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**

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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)
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- Constructive algorithms build-up a solution
- They usually rely on a greedy heuristic
- They are very fast
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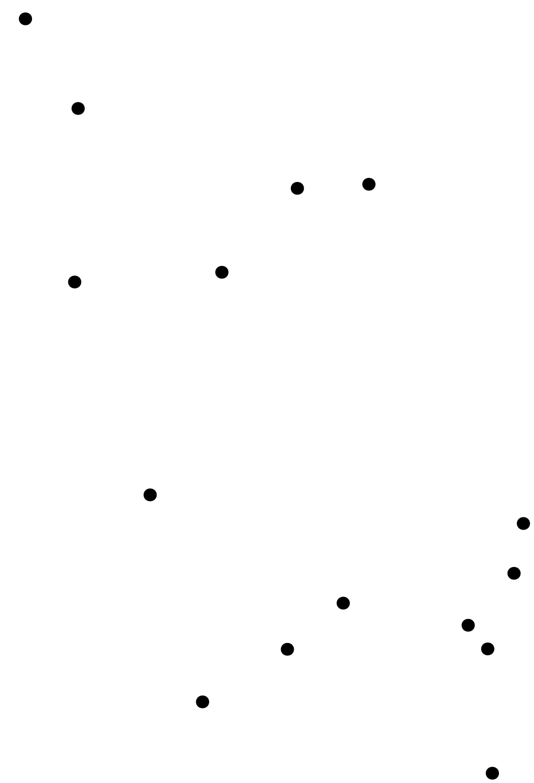

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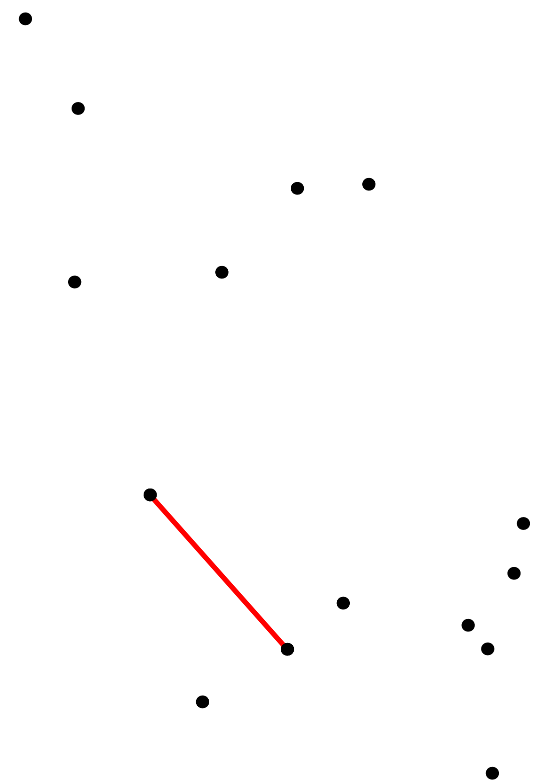

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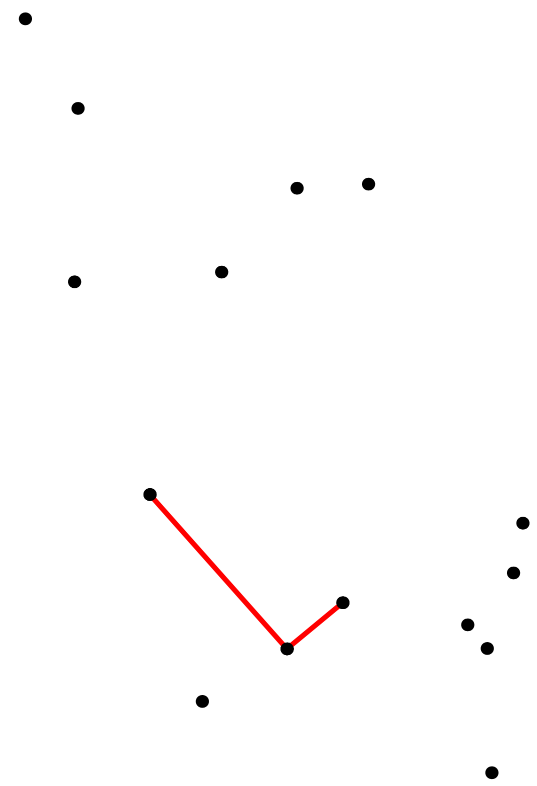

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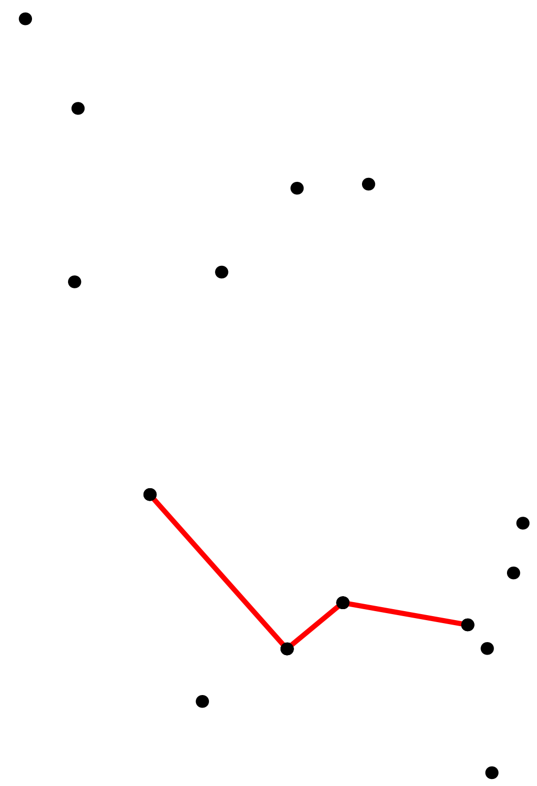

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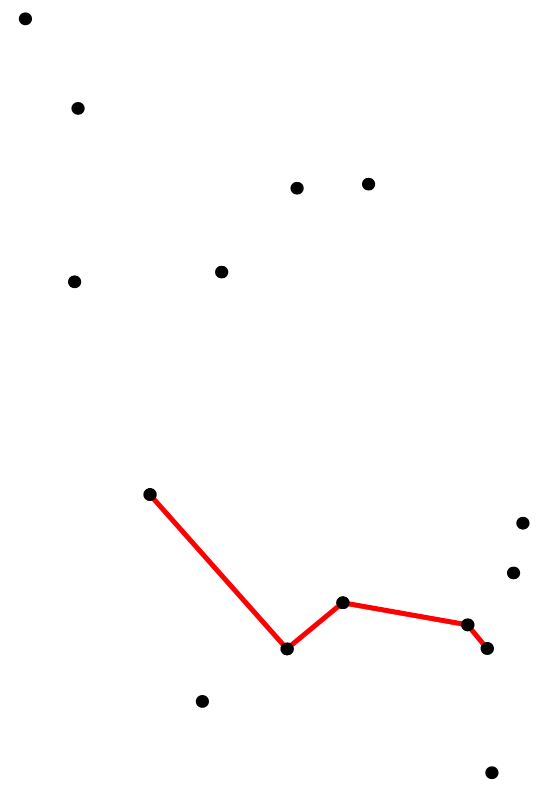

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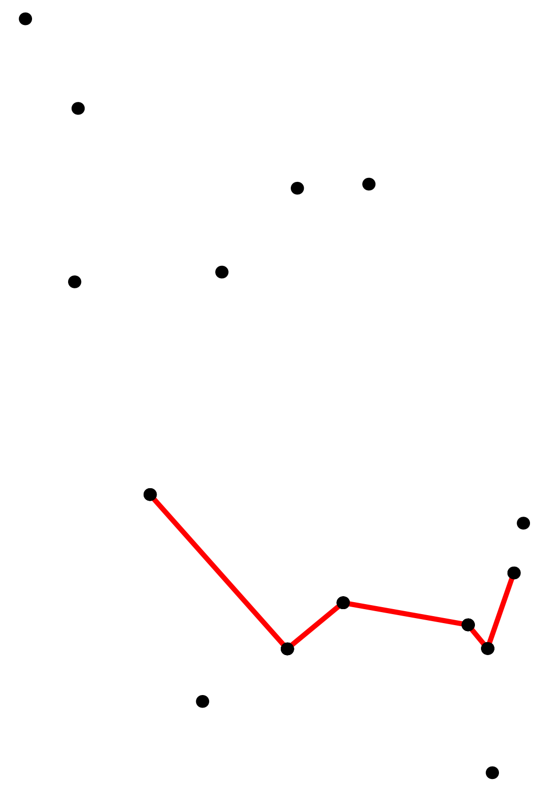

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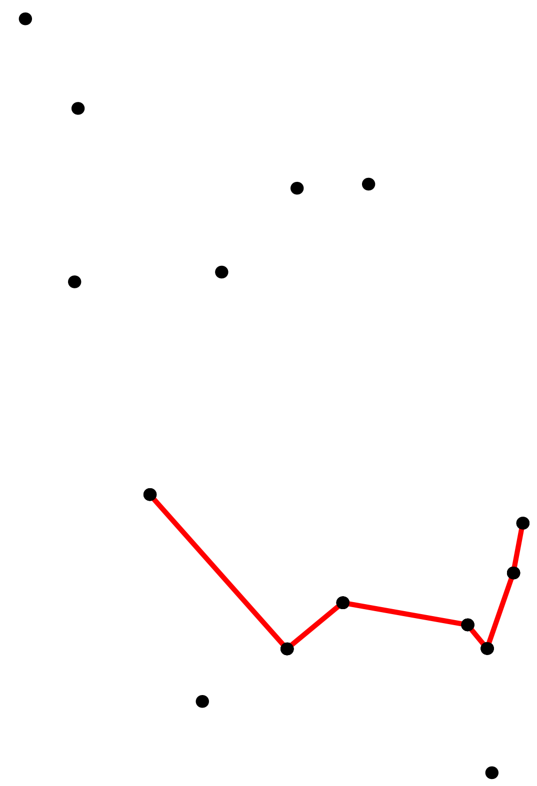

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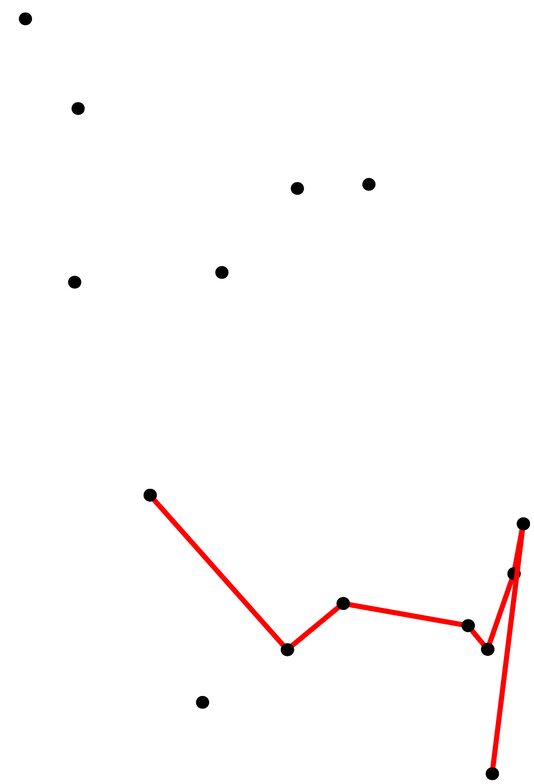

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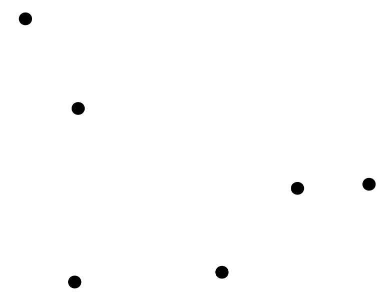

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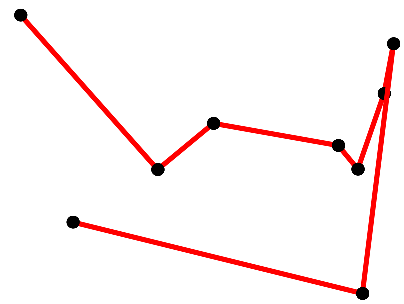

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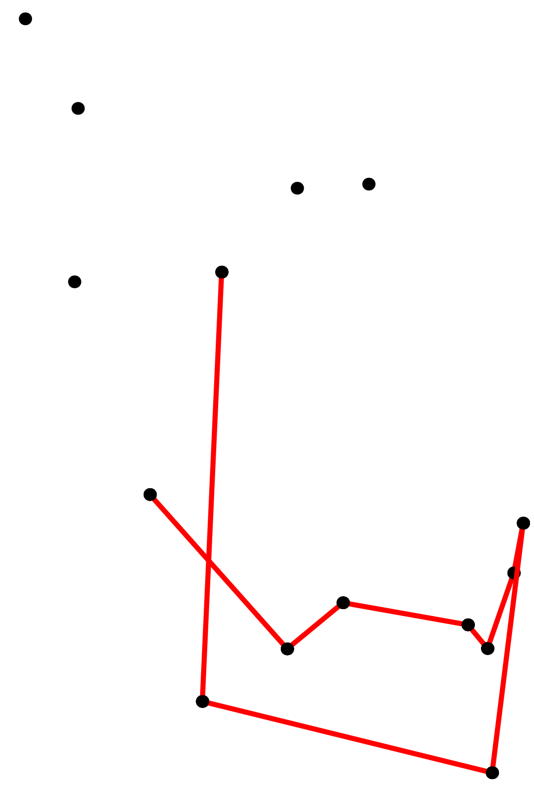

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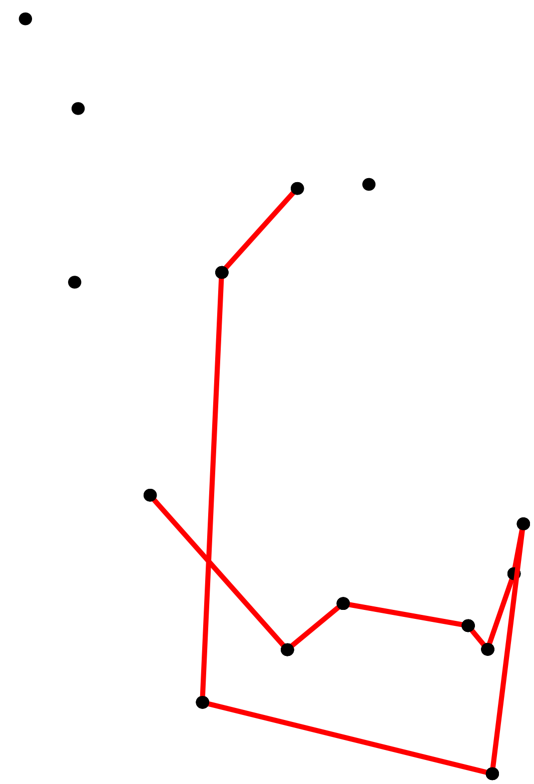

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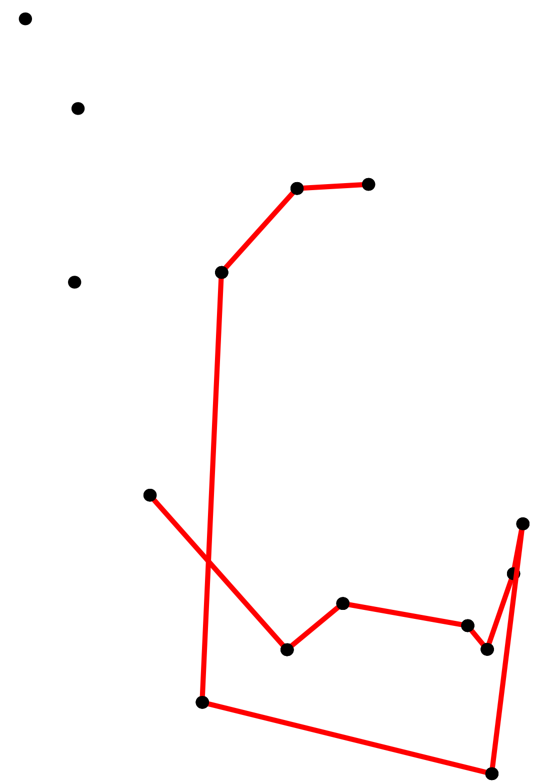

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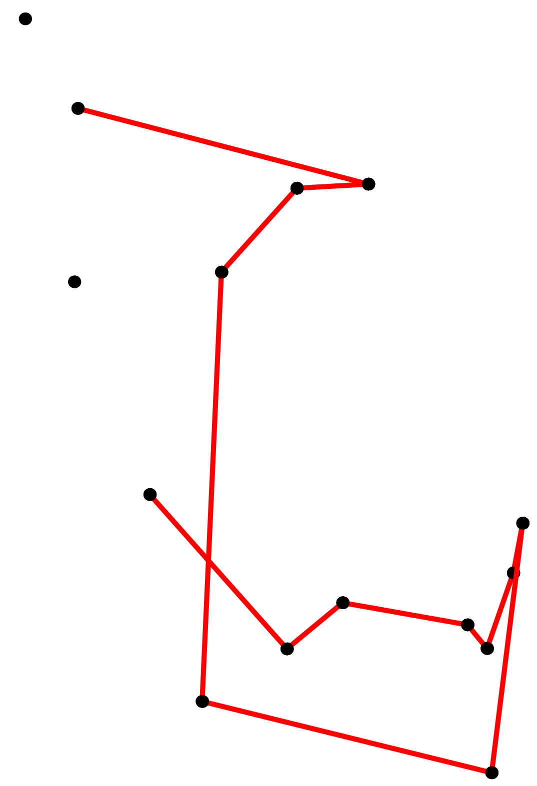

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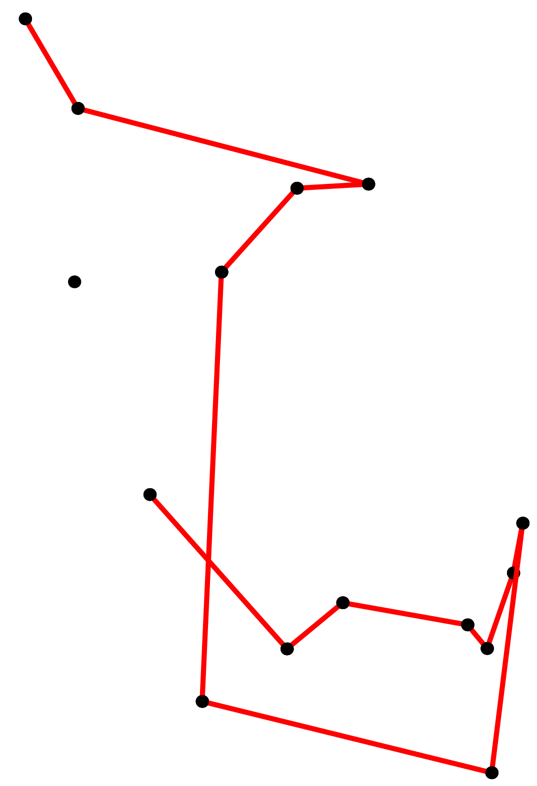

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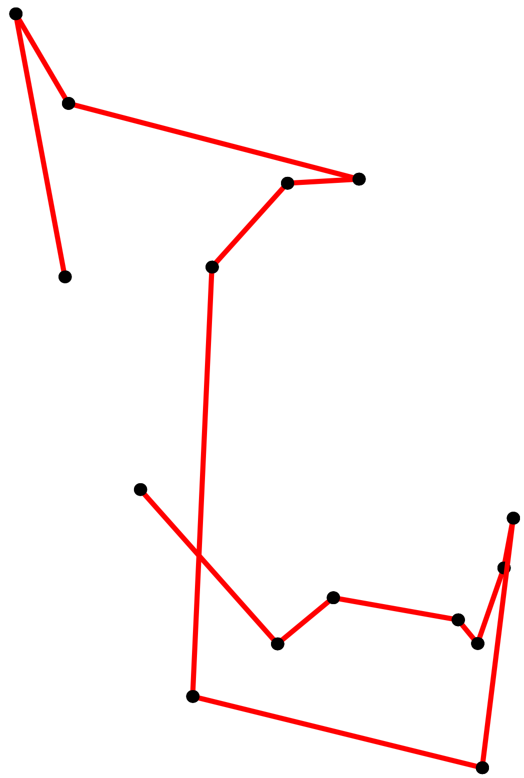

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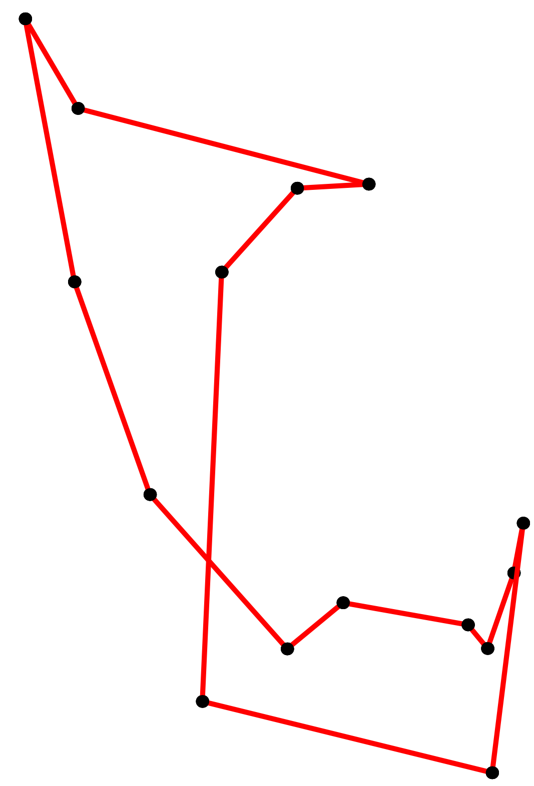

Neighbourhood search

- 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
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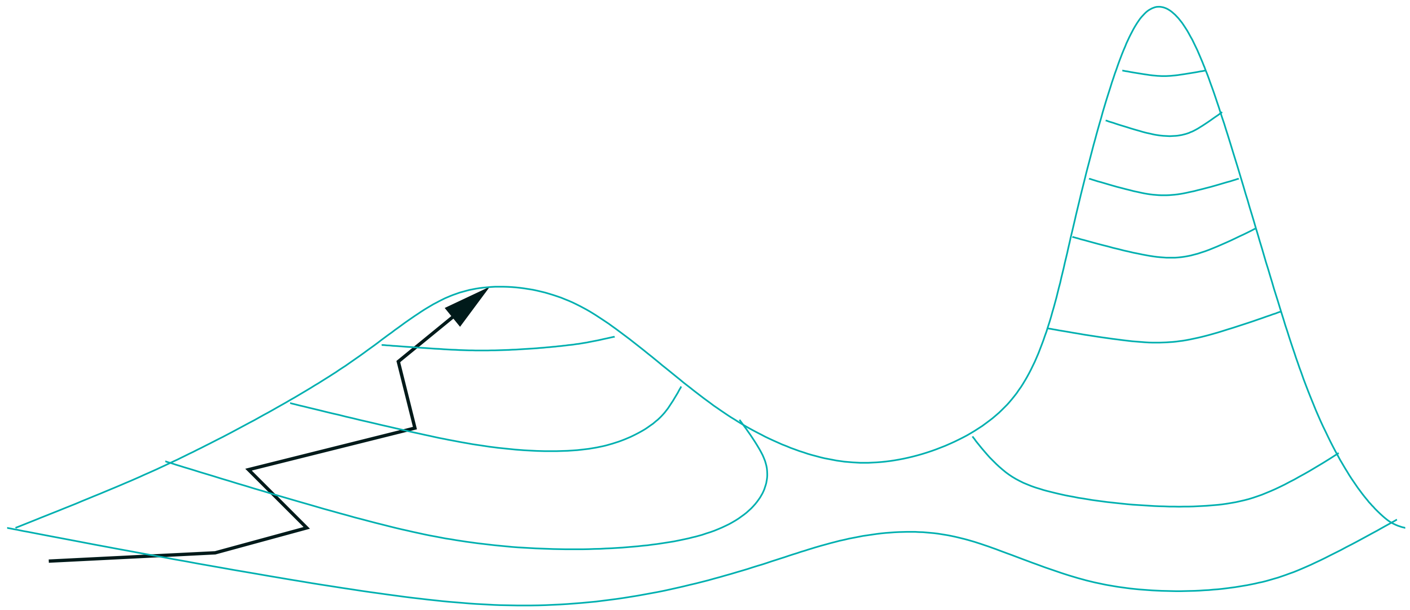
- Unfortunately, this doesn't always work

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



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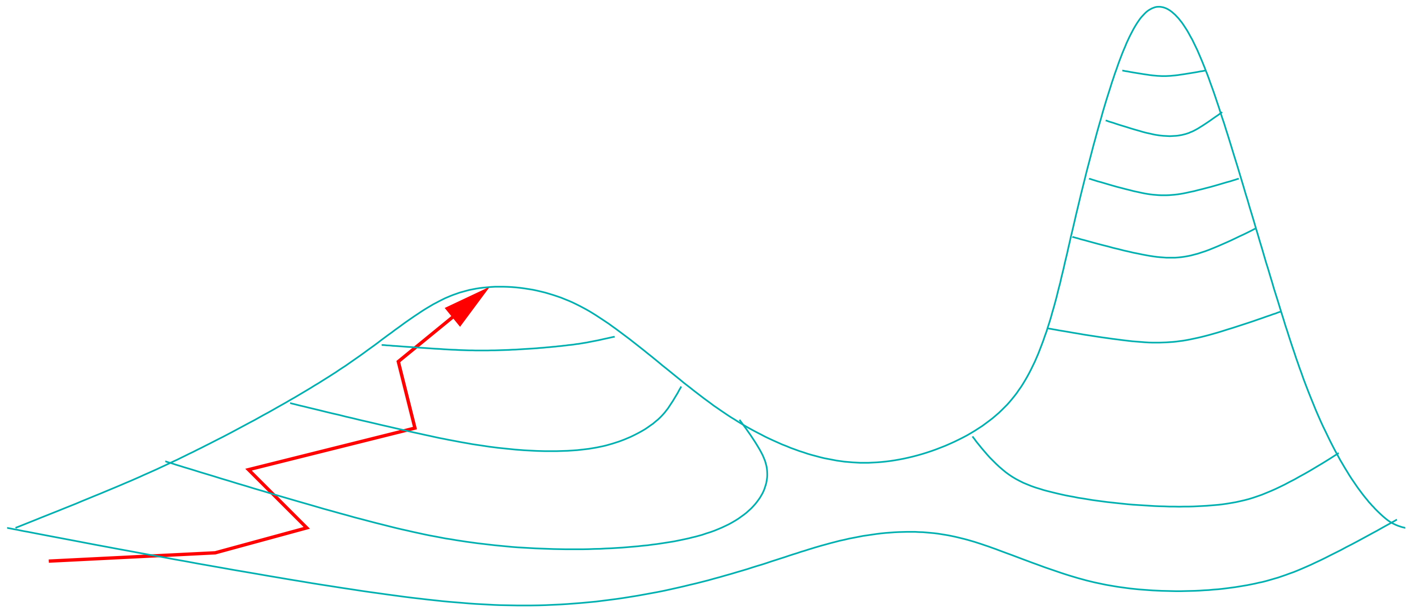

Simple Fixes

- 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 cites)

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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)

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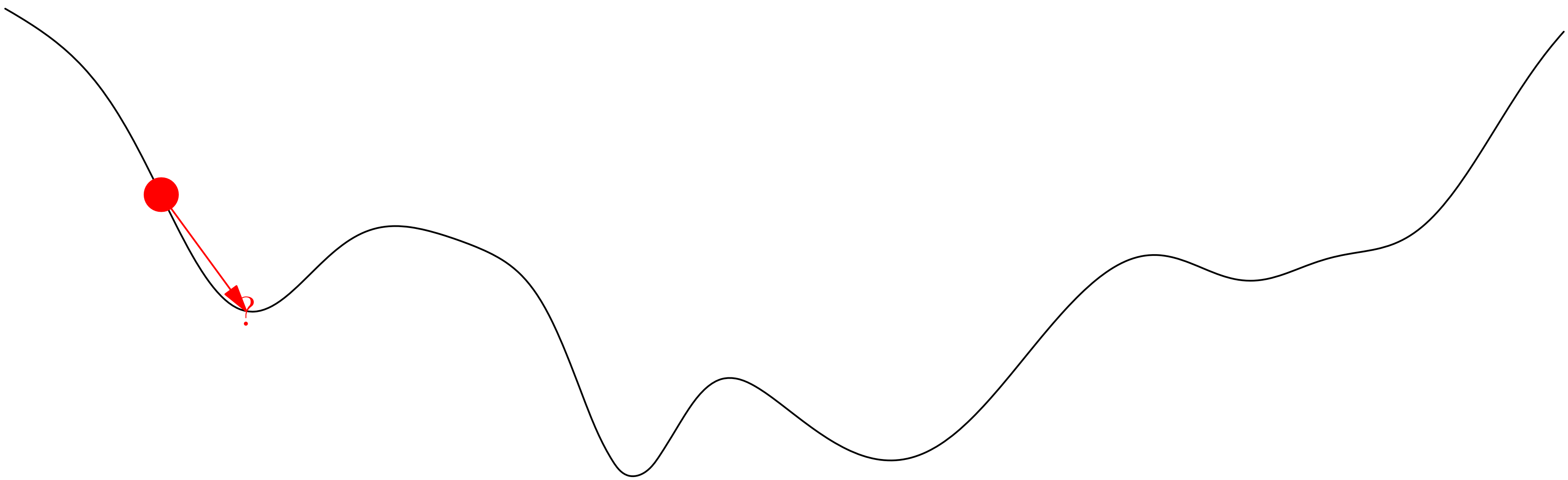

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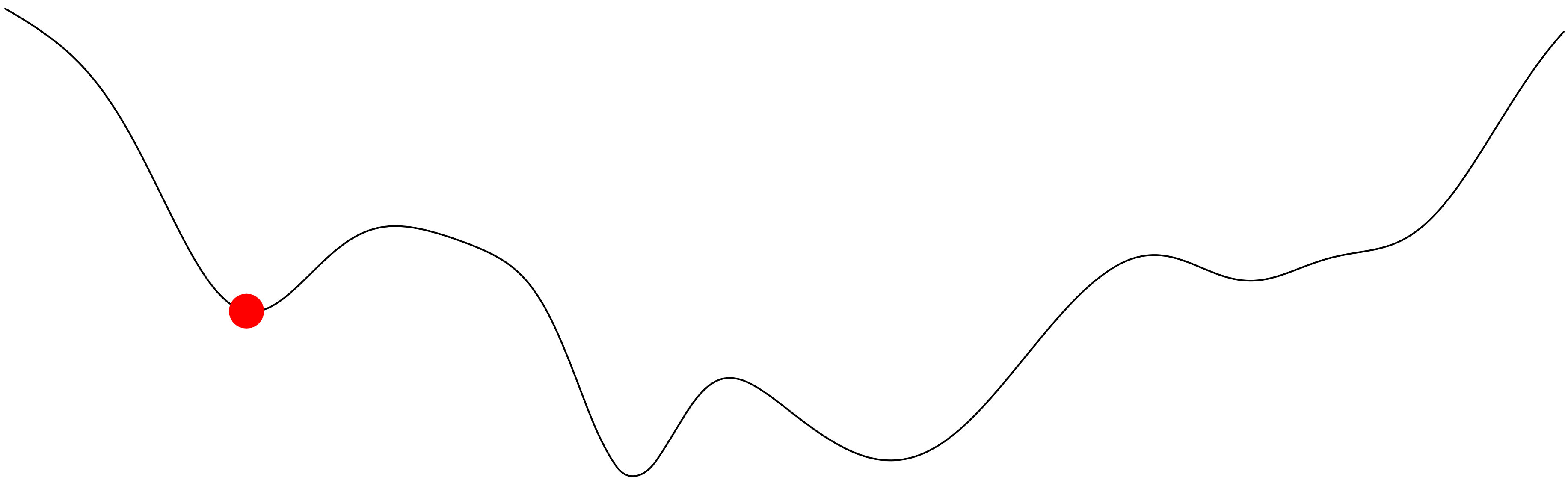

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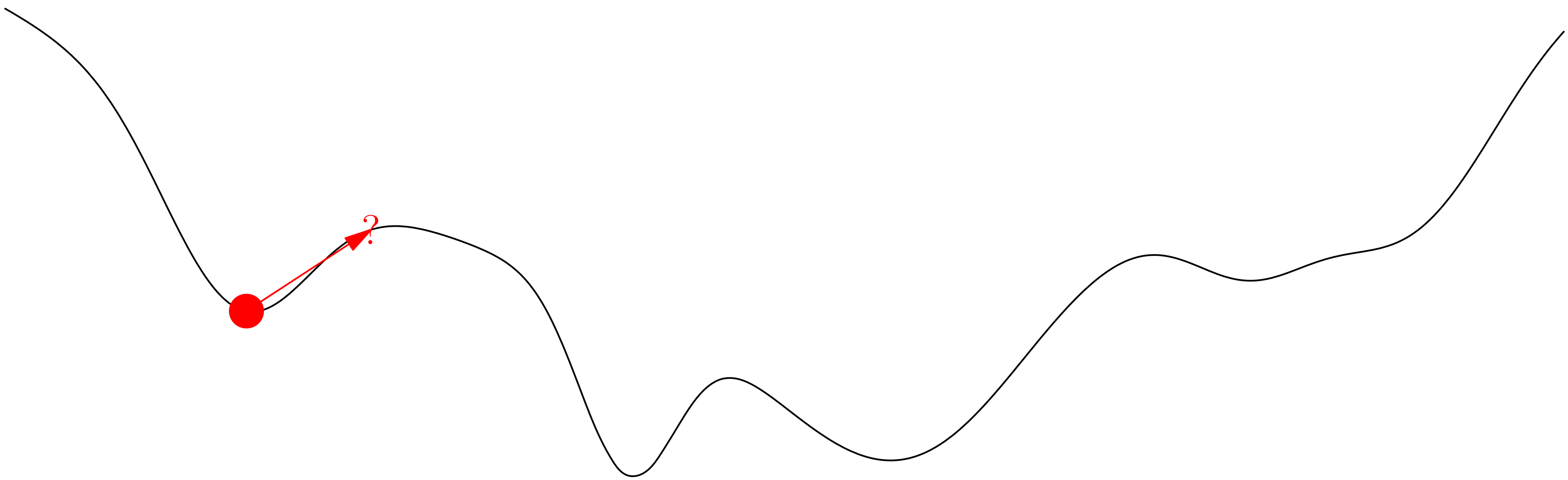

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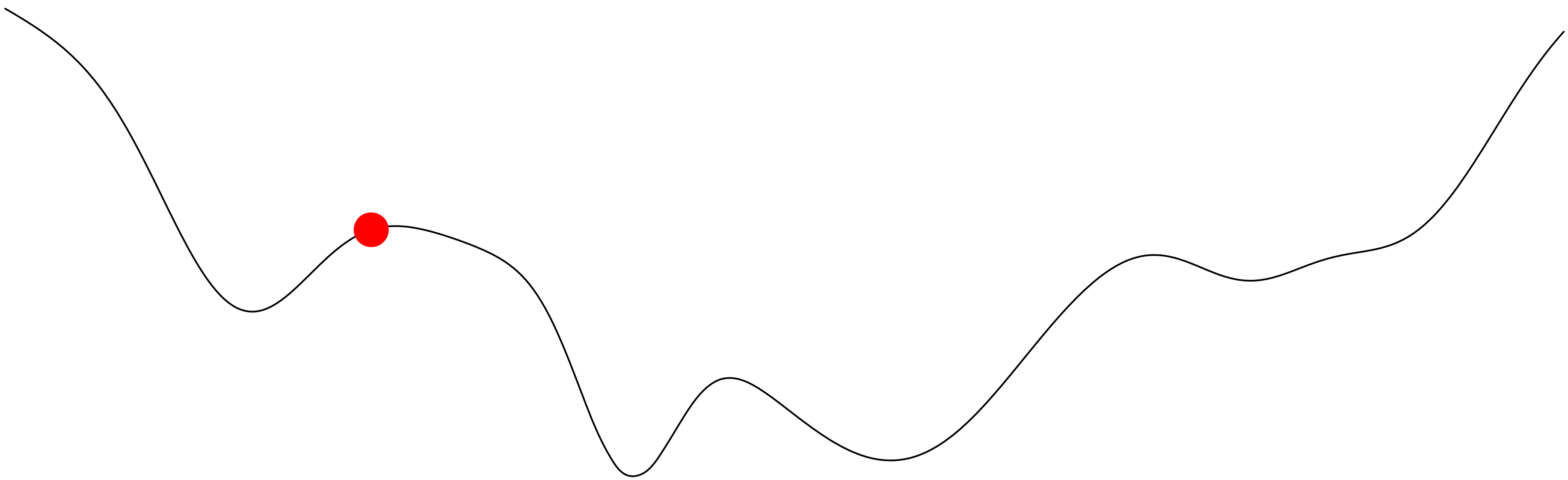

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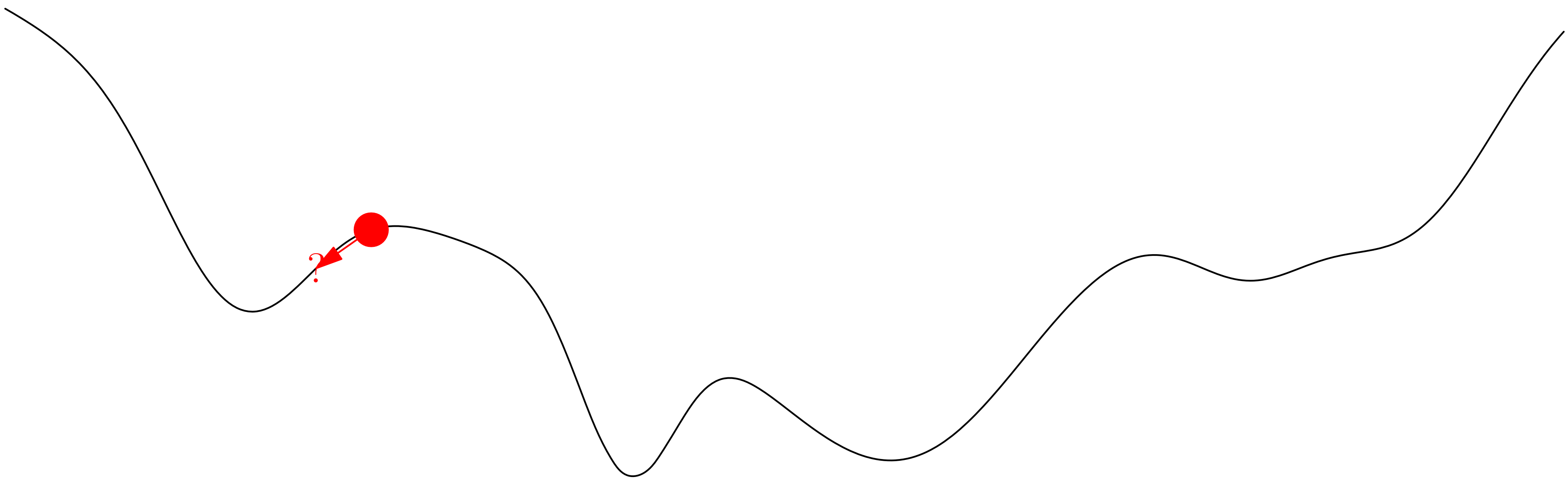

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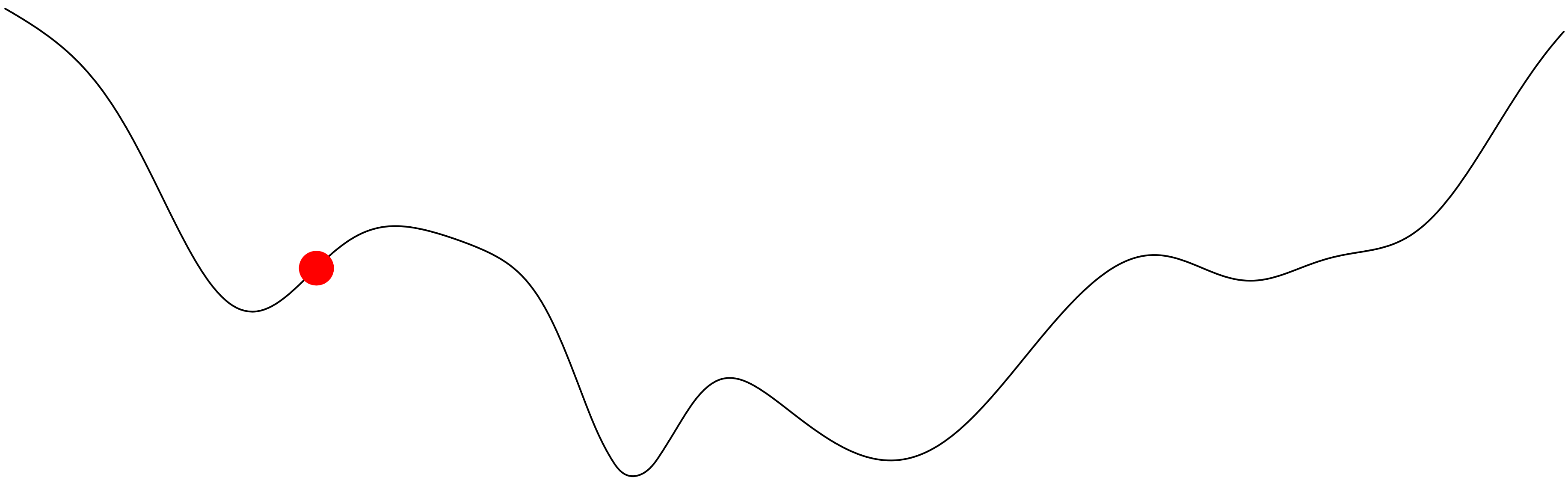

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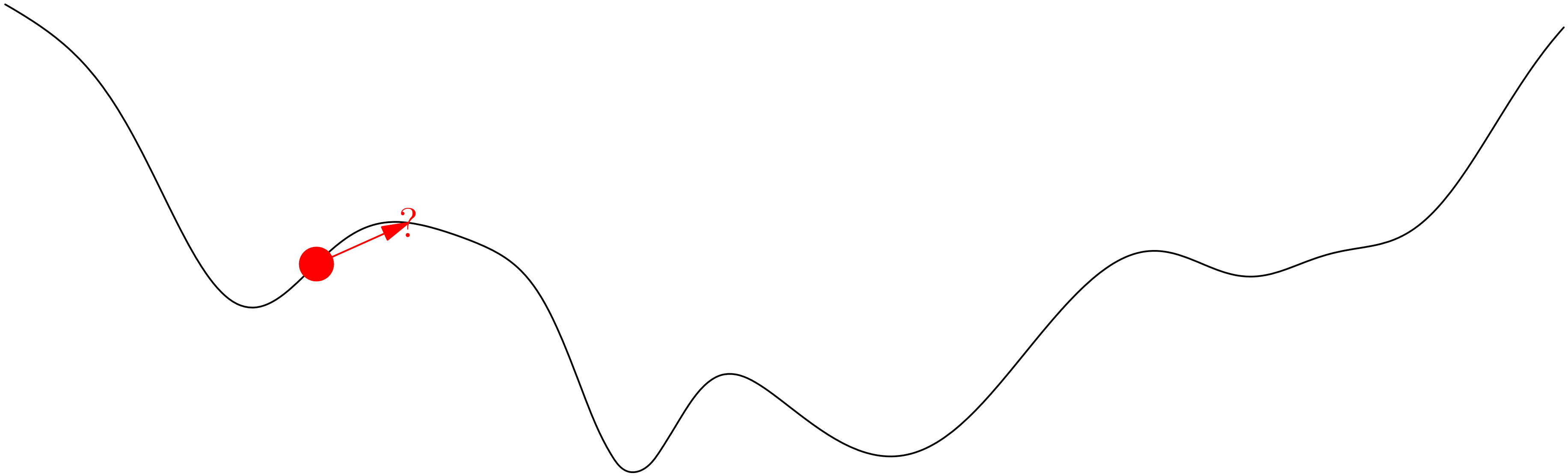

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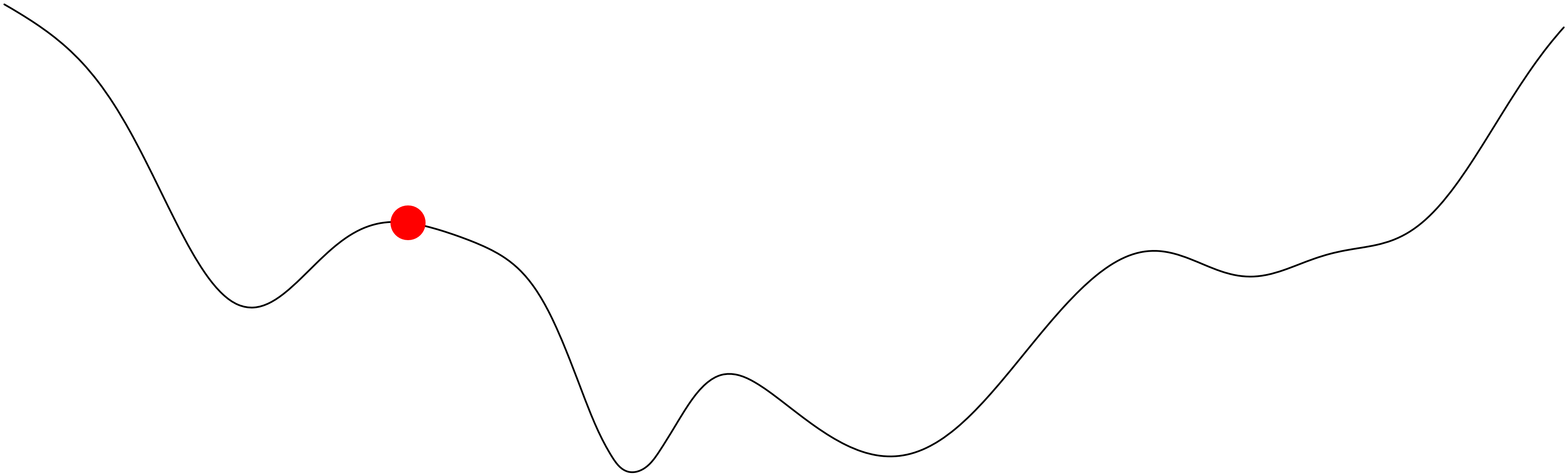

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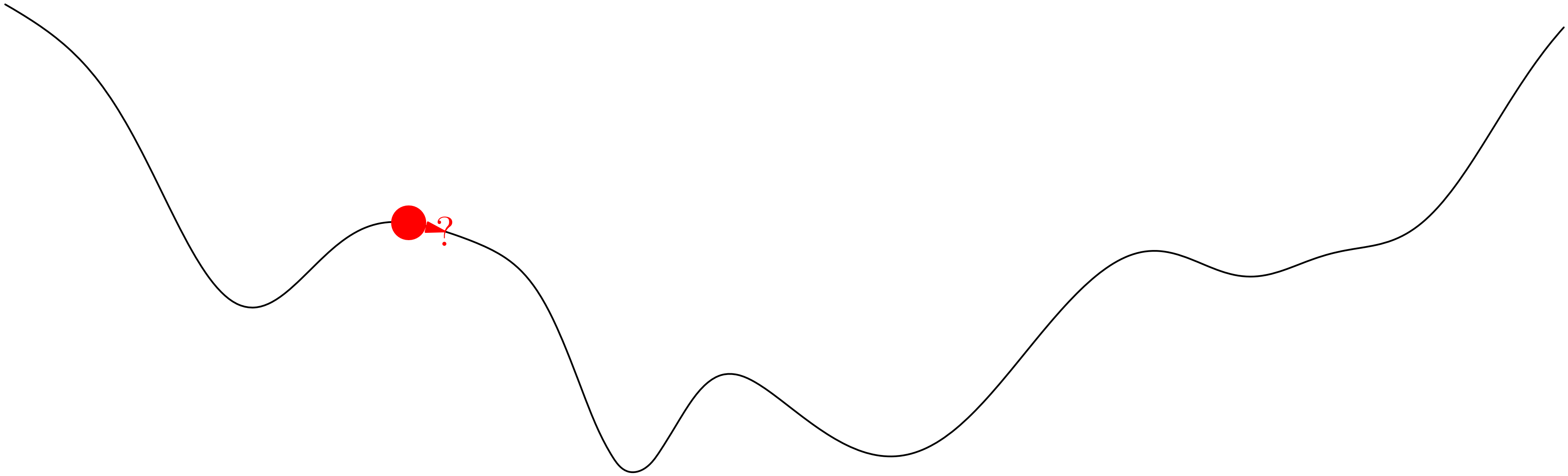

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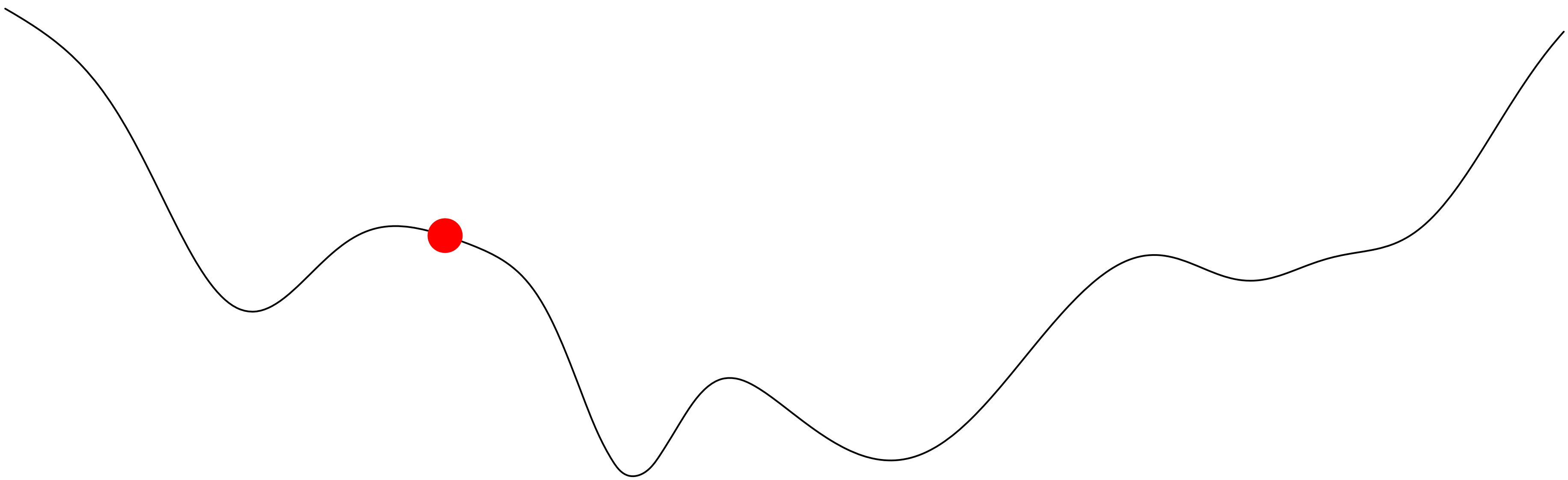

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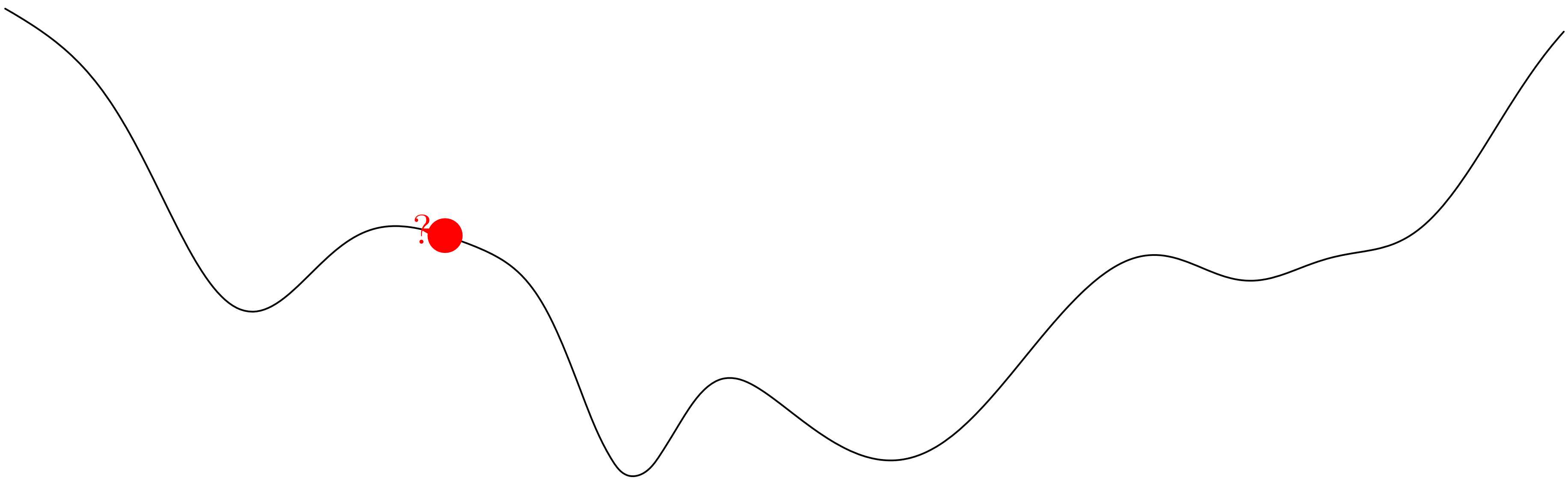

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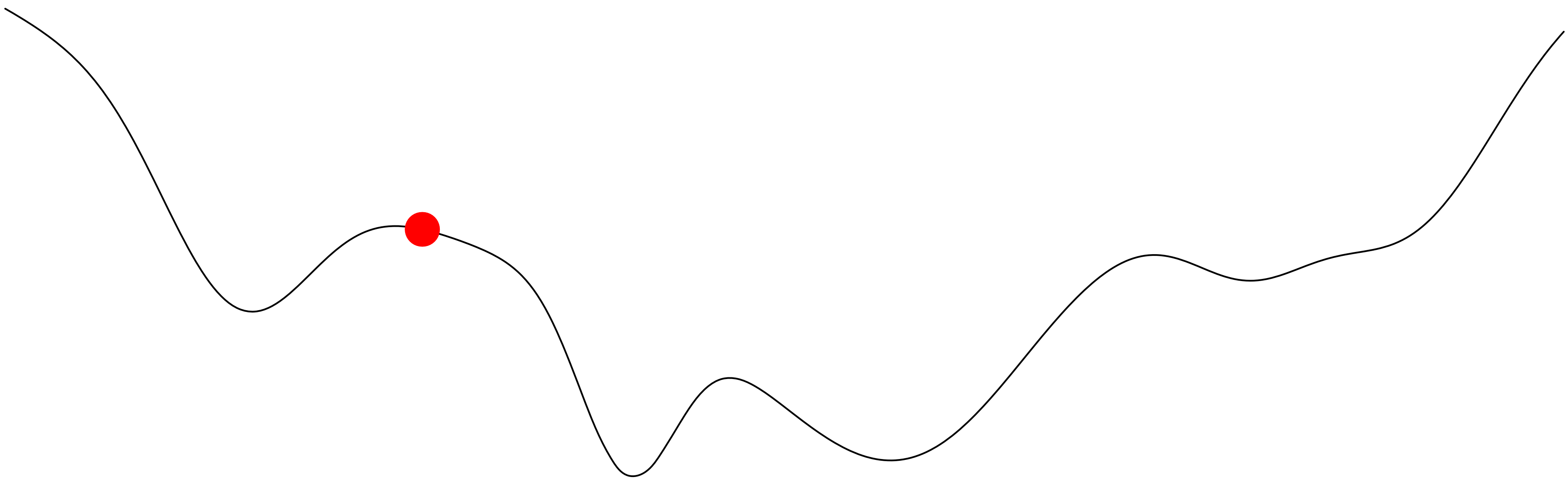

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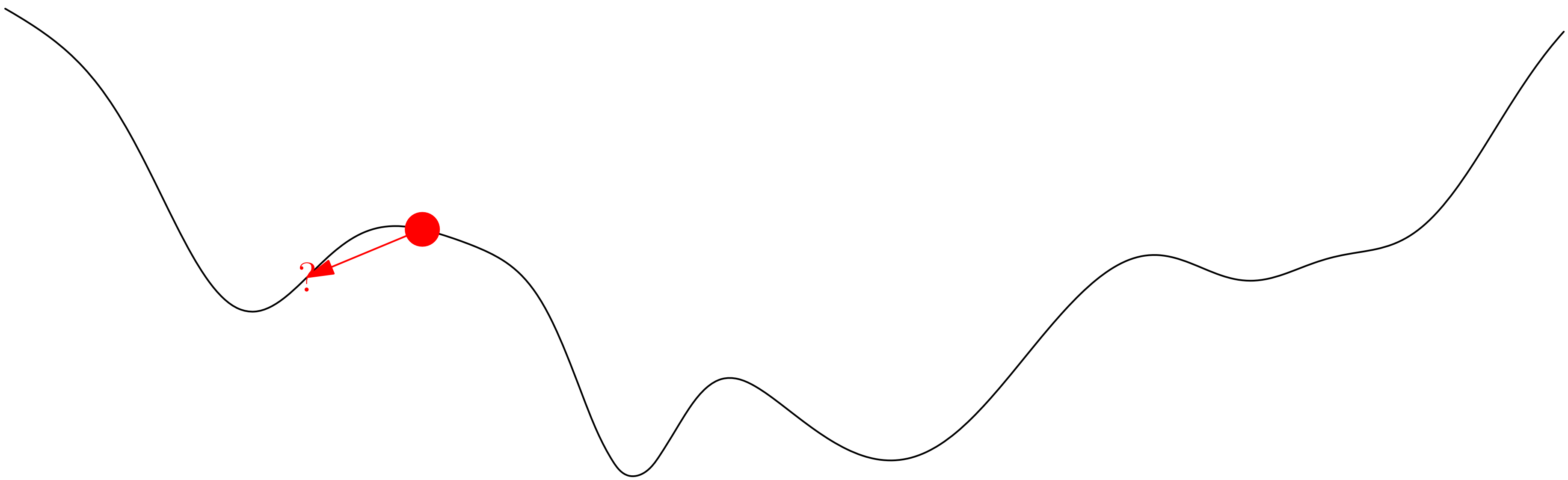

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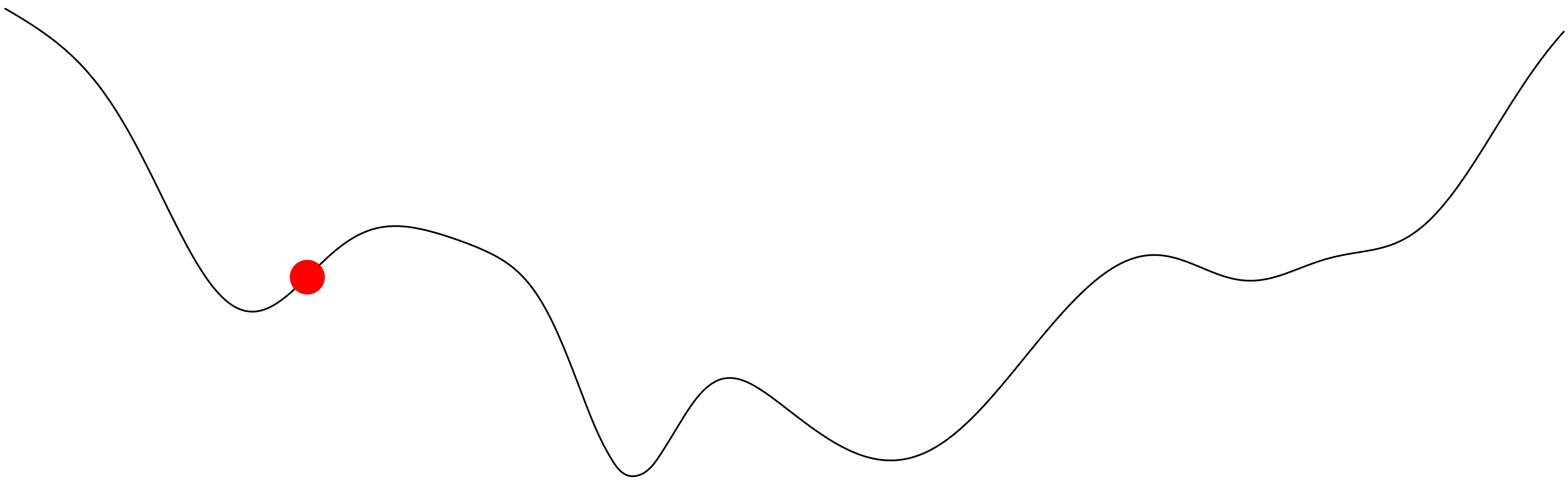

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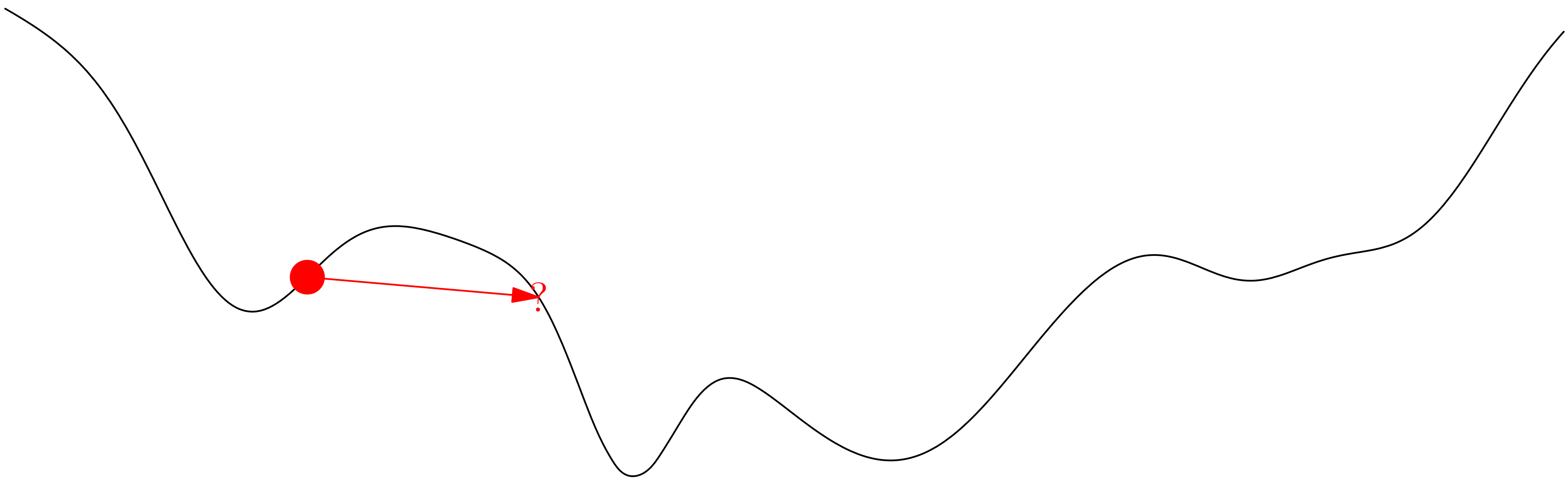

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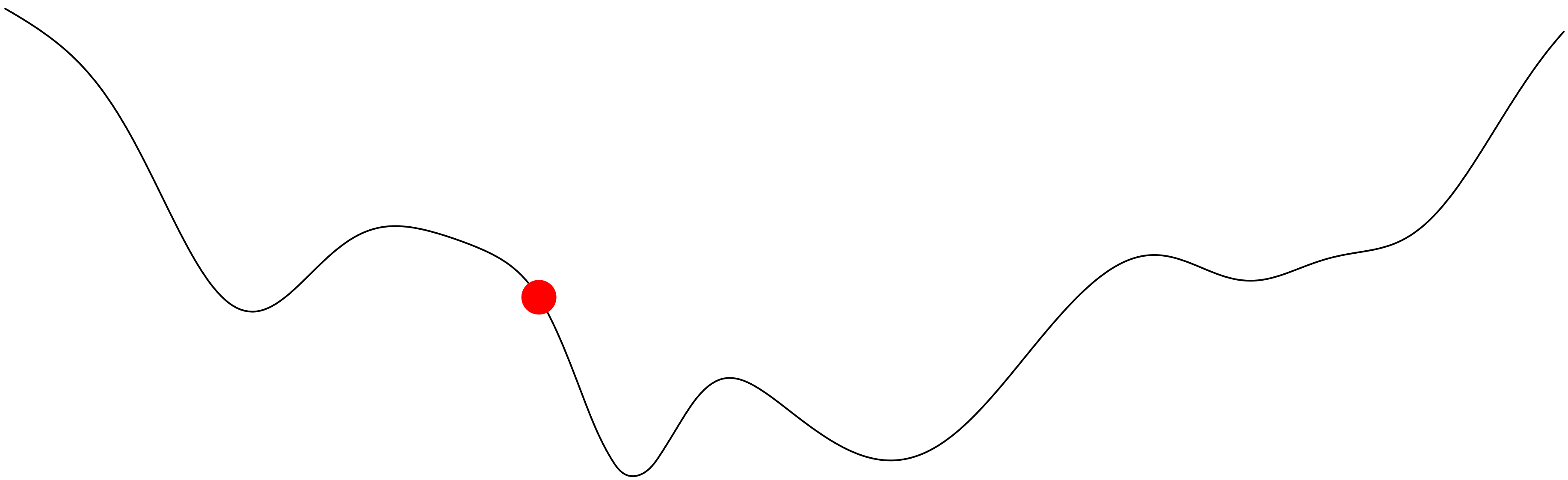

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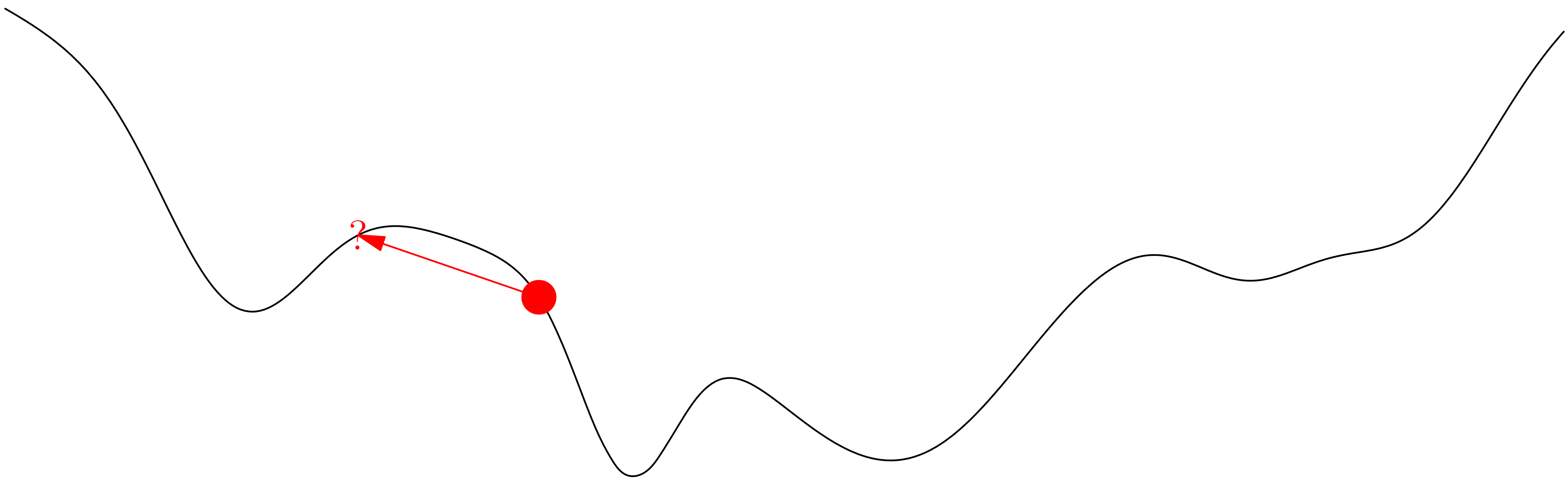

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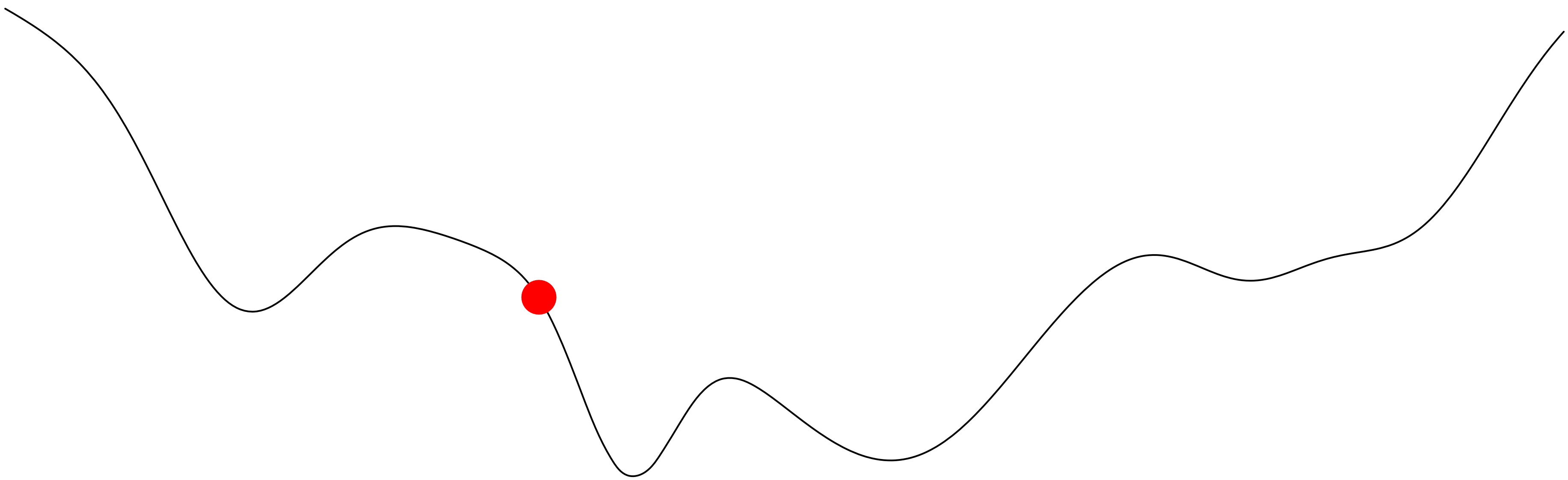

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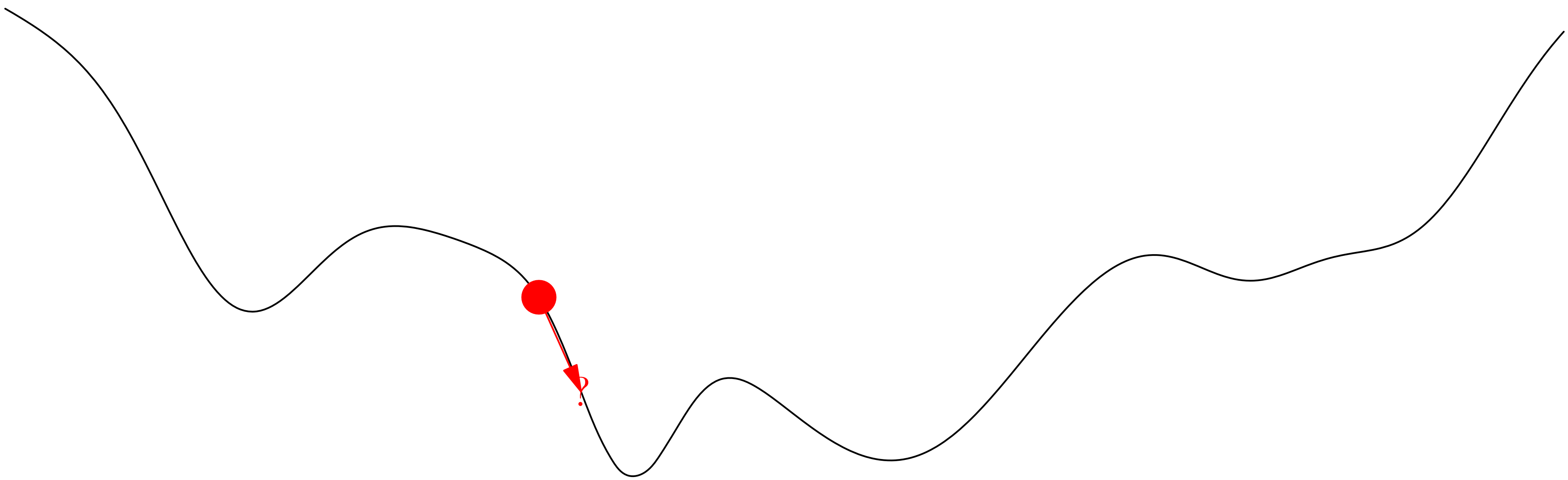

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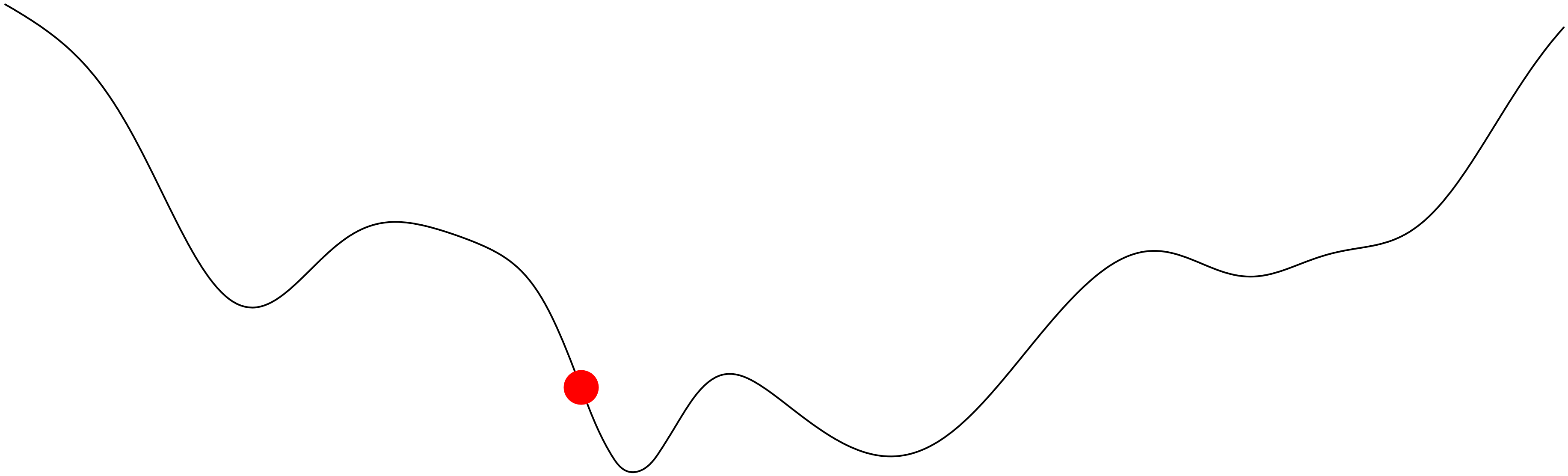

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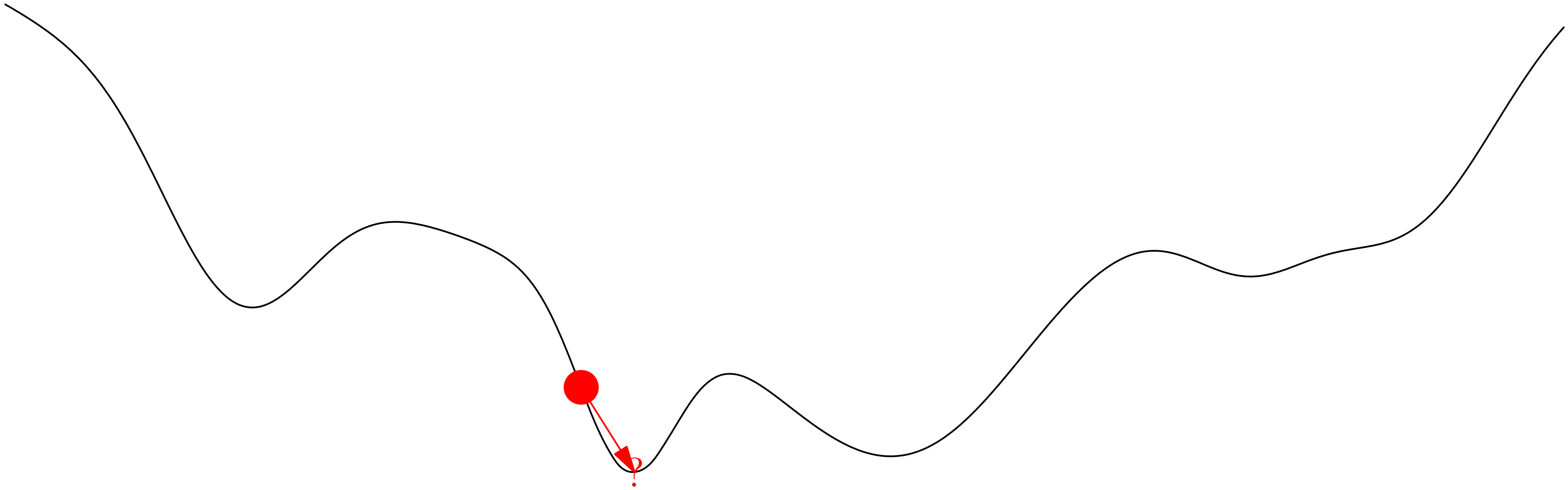

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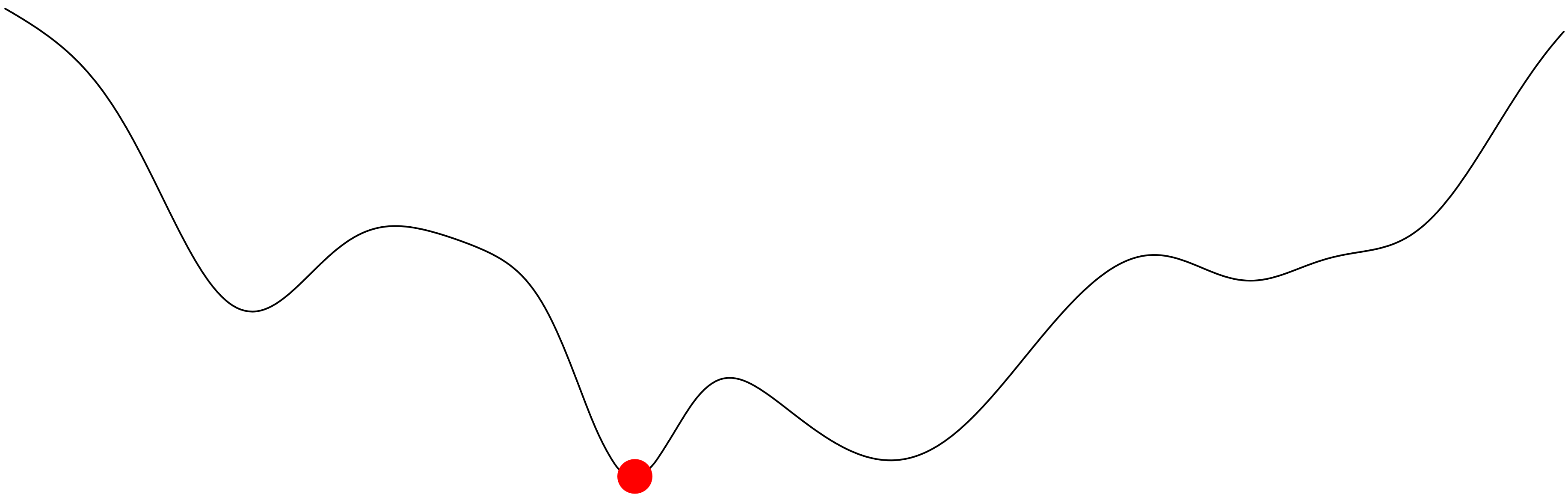

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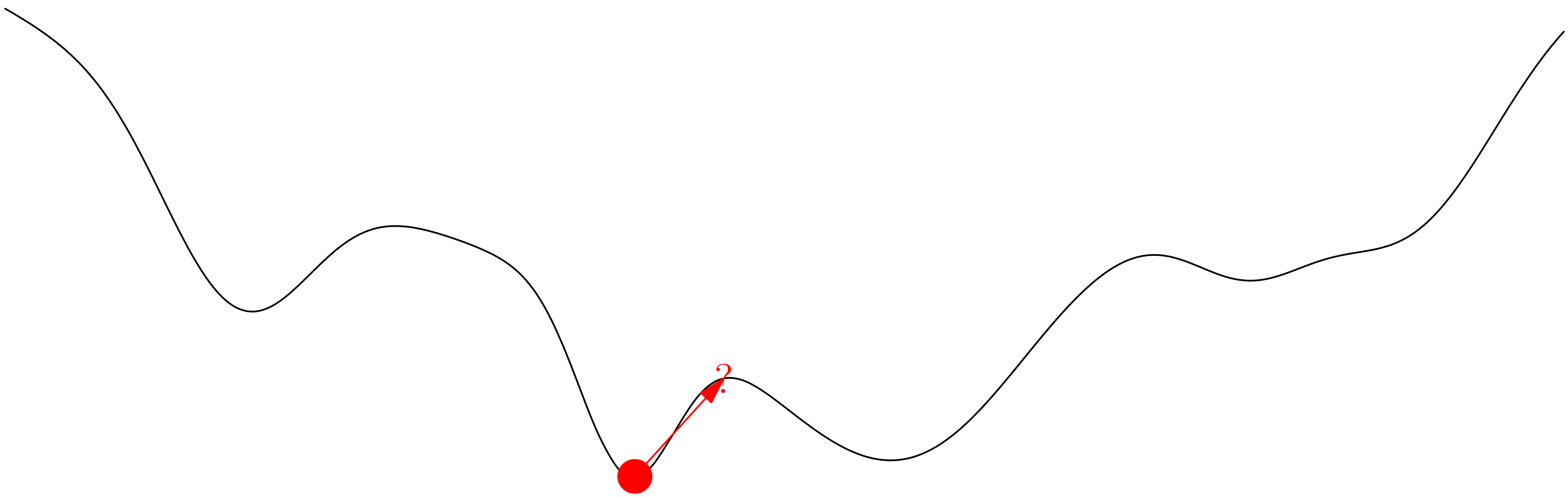

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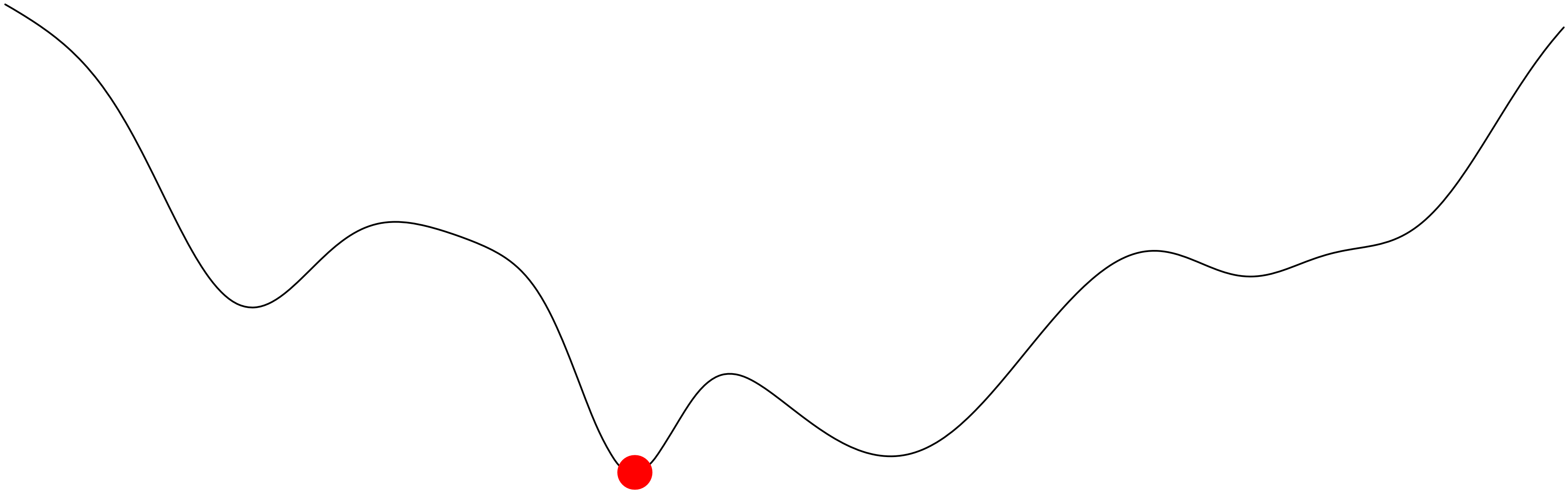

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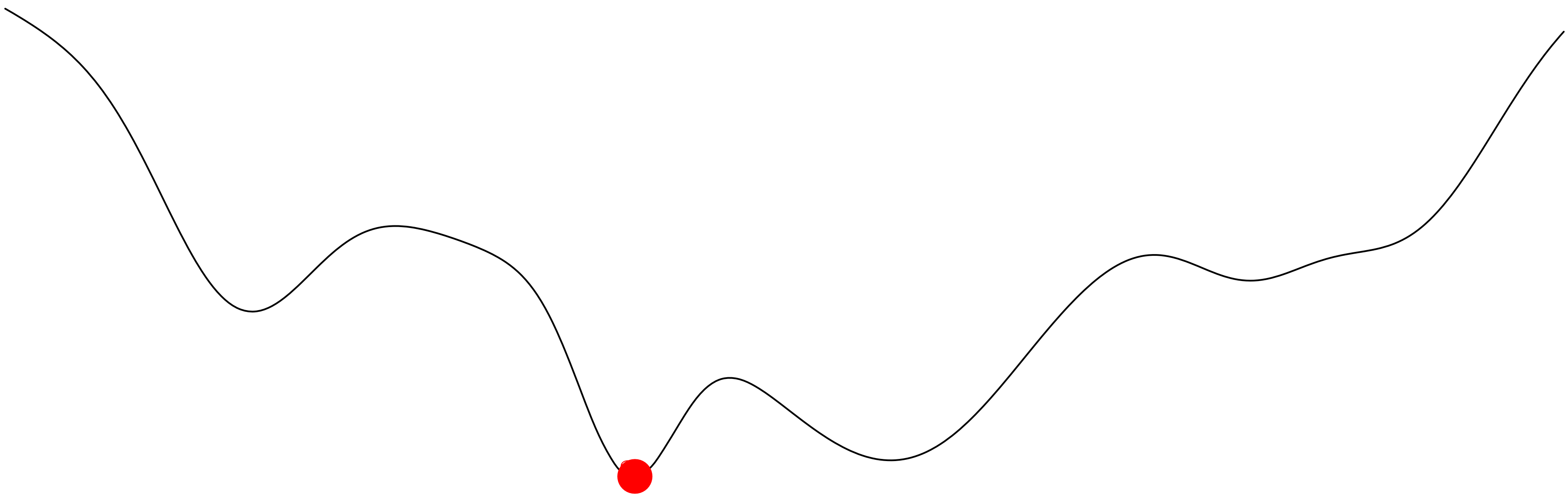

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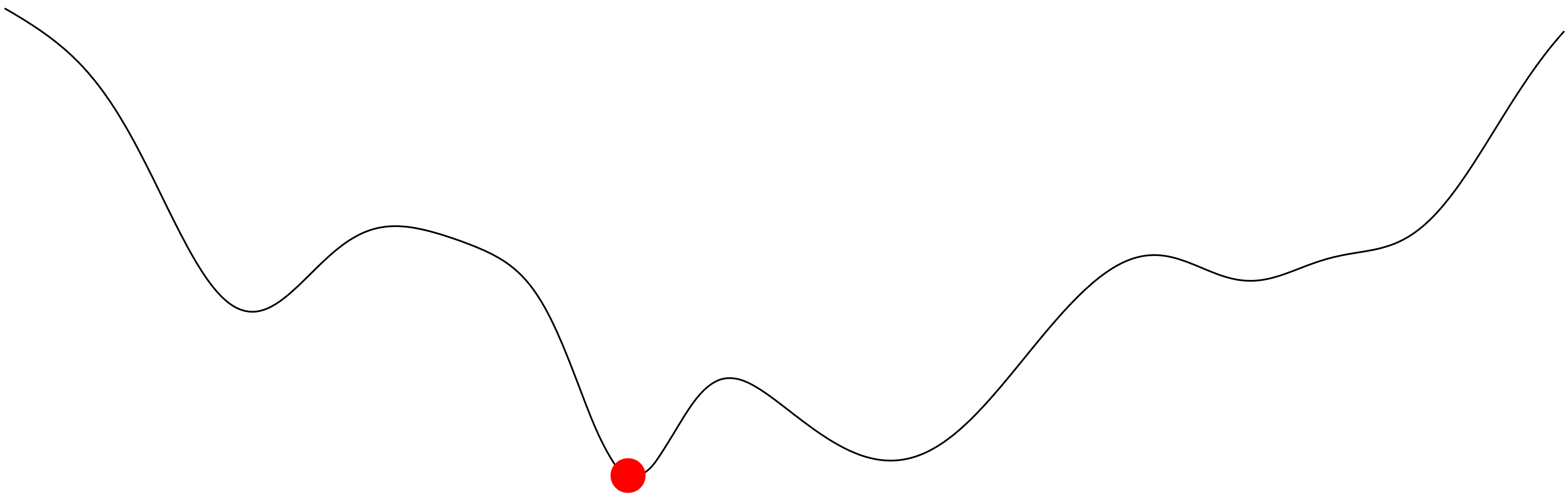

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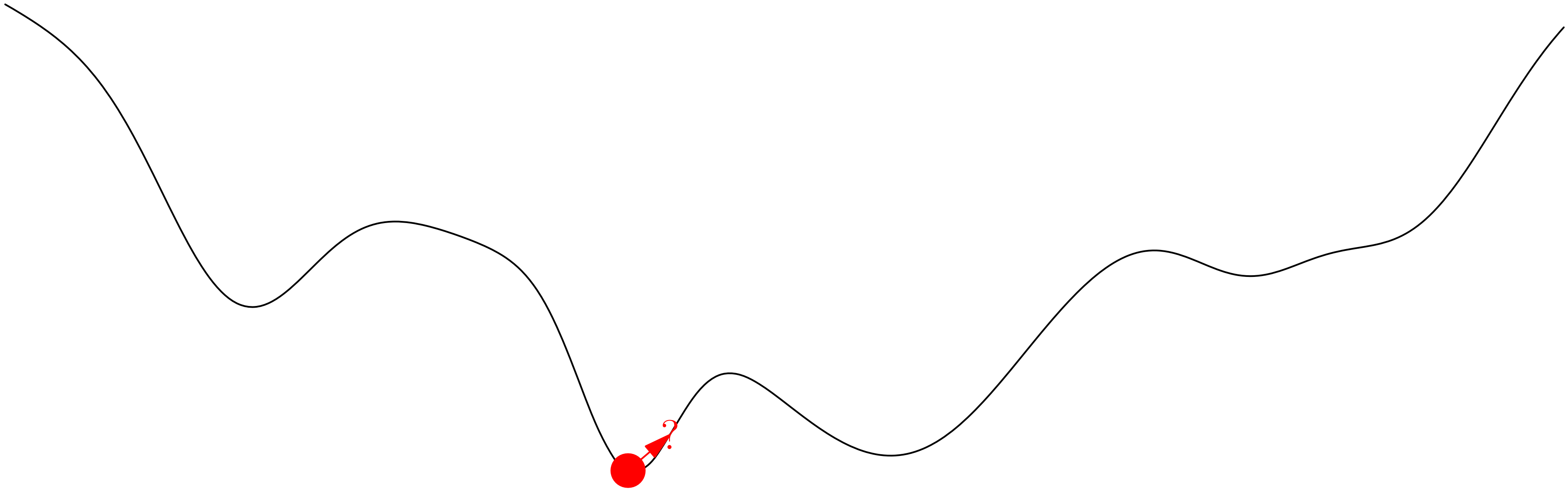

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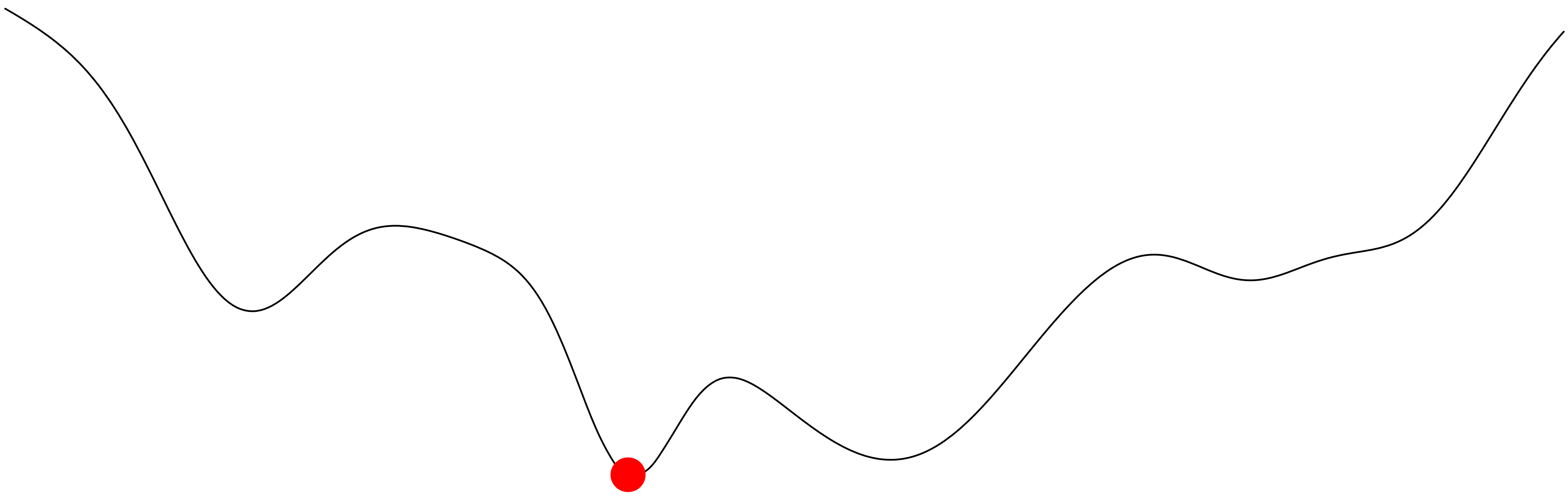

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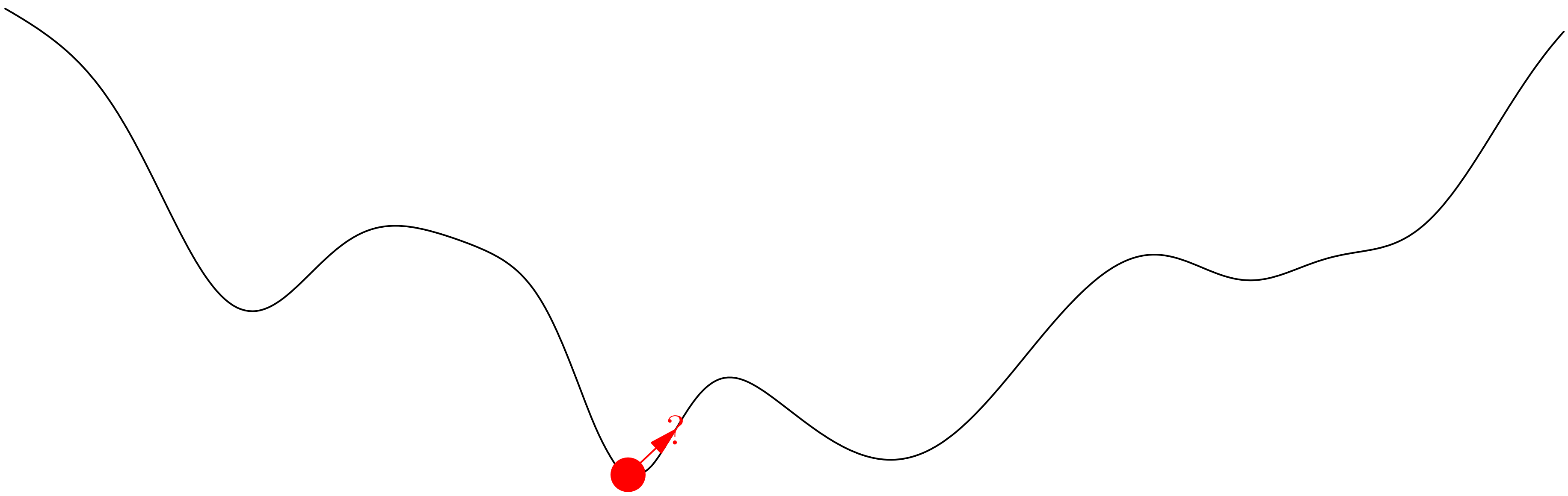

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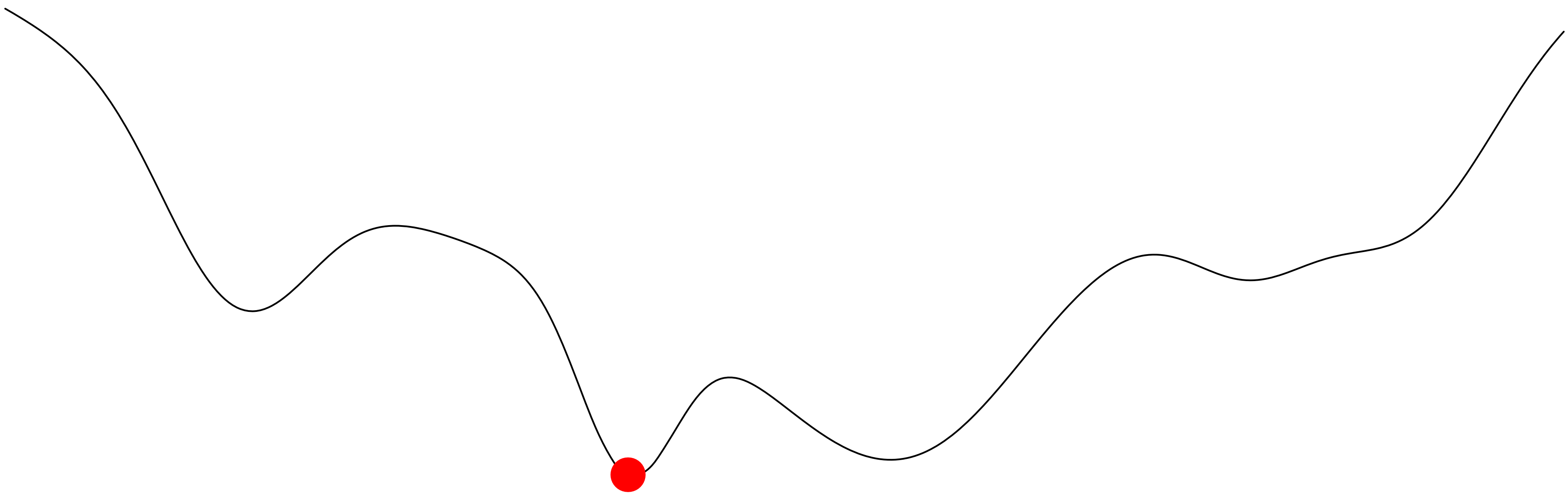

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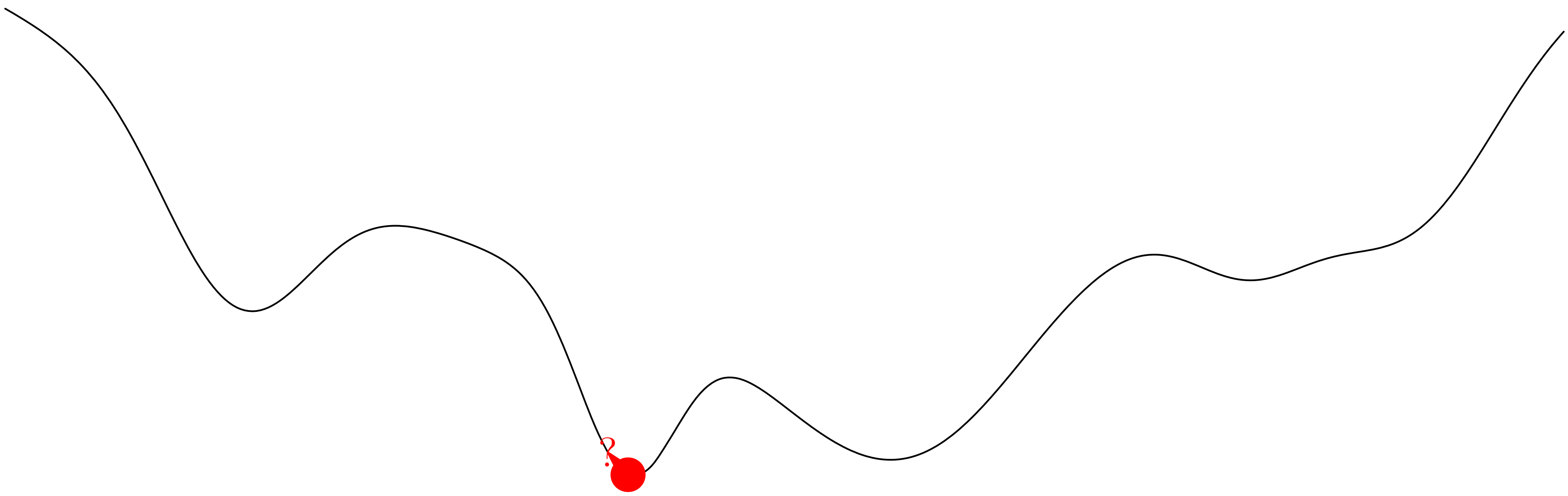

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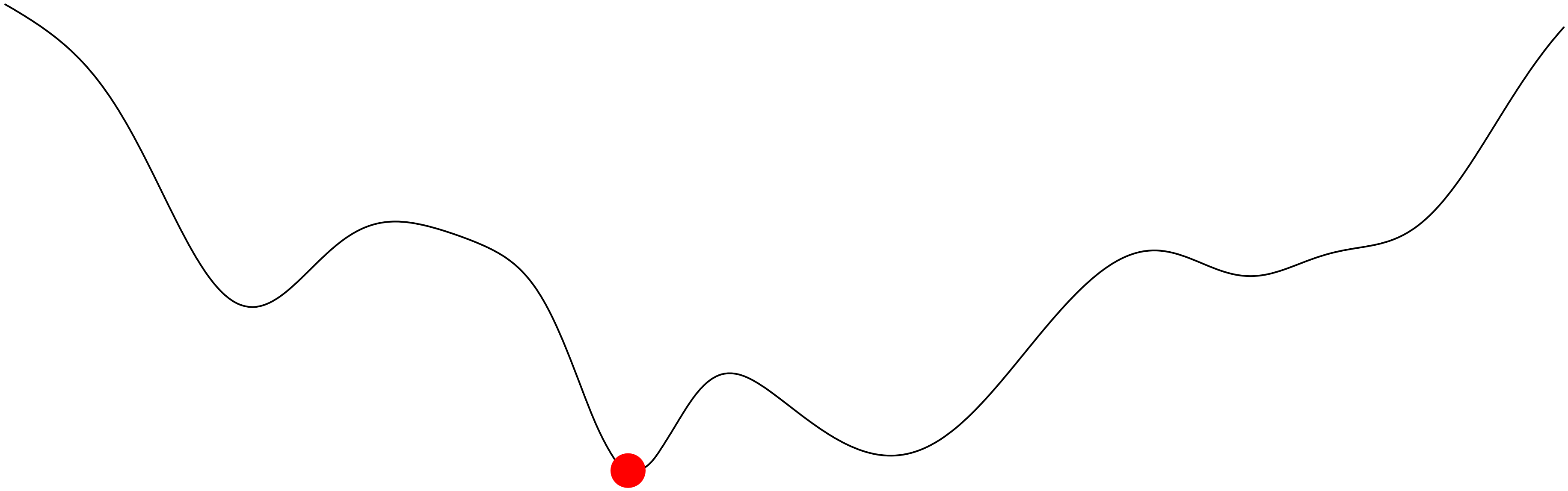

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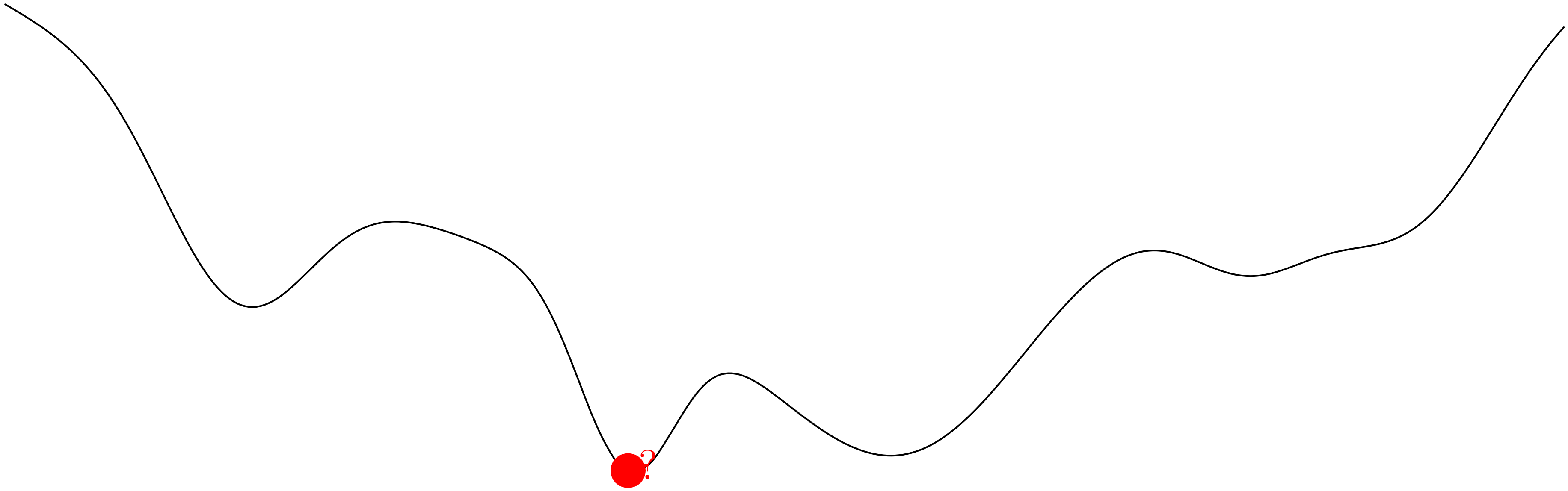

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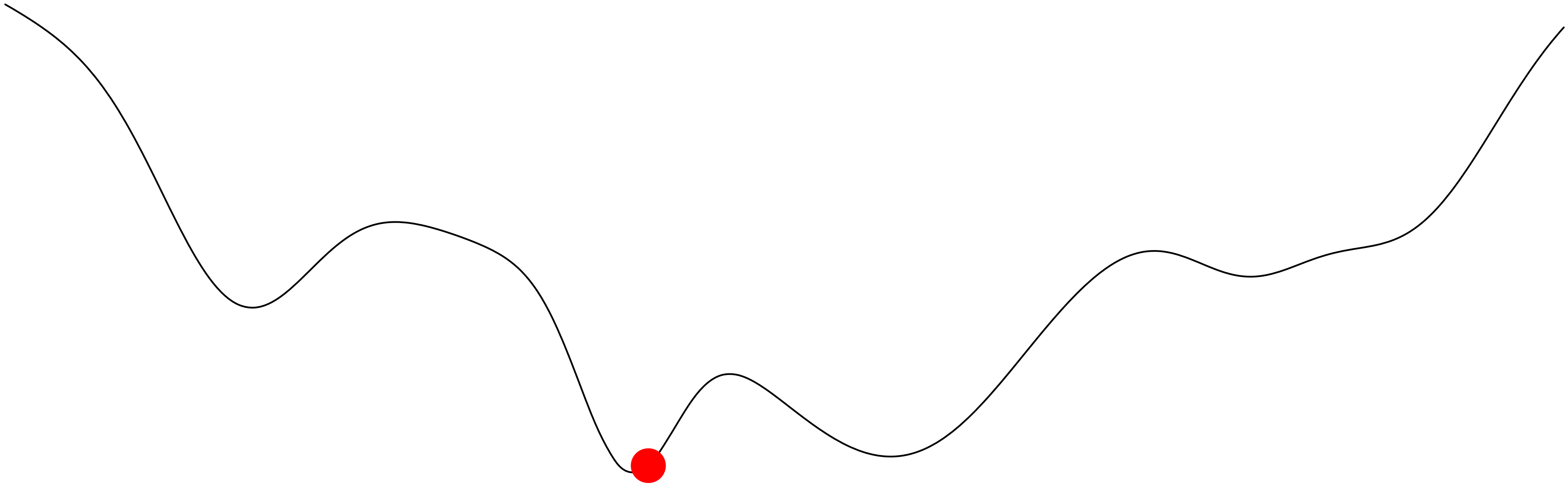

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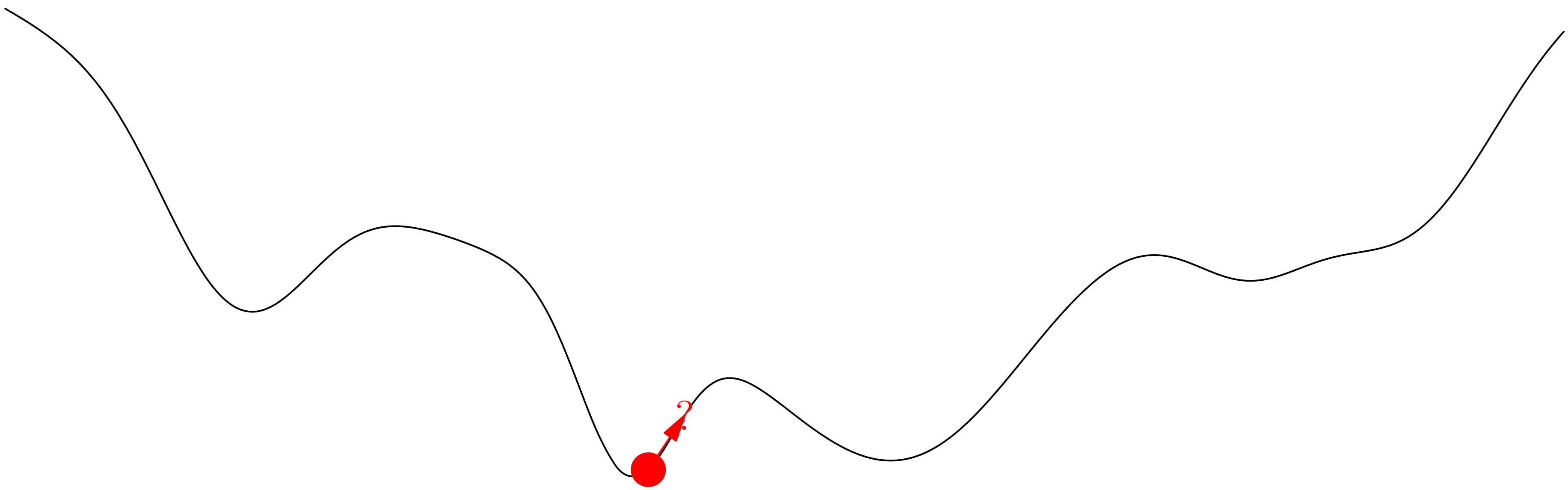

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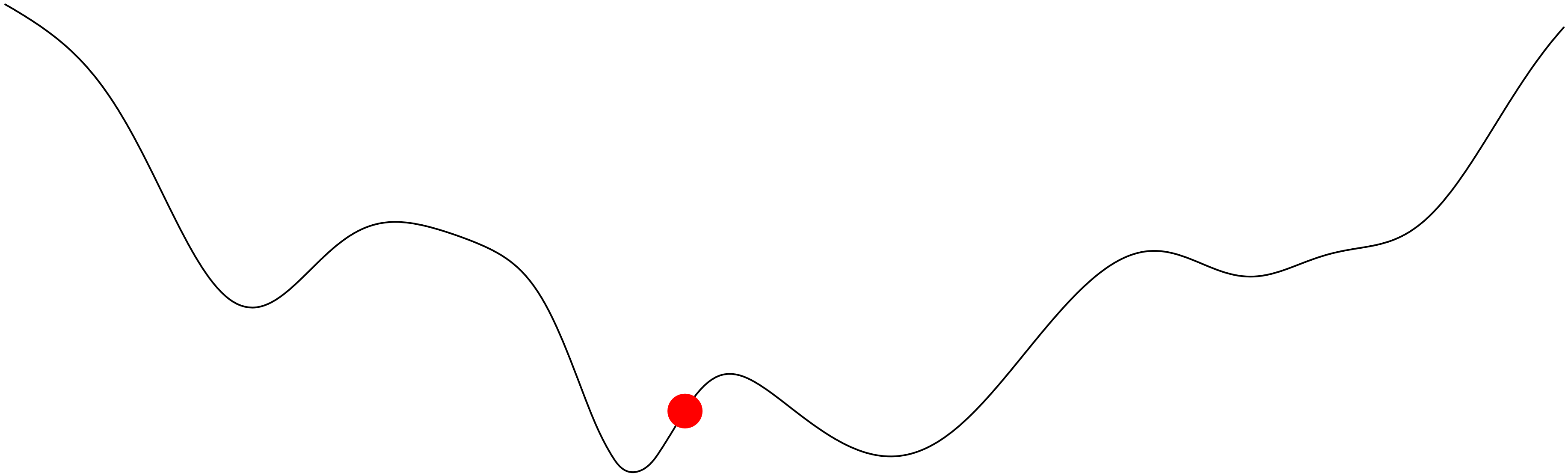

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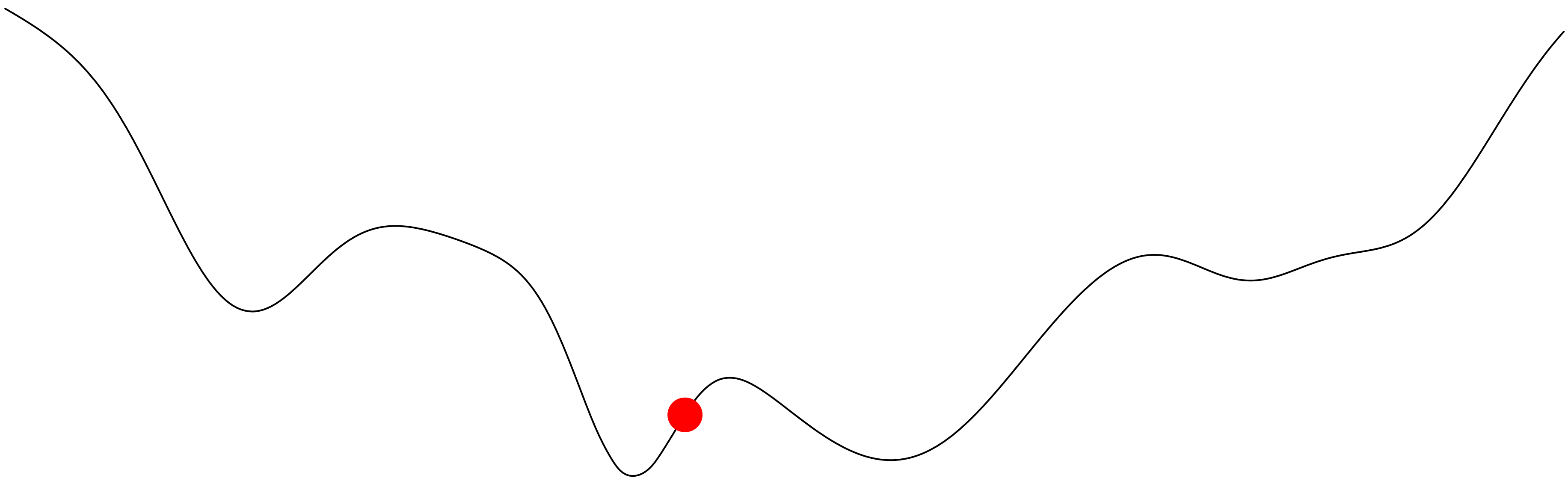

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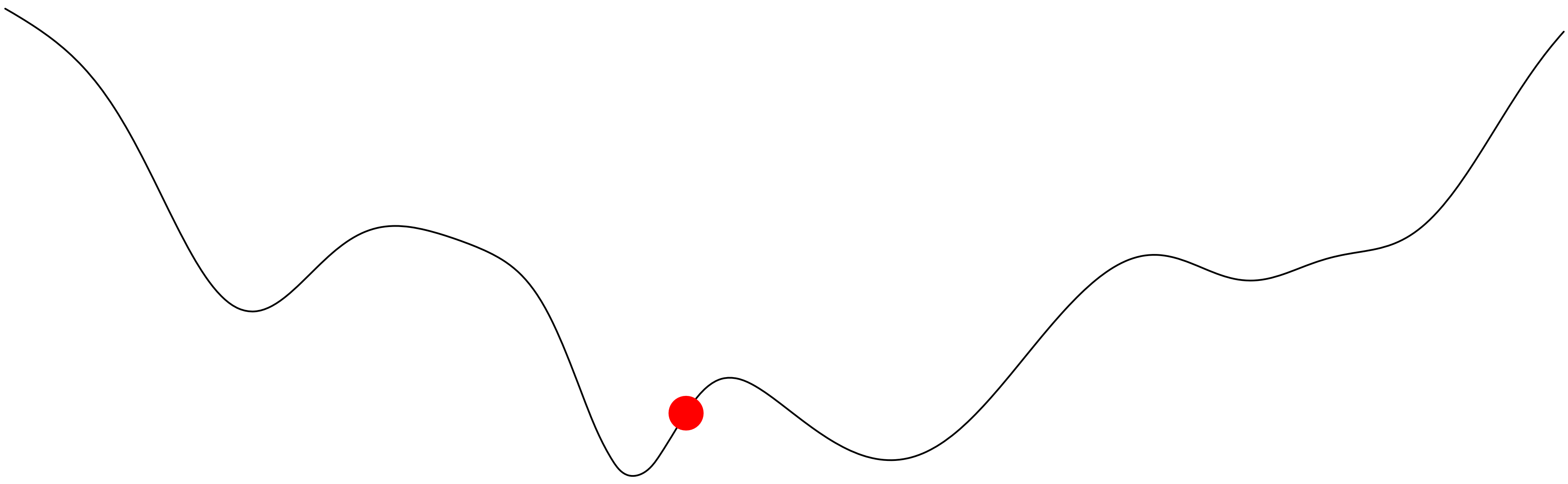

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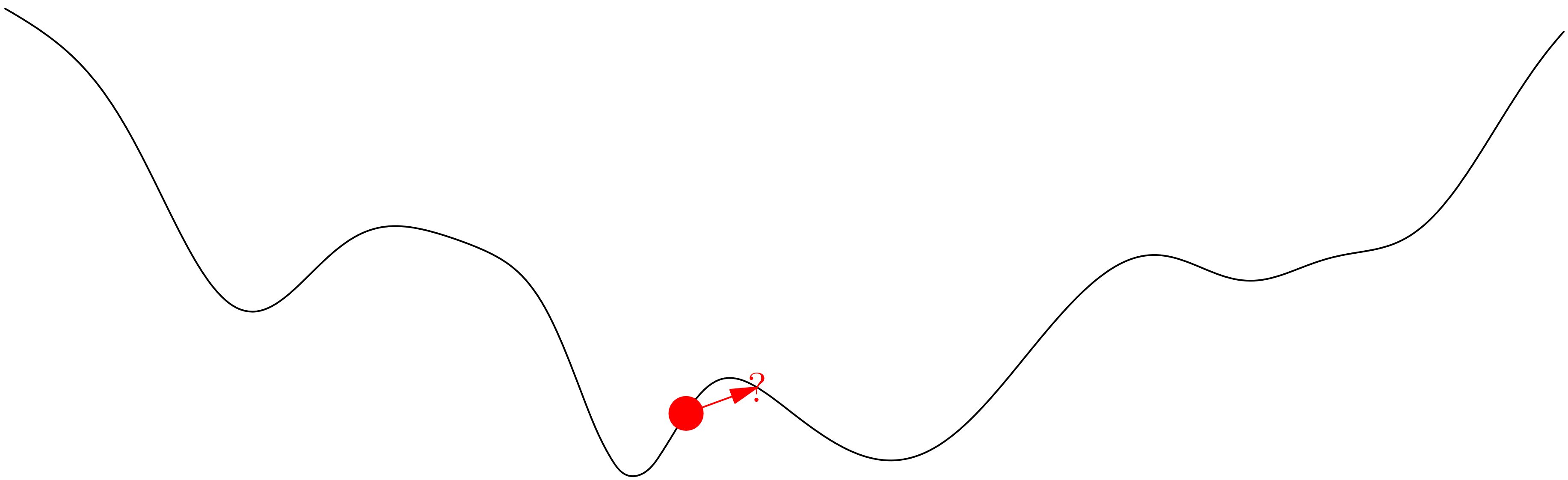

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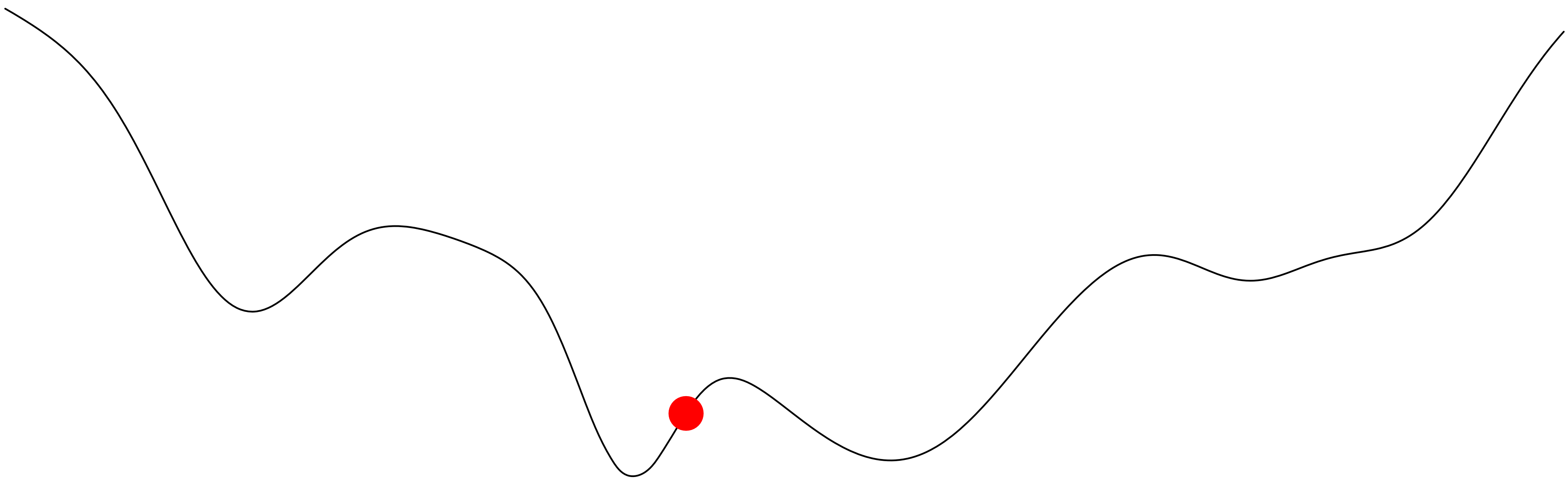

Simulated Annealing

- Algorithm to minimise energy $E(\boldsymbol{X})$ 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
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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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- 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
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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
- I'm going to present my, highly prejudiced view of what's important in making a GA work

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A Canonical GA

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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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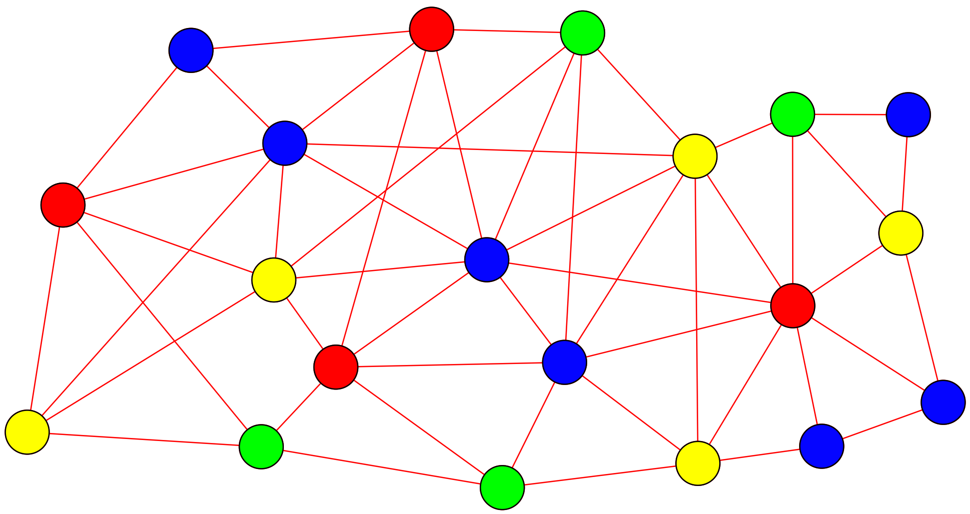
E.g. Graph Colouring



- 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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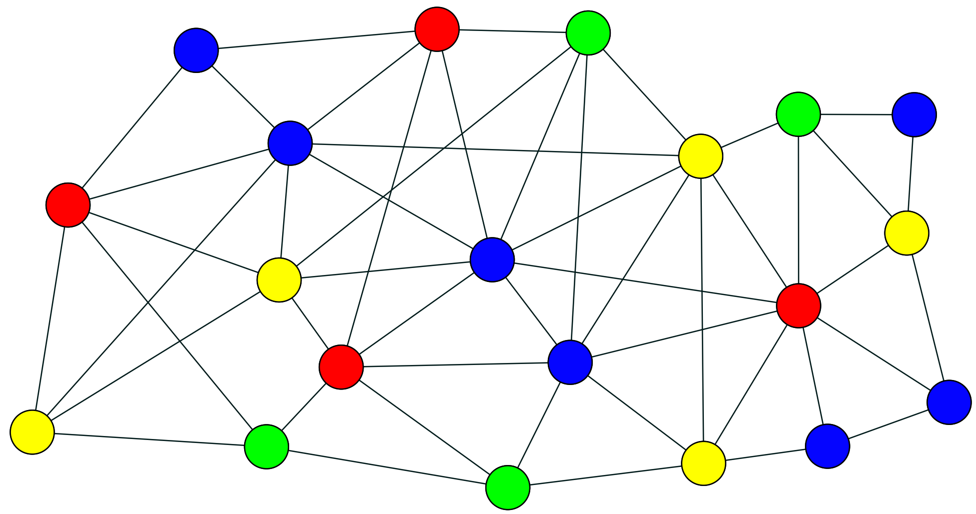

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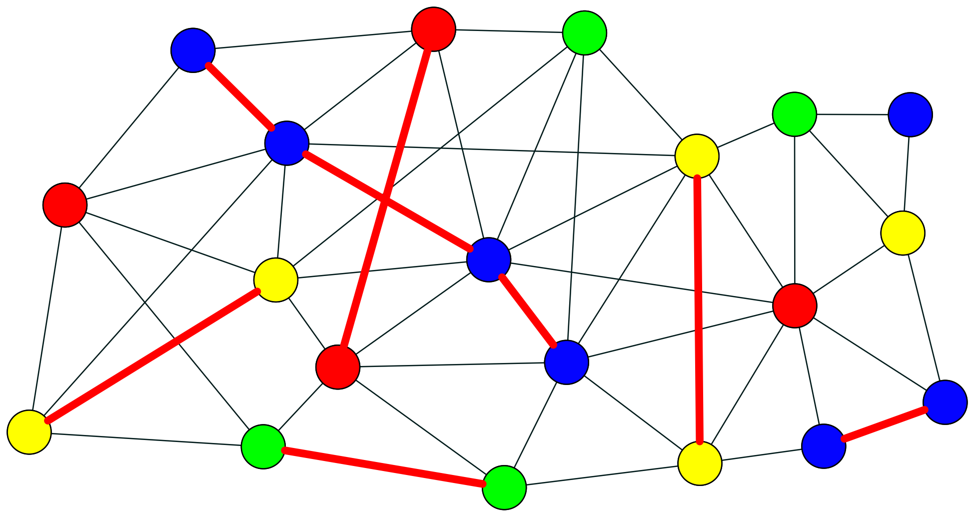

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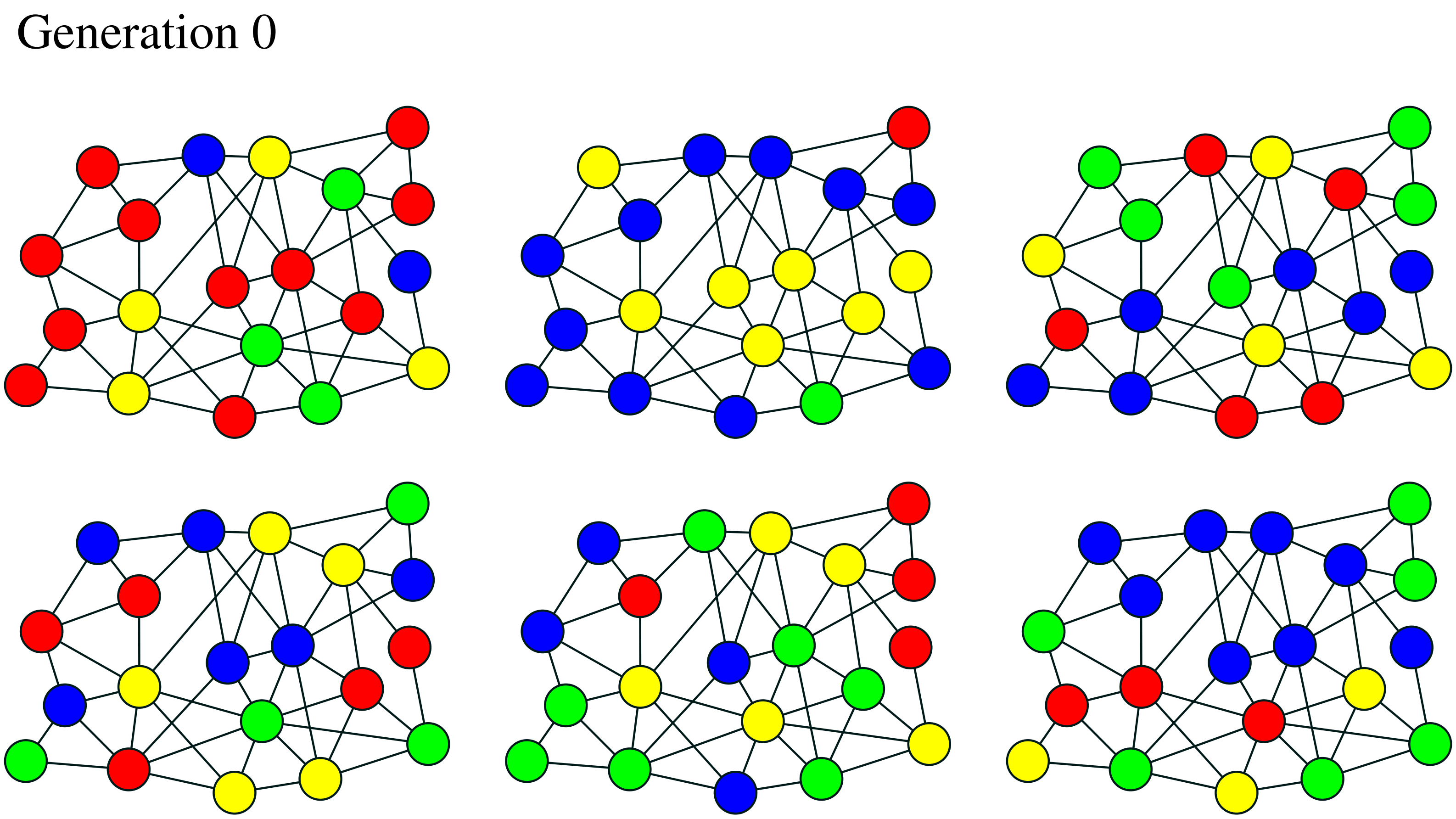

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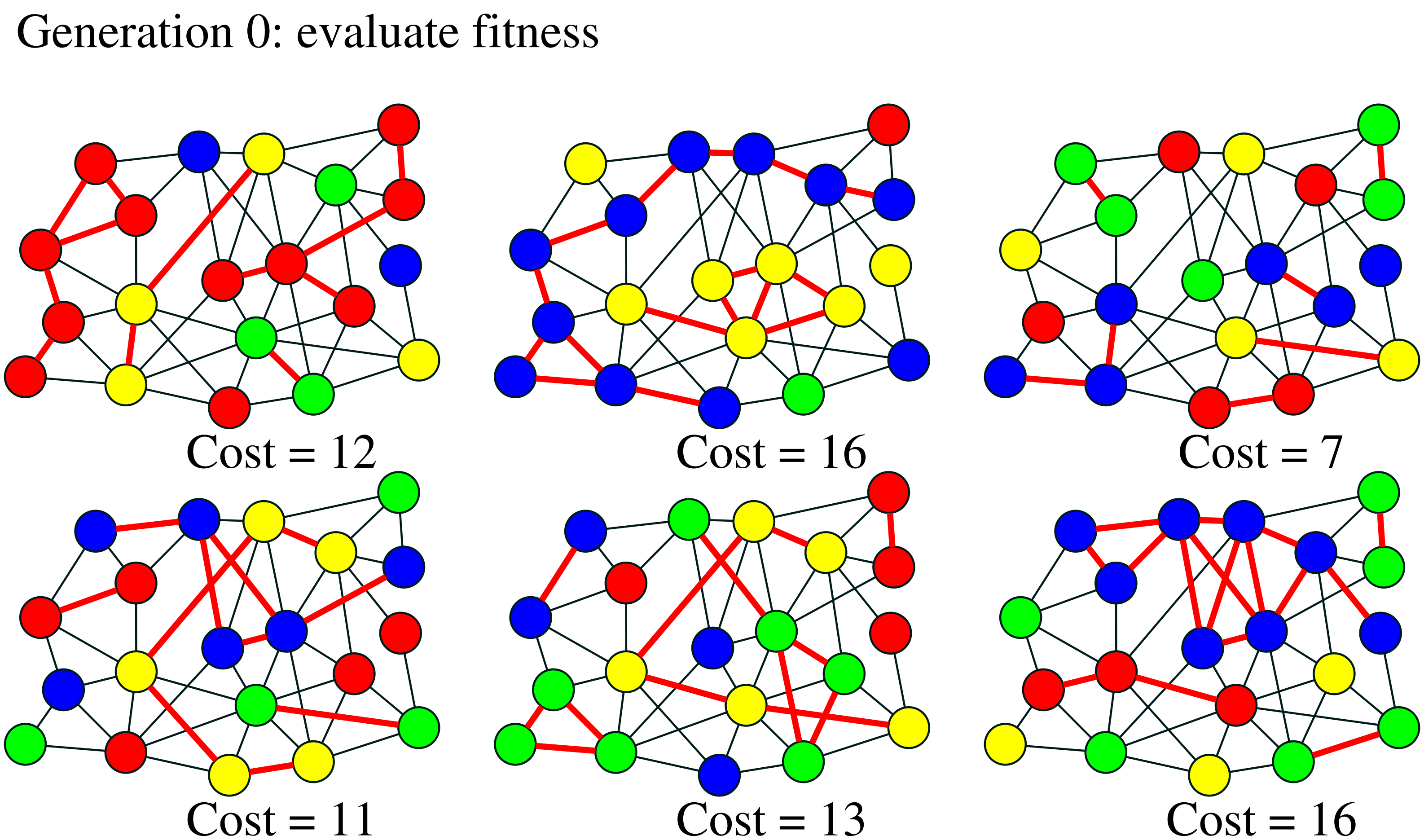

Selection

- 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)

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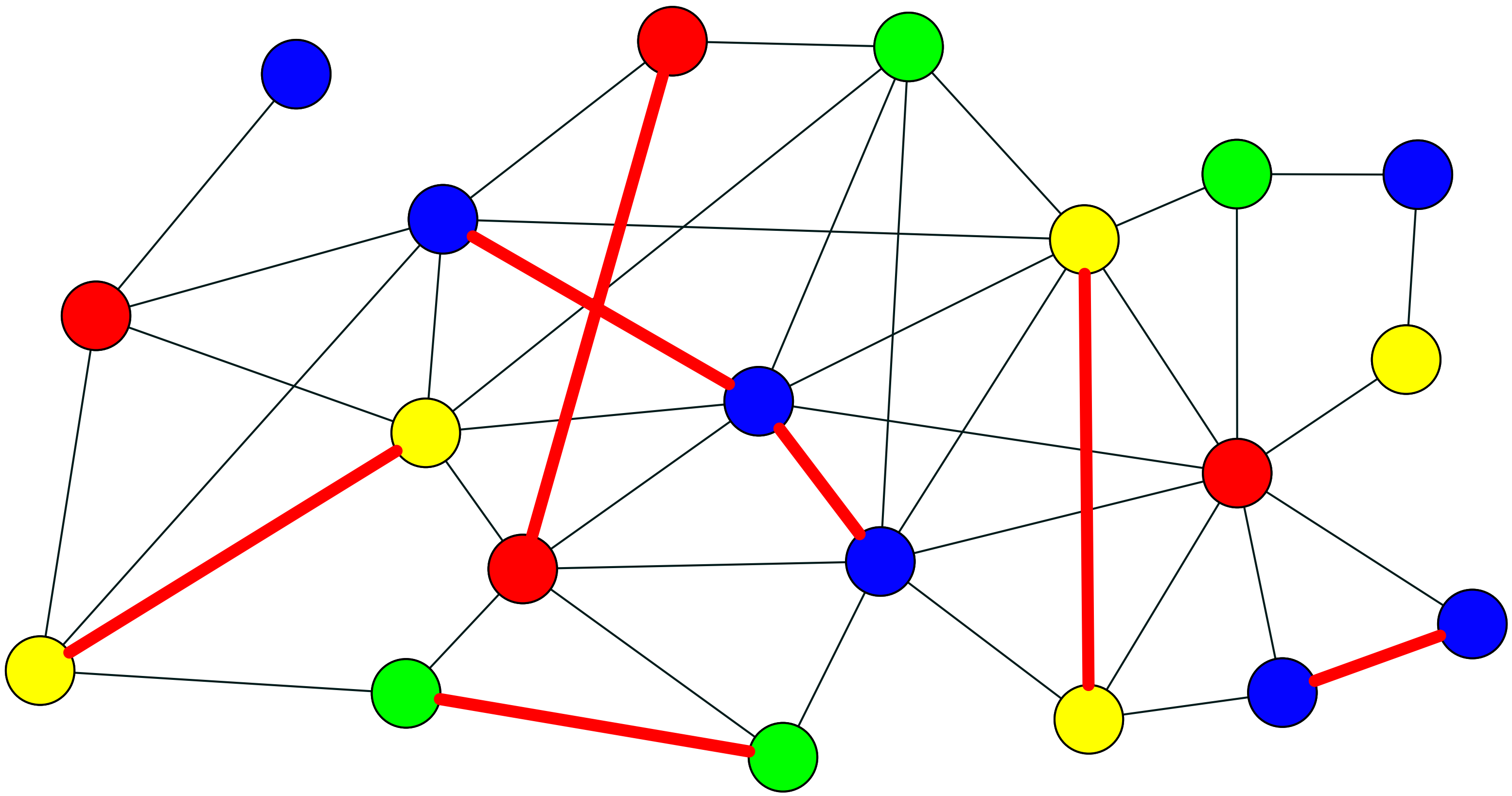

$\mathrm{cost}=7$

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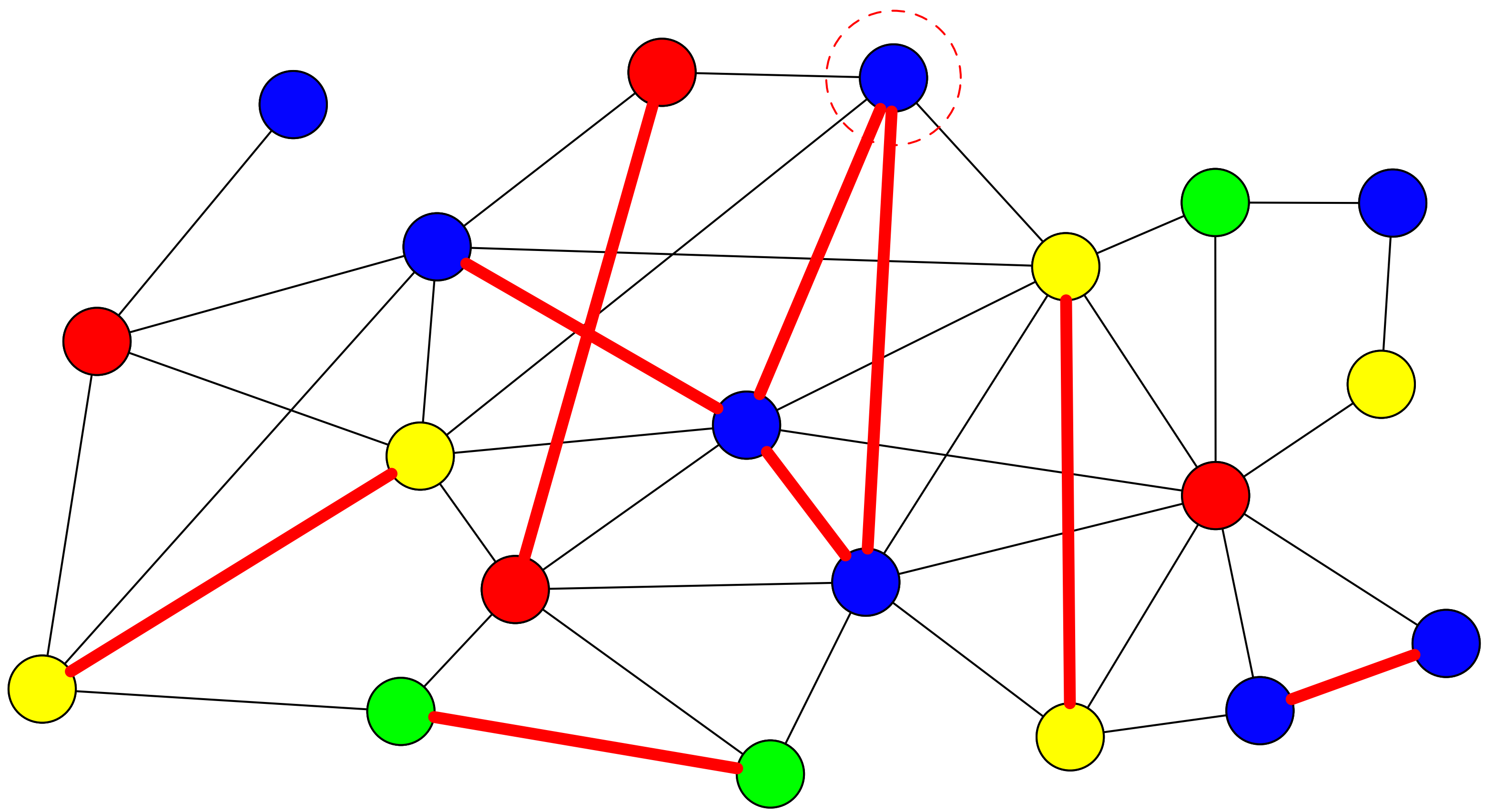

$$\text{cost} = 9$$

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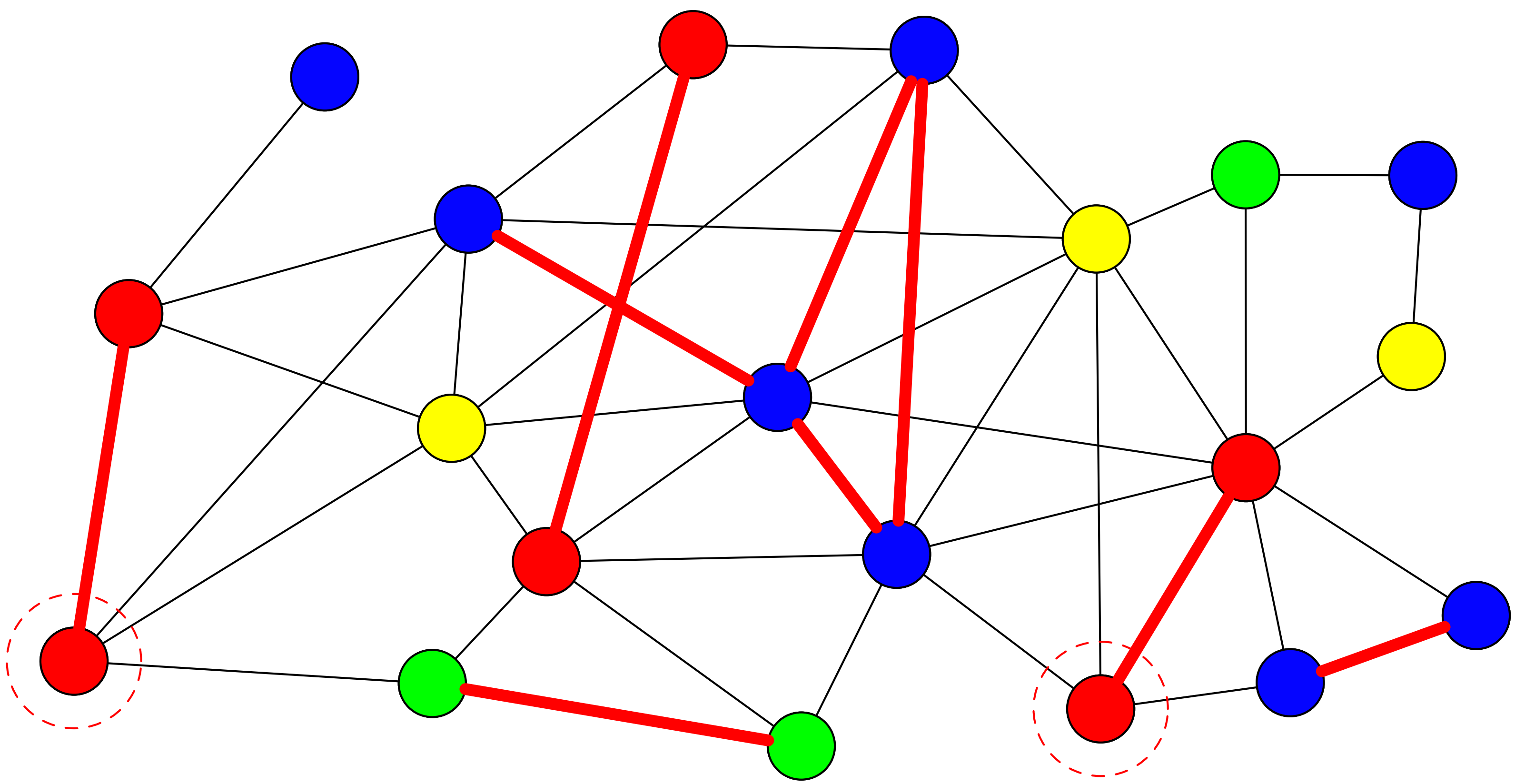

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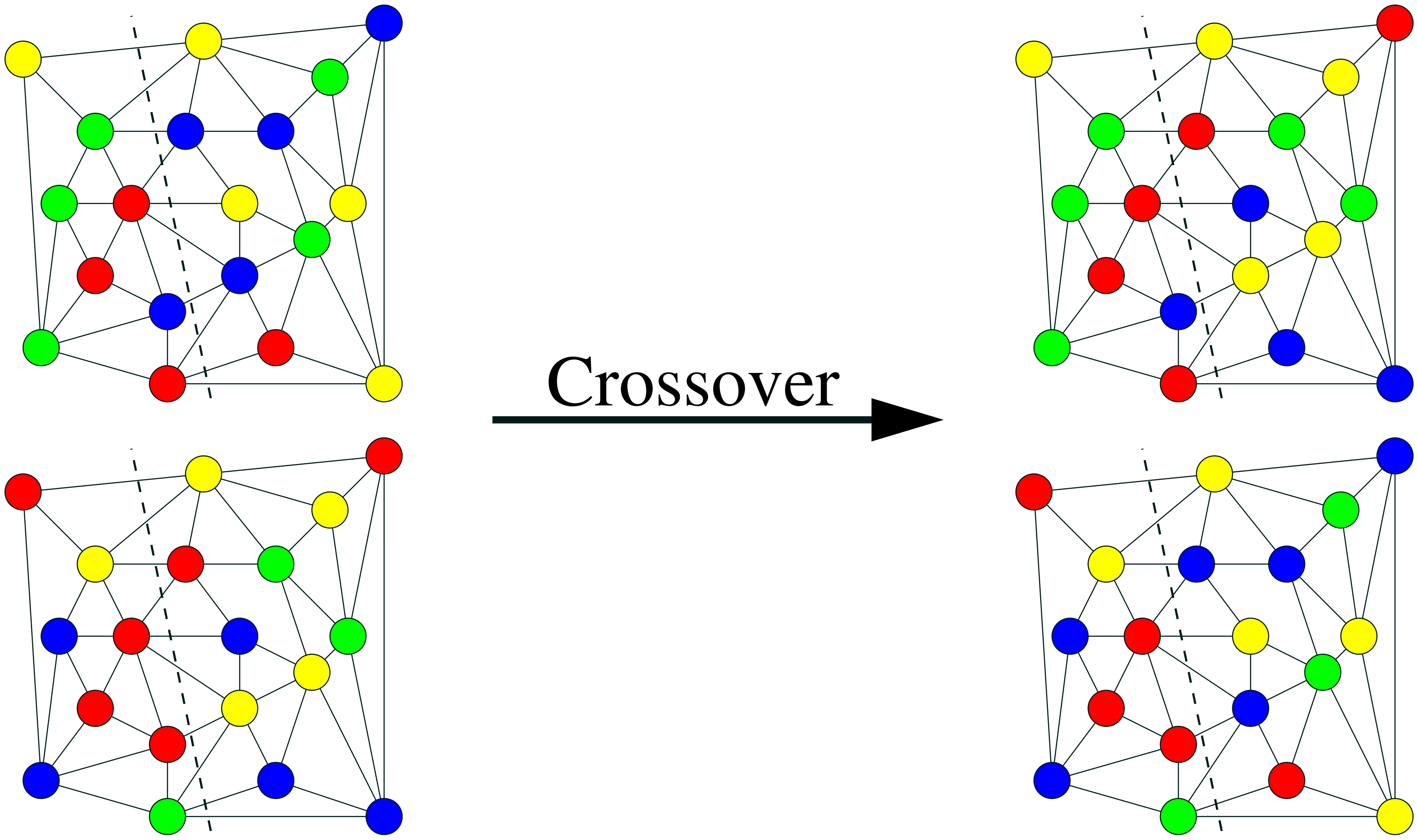

Crossover Operators

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

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

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

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

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

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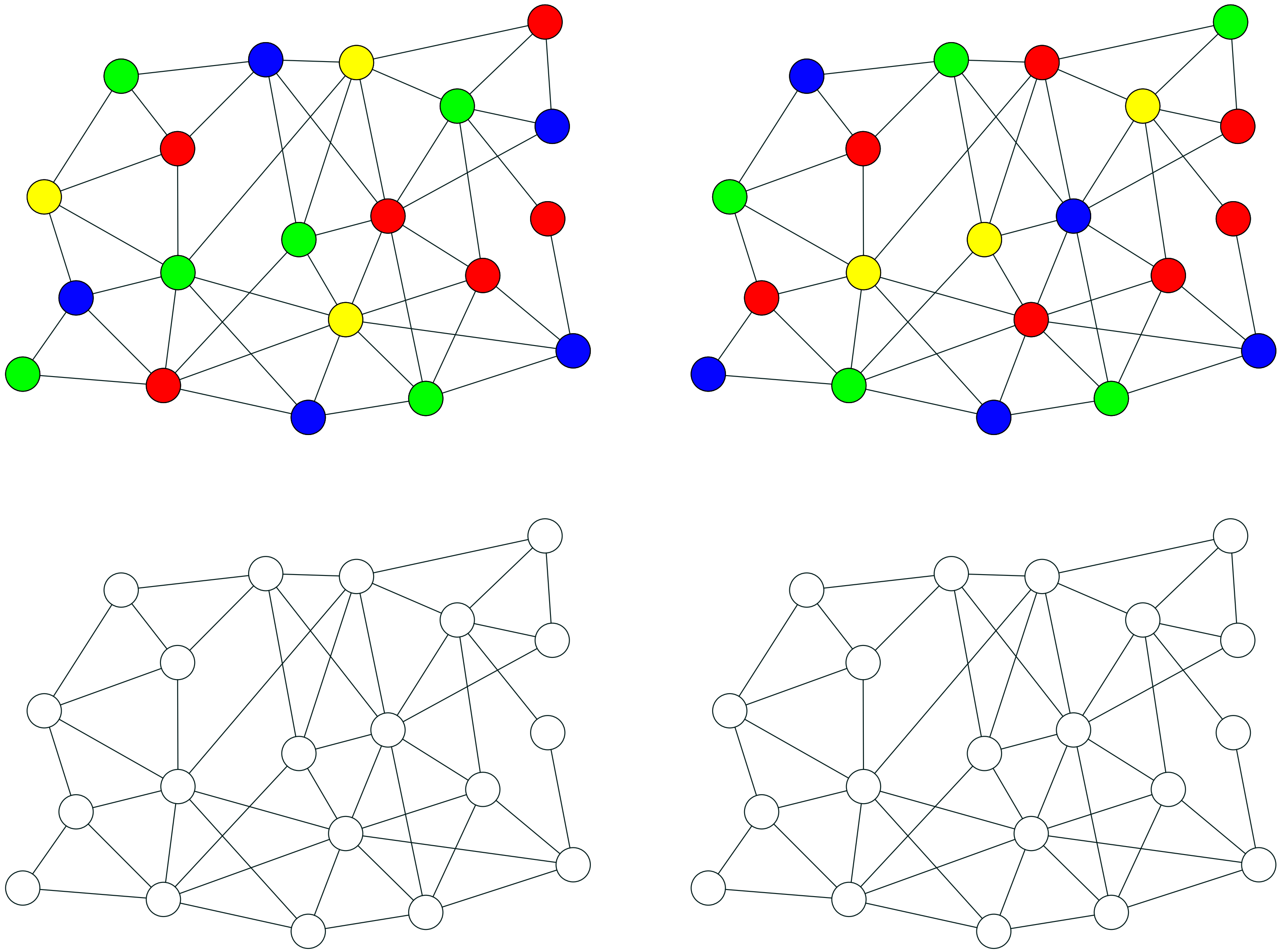
- Uniform Crossover
  - ⋆ Take two strings and create children by a random shuffle

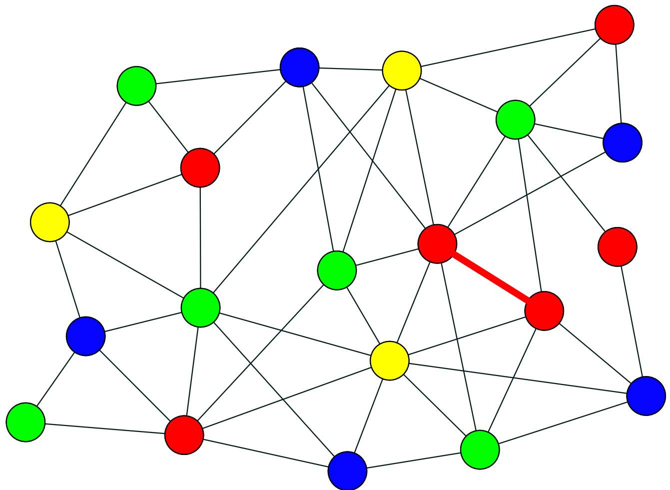
$$\left.\begin{array}{l}(GRBGBRBGGBGBG)\\(RRBRGBRGRBBGB)\end{array}\right\}\longrightarrow\left\{\begin{array}{l}(GRBRGBRGRGGGB)\\(RRBGBRBGGBBBG)\end{array}\right.$$

- Any of these crossover can be biased towards one parent

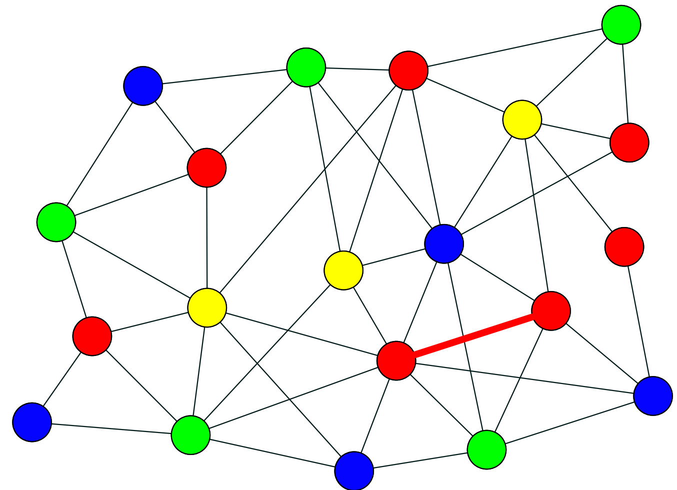
Cost of Crossover



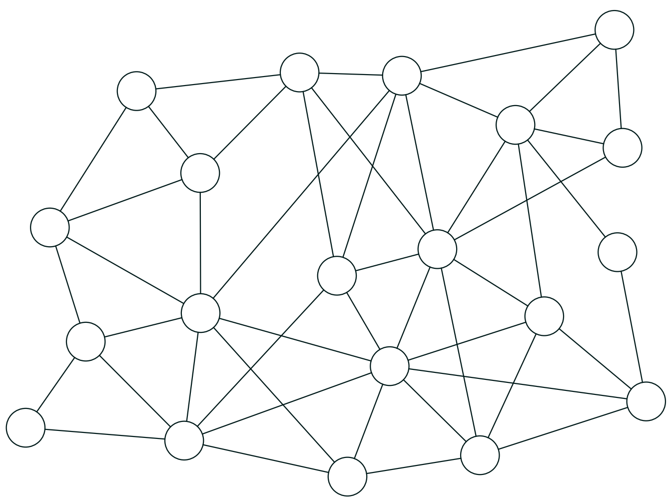
Cost of Crossover

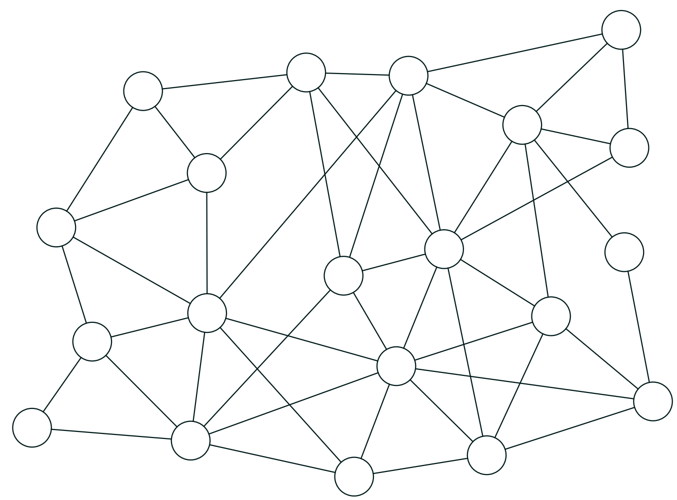


cost=1

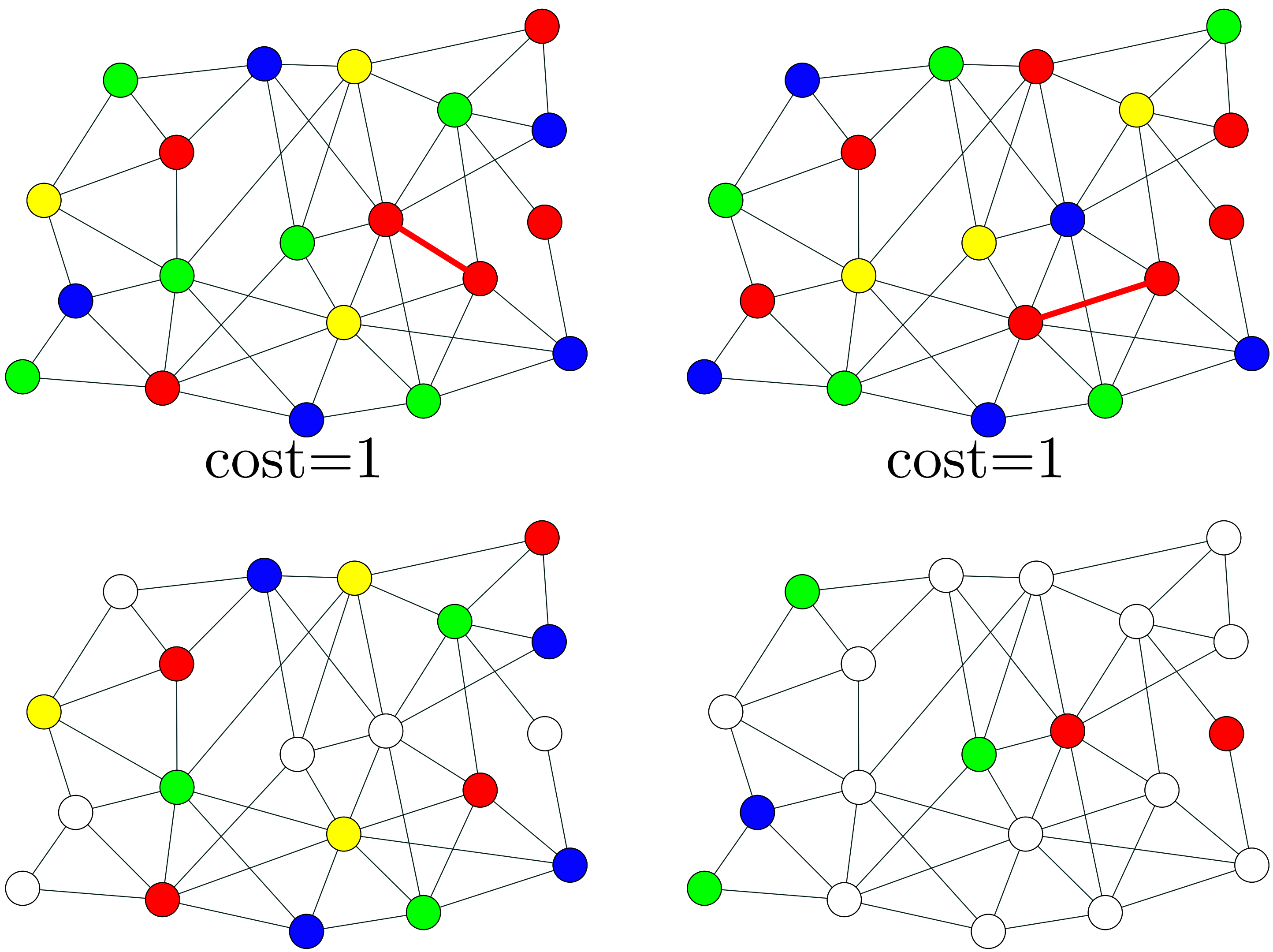


cost=1

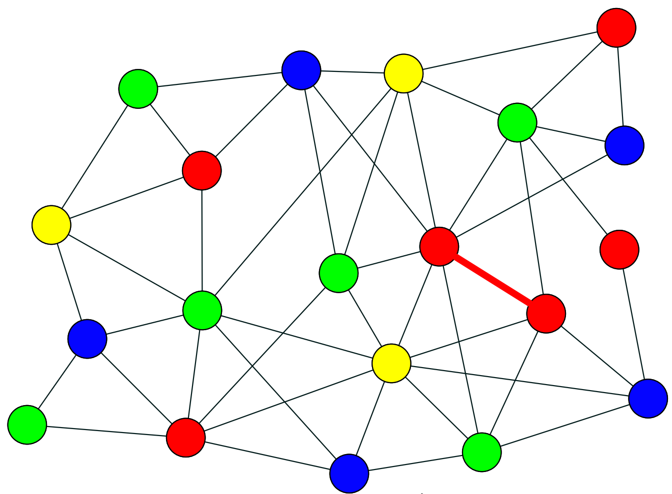




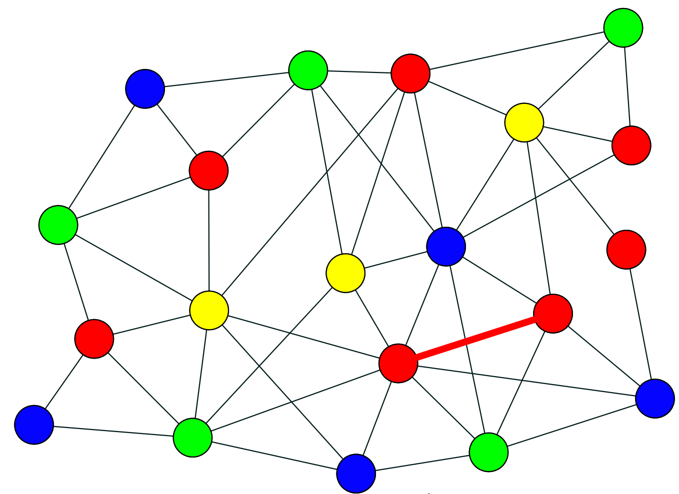
Cost of Crossover



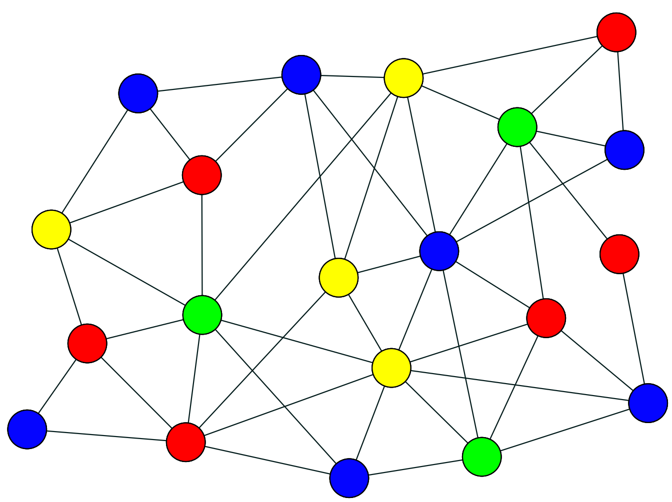
Cost of Crossover

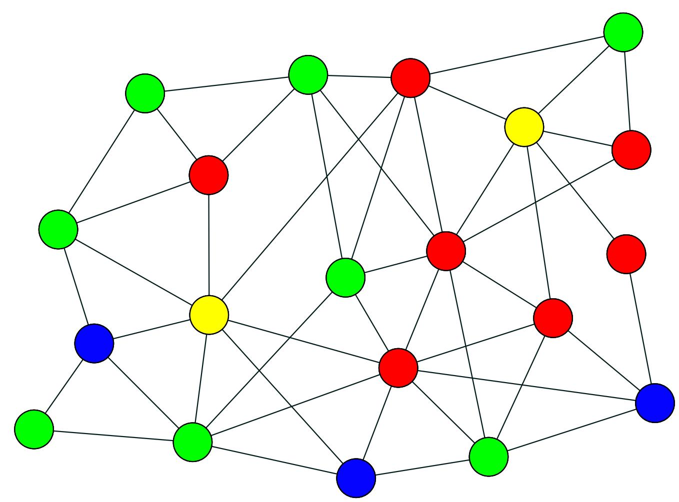


cost=1

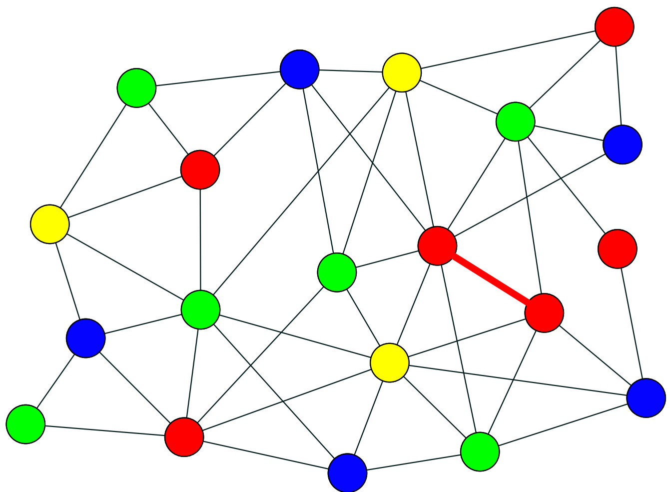


cost=1

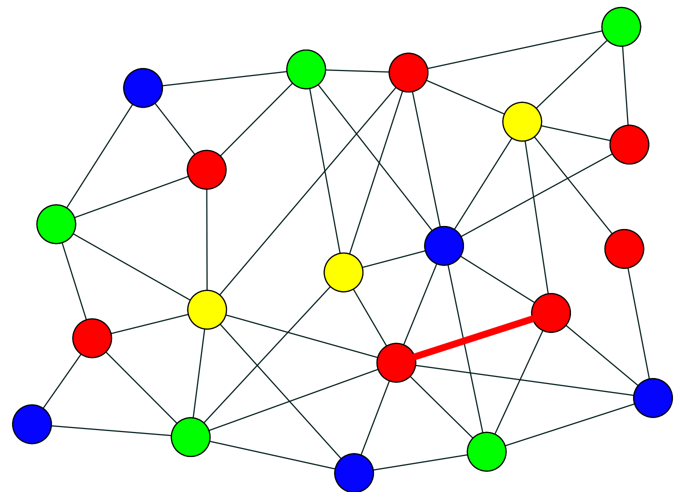




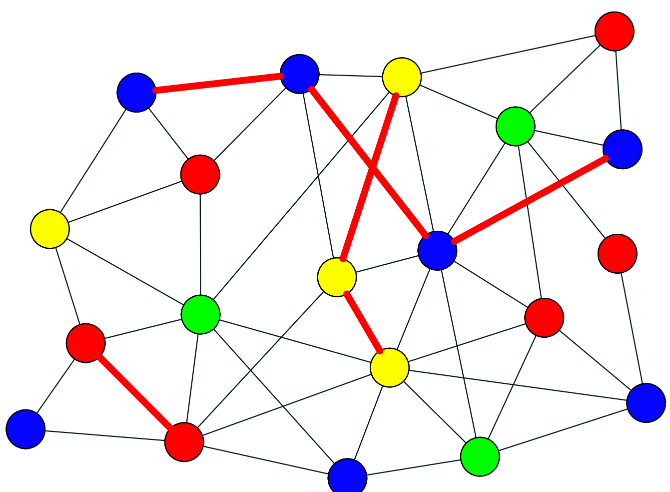
Cost of Crossover



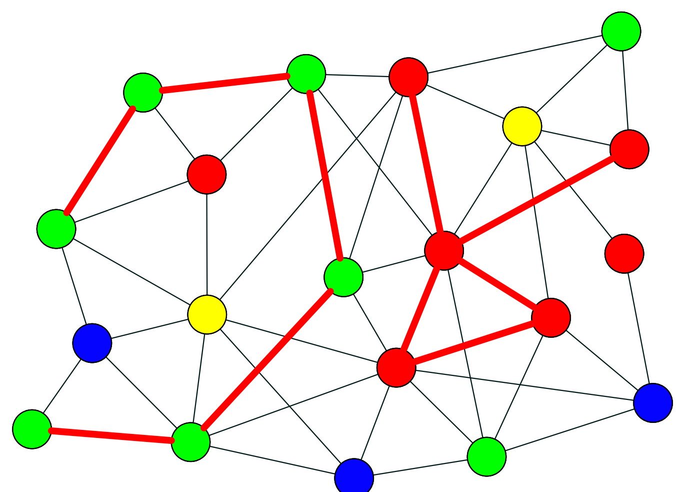
cost=1



cost=1



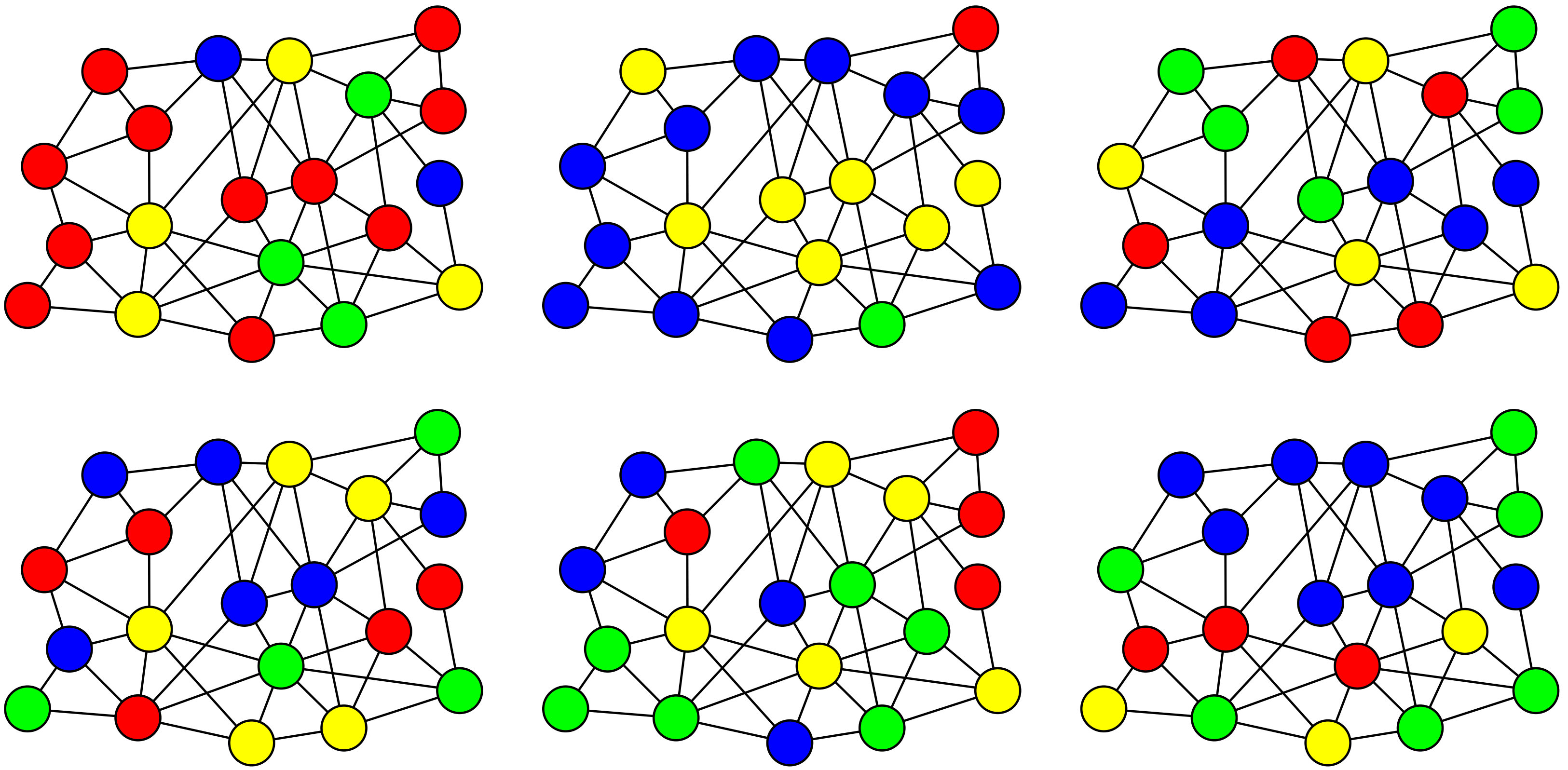
cost=6



cost=10

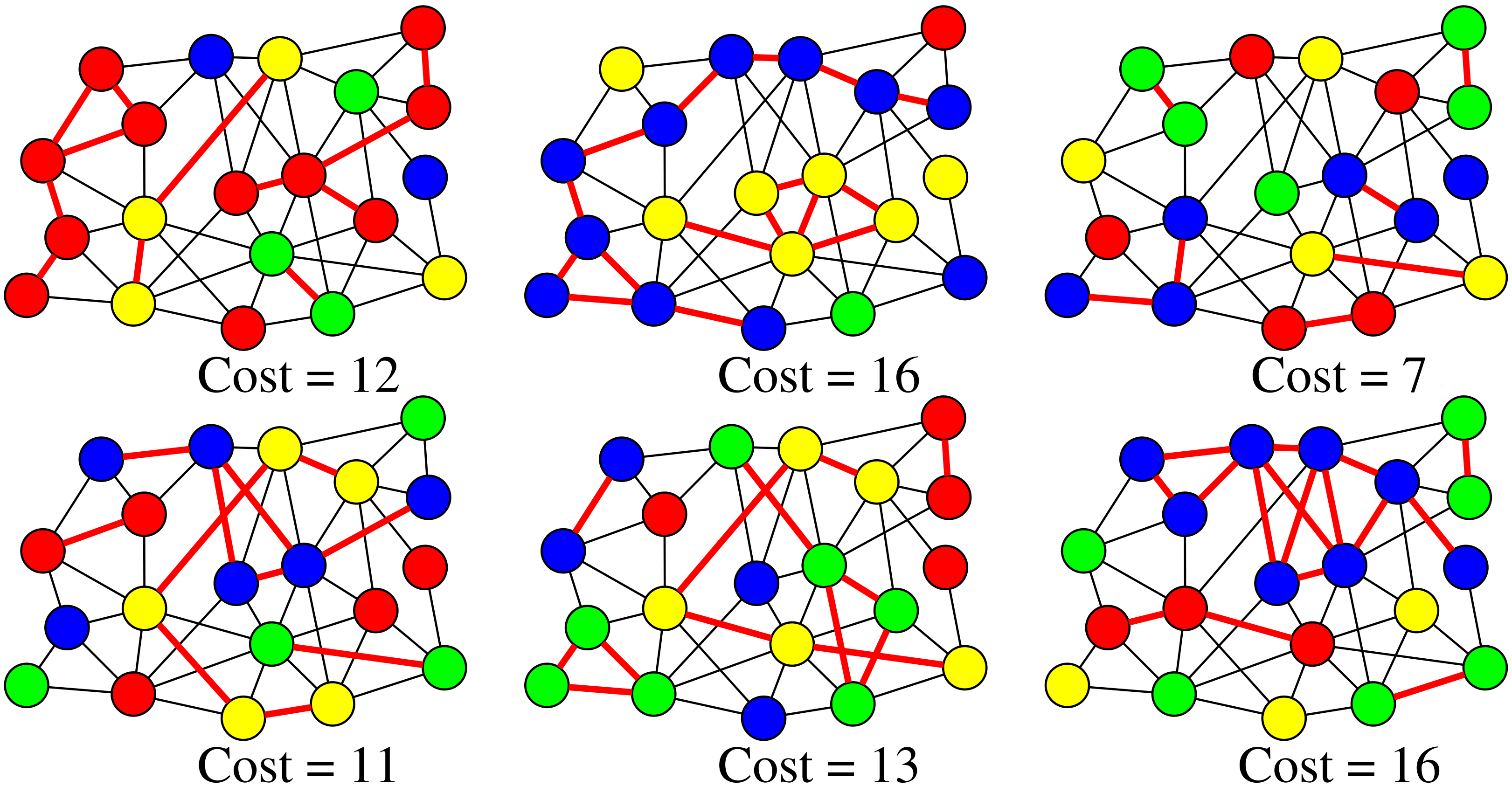
GA

Generation 0



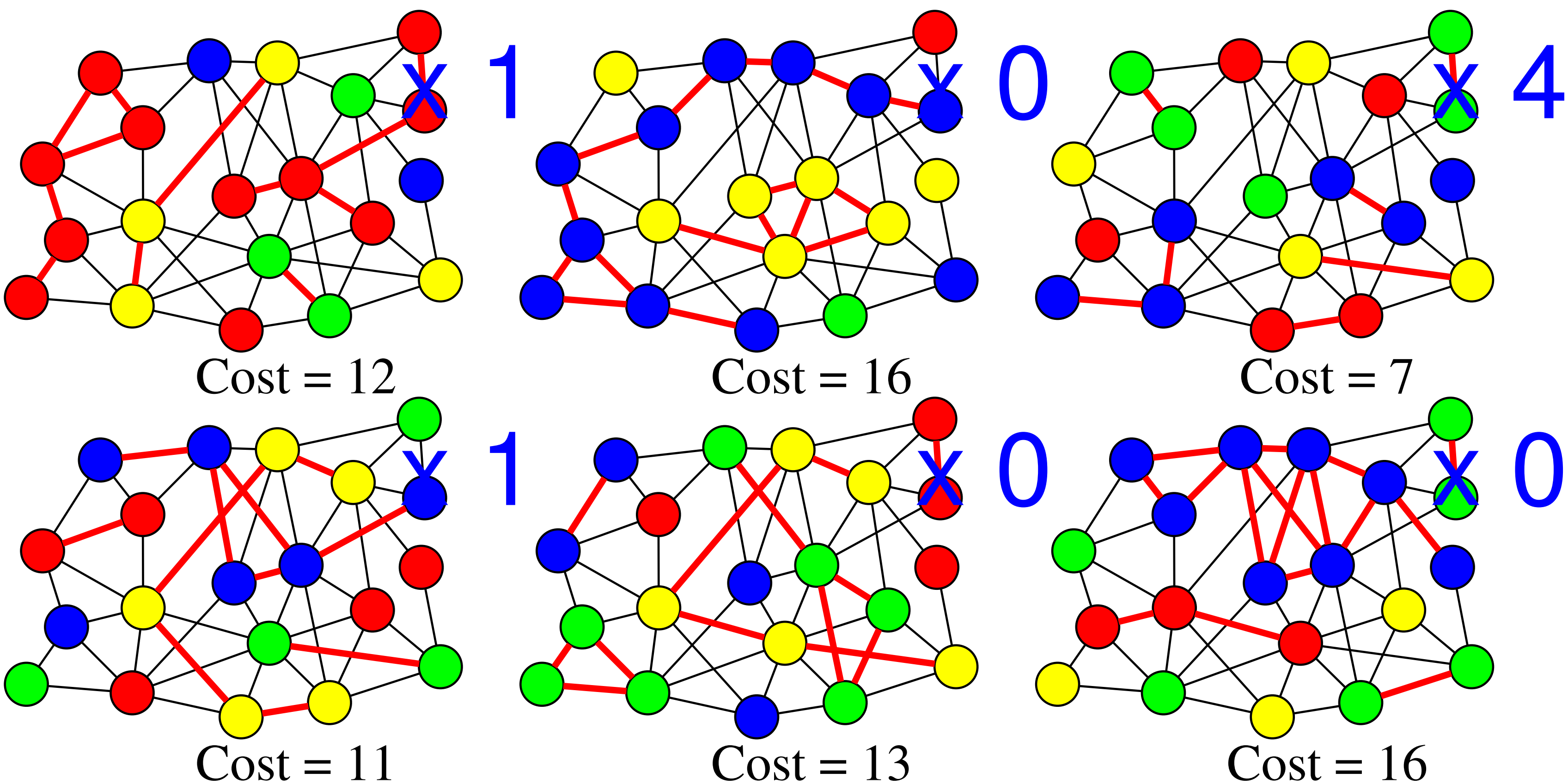
GA

Generation 0: evaluate fitness



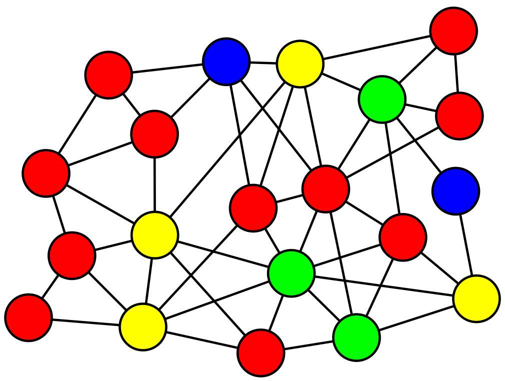
GA

Generation 0: selection

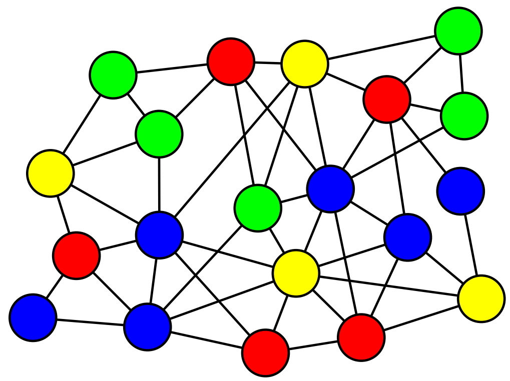


GA

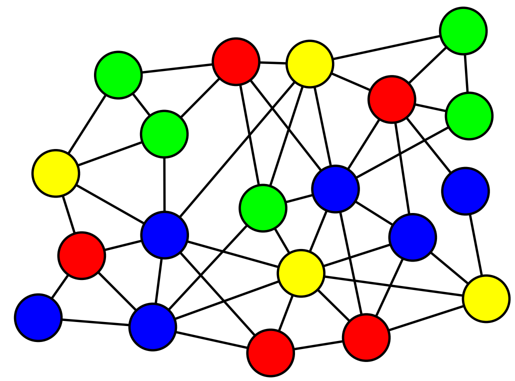
Generation 0: selection



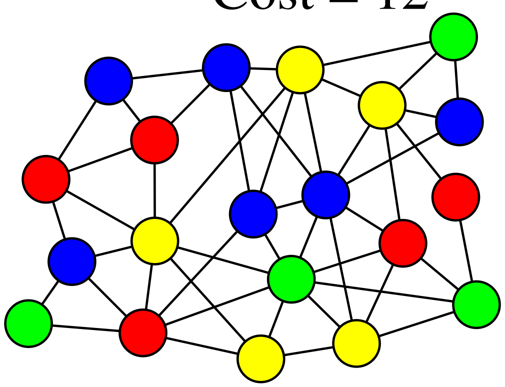
Cost = 12



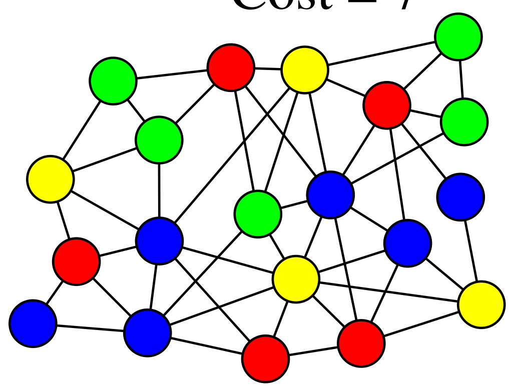
Cost = 7



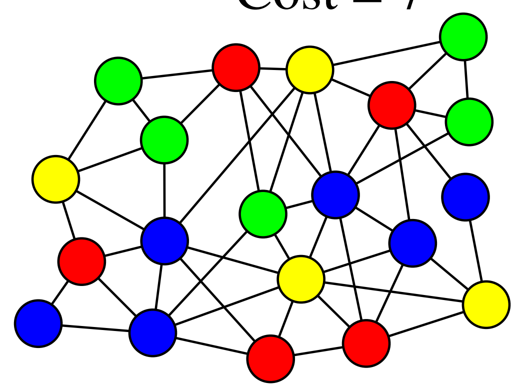
Cost = 7



Cost = 11



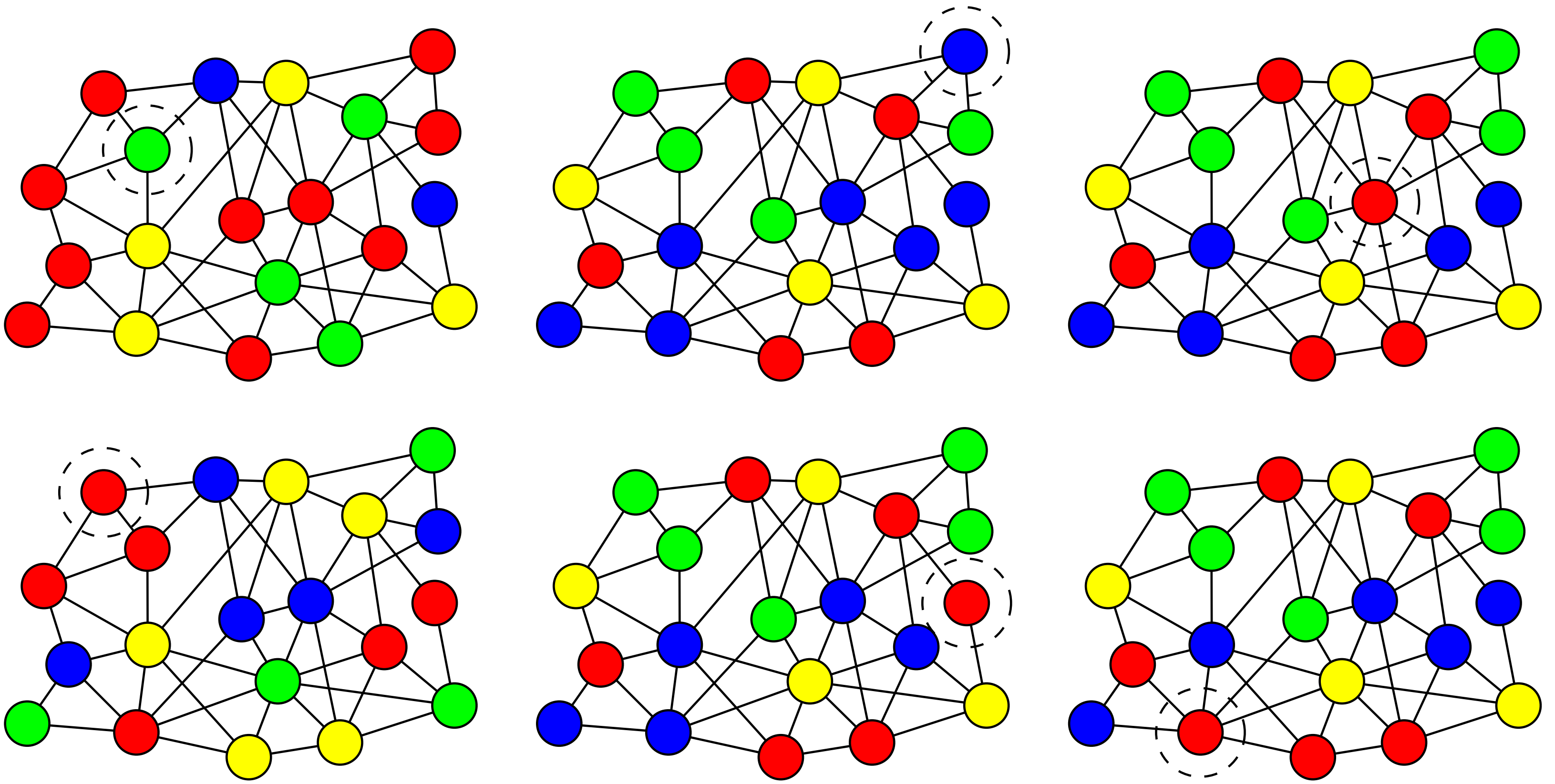
Cost = 7



Cost = 7

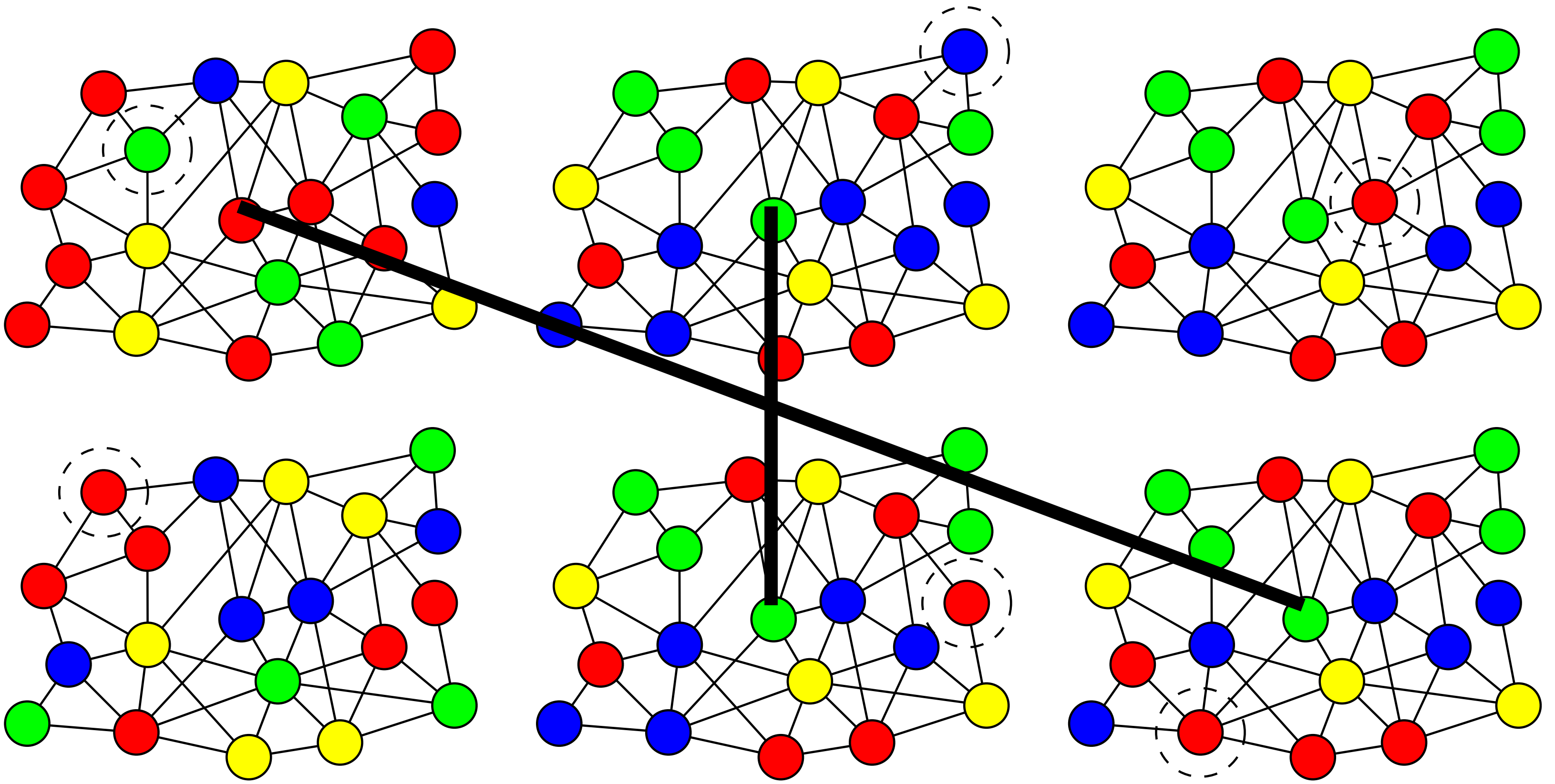
GA

Generation 0: mutation



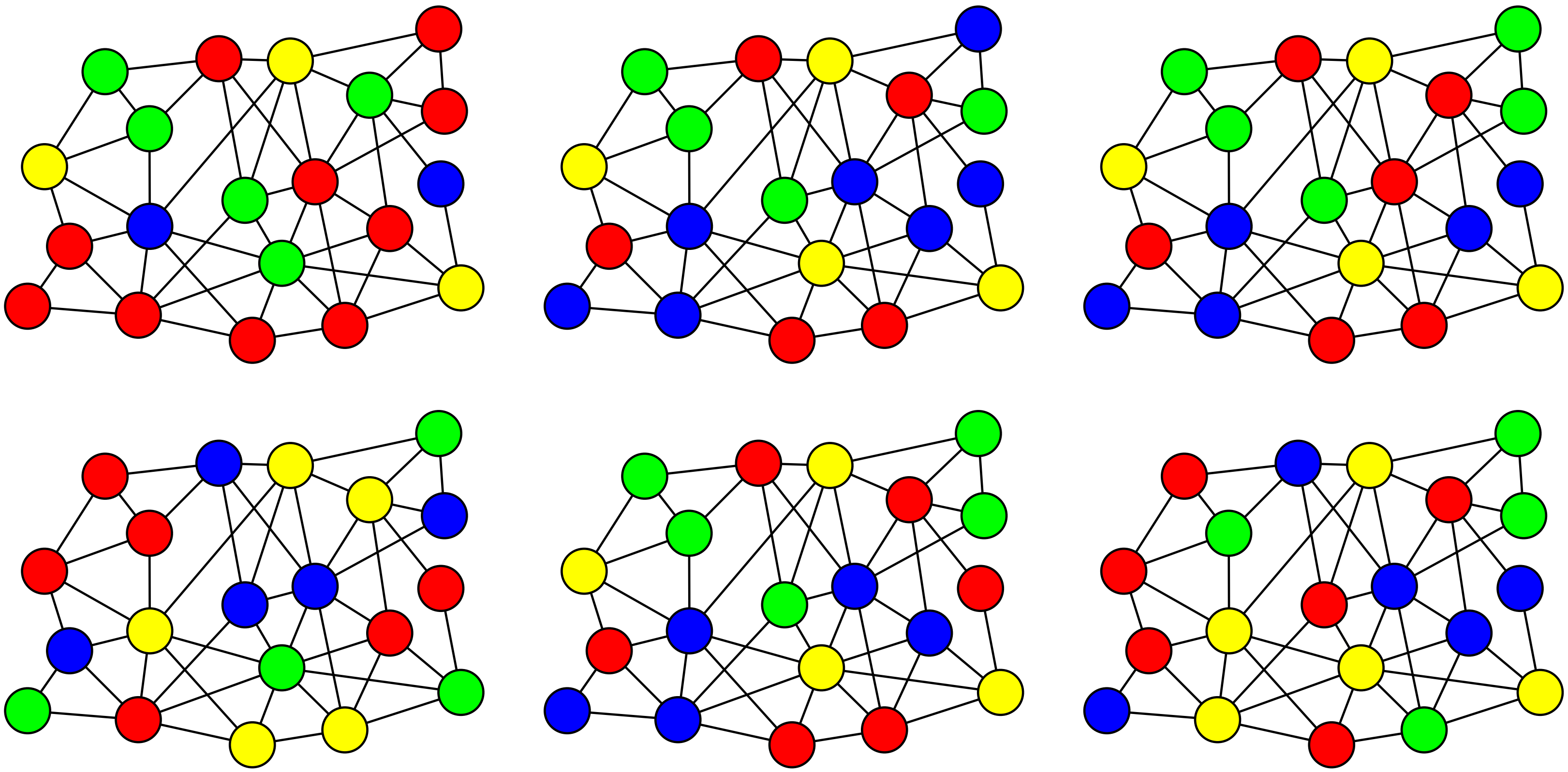
GA

Generation 0: crossover



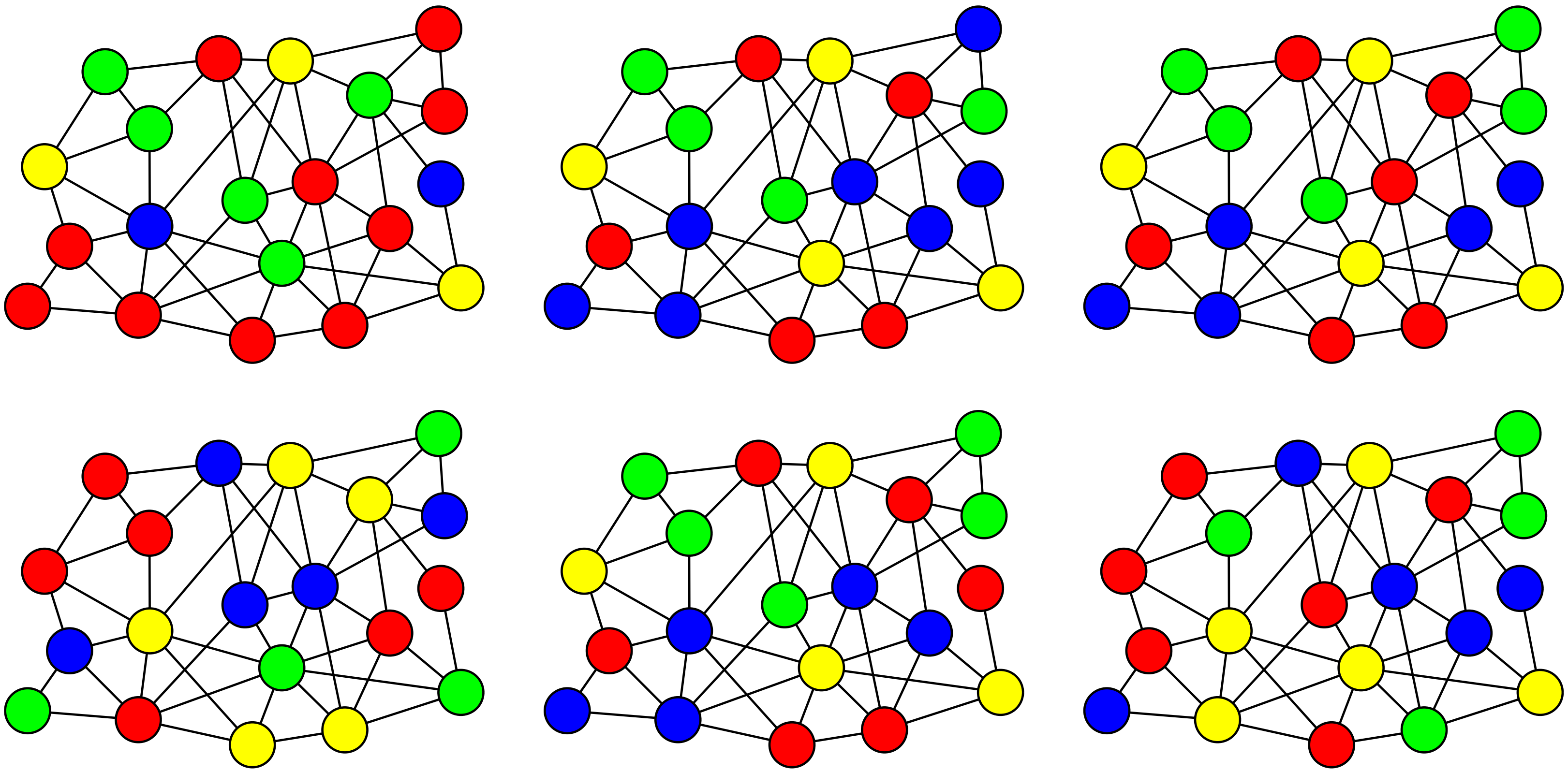
GA

Generation 0: crossover



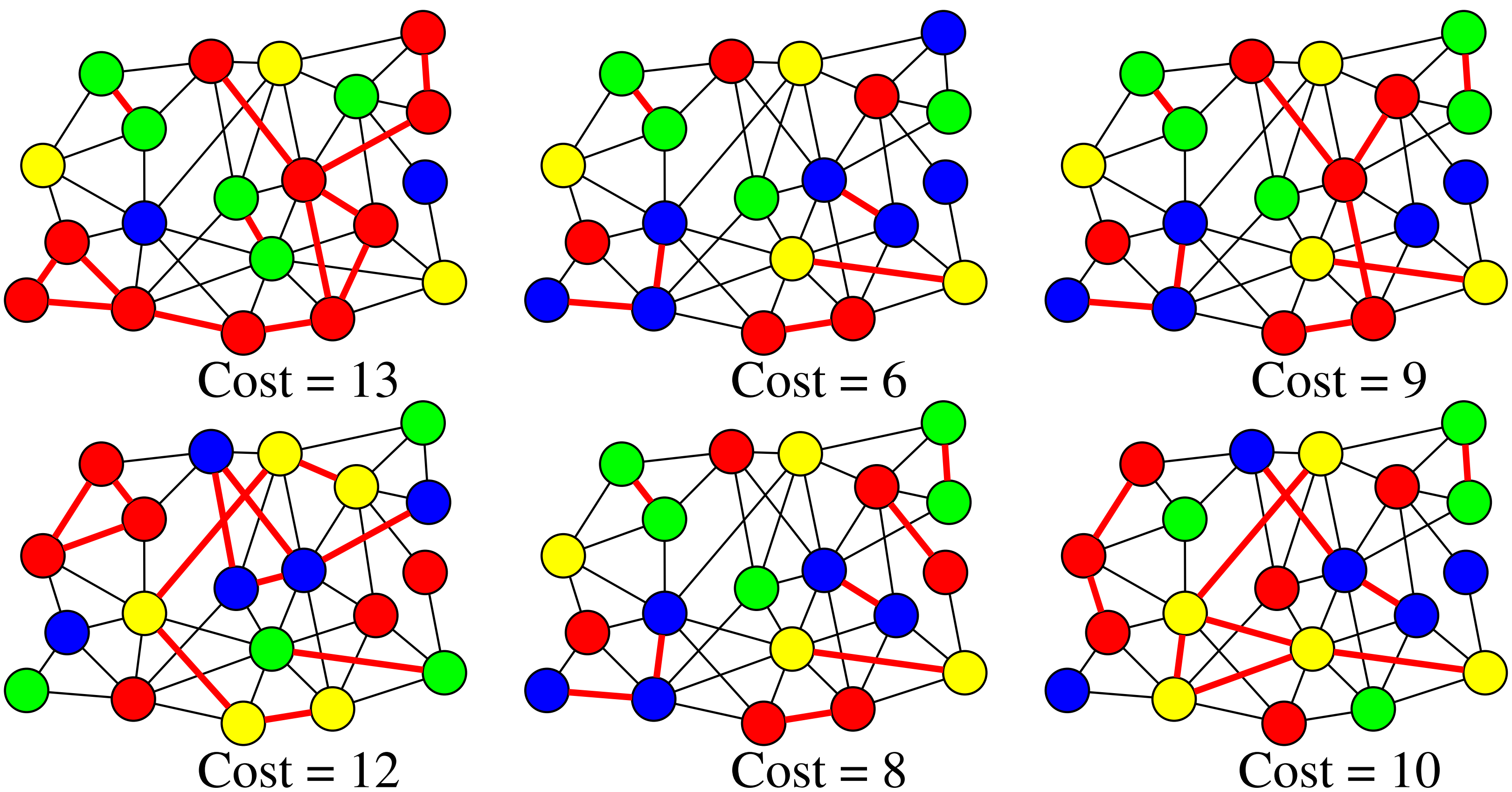
GA

Generation 1



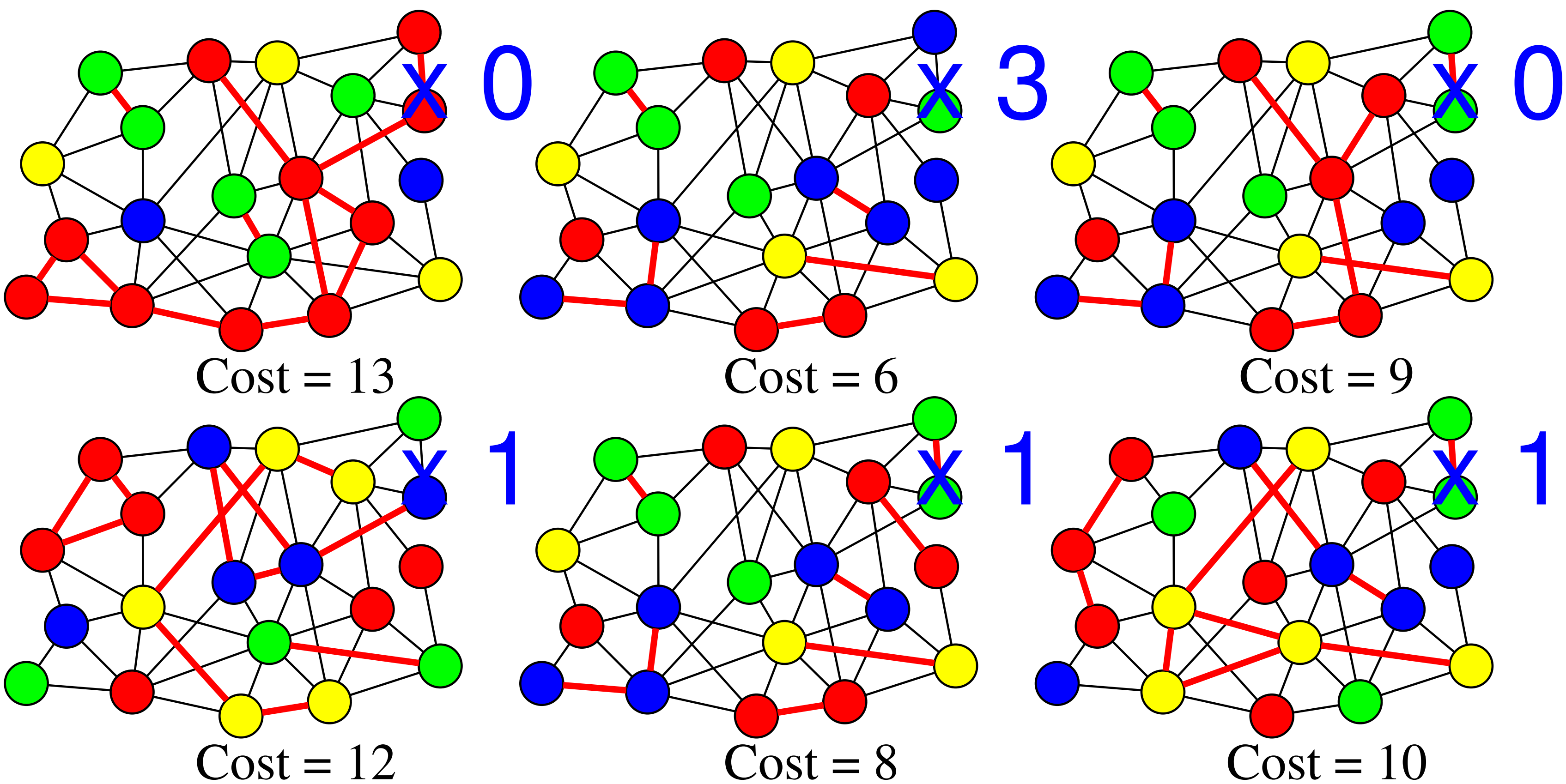
GA

Generation 1: evaluate fitness



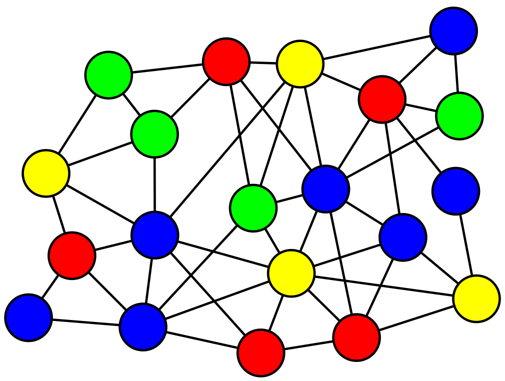
GA

Generation 1: selection

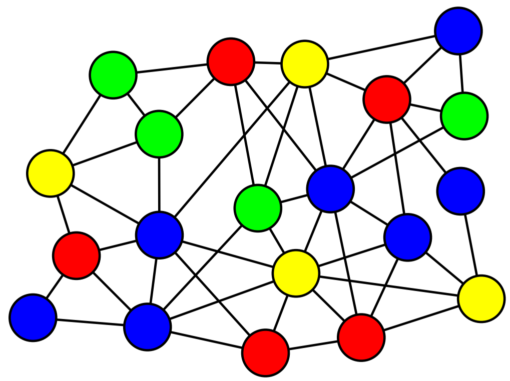


GA

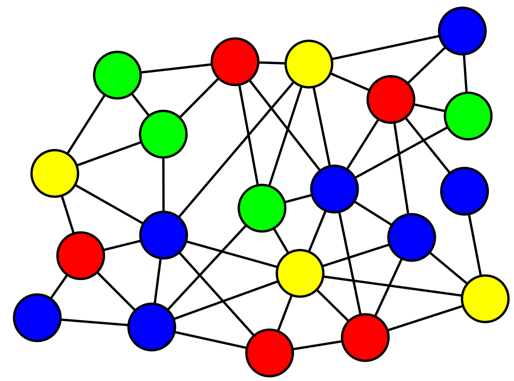
Generation 1: selection



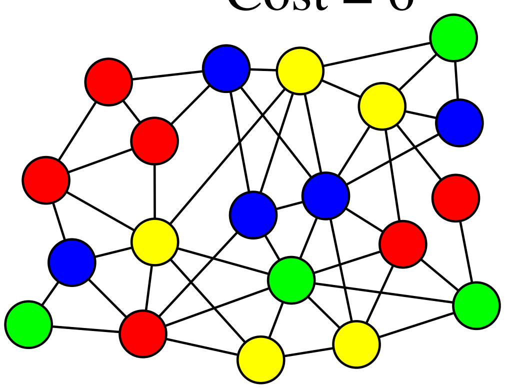
Cost = 6



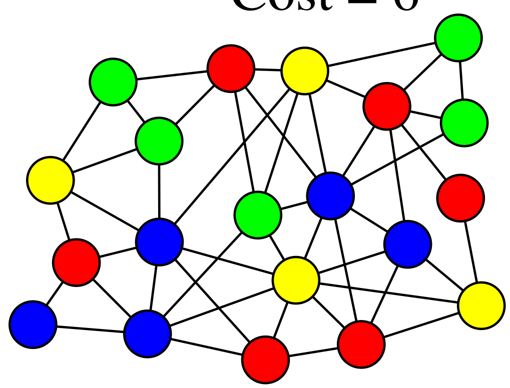
Cost = 6



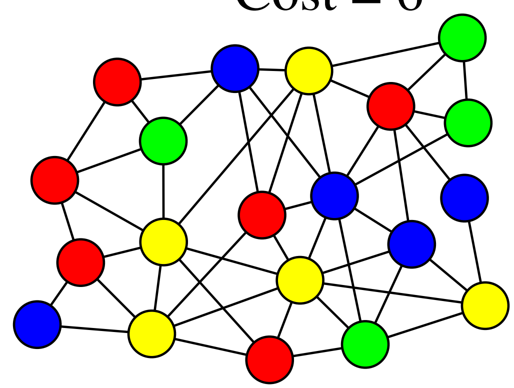
Cost = 6



Cost = 12



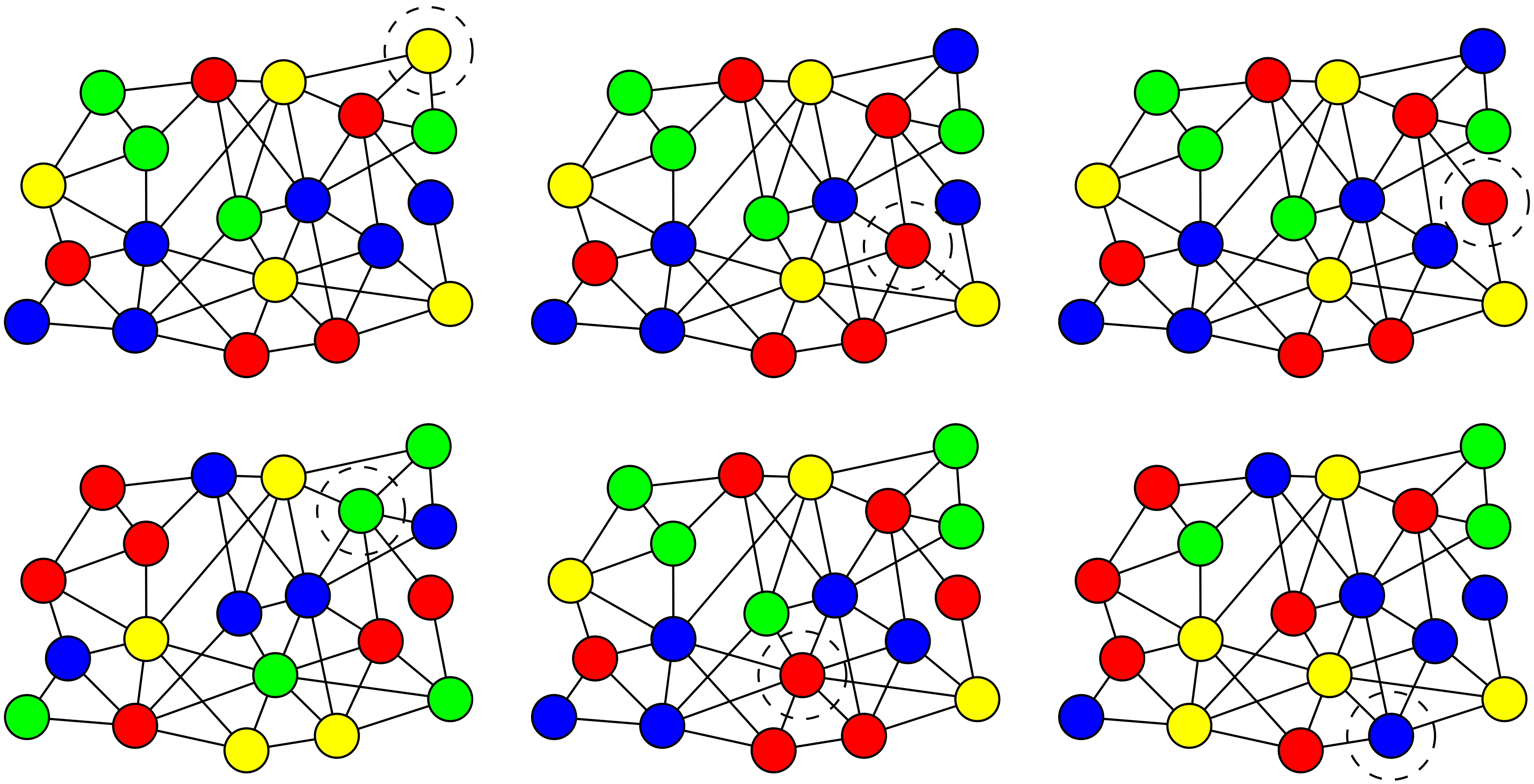
Cost = 8



Cost = 10

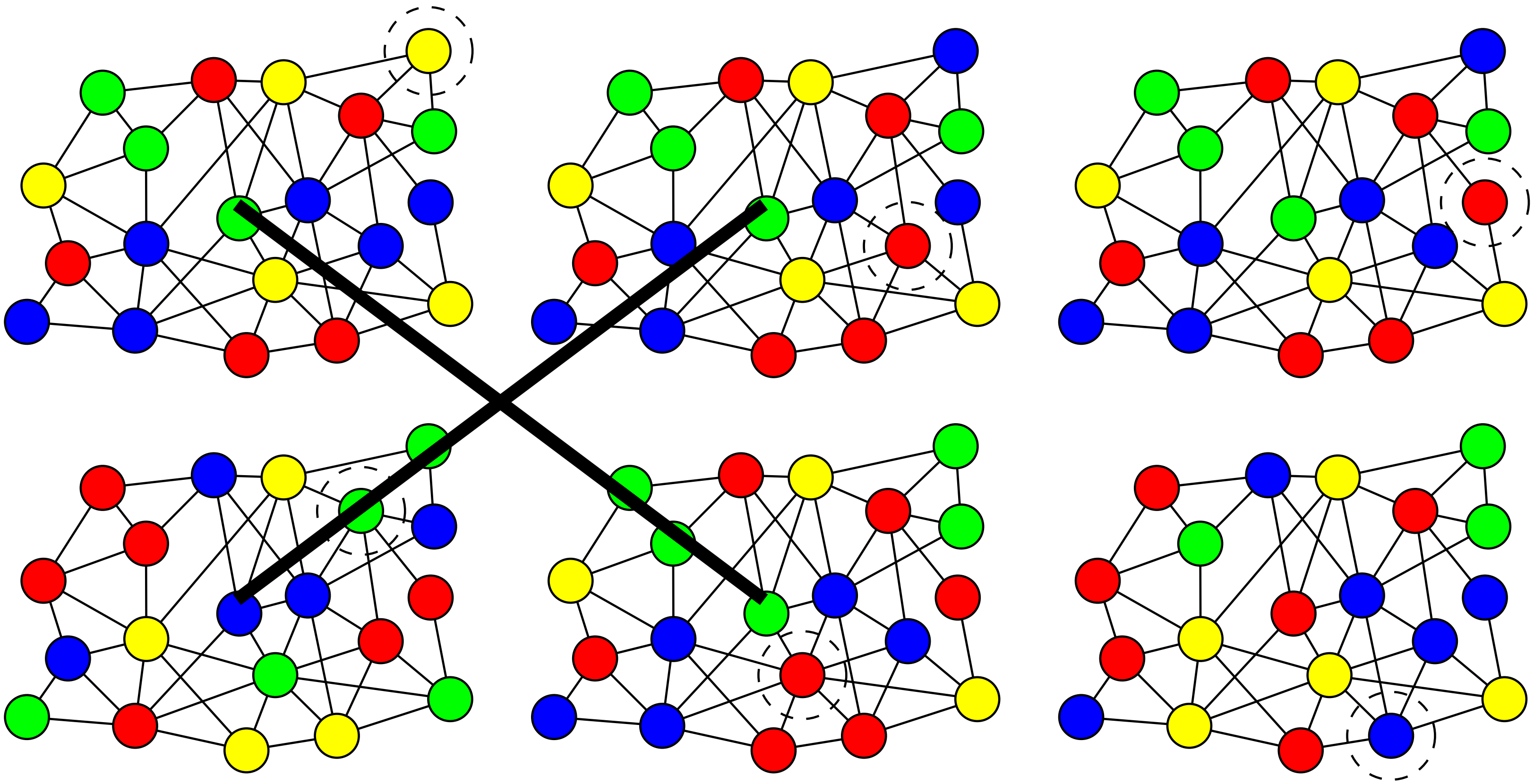
GA

Generation 1: mutation



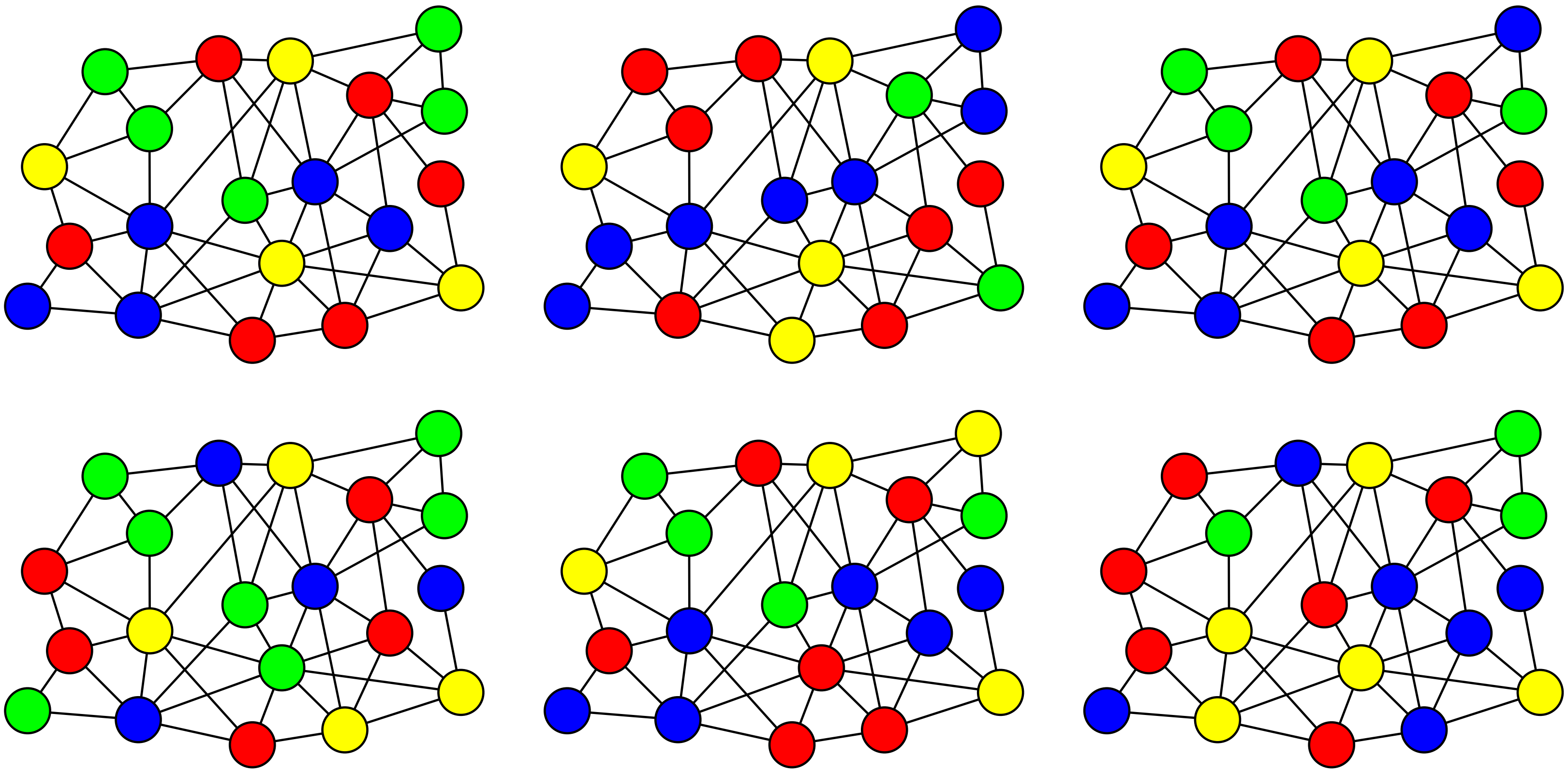
GA

Generation 1: crossover



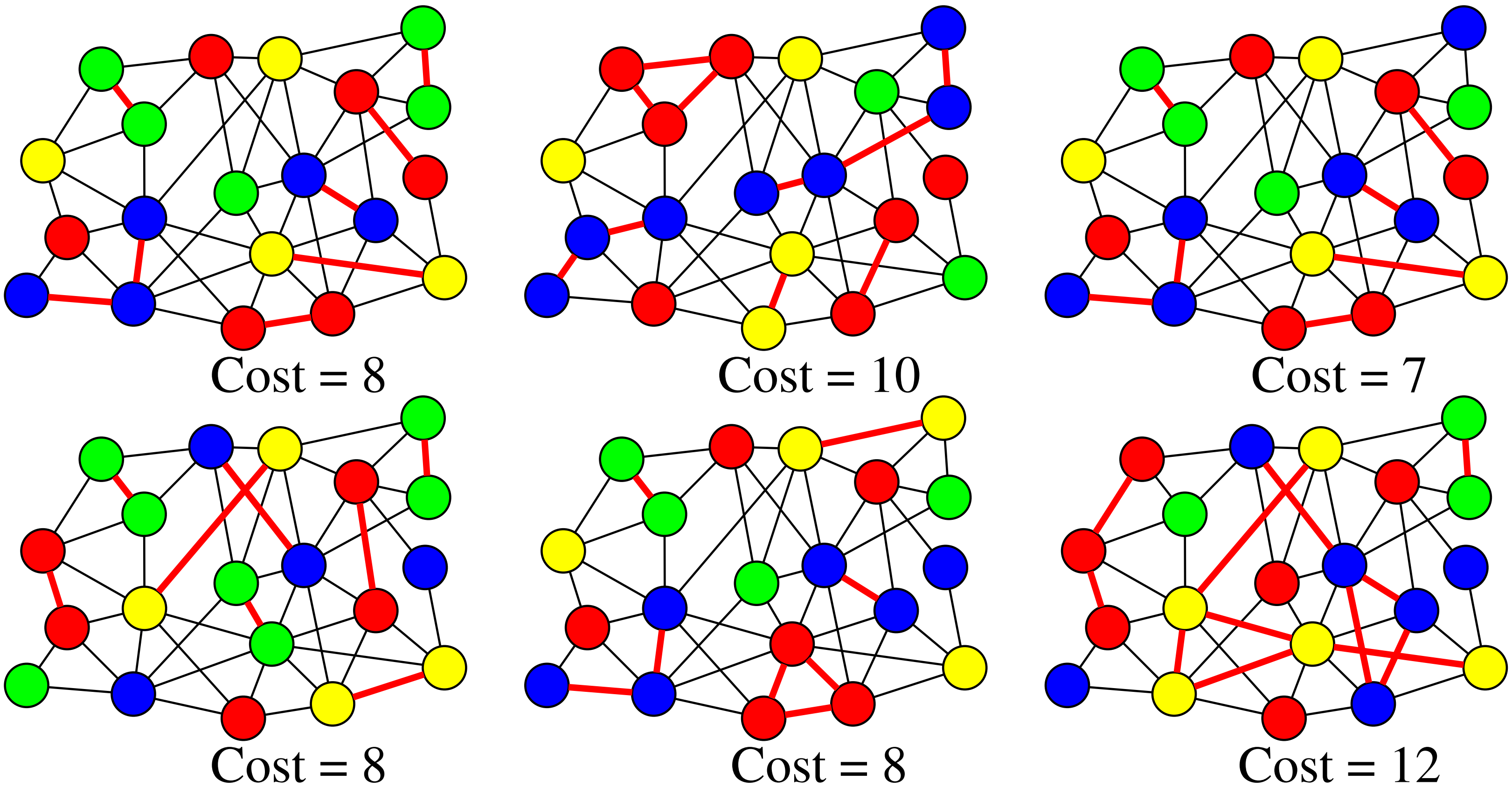
GA

Generation 1: 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

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

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(\cdots, R, \cdots) & (\cdots, B, \cdots) & (\cdots, G, \cdots) \\
(\cdots, B, \cdots) & (\cdots, G, \cdots) & (\cdots, B, \cdots) \\
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Galinier and Hao's Crossover Operator

- Choose two parents
- Sort nodes into colour-groups

	Parent 1	Parent 2
B	$\{1,3,4,8,\ldots\}$	$\{3,5,7,10,\ \ldots\}$
G	$\{2,6,7,10,\ldots\}$	$\{1,11,12,13,\ \ldots\}$
R	$\{5,9,11,12,\ldots\}$	$\{2,3,6,8,\ \ldots\}$
$\vdots$	$\vdots$	$\vdots$

- 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.

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Galinier and Hao's Crossover Operator

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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, . . . }
⋮	⋮	⋮

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$\vdots$	$\vdots$	$\vdots$

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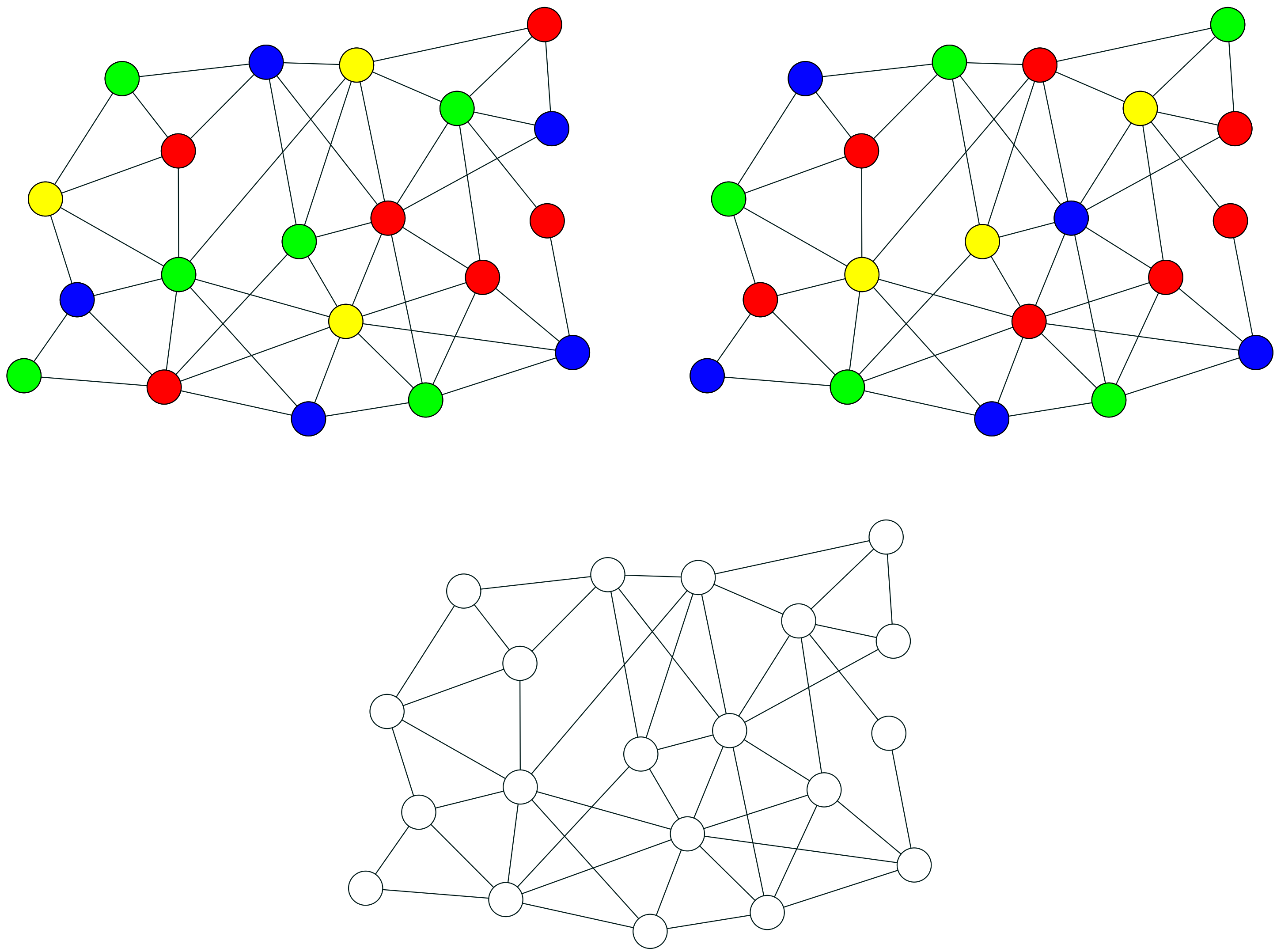
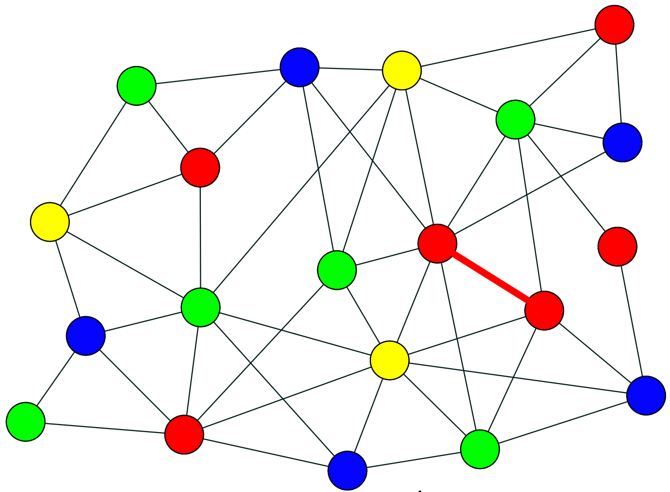
- etc.

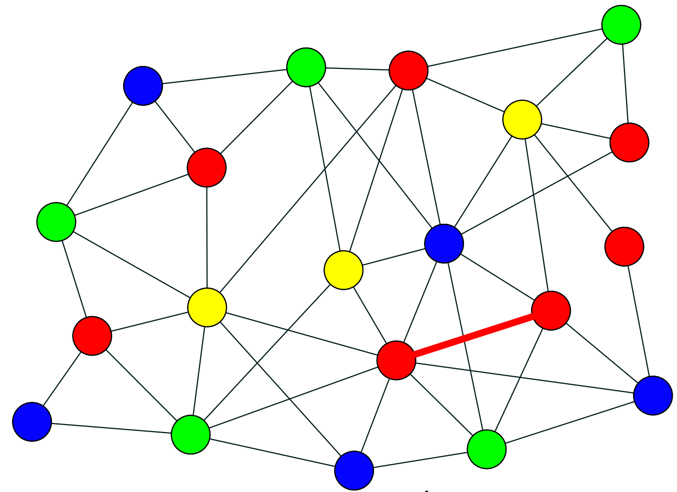
Cost of Crossover



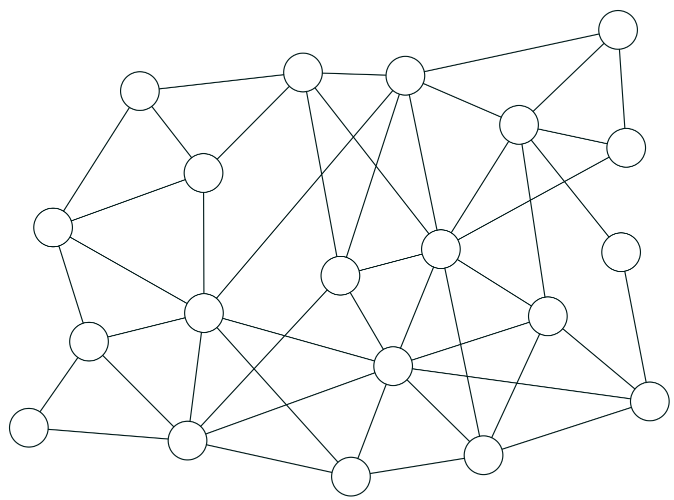
Cost of Crossover



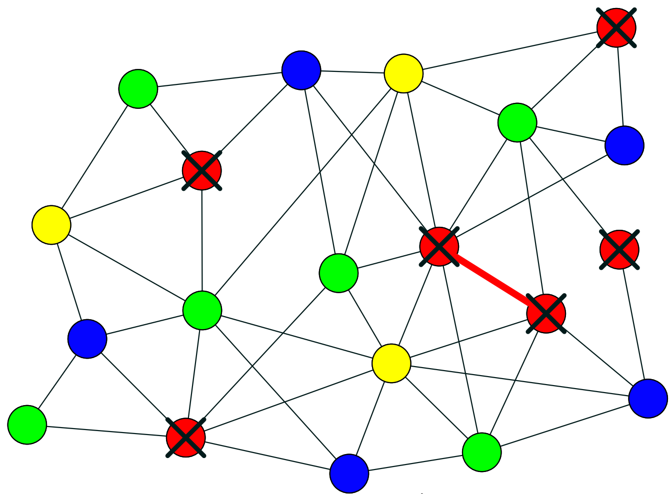
cost=1



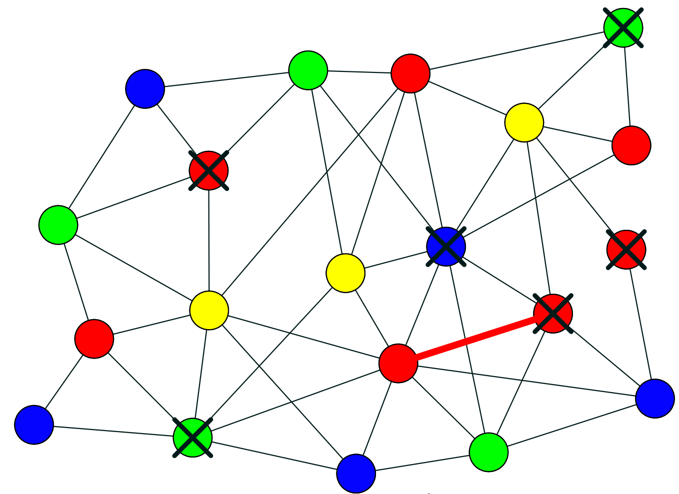
cost=1



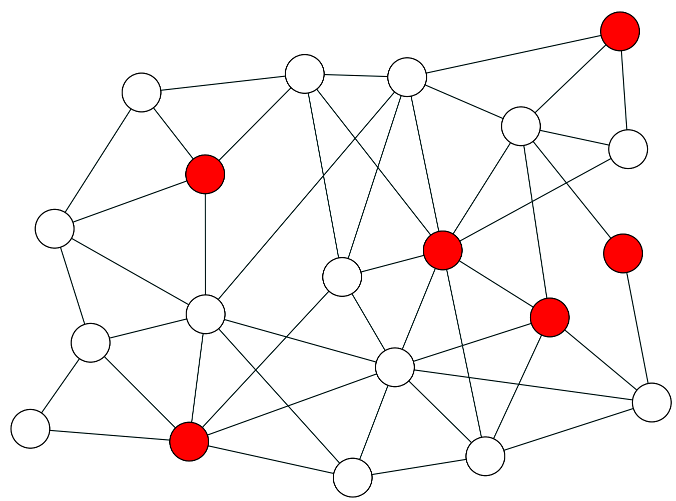
Cost of Crossover



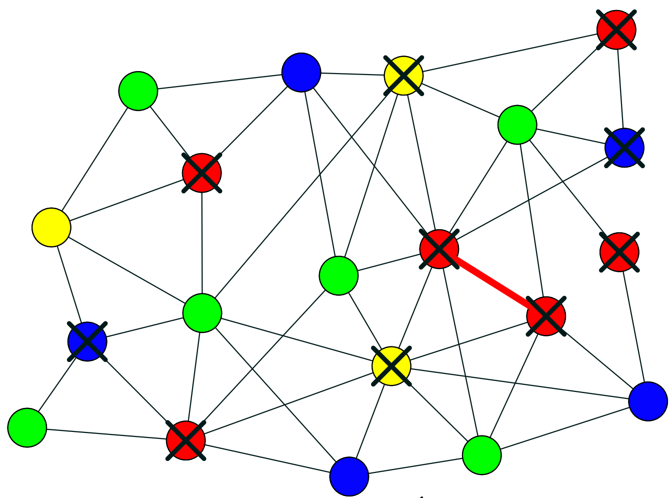
cost=1



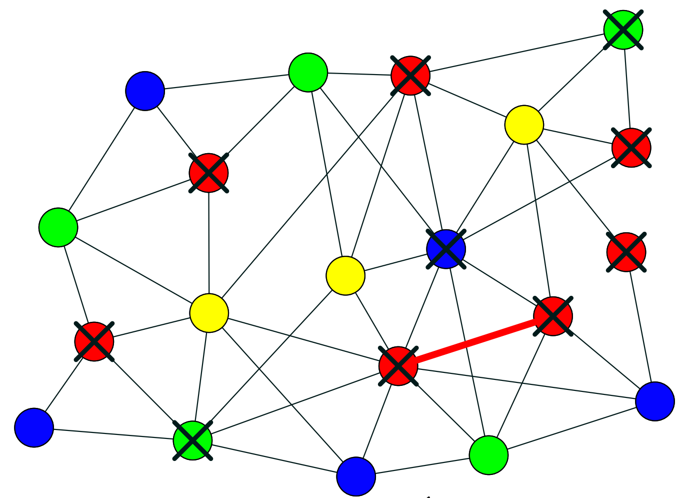
cost=1



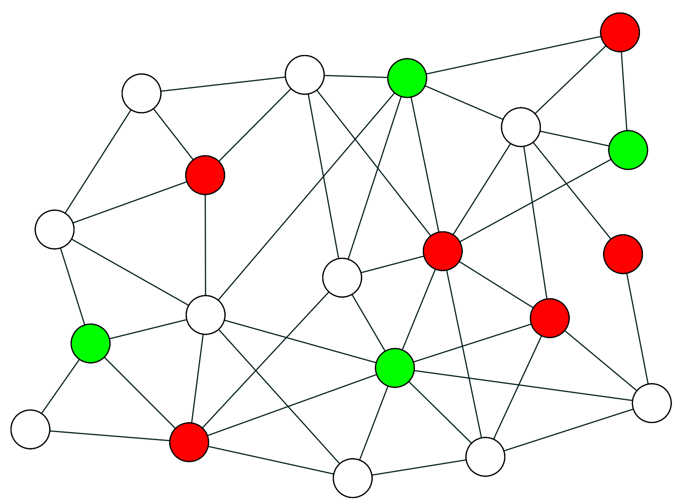
Cost of Crossover



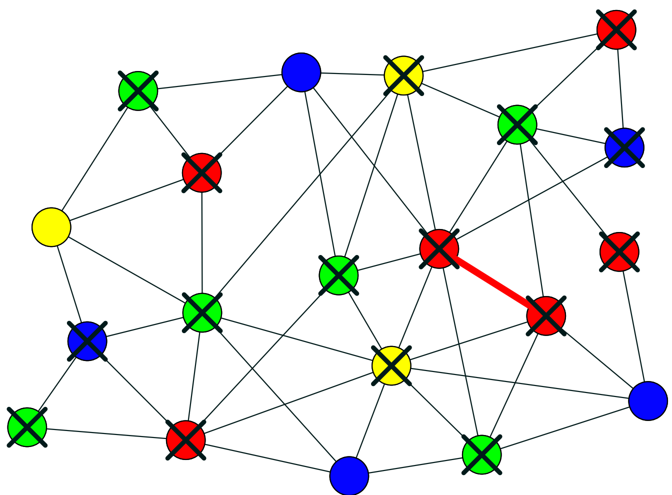
cost=1



cost=1



Cost of Crossover



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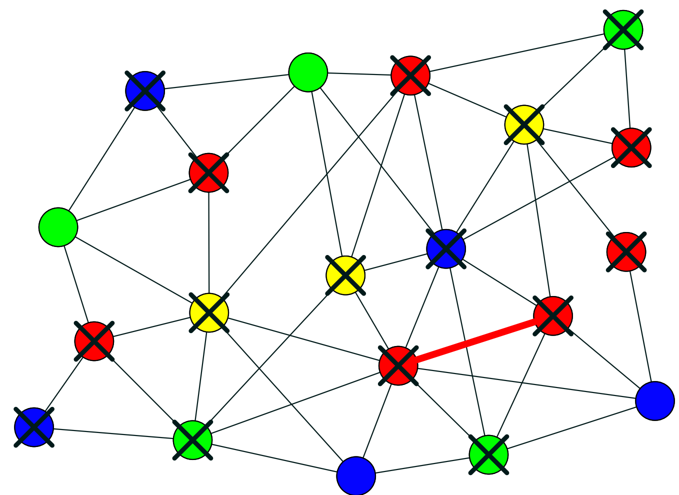

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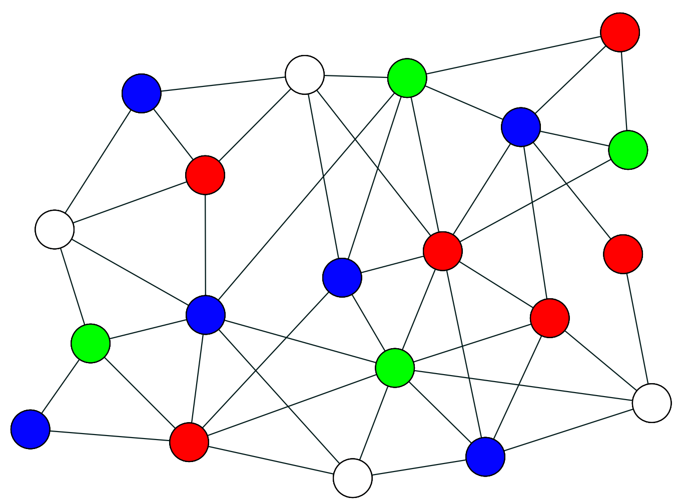

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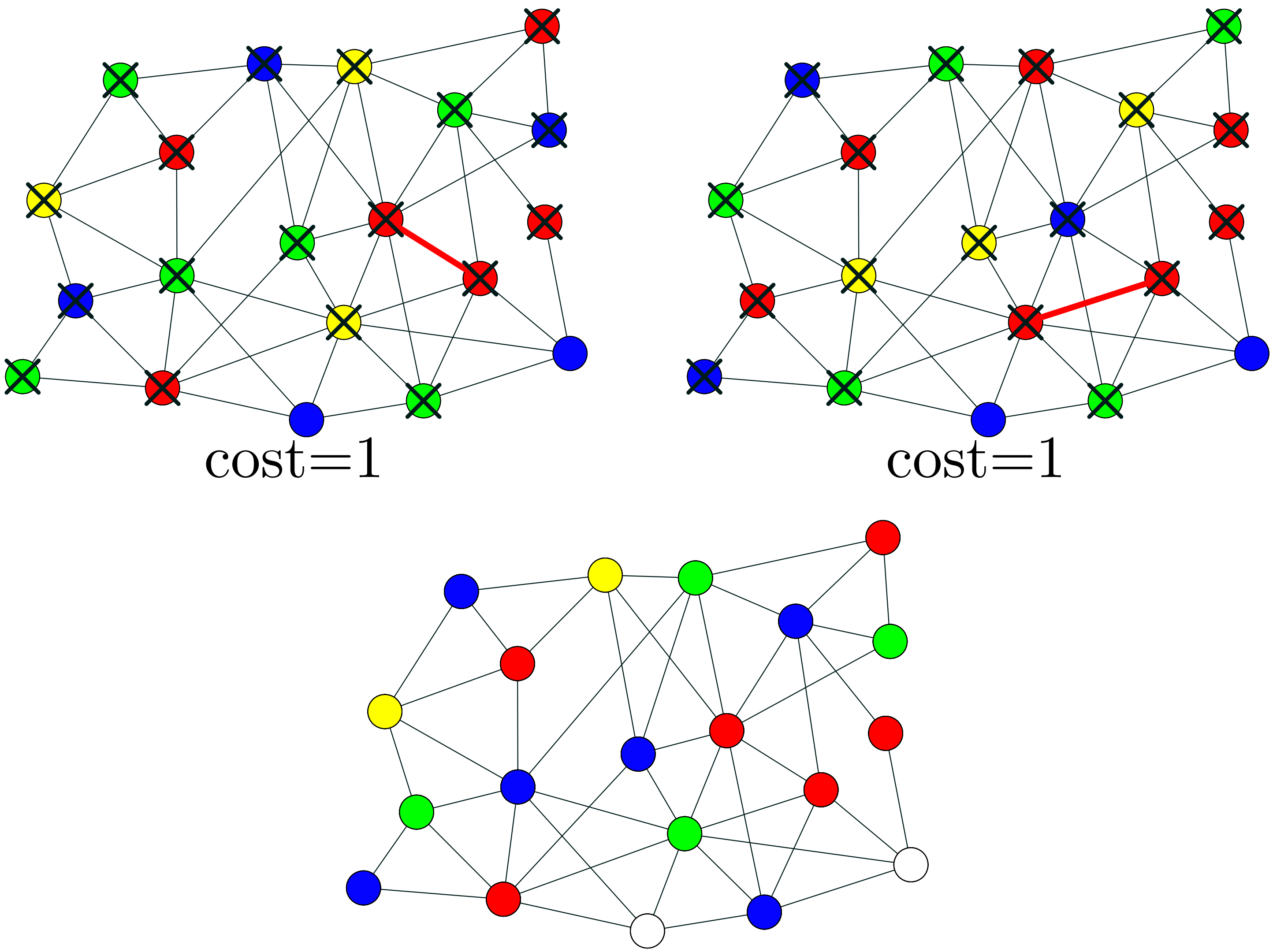

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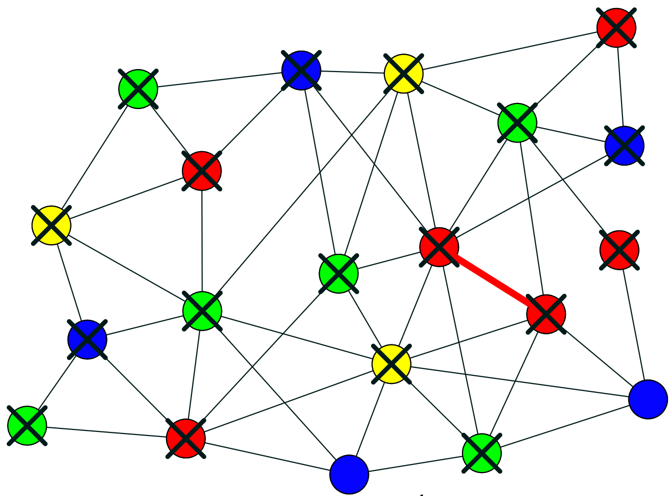

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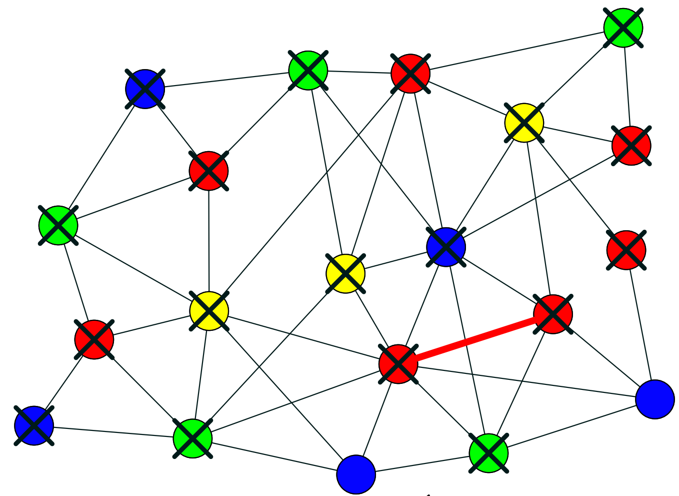

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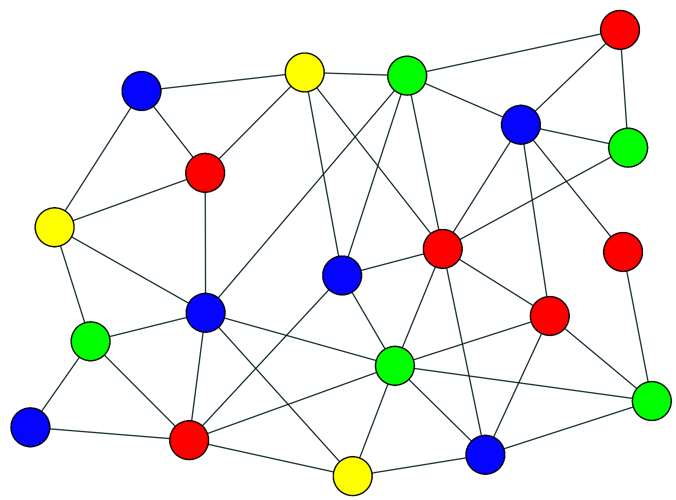

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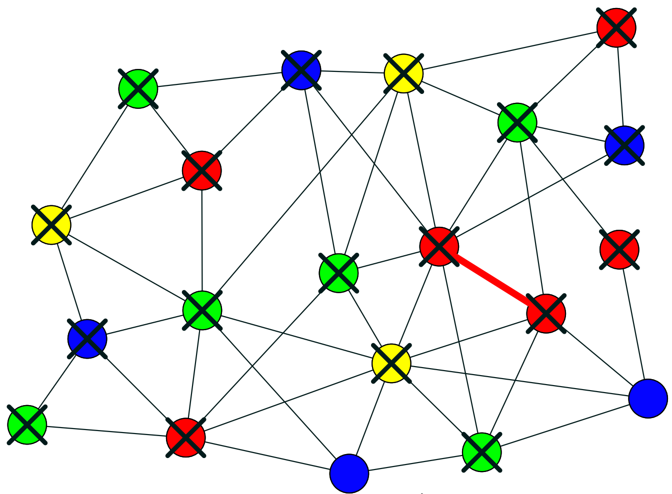

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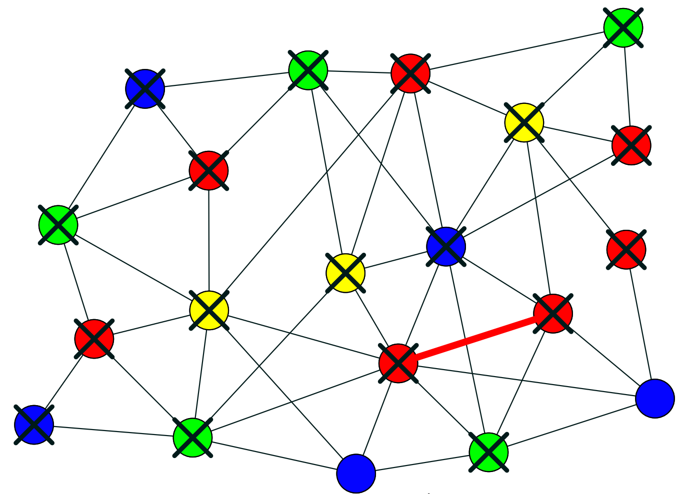

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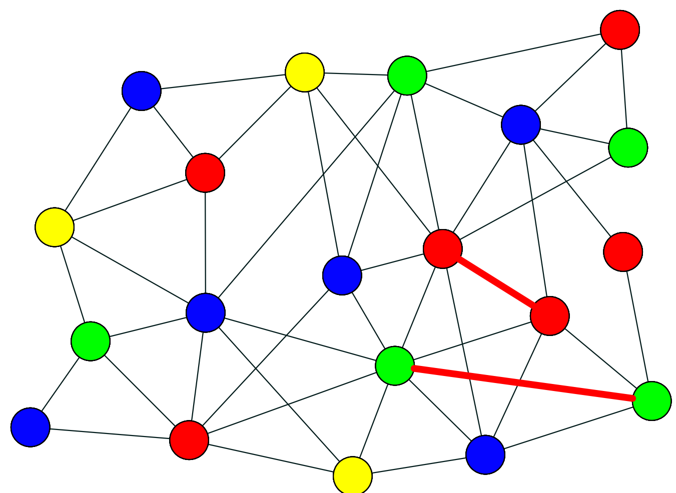

cost=2

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
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- Many other EAs including particle swarm optimisations (PSO), ant colony optimisation (ACO), evolutionary strategies, . . .

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- The best heuristic depends on the application
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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
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