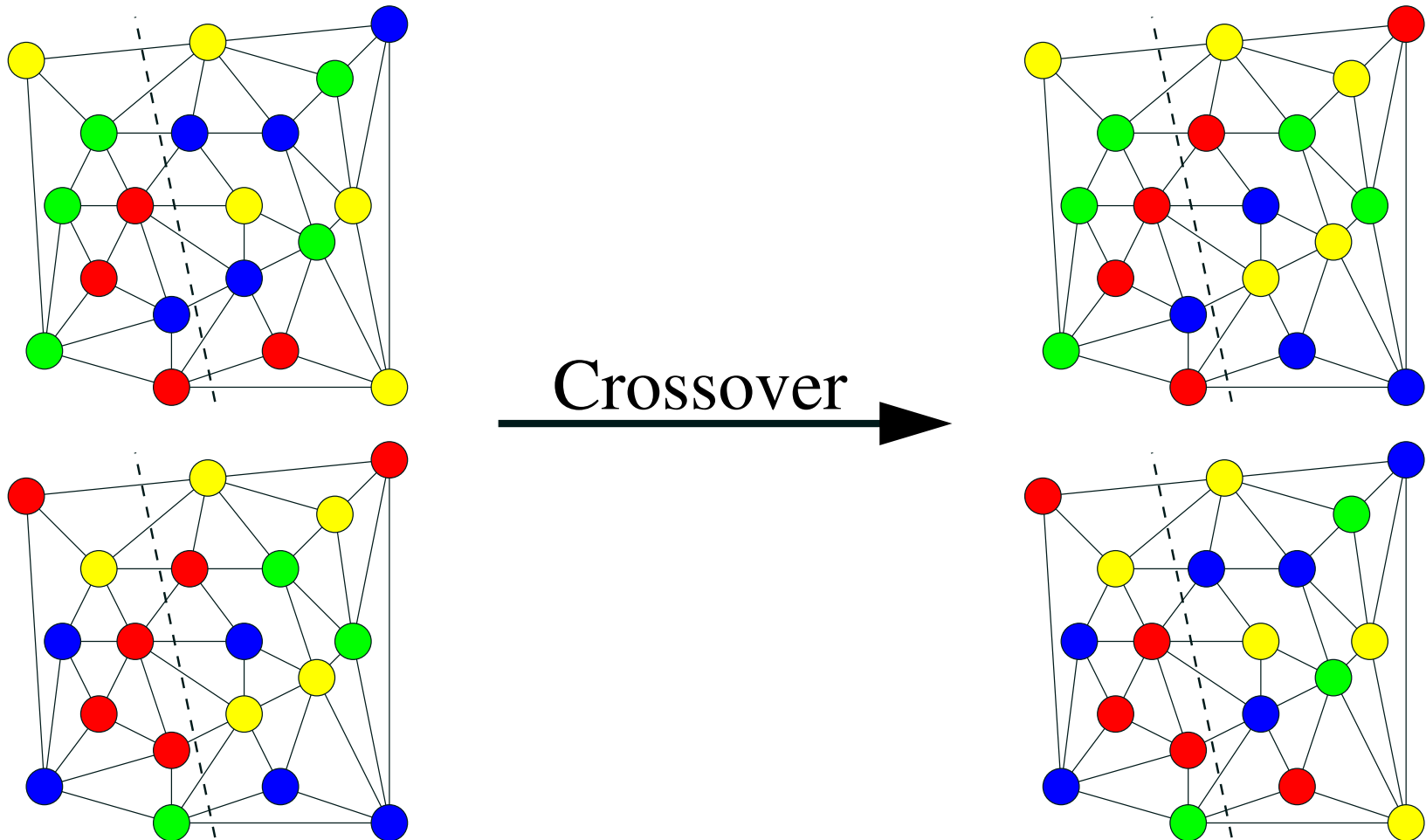


Crossover

Take two solutions and combine them to form a new solution

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Crossover Operators

- Single-point crossover

- ★ Take two strings and cut them at some random site

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

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- Uniform Crossover

- ★ Take two strings and create children by a random shuffle

$$\left(\begin{array}{c} GRBGBR RBGGBGBG \\ \hline RRBRGB RGRBBGB \end{array} \right) \longrightarrow \left\{ \begin{array}{c} GRBRGBRGRGGGB \\ \hline RRBGBRRBGGBBBG \end{array} \right.$$

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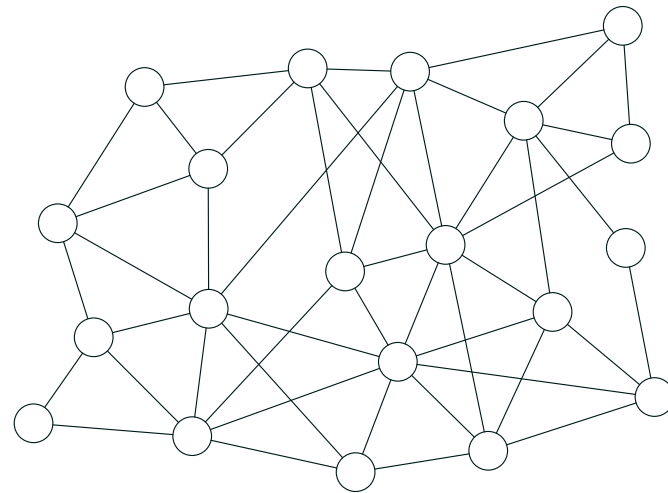
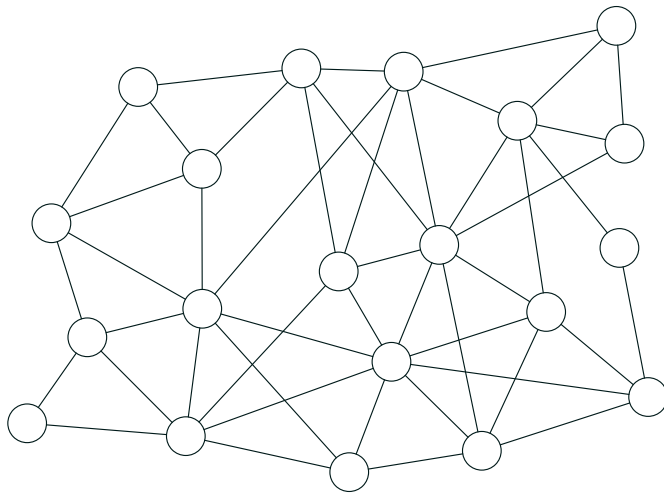
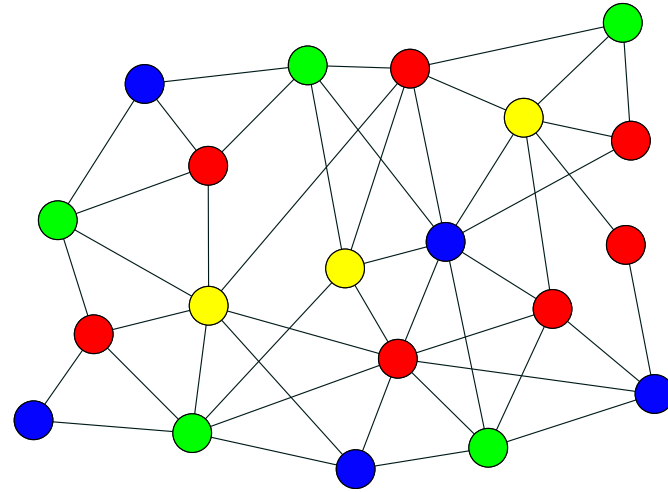
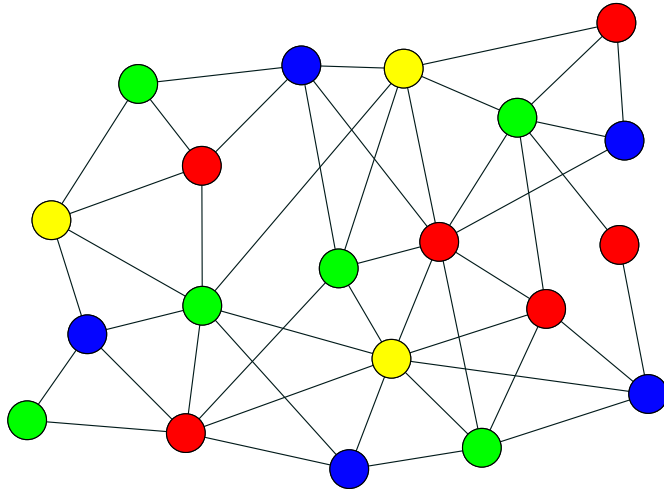
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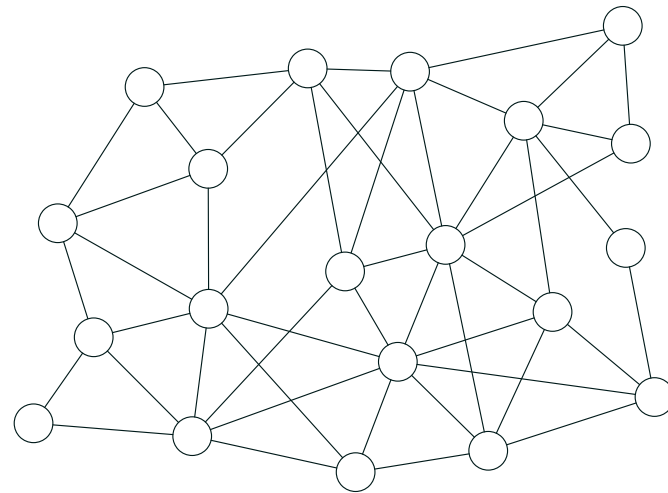
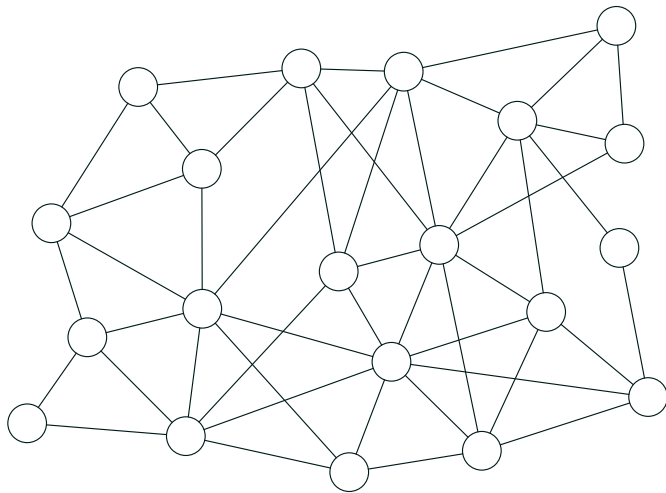
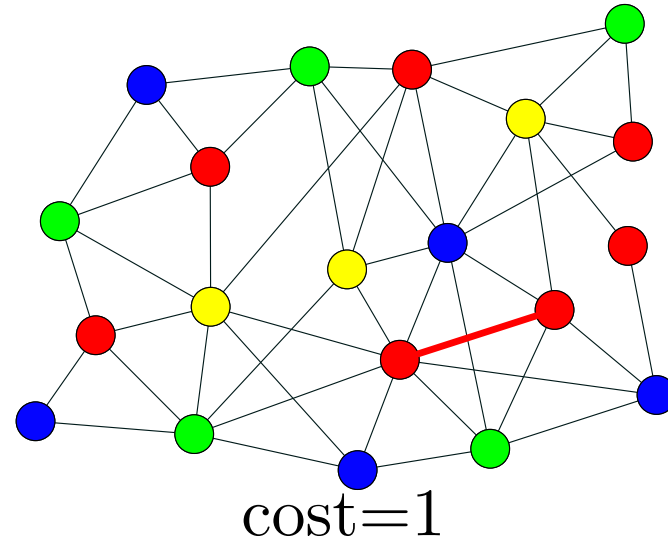
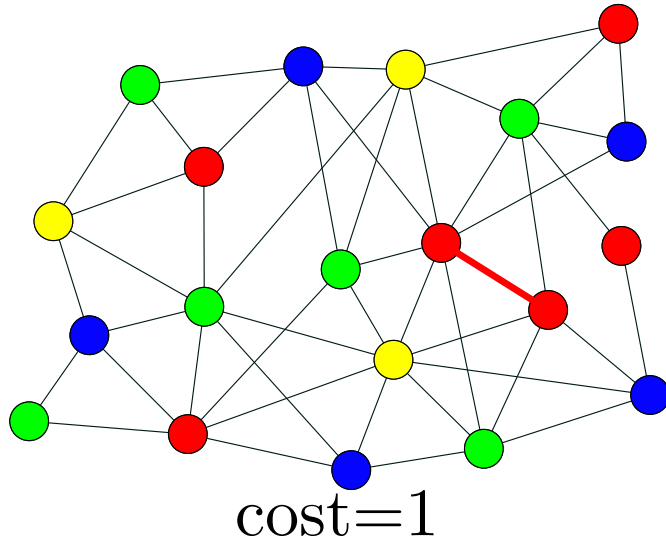
$$\left(\begin{array}{c} GRBGBR RBGGBGBG \\ \hline RRBRGB RGRBBGB \end{array} \right) \longrightarrow \left\{ \begin{array}{c} GRBRGBRGRGGGB \\ \hline RRBGBRRBGGBBBG \end{array} \right.$$

- Any of these crossover can be biased towards one parent

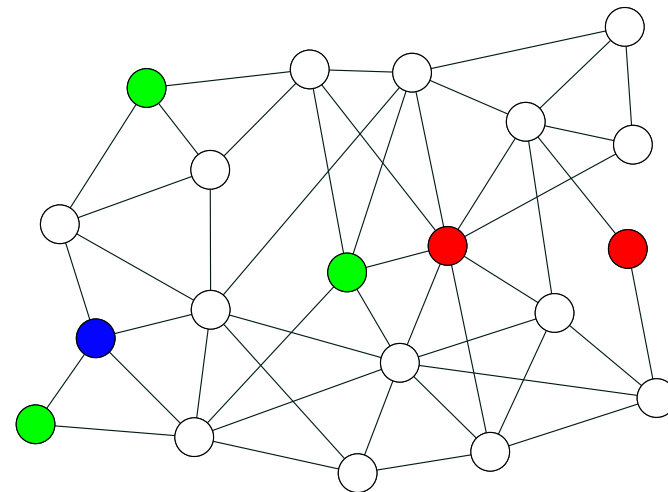
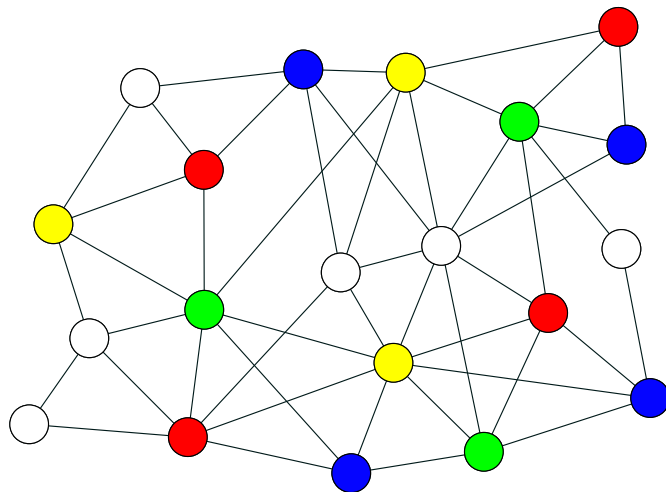
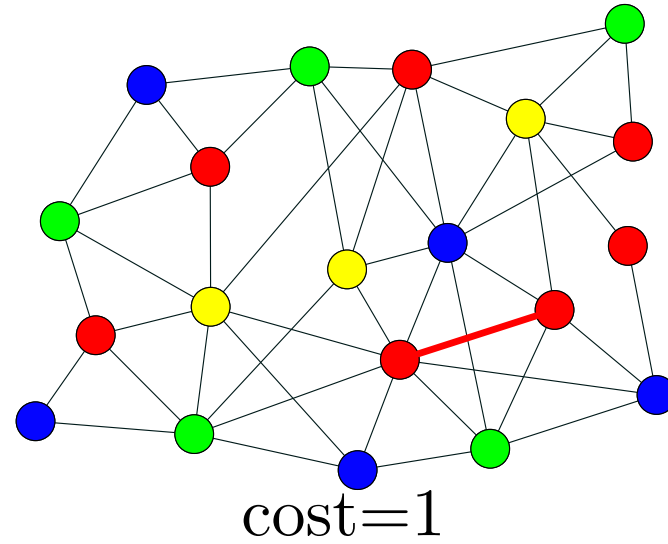
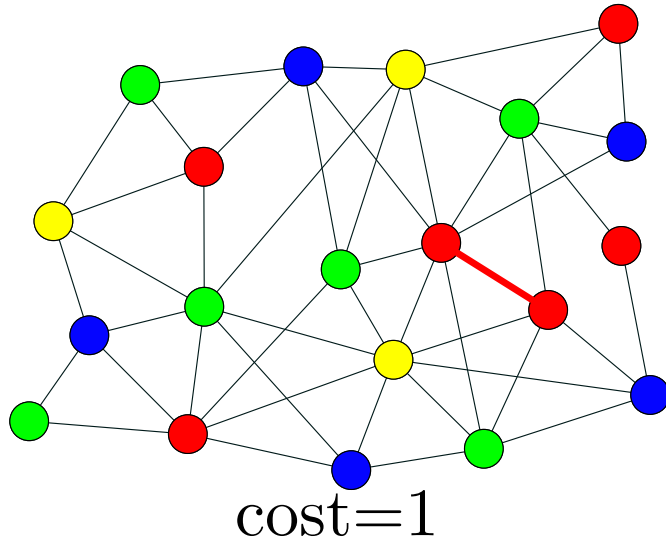
Cost of Crossover



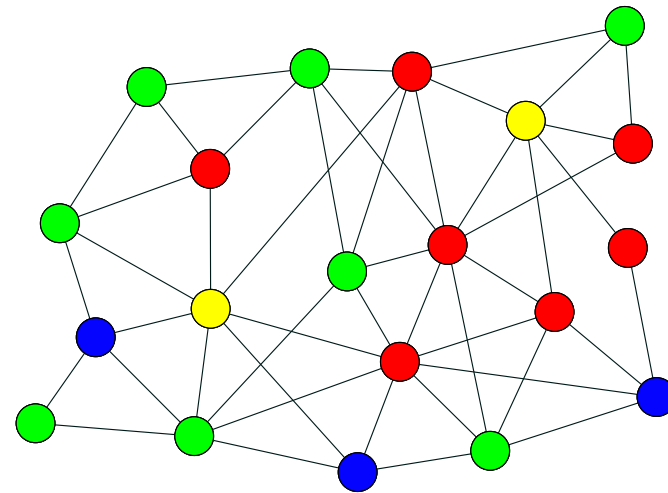
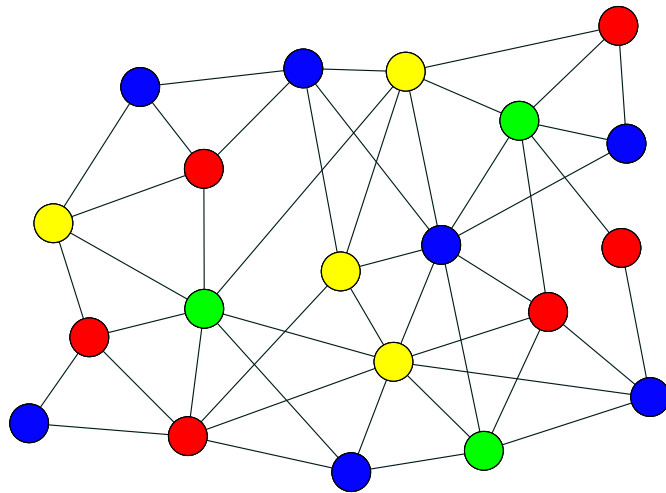
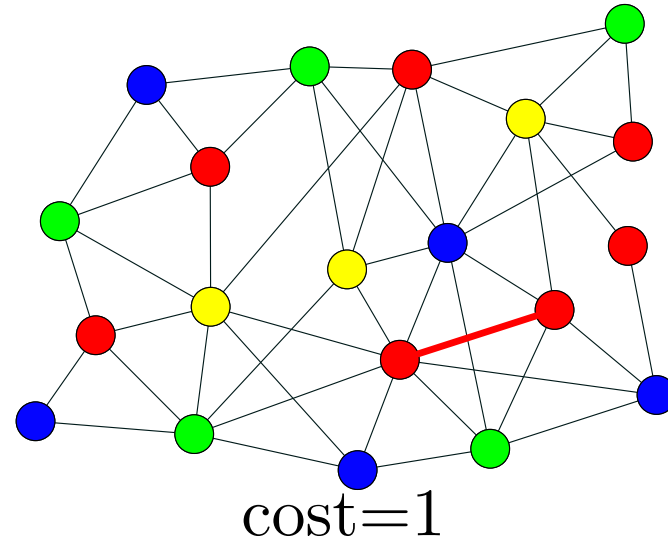
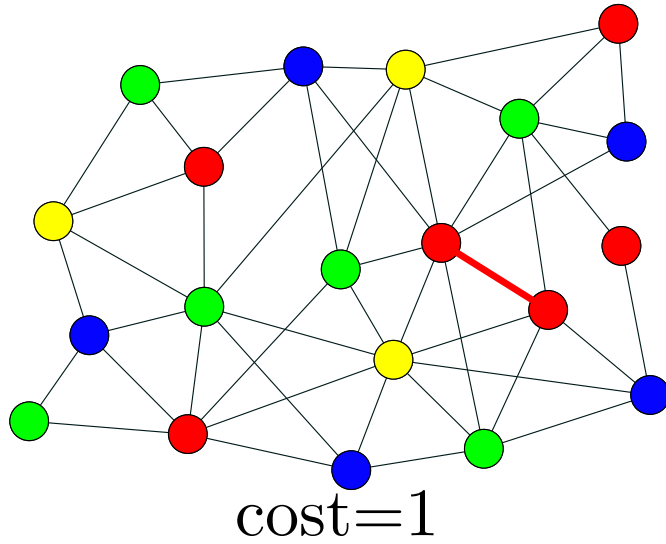
Cost of Crossover



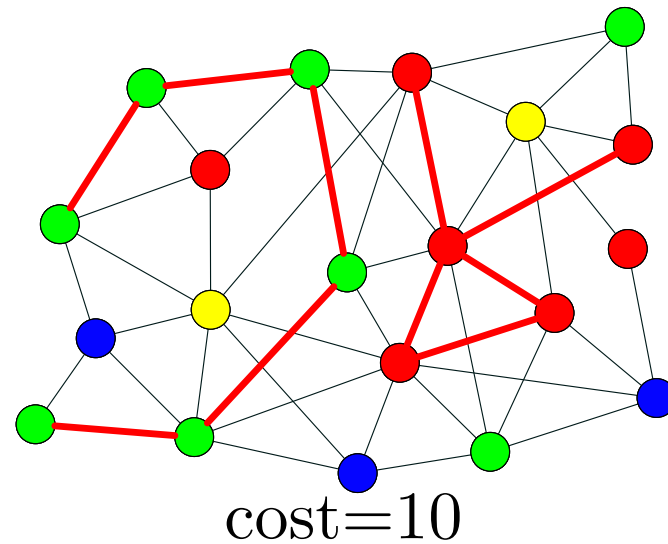
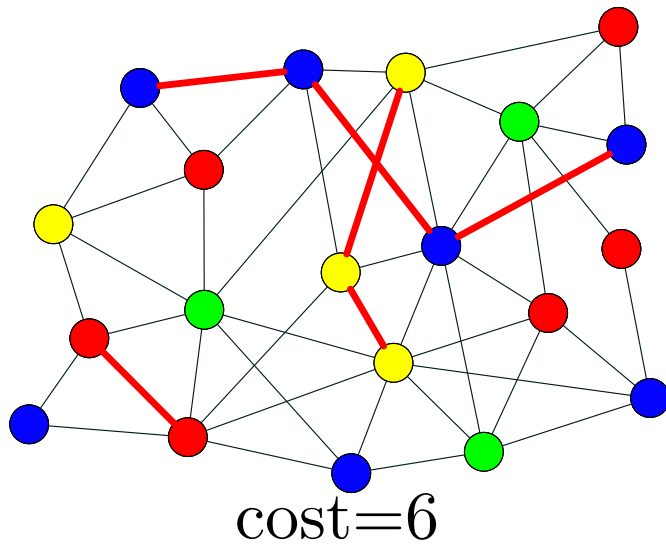
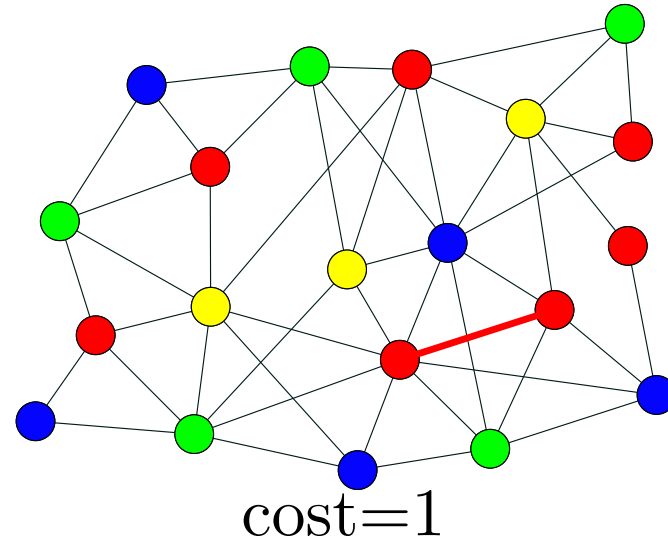
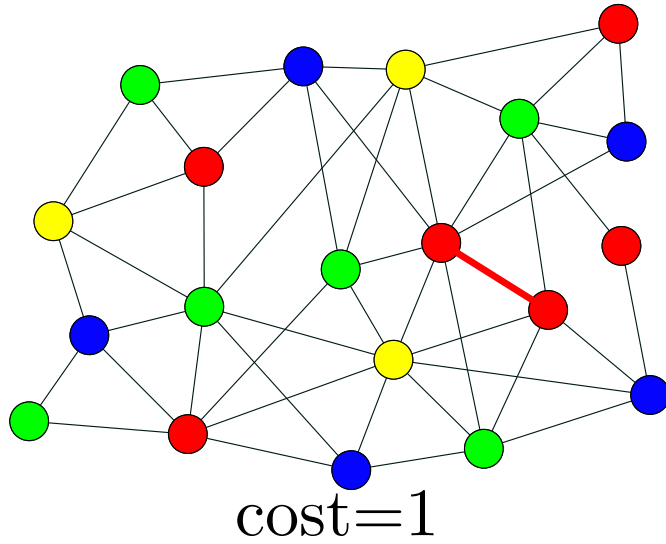
Cost of Crossover



Cost of Crossover

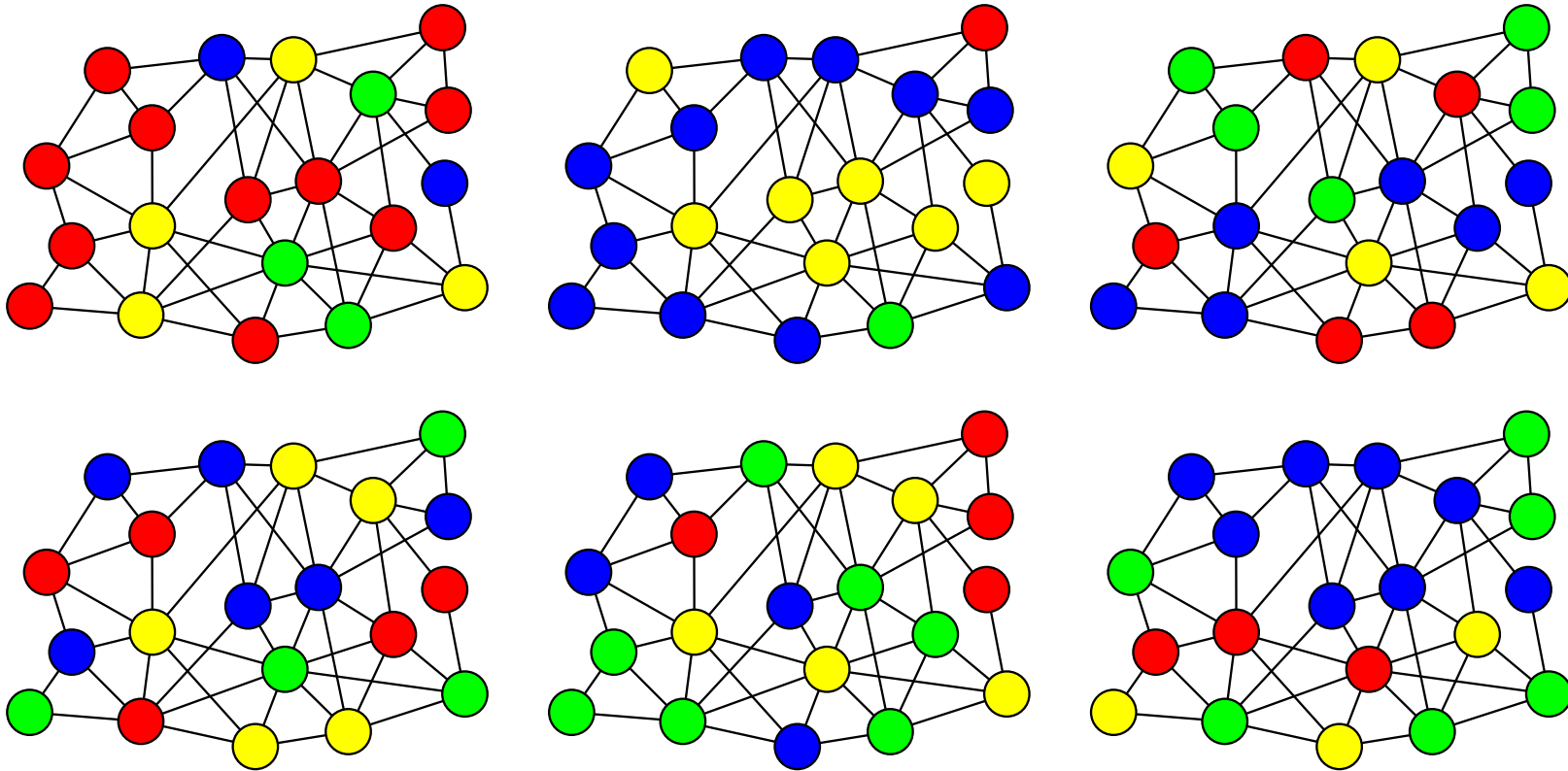


Cost of Crossover



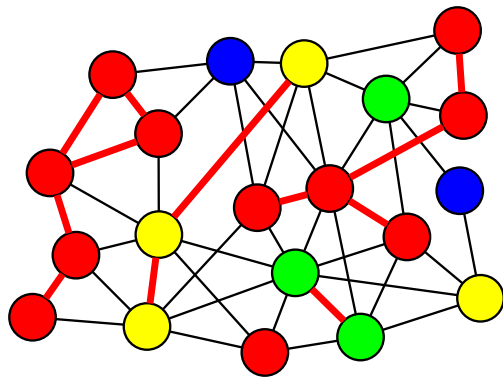
GA

Generation 0

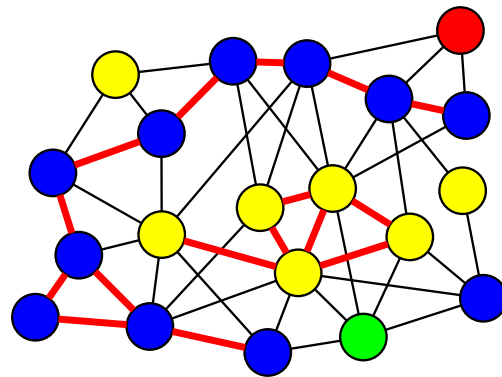


GA

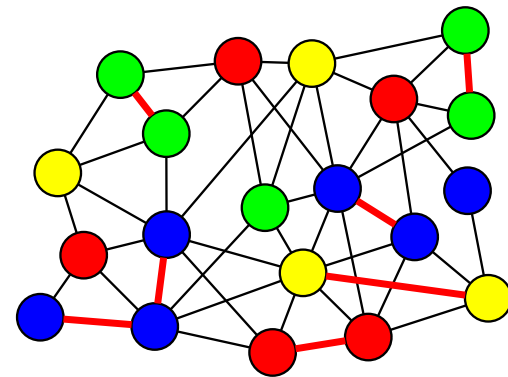
Generation 0: evaluate fitness



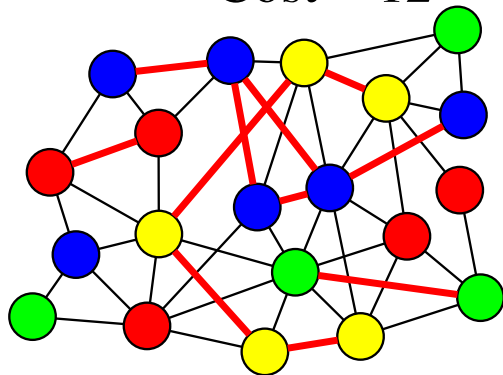
Cost = 12



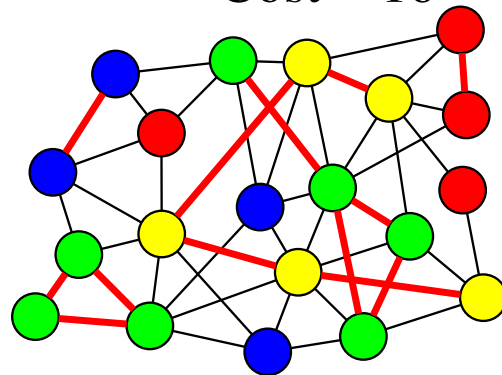
Cost = 16



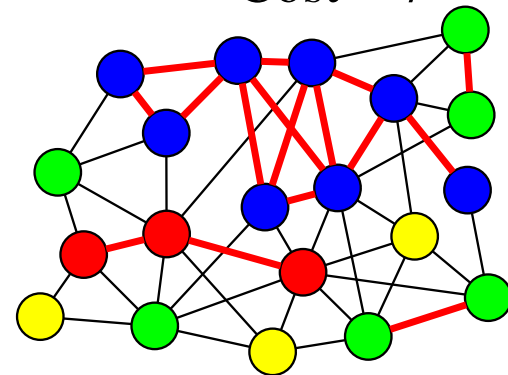
Cost = 7



Cost = 11



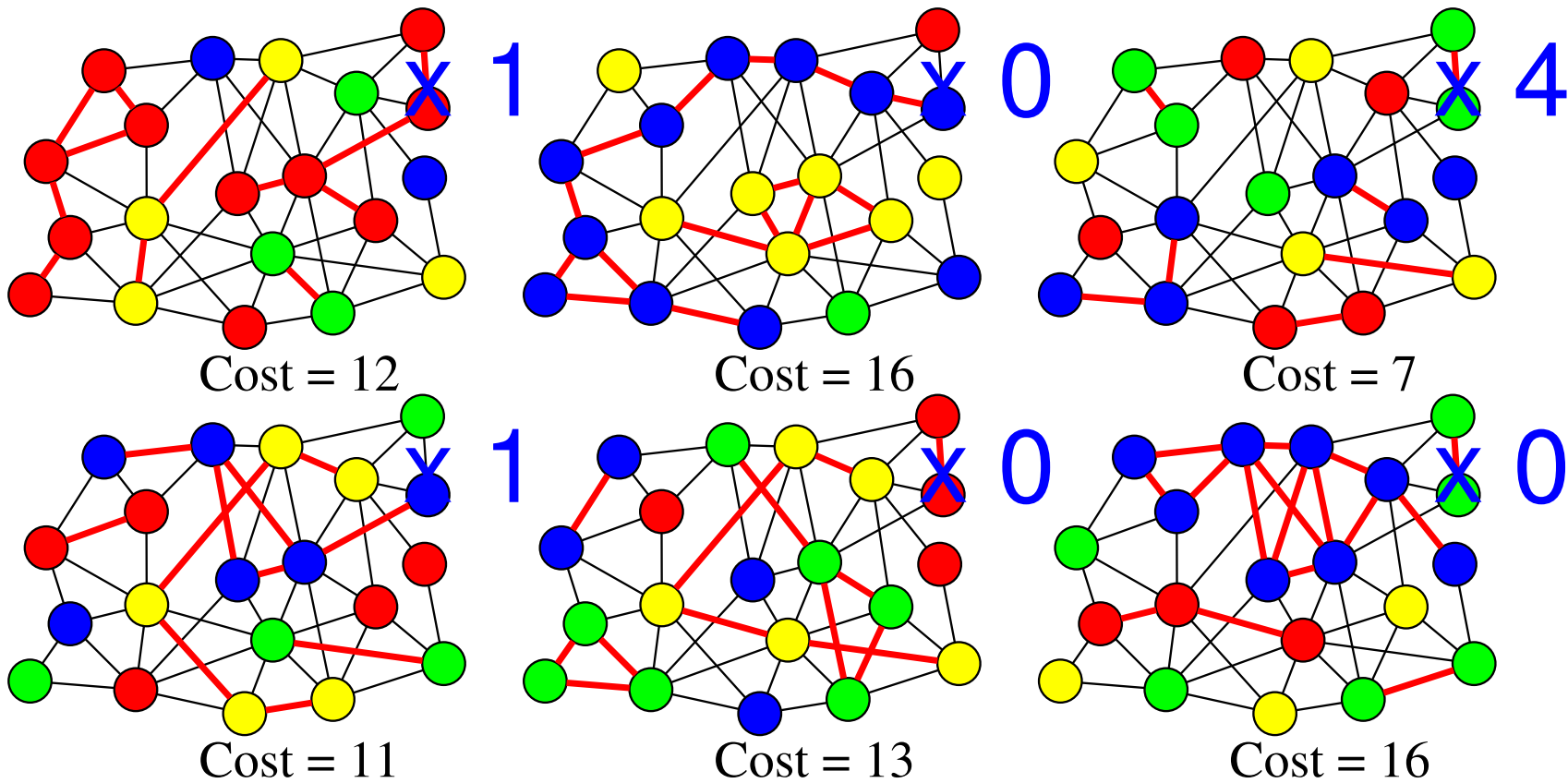
Cost = 13



Cost = 16

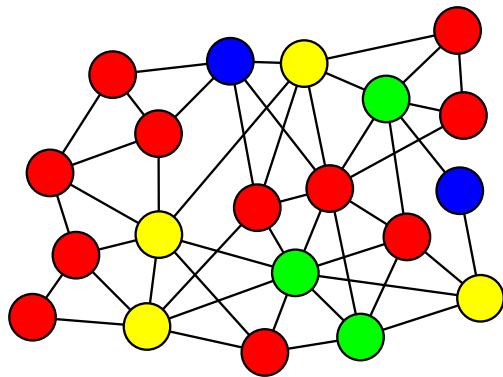
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Generation 0: selection

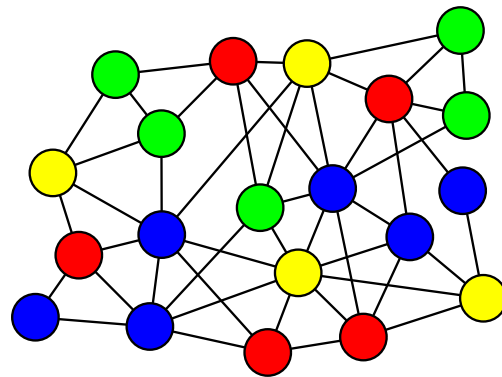


GA

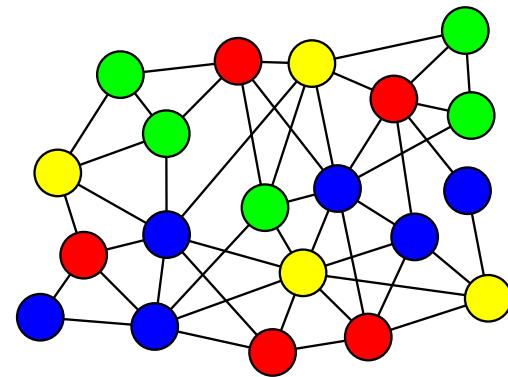
Generation 0: selection



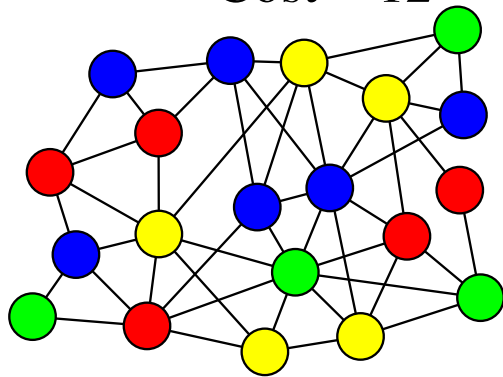
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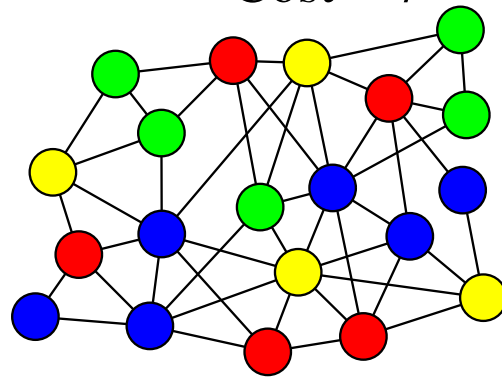
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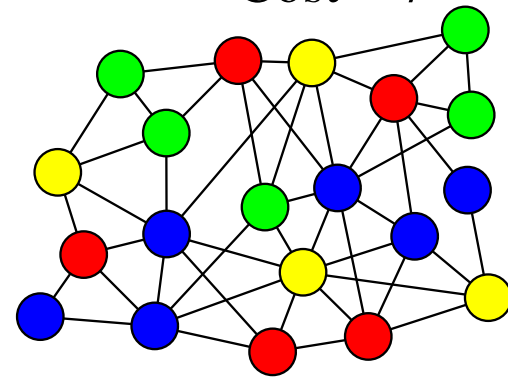
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Cost = 11



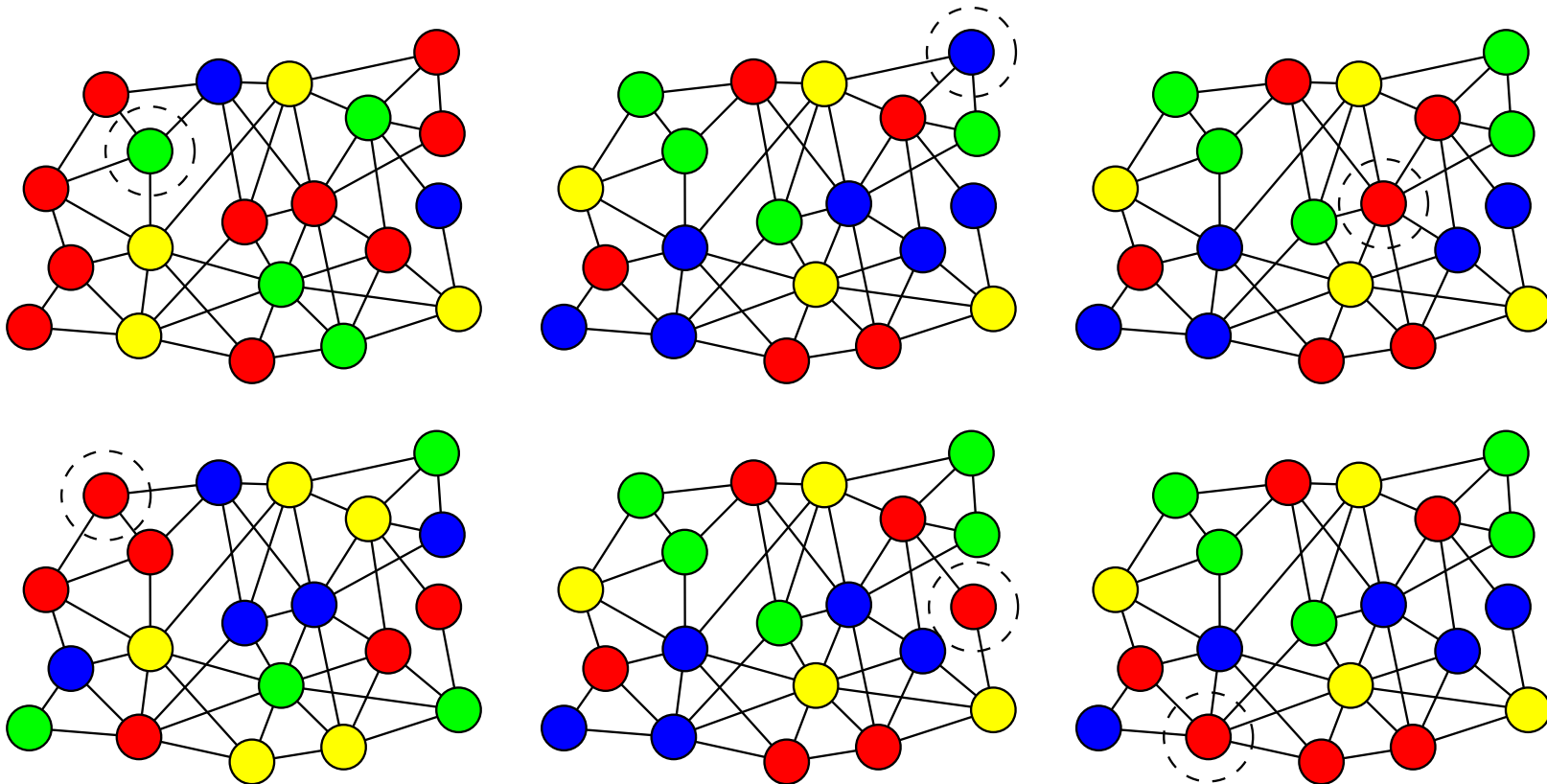
Cost = 7



Cost = 7

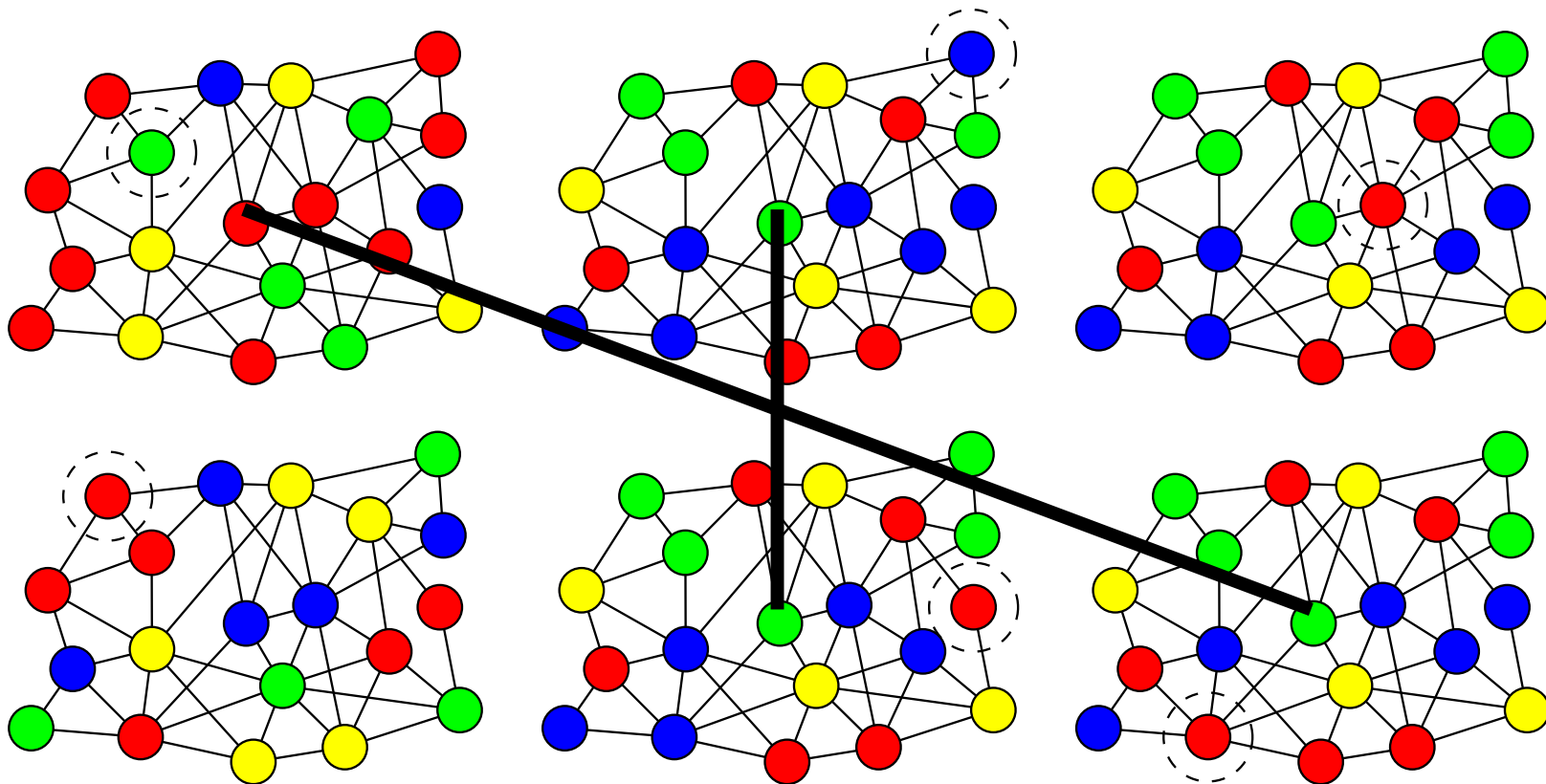
GA

Generation 0: mutation



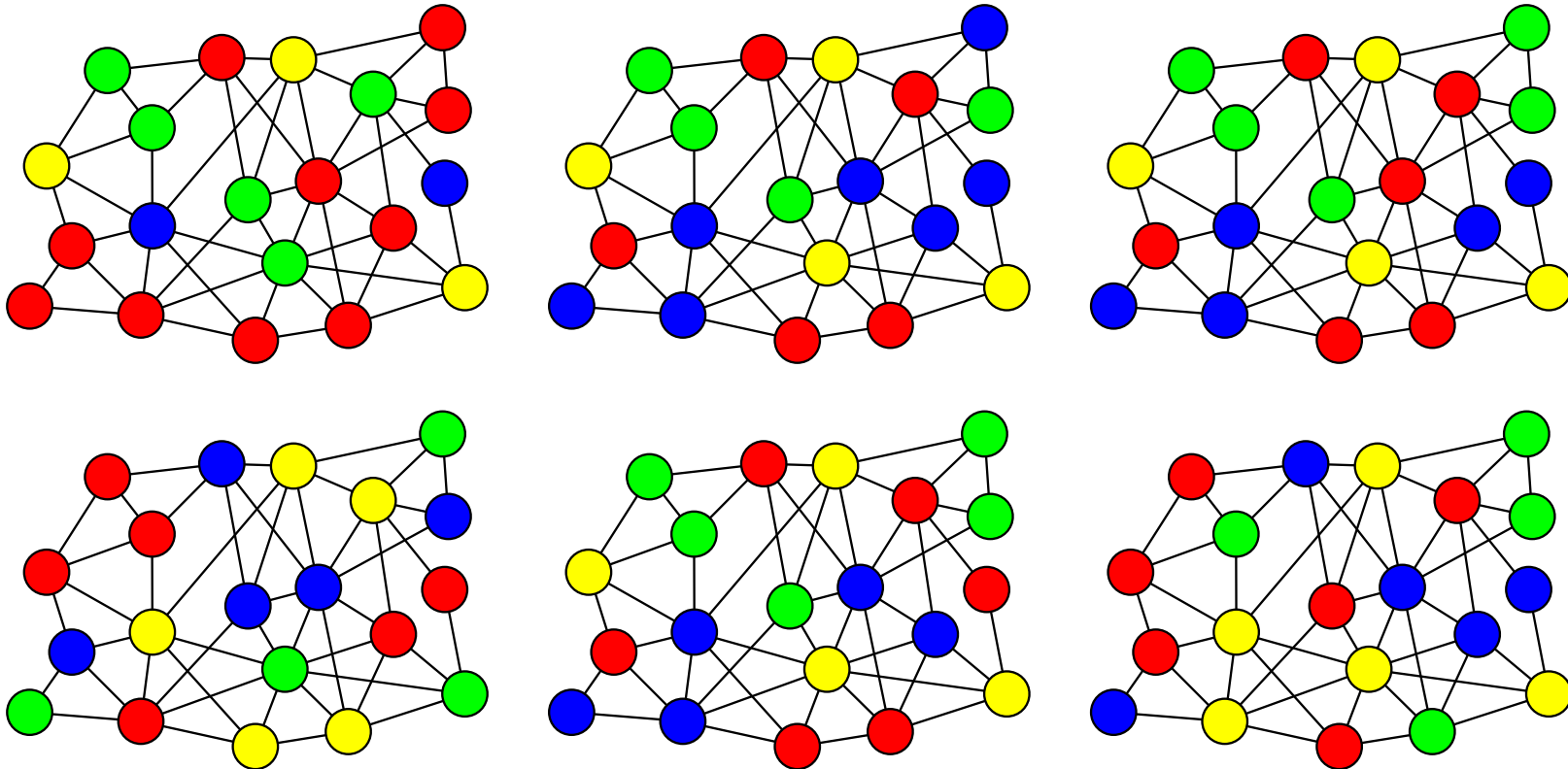
GA

Generation 0: crossover



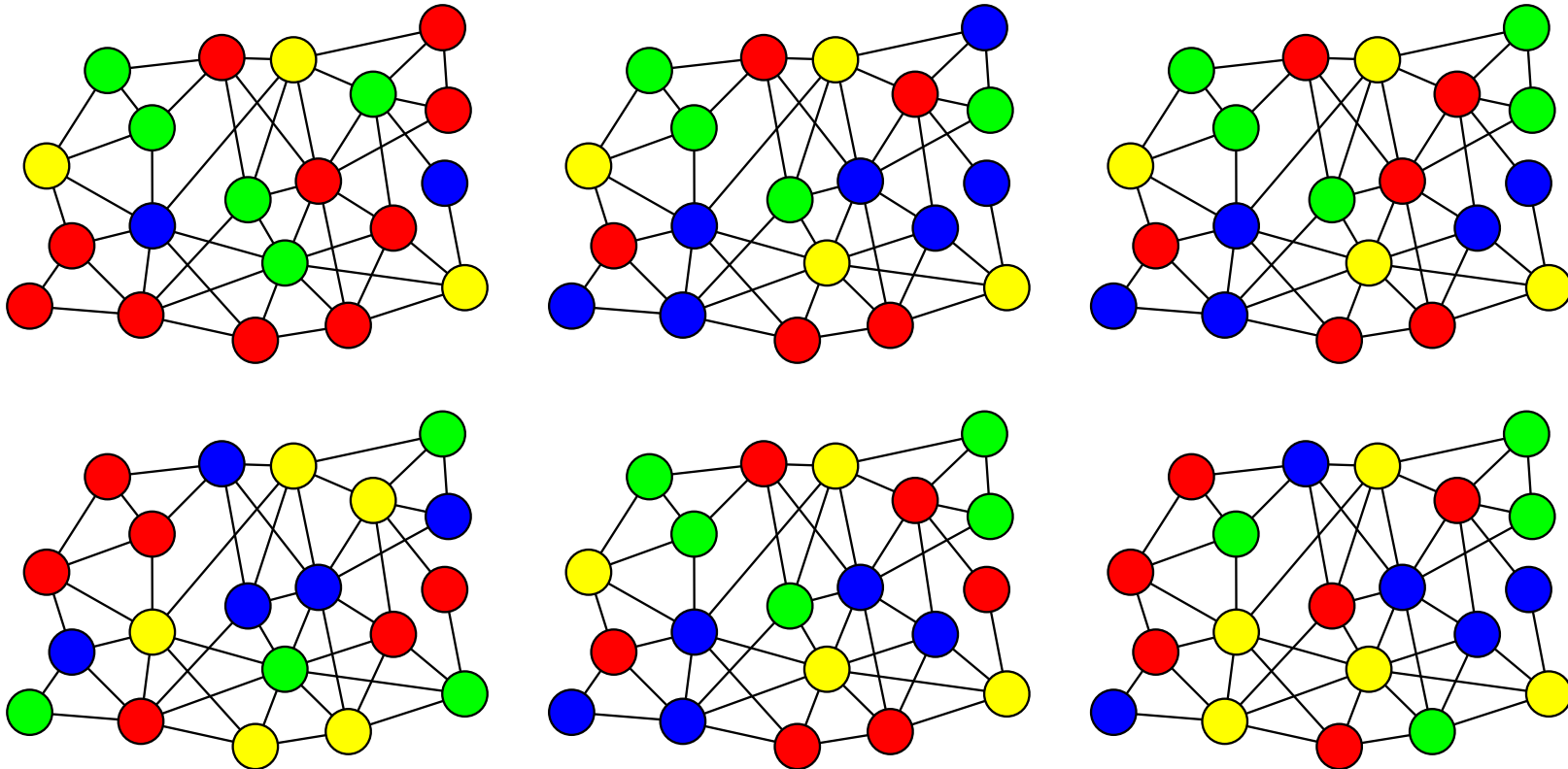
GA

Generation 0: crossover



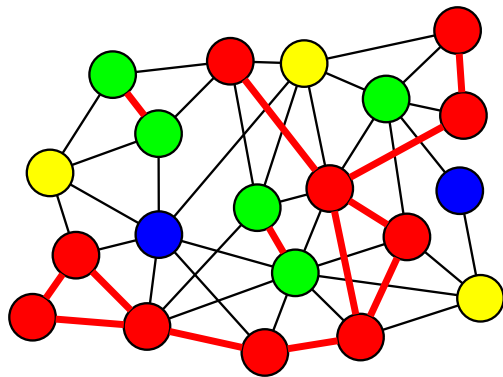
GA

Generation 1

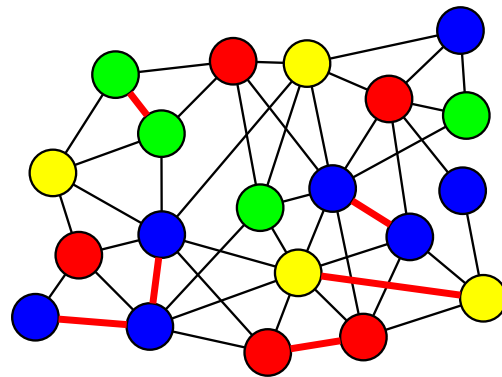


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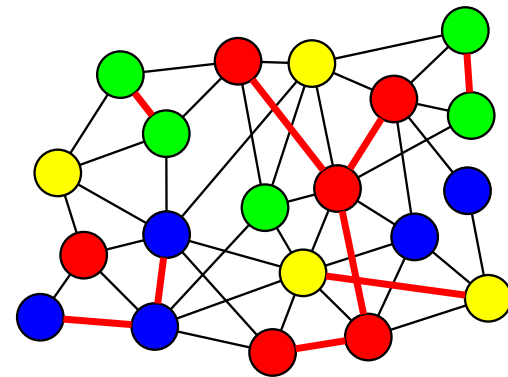
Generation 1: evaluate fitness



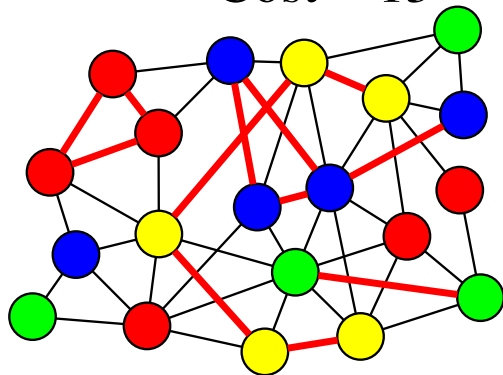
Cost = 13



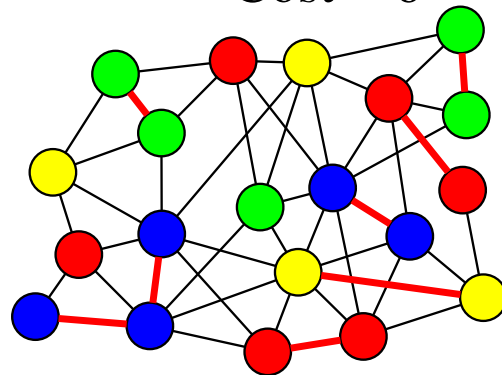
Cost = 6



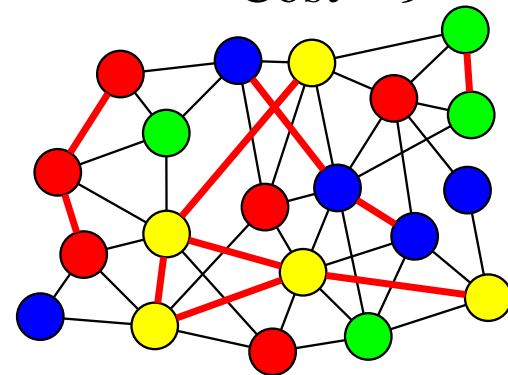
Cost = 9



Cost = 12



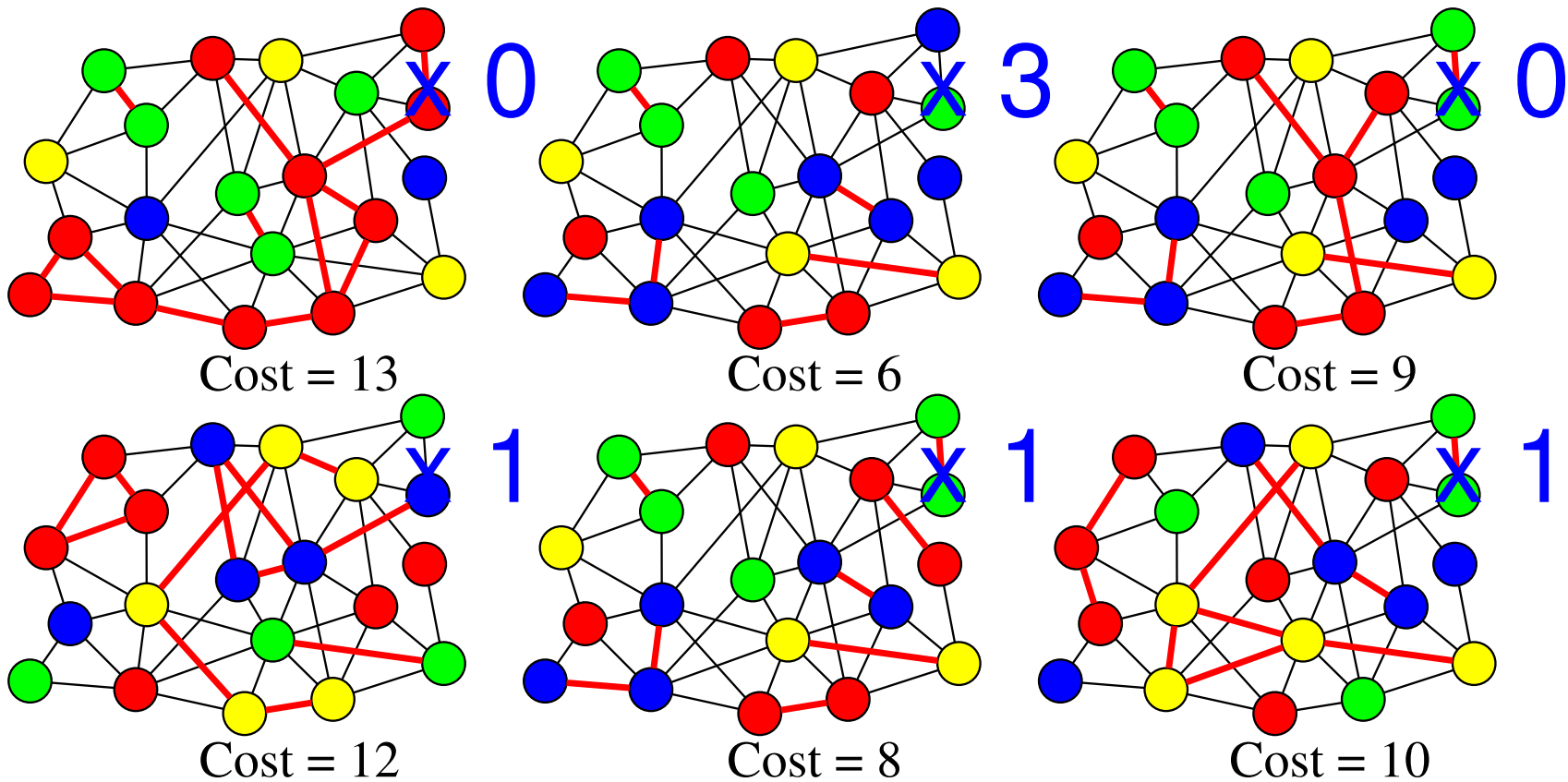
Cost = 8



Cost = 10

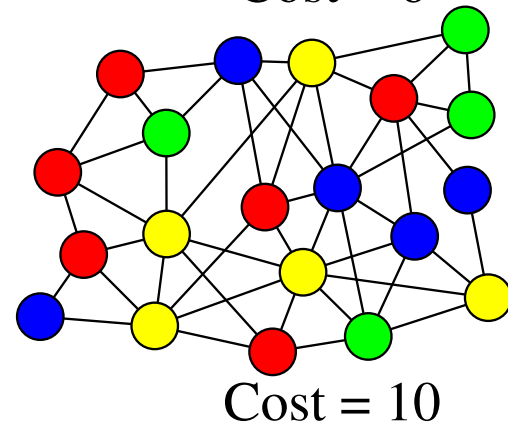
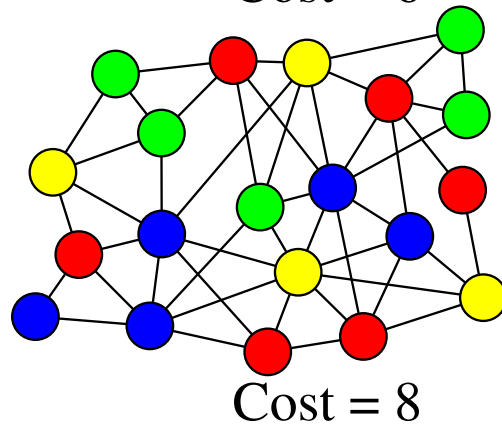
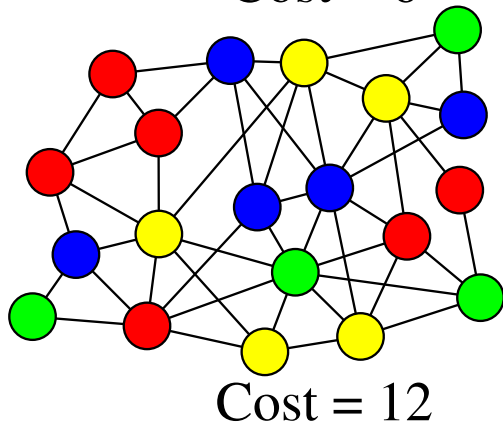
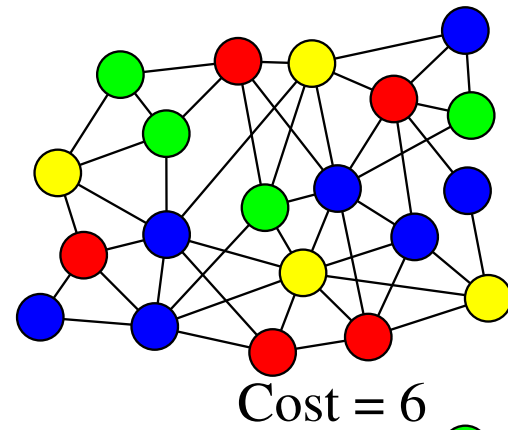
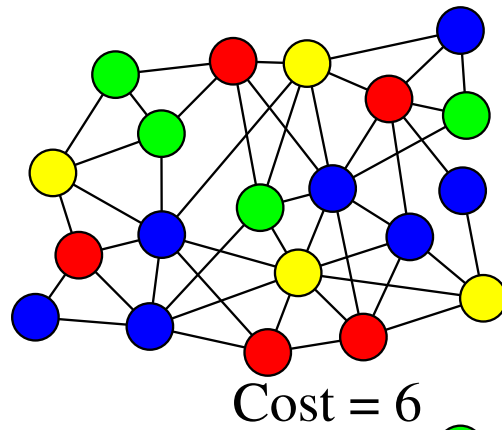
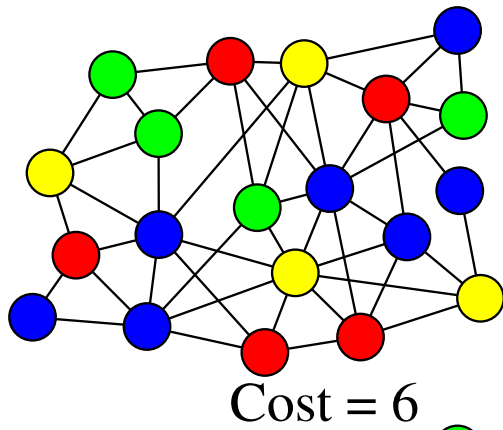
GA

Generation 1: selection



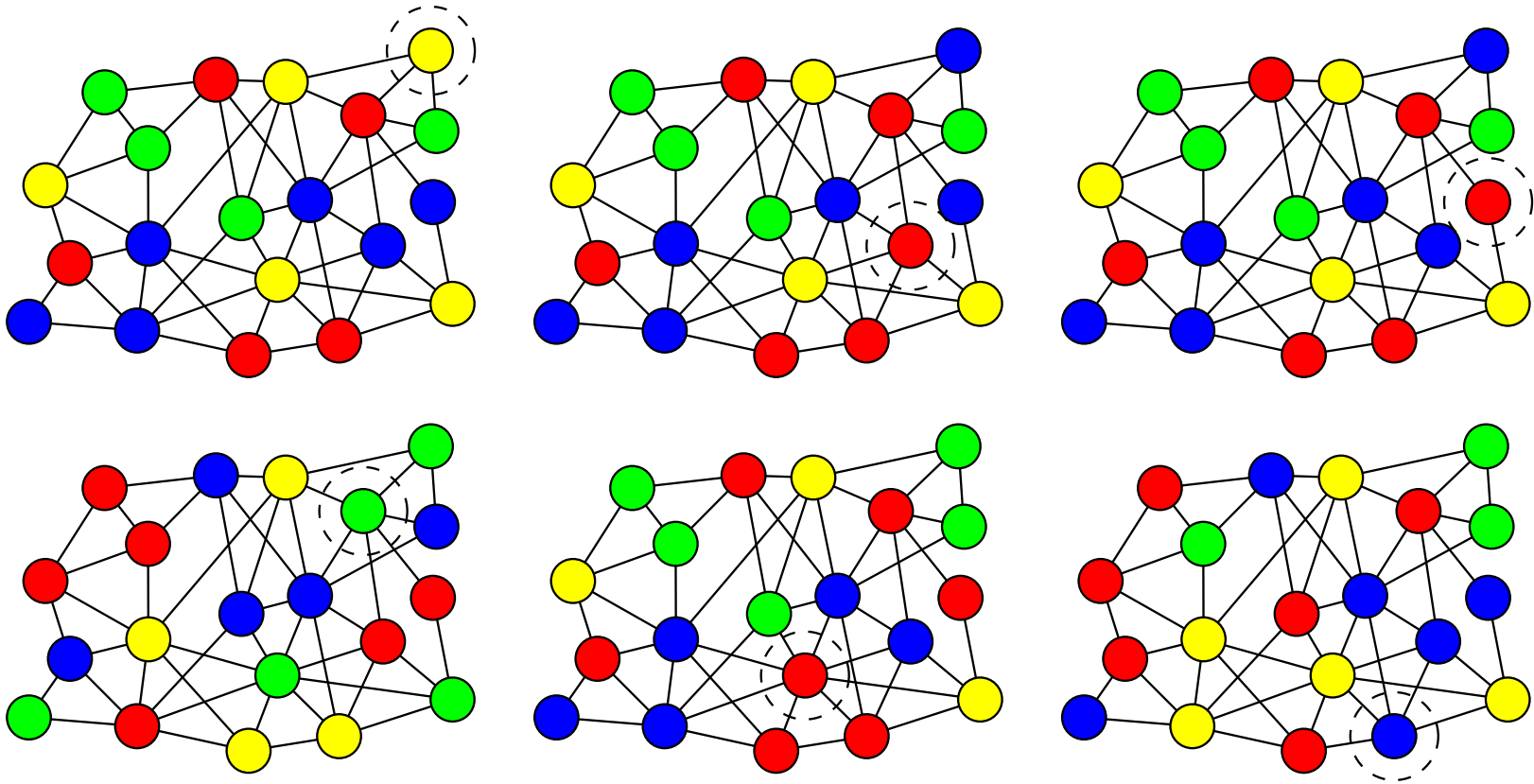
GA

Generation 1: selection



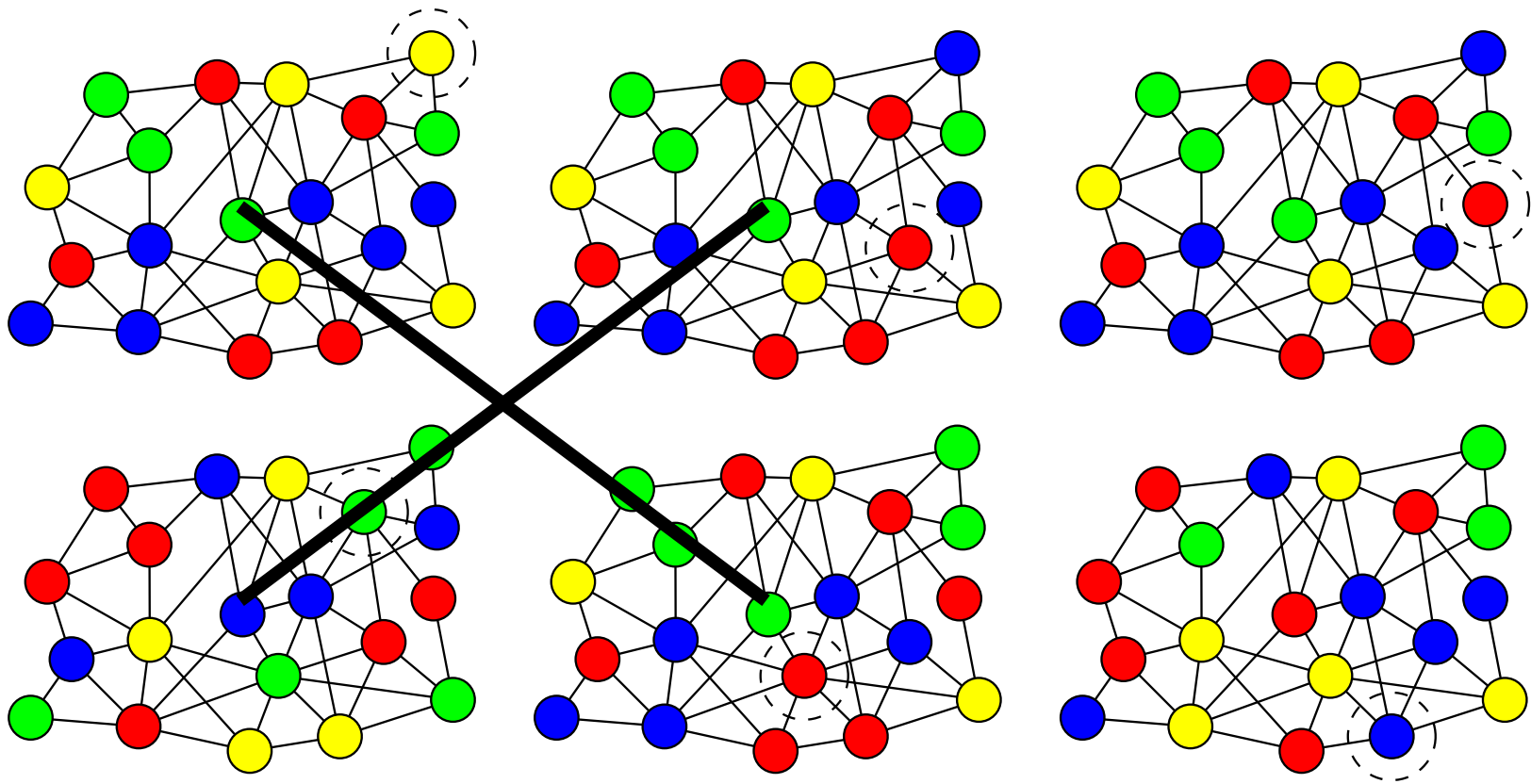
GA

Generation 1: mutation



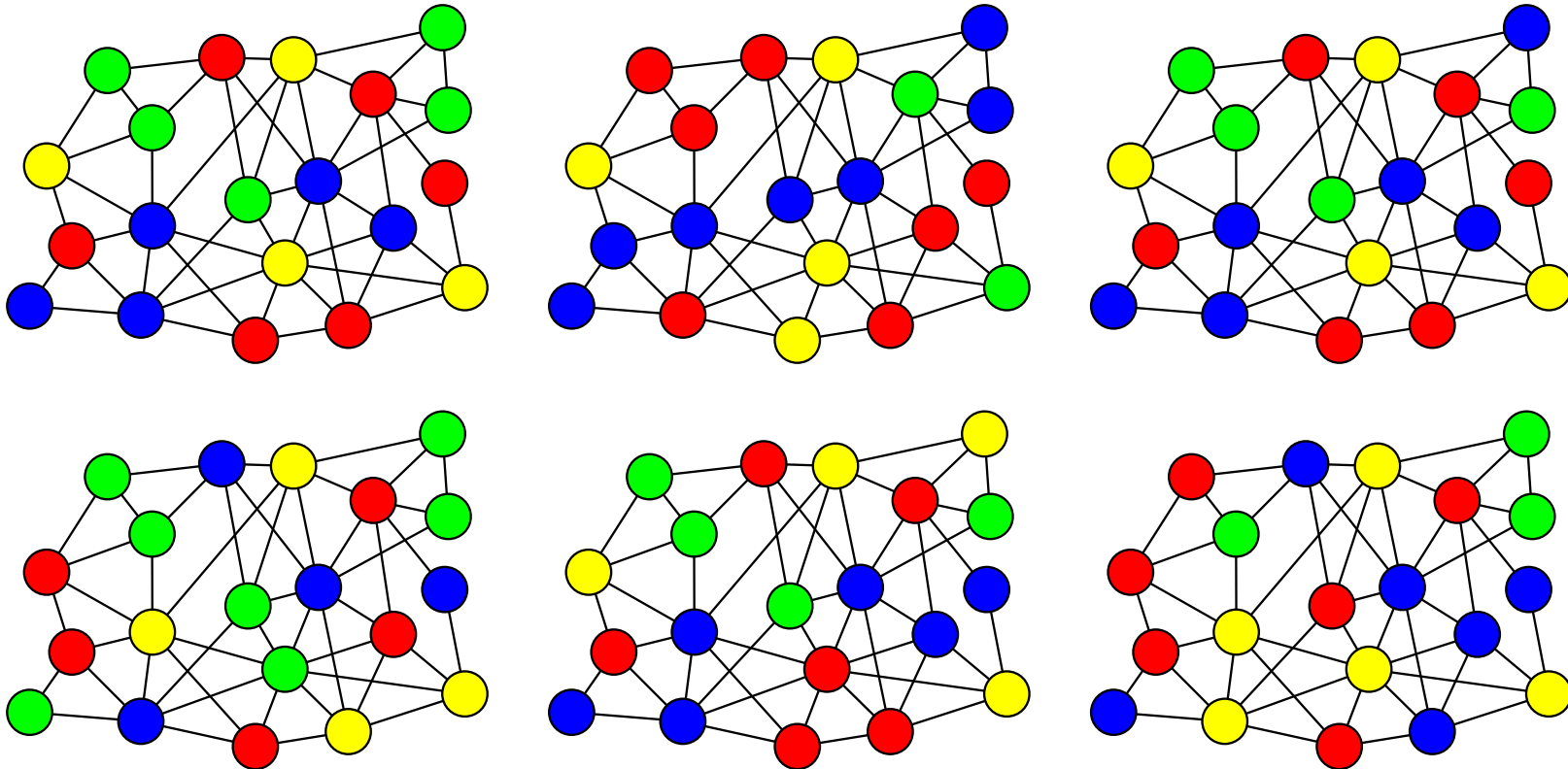
GA

Generation 1: crossover



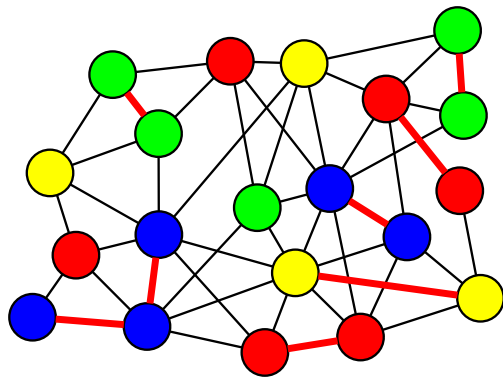
GA

Generation 1: crossover

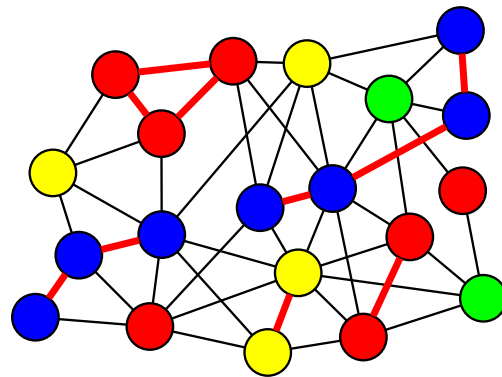


GA

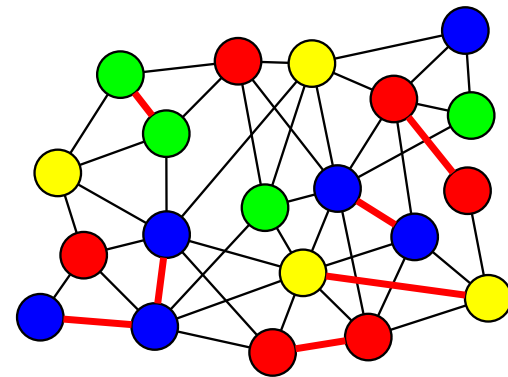
Final Population



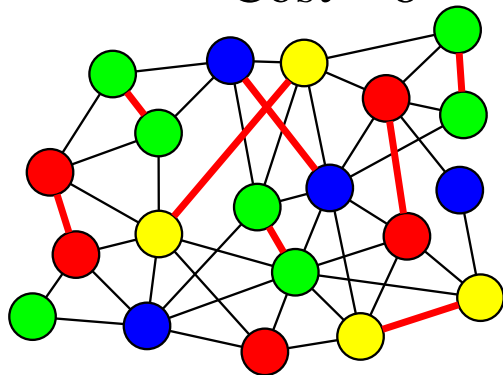
Cost = 8



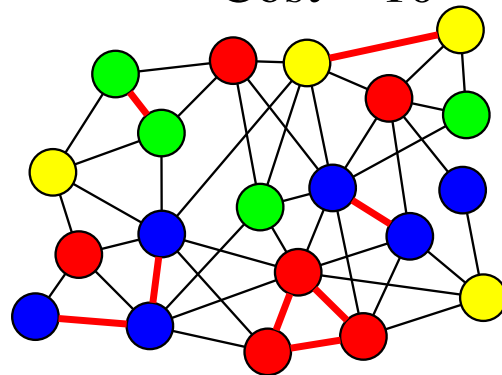
Cost = 10



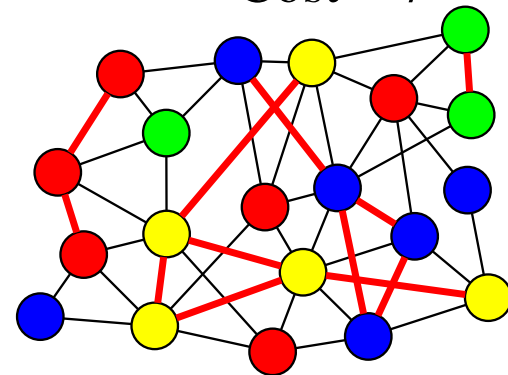
Cost = 7



Cost = 8



Cost = 8



Cost = 12

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

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(\dots, B, \dots) (\dots, R, \dots) (\dots, G, \dots)
 (\dots, R, \dots) (\dots, B, \dots) (\dots, G, \dots)
 (\dots, B, \dots) (\dots, G, \dots) (\dots, B, \dots)
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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
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- etc.

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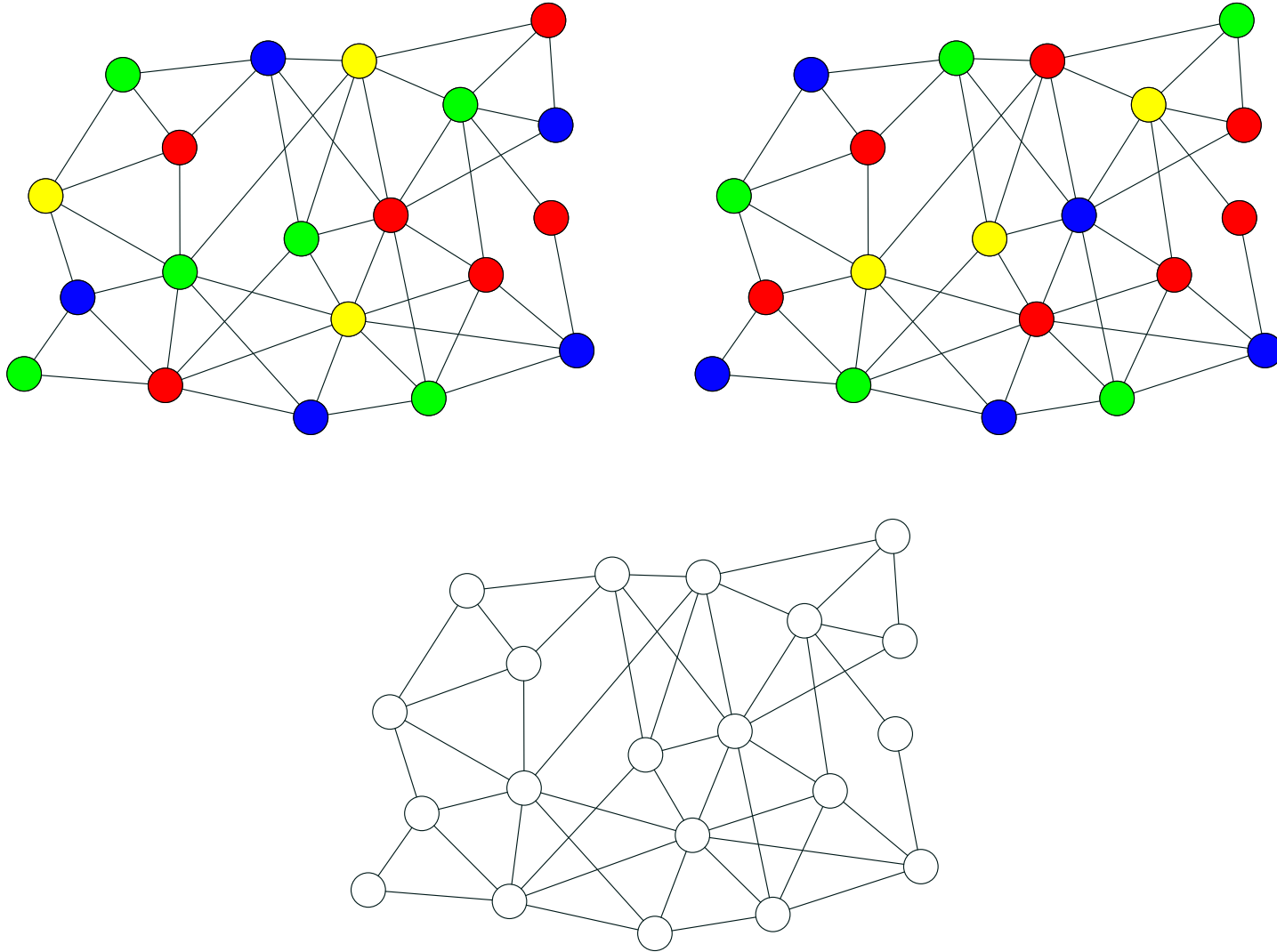
Galinier and Hao's Crossover Operator

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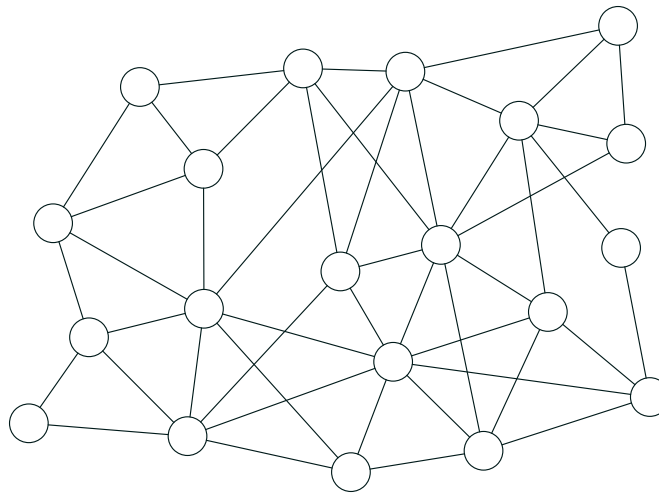
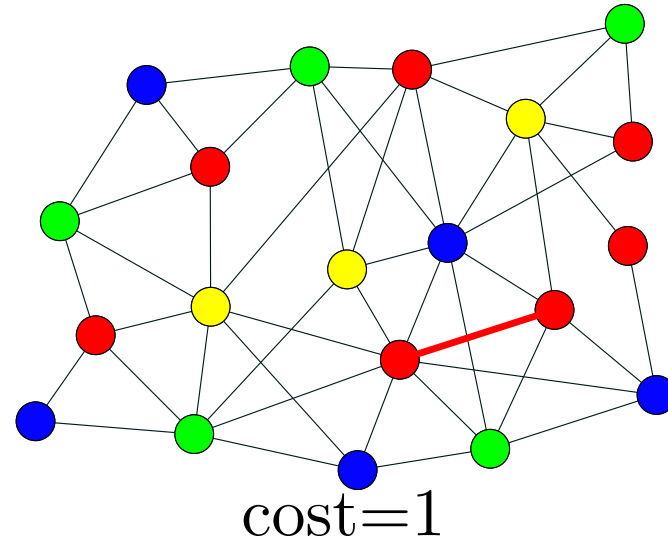
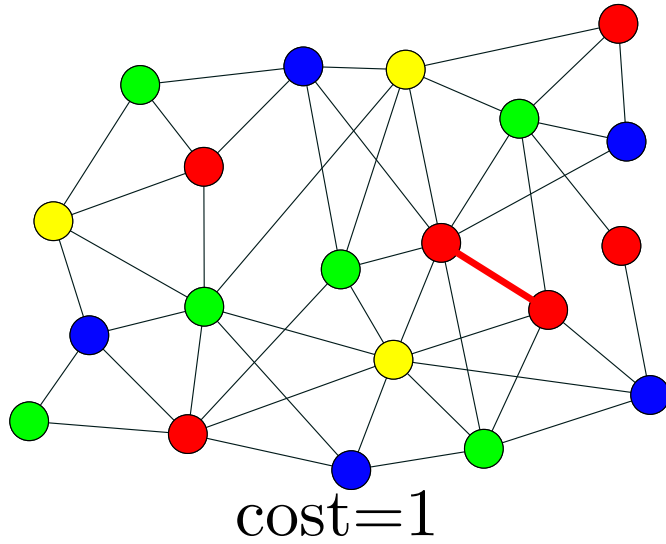
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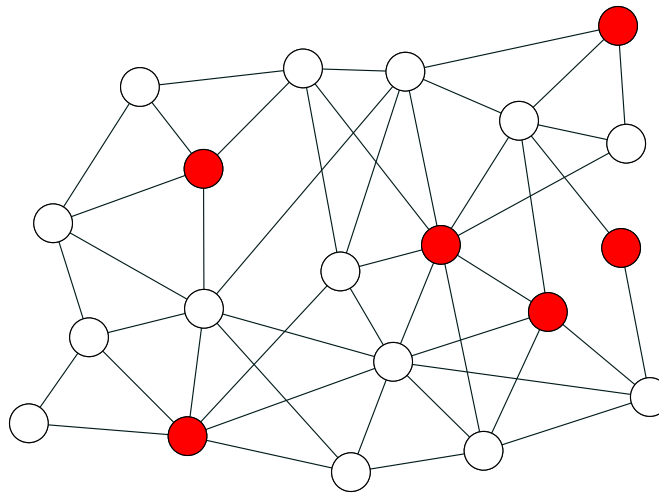
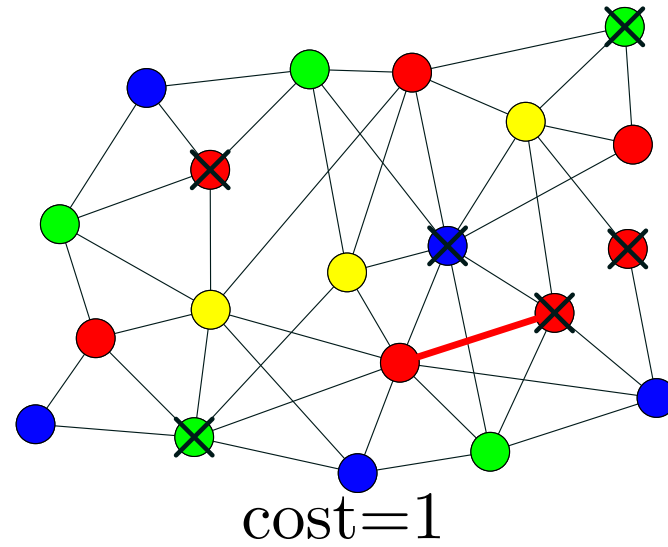
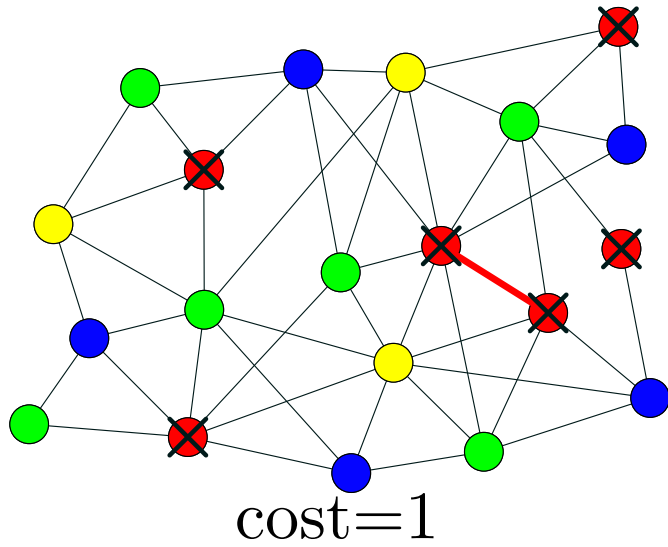
Cost of Crossover



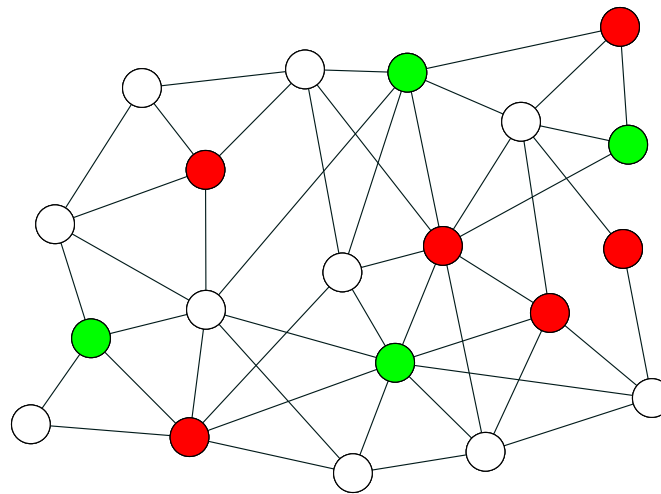
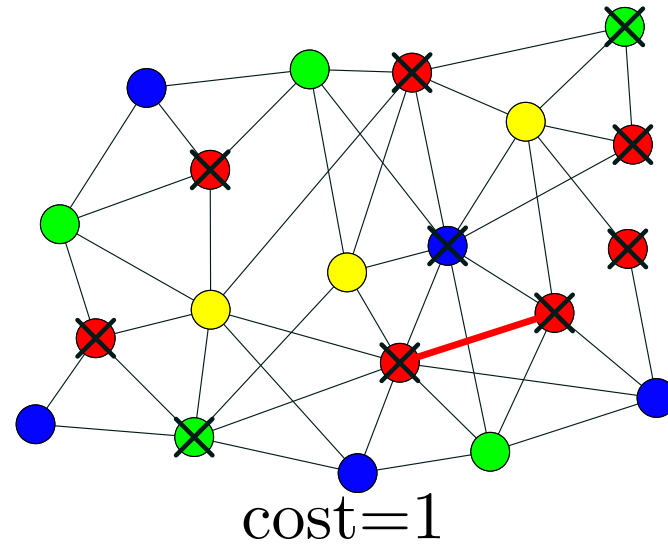
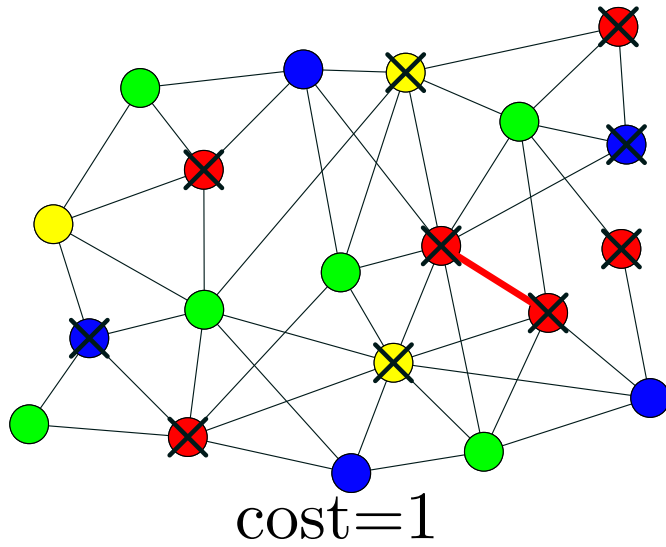
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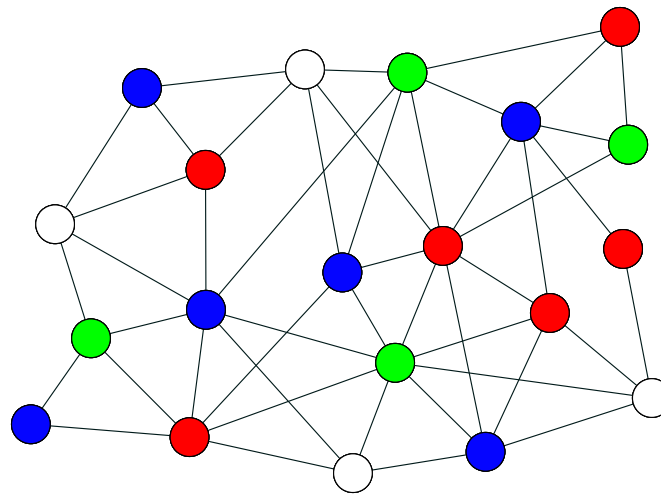
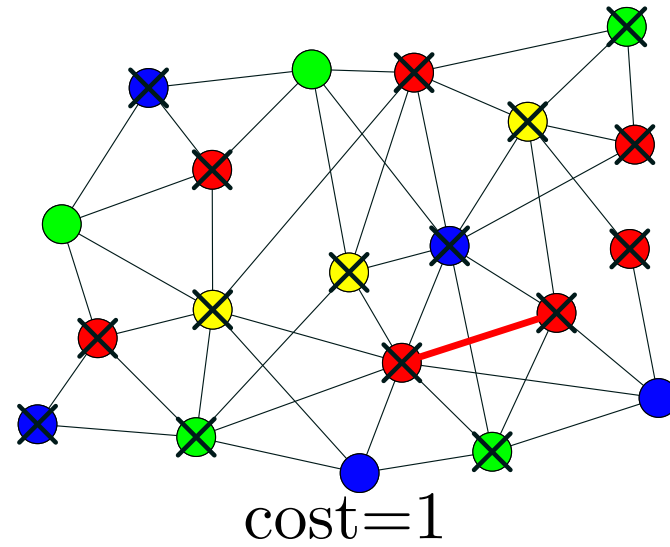
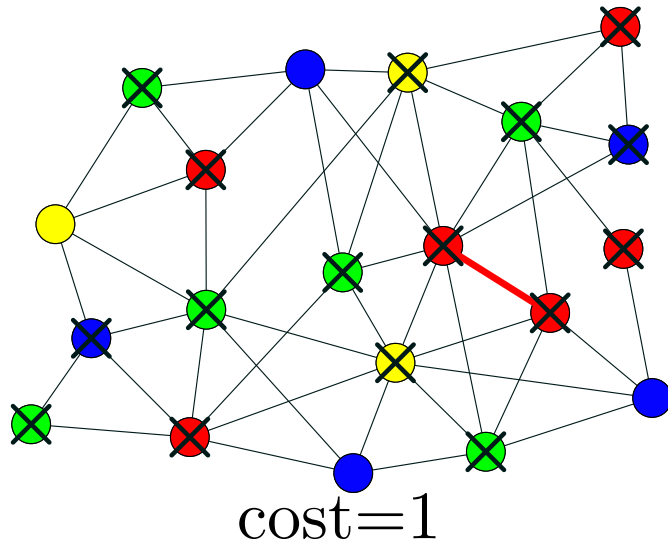
Cost of Crossover



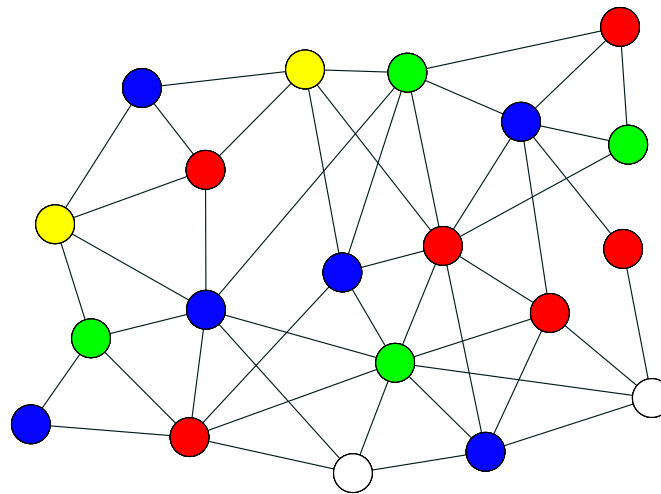
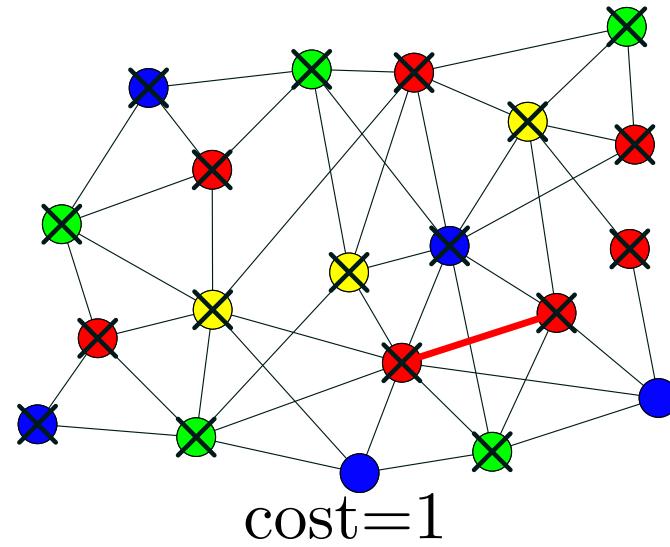
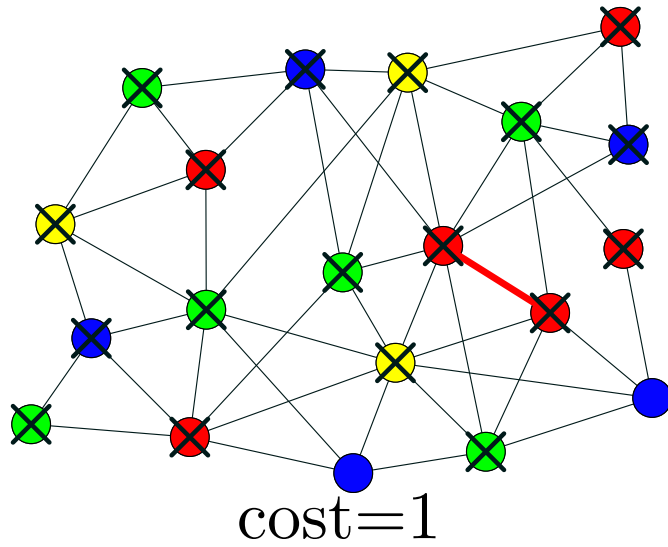
Cost of Crossover



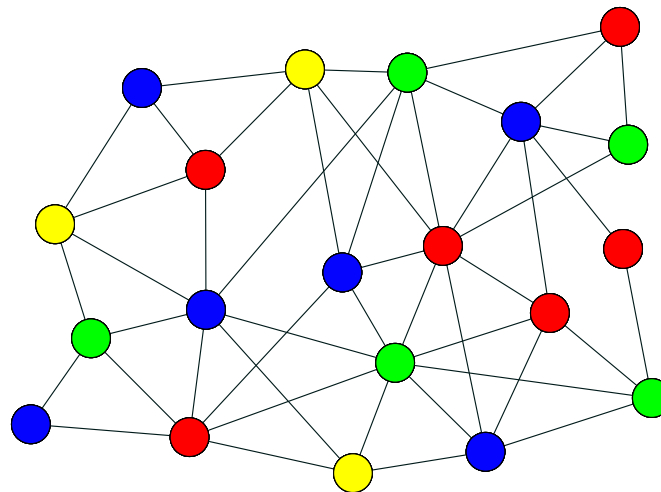
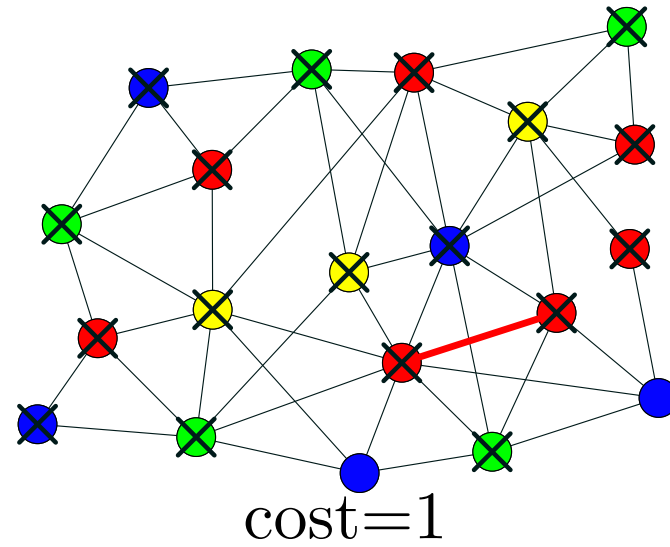
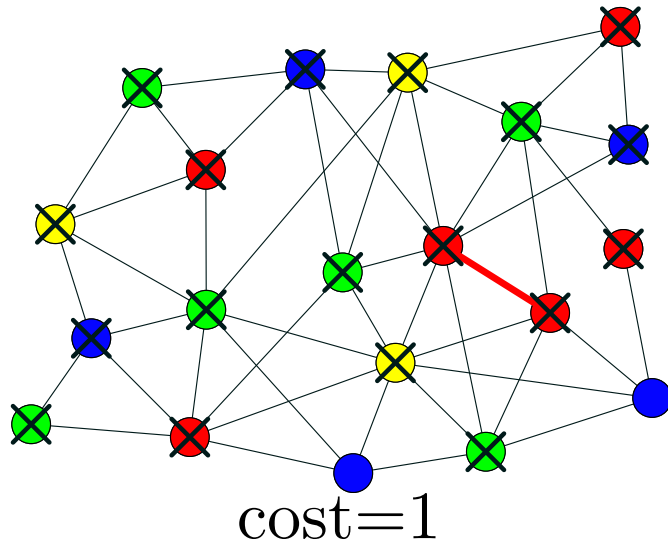
Cost of Crossover



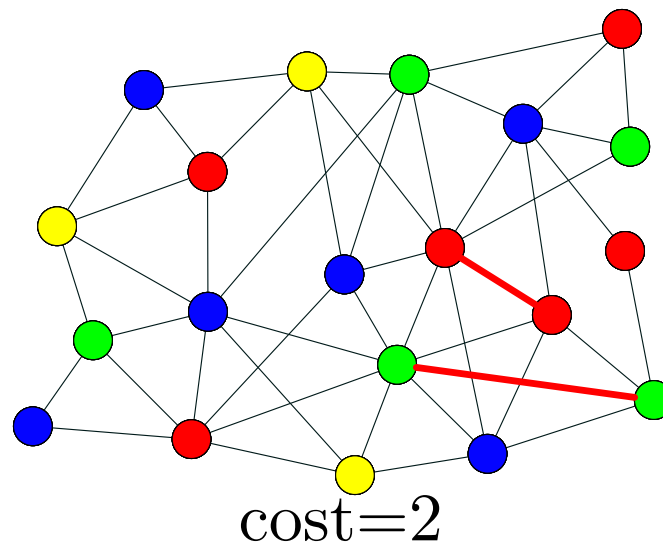
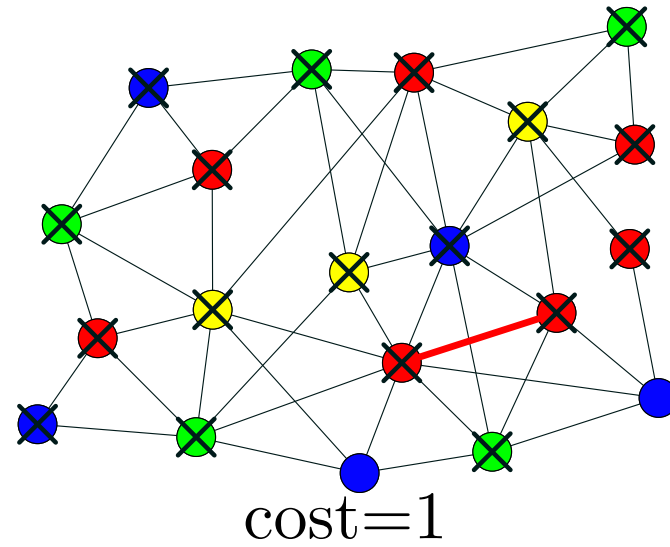
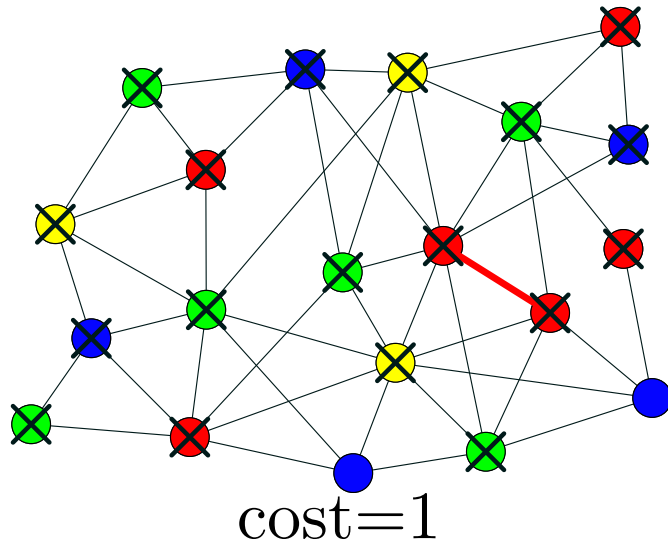
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Other Heuristics

- 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, . . .

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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
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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

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