Local and Global Search

Parts adapted from:

- Chapter 4 of AI 2E by David Poole and Alan Macworth;
- AI a modern approach by Stuart Russel and Peter Norvig

Optimisation problems

Optimisation problem: given

- a set of variables and their domains; and
- an objective function (aka cost function),

find an assignment (of a value to each variables) that optimises (maximise or minimises) the value of the objective function.

- Optimisation usually involves searching.
- CSPs and Optimisation Problems can be converted (reduced) to each other.
- There are special algorithms for certain kind of optimisation problems (e.g. linear programming, convex optimisation).
- In this lecture we look at two families of algorithms (local and global) for general optimisation problems.

Note: there is also a *constrained optimisation problem*, where the goal is to find an assignment that satisfies a given set of constraints and maximises/minimises a given objective function.

Local search for optimisation

- A ***local search*** algorithm is an iterative algorithm that keeps a single current state, and in each iteration tries to improve it by moving to one of its neighbouring states.

- Two key aspects to decide:

  - Neighbourhood: which states are the neighbours of a given state

  - Movement: which neighbouring state should the algorithm go to

- Asearch algorithm is considered to be greedy if it always moves to the best neighbour. Two variants happen to have special names:

  - *hill climbing* (or greedy ascent) for maximisation

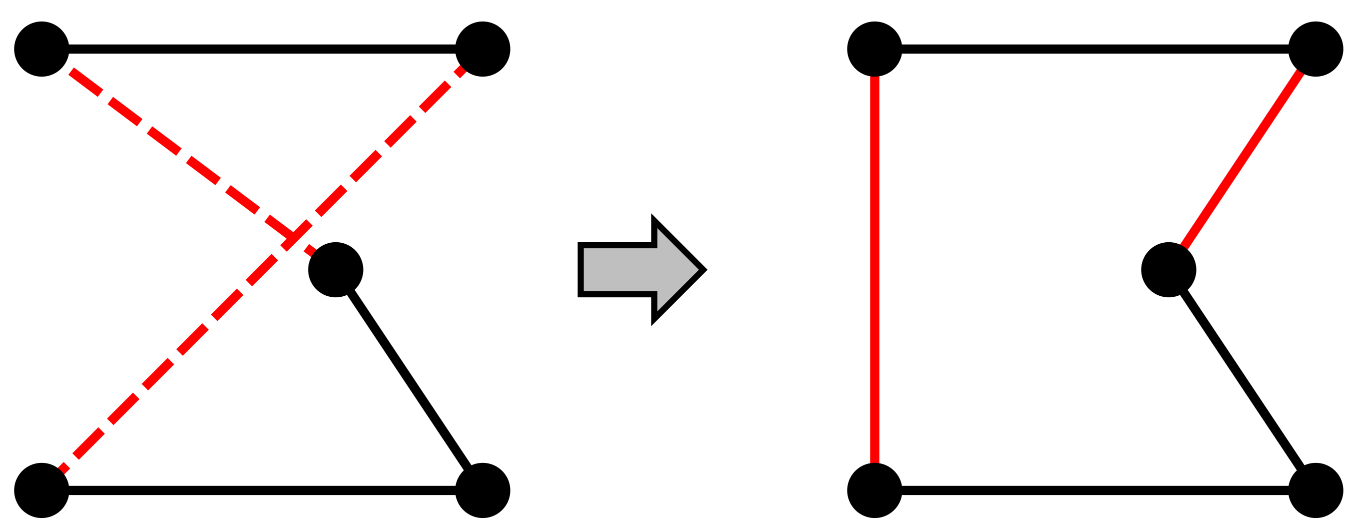
  - *greedy descent* for minimisation.

Example: Local Search for TSP

- Traveling Salesperson Problem (TSP): Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

- Start with any complete tour, in each iteration perform pairwise exchanges if it improves the total cost.

- Variants of this approach can get close to optimal solution quickly (even with a large number of cities).



Local search for CSPs

- A constrained satisfaction problem (CSP) can be reduced to an optimisation problem.
- Given an assignment, a **conflict** is an unsatisfied constraint.
- The goal is to find an assignment that does not produce any conflict (i.e. all the constraints are satisfied).
- Heuristic (or cost or objective) function: the number of conflicts produced by an assignment.
- Optimisation problem: find an assignment that minimises this heuristic function.

Local Search for CSP: Neighbourhood

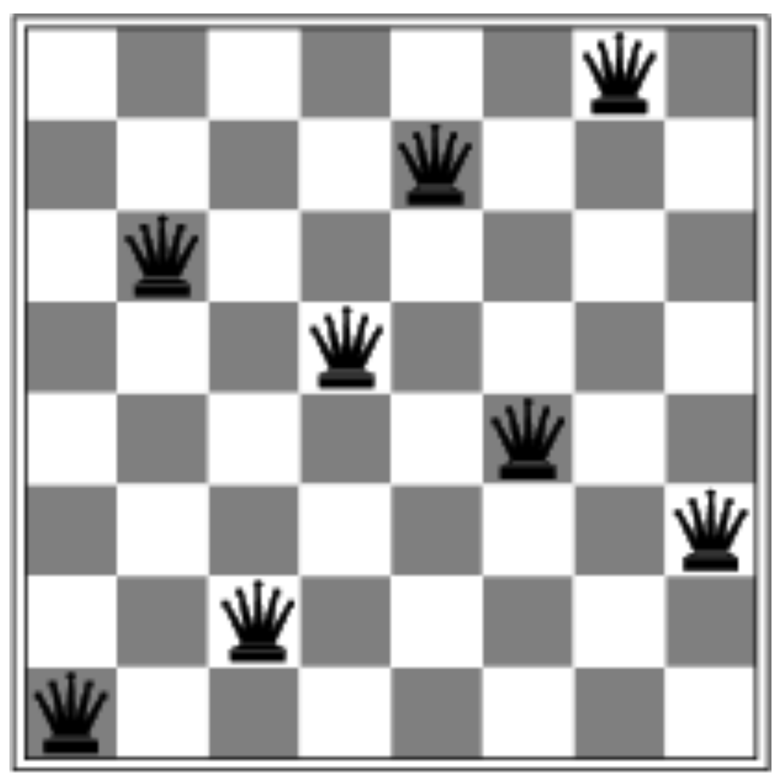
Neighbours of a given state (assignment) can be defined in many ways. Examples:

- All possible assignments except the current one (poor definition - why?)
- Select a variable that appears in any conflict. Neighbours are assignments in which that variable takes a different value from its domain.
- Select a variable in the current assignment that participates in the most number of conflicts. Neighbours are assignments in which that variable takes a different value from its domain.

Example: local search for *n*-queens problem

- Aim: Put n queens on an $n \times n$ board with no two queens attacking each other.

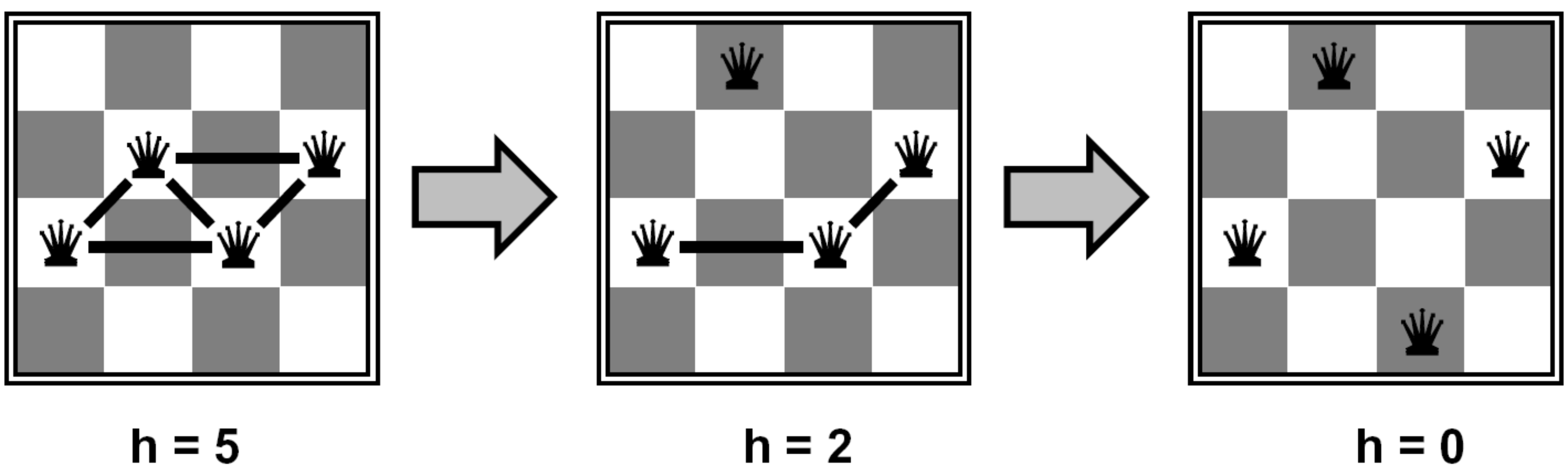
- The objective (heuristic) function to minimise: number of conflicts.



$h = 1$

Example: 4-Queens

- States: 4 queens in 4 columns ($4^4 = 256$ states)
- Obtaining neighbours: move each queen in its own column
- Objective function to minimise: h(board) = number of pairs of queens that are attacking each other (number of conflicts)



Example: neighbours

- Objective function (conflict count): number of pairs of queens that are attacking each other.

- Number of conflicts in the current state: 17

Local Search Issues

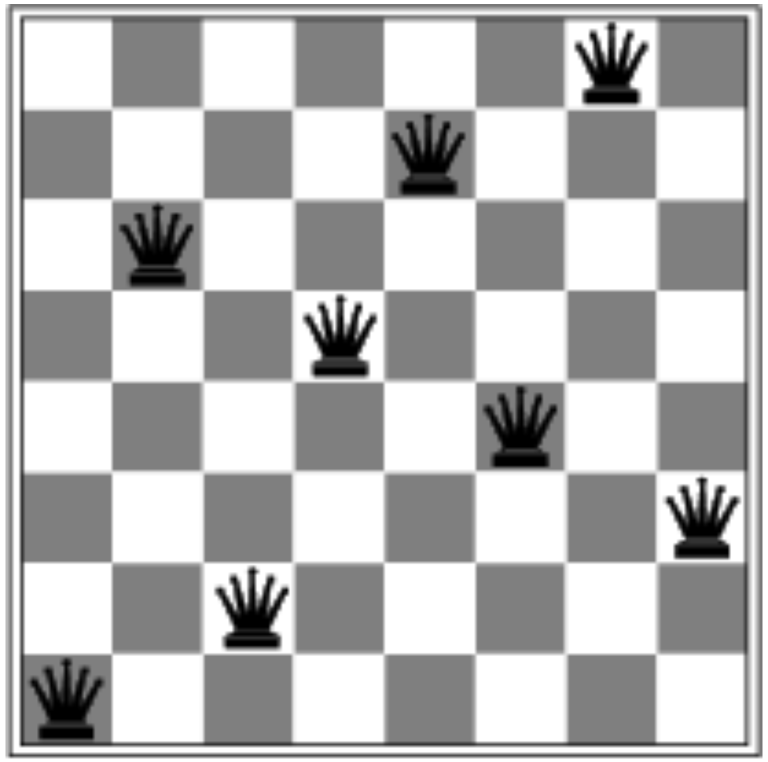
- Local search can get stuck in local optima or flat ares of the landscape of the objective function.

- Randomised greedy descent can help sometimes:

    - **random step**: move to a random neighbour.

    - **random restart**: reassign random values to all variables.

    - these make the search ***global***.



a local minimum with a conflict count of 1.

Parallel search

- A total assignment is called an **individual**.
- Idea: maintain a population of *k* individuals instead of one.
- At every stage, update each individual in the population. Whenever an individual is a solution, it can be reported.
- Like *k* restarts, but uses *k* times the minimum number of steps.
- A basic form of global search.

Simulated Annealing

- Pick a variable at random and a new value at random.
- If it is an improvement, adopt it.
- If it isn't an improvement, adopt it probabilistically depending on a temperature parameter, T.
  - With current assignment n and proposed assignment n' we move to n' with probability $e^{(h(n)-h(n'))/T}$
- Temperature can be reduced.

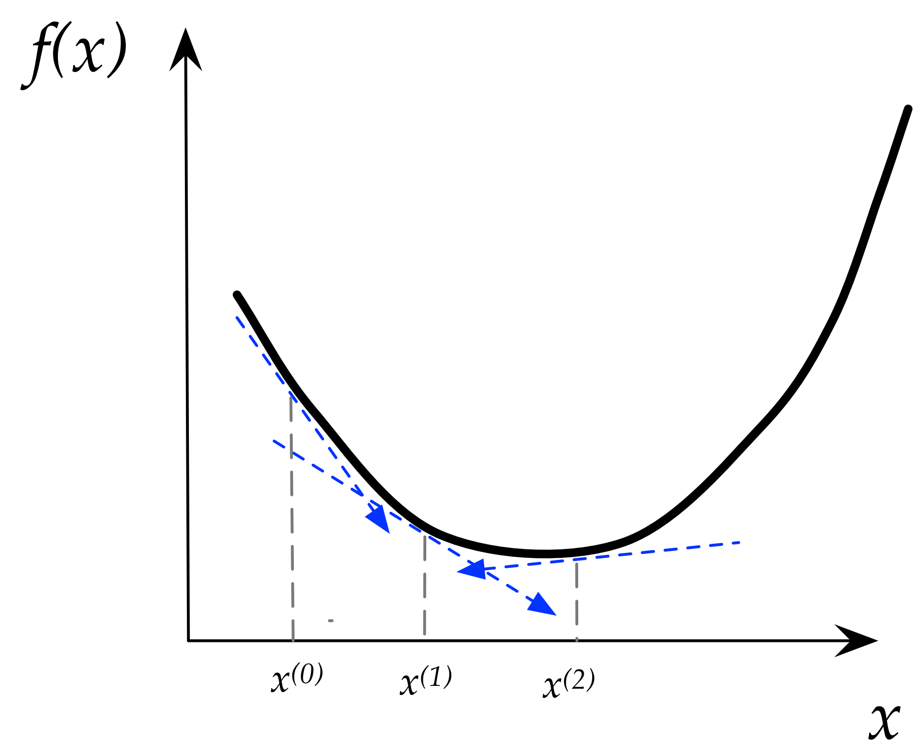
Probability of accepting a change:

Temperature	1-worse	2-worse	3-worse
10	0.91	0.81	0.74
1	0.37	0.14	0.05
0.25	0.02	0.0003	0.000005
0.1	0.00005	0	0

Gradient Descent

- A widely-used local search algorithm in numeric optimisation (e.g. in machine learning)
- Used when the variables are numeric and continuous.
- The objective function must be differentiable (mostly).

Guess $\mathbf{x}^{(0)}$, set $k \leftarrow 0$
while $||\nabla f(\mathbf{x}^{(k)})|| \geq \epsilon$ **do**
$\quad \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - t_k \nabla f(\mathbf{x}^{(k)})$
$\quad k \leftarrow k + 1$
end while
return $\mathbf{x}^{(k)}$



Evolutionary Algorithms

References:

A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing, Springer

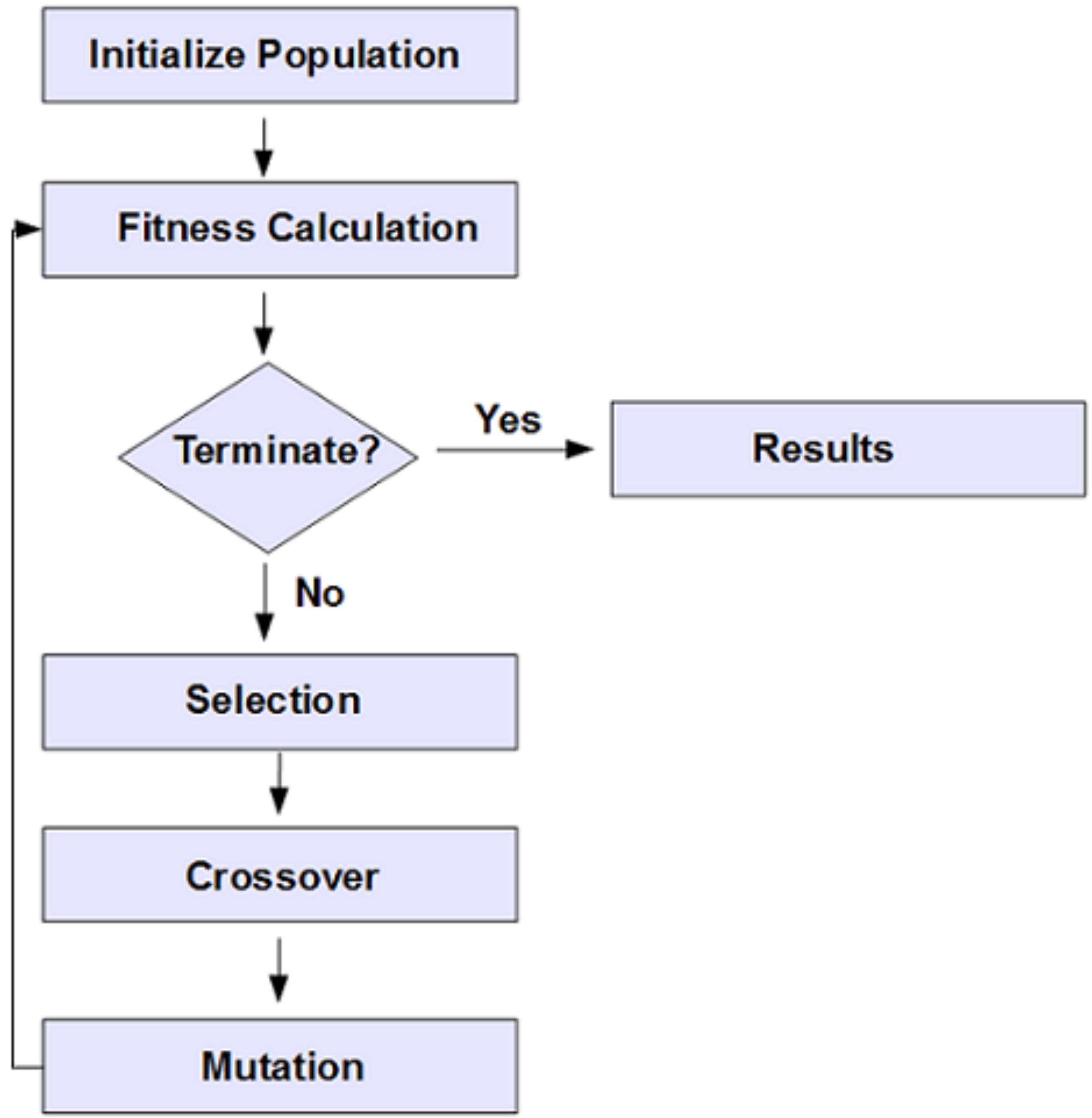
K. A. De Jong, Evolutionary Computation, MIT Press

J. C. Spall
Introduction to Stochastic Search and Optimization, John Wiley and Sons

Genetic (Evolutionary) Algorithms

- Genetic Algorithms (GAs) and the whole family of Evolutionary Algorithms (EAs) are inspired by natural selection.
- They are in the global search family.
- The algorithm maintains a population of *individuals* (aka chromosomes) which evolves over time.
- We can make an individual to represent anything we want (e.g. for CSP it would be an assignment or list of values)
- A *fitness function* is needed. The function takes an individual as input and returns a numeric value indicating how good/bad the individual is.
- A mechanism is needed to create an initial population (usually randomly)
- A mechanism is needed to "evolve" the current generation (population) to the next one. This involves the following mechanisms (also called operators or functions):
  - selection (decide which individuals survive or can reproduce/breed)
  - crossover (given a number of parent individuals, create a number of children)
  - mutation (make some random changes to individuals)

GA: Flowchart



Evaluation: Fitness Function

Purpose:

- Parent selection
- Measure for convergence
- For Steady state: Selection of individuals to die
- Should reflect the value of the chromosome (individual)
- It is a critical part of any EA / GA

Selection

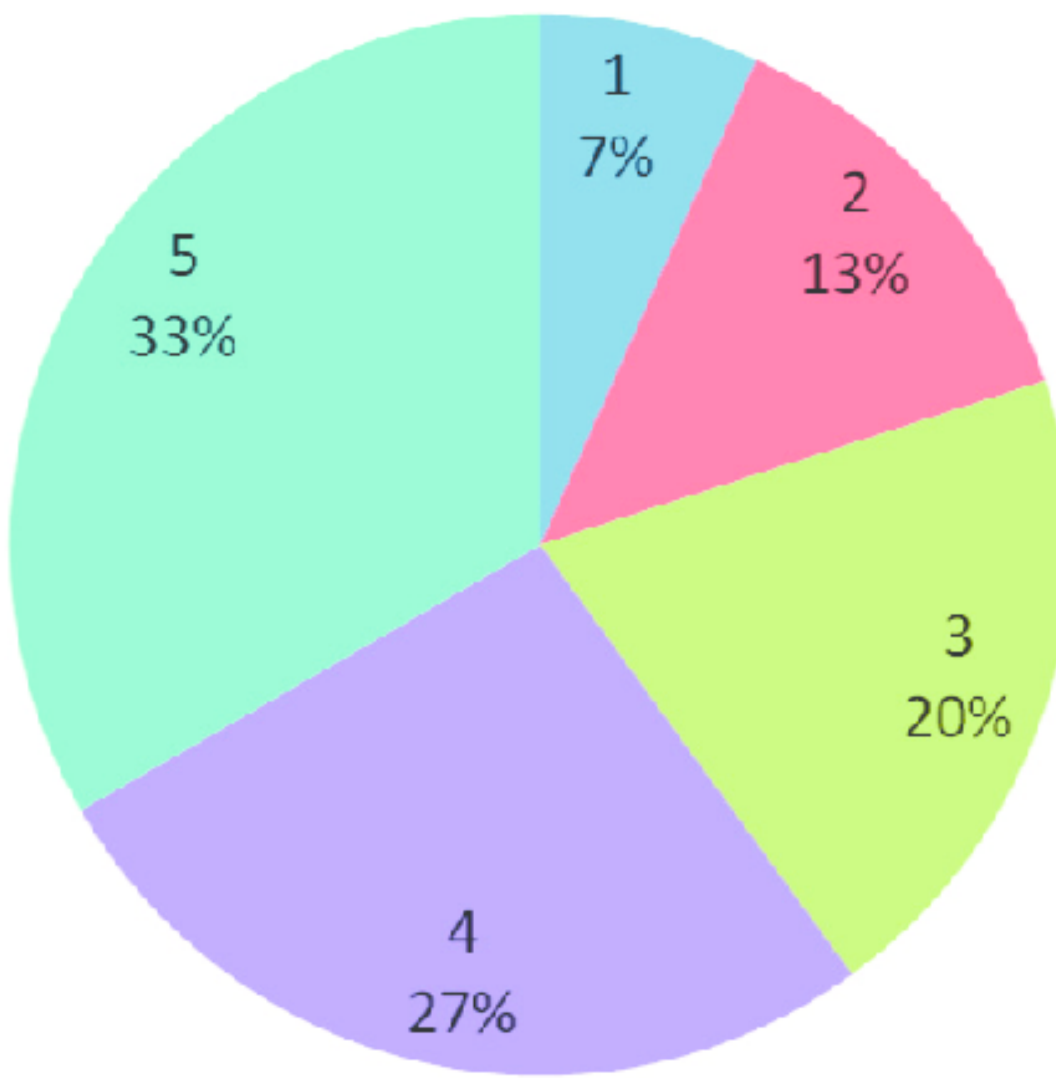
Main idea: better individuals should have higher chance of surviving and breeding.

Types:

- Roulette wheel selection
- Tournament selection
- … any mechanism that somehow overall achieves the main idea.

Roulette Wheel Selection

- Chances proportional to fitness
- Assign to each individual a part of the roulette wheel
- Spin the wheel *n* times to select *n* individuals



Individual	Fitness
1	1.0
2	2.0
3	3.0
4	4.0
5	5.0

Roulette Wheel Selection: Example

- Sum the fitness of all individuals, call it T
- Generate a random number N between 1 and T
- Return individual whose fitness added to the running total is equal to or larger than N
- Chance to be selected is exactly proportional to fitness
- Individual: 1, 2, 3, 4, 5, 6
- Fitness: 8, 2, 17, 7, 4, 11
- Running total: 8, 10, 27, 34, 38, 49
- N: 23
- Selected: 3

Selection: Tournaments

- *n* individuals are randomly chosen; the fittest one is selected as a parent.
- *n* is the “size” of the tournament.
- By changing the size, selection pressure can be adjusted.

Elitism

- Always keep at least one copy of the fittest individual so far

- Results in non-decreasing fitness (of the best individual in the population) over generations

- Widely used in population models

Reproduction Operators

Selected individuals will be, with different proportions:

- copied to the next generation (unchanged);

- combined with each other (with crossover) to generate child individuals (offsprings) for the next generation; or

- mutated for the next generation.

Crossover

- Some portion of the next generation is created by combining selected parents and creating offsprings.
- Usually two parents produce two offspring.
- Typically the probability of crossover (proportion of the next population created by crossover) is between 0.6 and 1.0

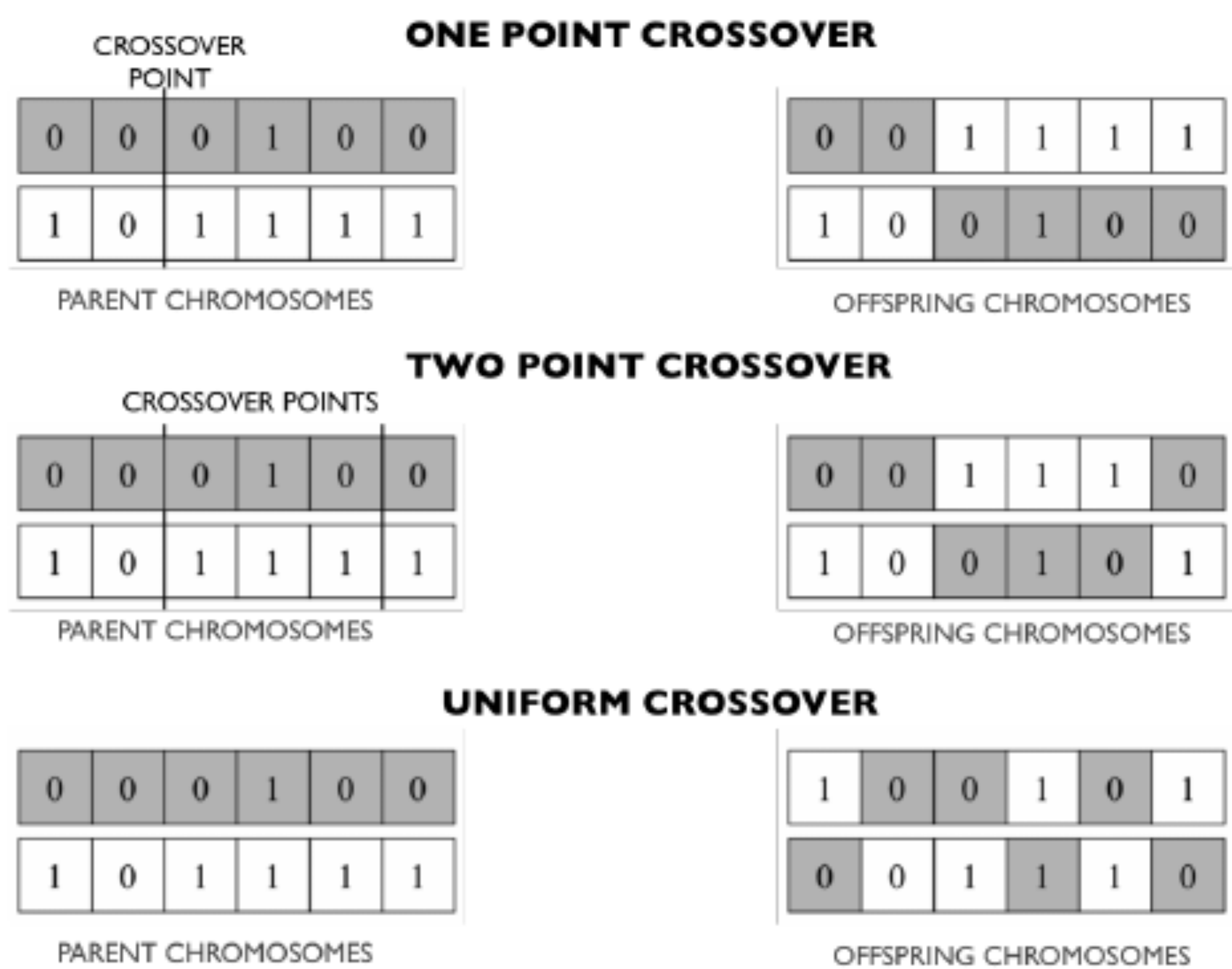
Mutation

- Some portion of the next generation is created by mutation.
- In mutation a few “genes“ of an individual is changed randomly (e.g. for CSP the value of a variable changes to another random value in its domain)
- Usually the probability of mutation is low - typically less than 5%

Crossover

Often individuals are represented as a sequence (tuple) of values (e.g. zeros and ones). With this representation, cross over can be performed very easily:

- Generate 1, 2, or a number of random *crossover points*.
- Split the parents at these points.
- Create offsprings by exchanging alternate segments.



Mutation

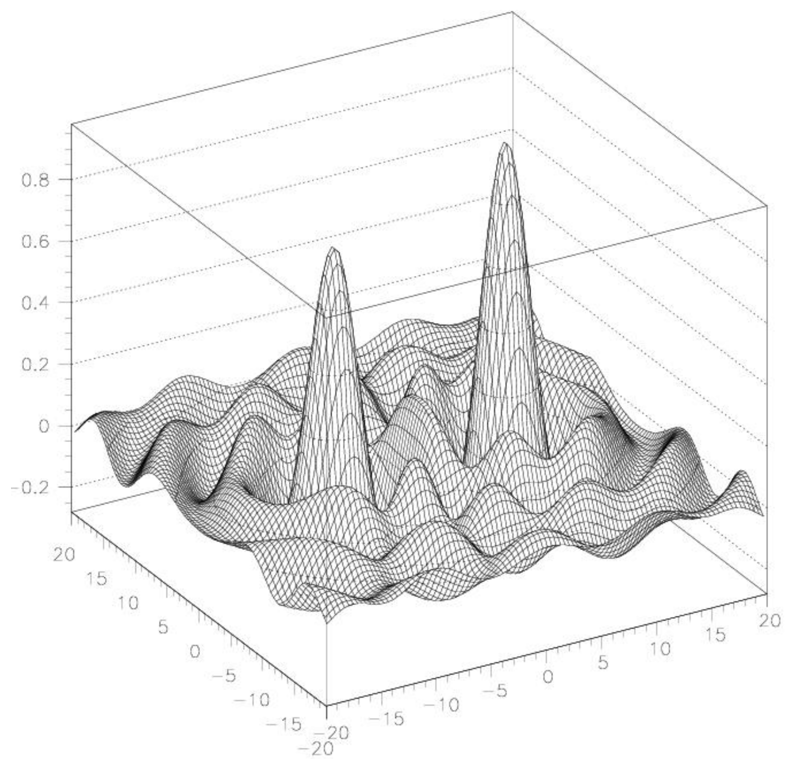
With sequential representation (e.g. tuples), mutation is performed by selecting 1 or more random locations (indices) and changing the values at those locations to some random value (from the domain).

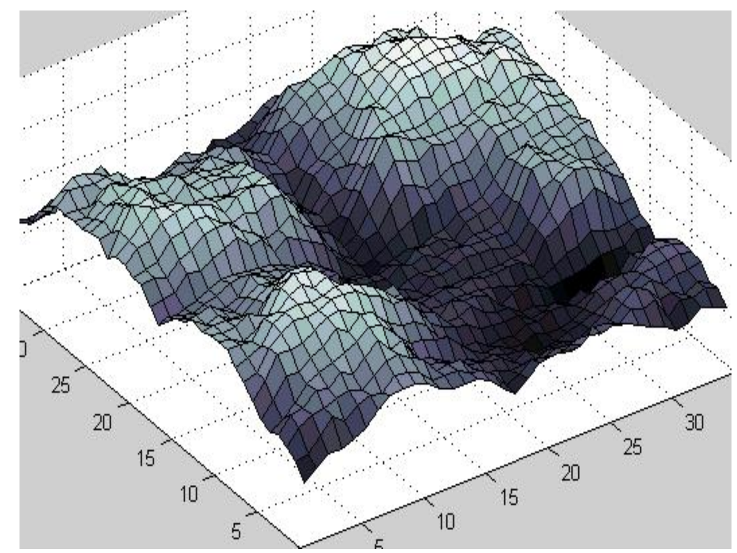
Mutation vs Crossover

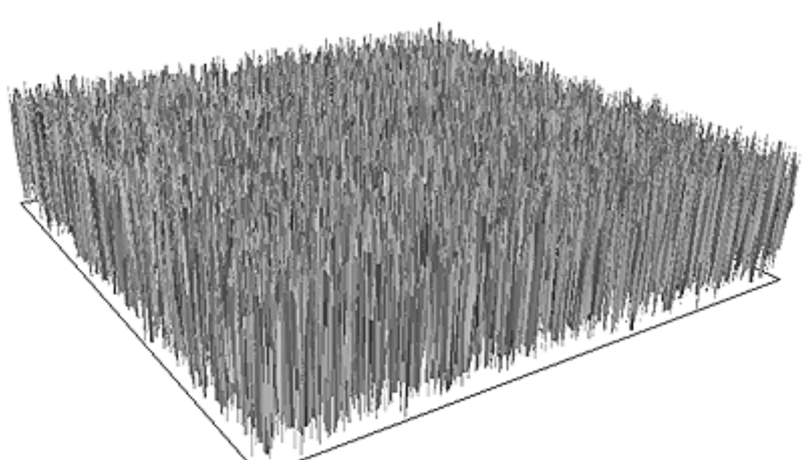
- Purpose of crossover: combining somewhat good candidates in the hope of producing better children
- Purpose of mutation: bring diversity (new “ideas”)
- It is good to have both.
- Mutation-only-EA is possible, crossover-only-EA would not work.

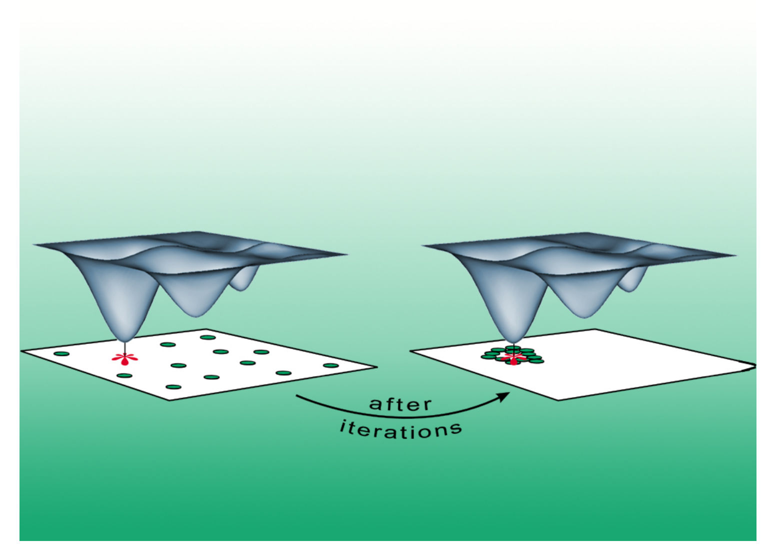
Fitness landscapes

- EAs are known to be able to handle relatively challenging fitness landscapes.
- Example fitness landscapes where the search space has two continuous variables are shown below.
    - The vertical axis is the value of the objective function.
    - Neighbours of a point are its surrounding points on the 2D plane.



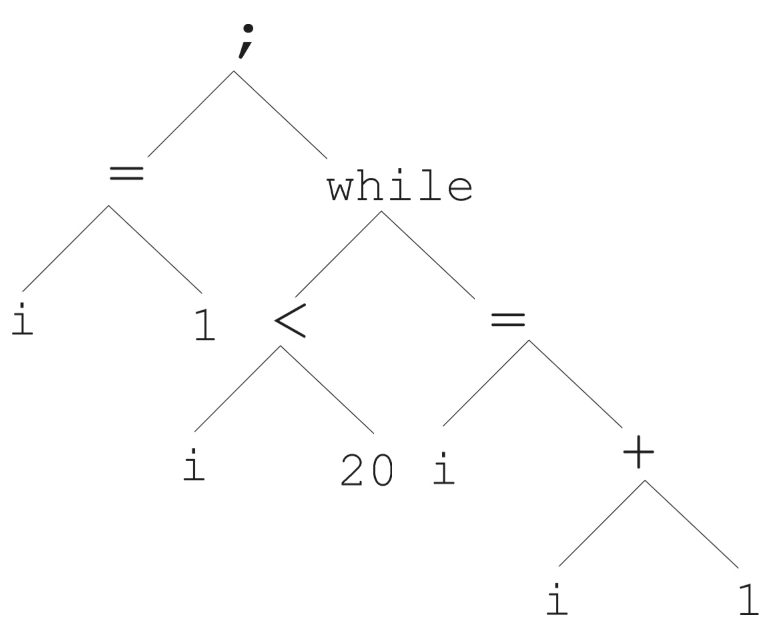




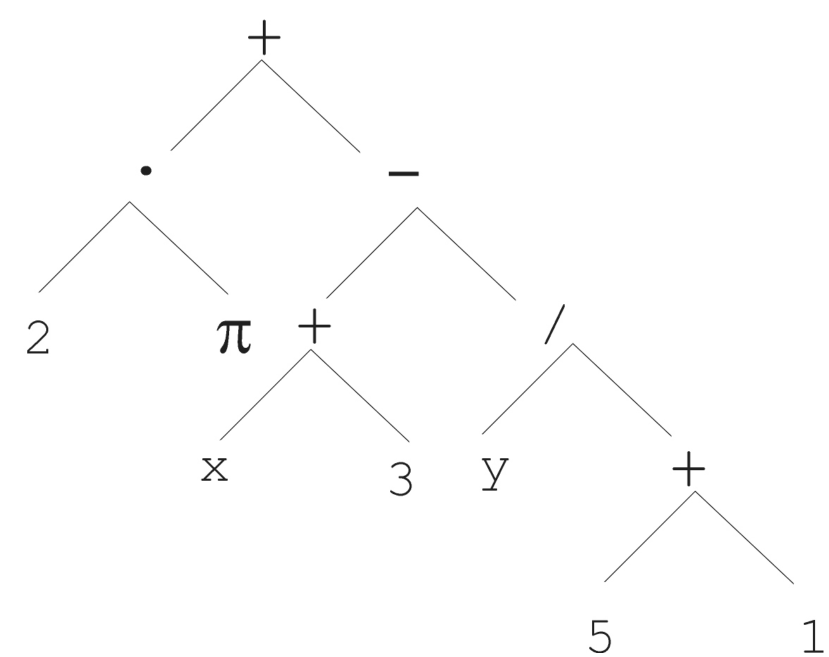


Tree representation

- Individuals can have more sophisticated structures
- For example when we need to do optimisation (search) in the space of computer programs or expressions, a tree representation can be used. Trees can be represented as nested lists.
- The following shows two example trees representing statements and expressions.



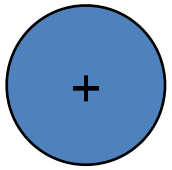

```
i =1;
while (i < 20)
{
        i = i +1
}
```



$$2 \cdot \pi + \left((x+3) - \frac{y}{5+1} \right)$$

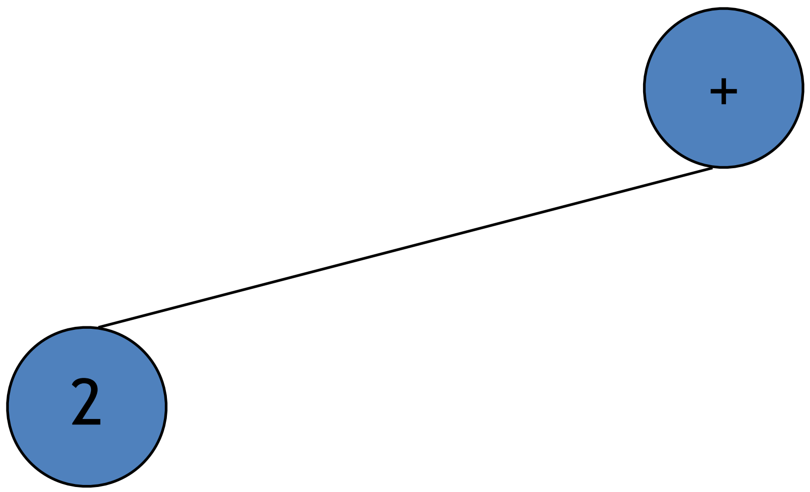
Randomly Generating Programs

(+ …)



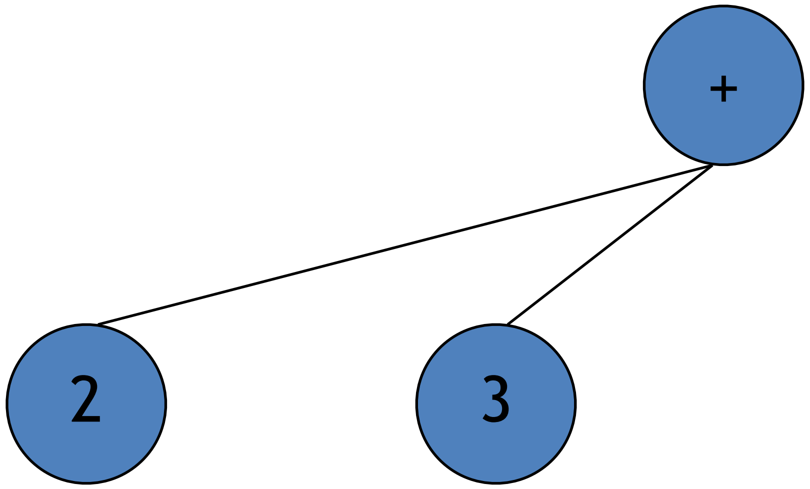
Randomly Generating Programs

(+ 2 ...)



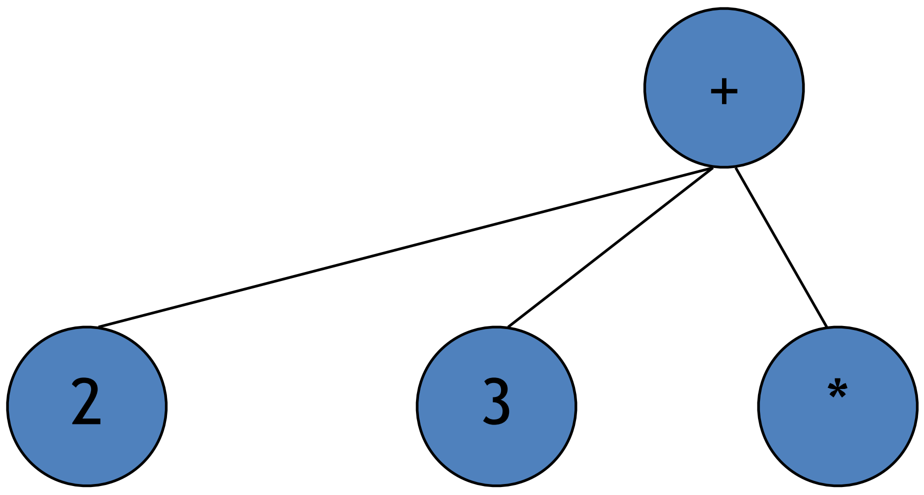
Randomly Generating Programs

(+ 2 3 …)



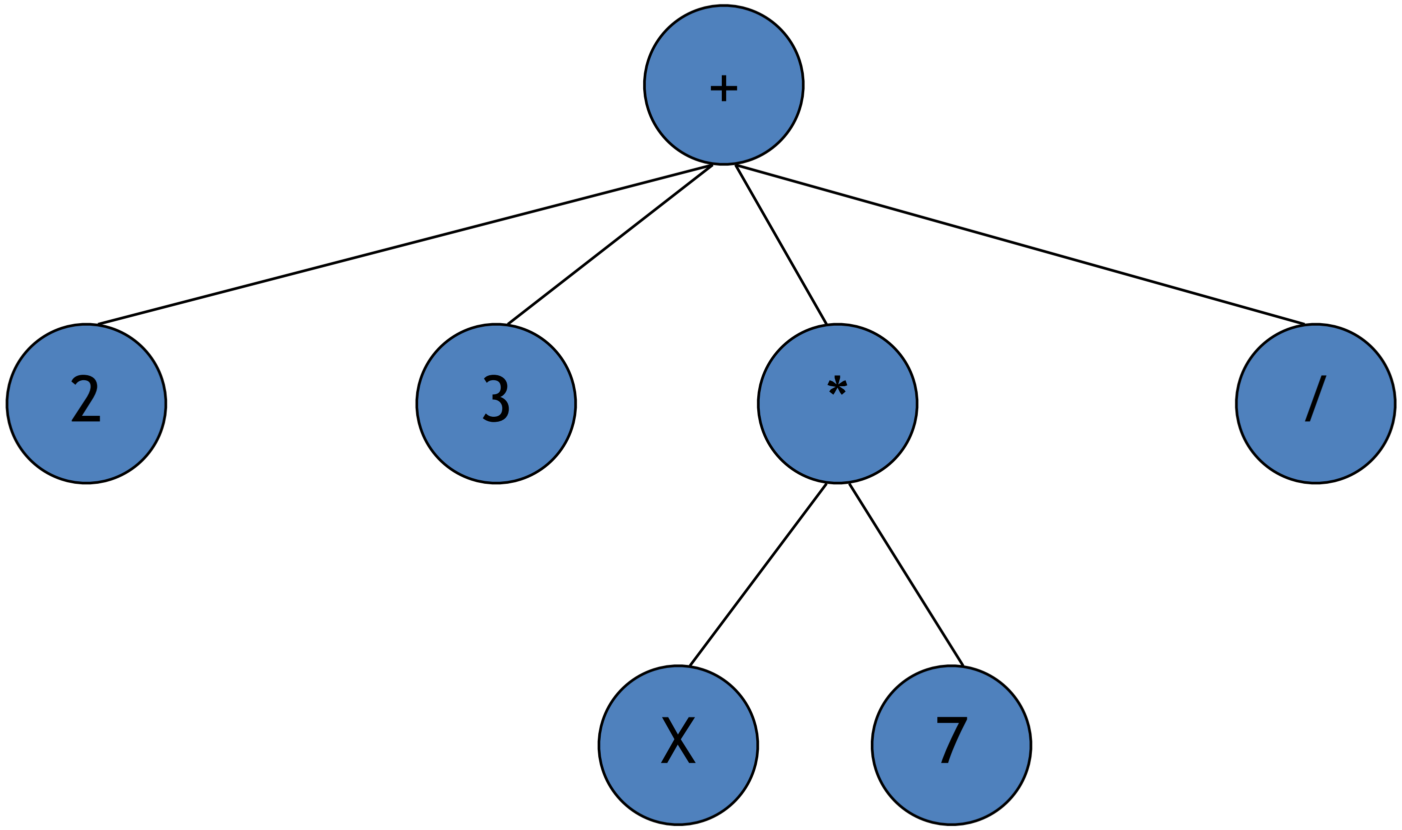
Randomly Generating Programs

(+ 2 3 (* …) …)



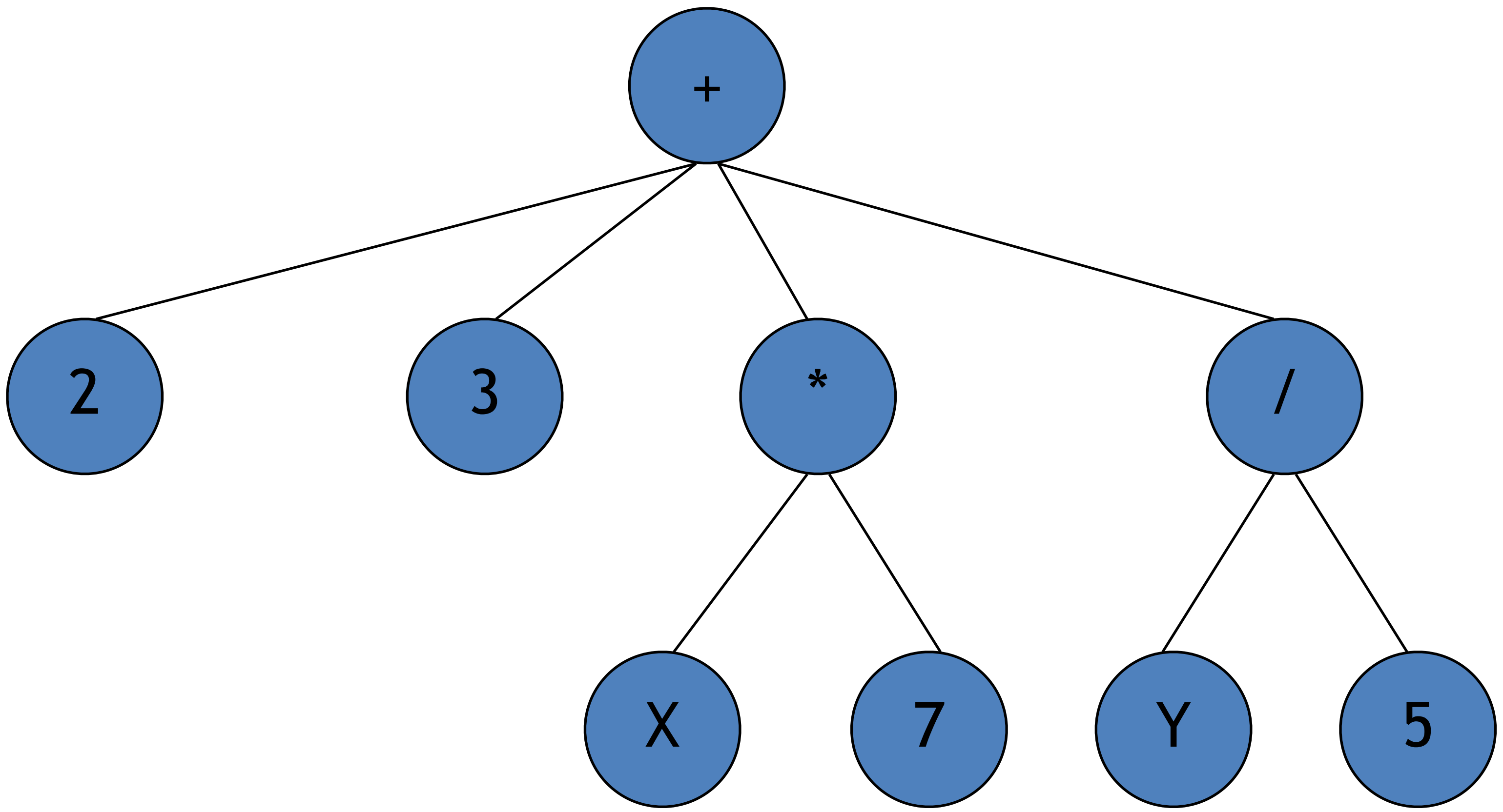
Randomly Generating Programs

(+ 2 3 (* X 7) (/ …))



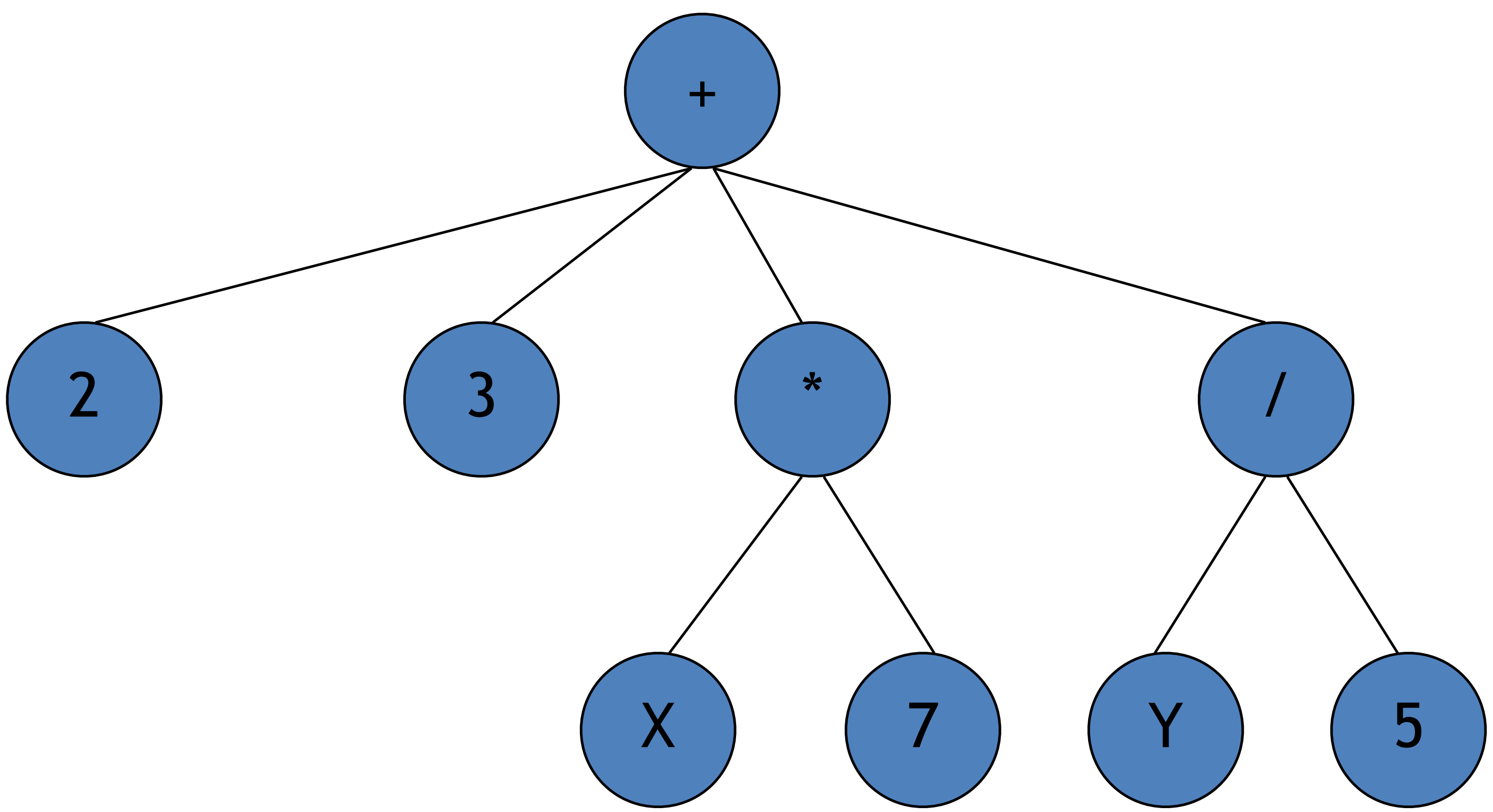
Randomly Generating Programs

(+ 2 3 (* X 7) (/ Y 5))



Mutation

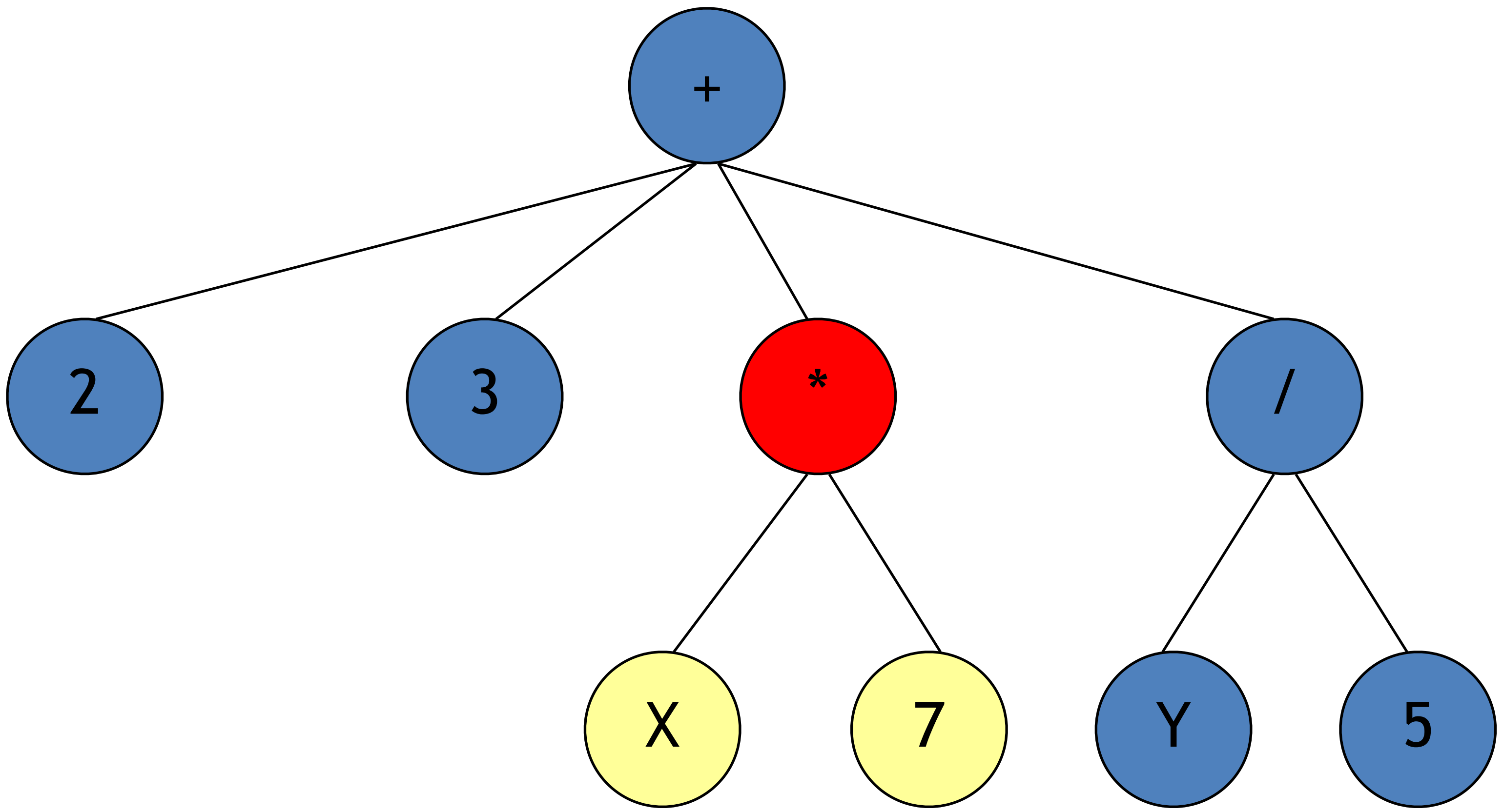
(+ 2 3 (* X 7) (/ Y 5))



Mutation

First pick a random point (node)

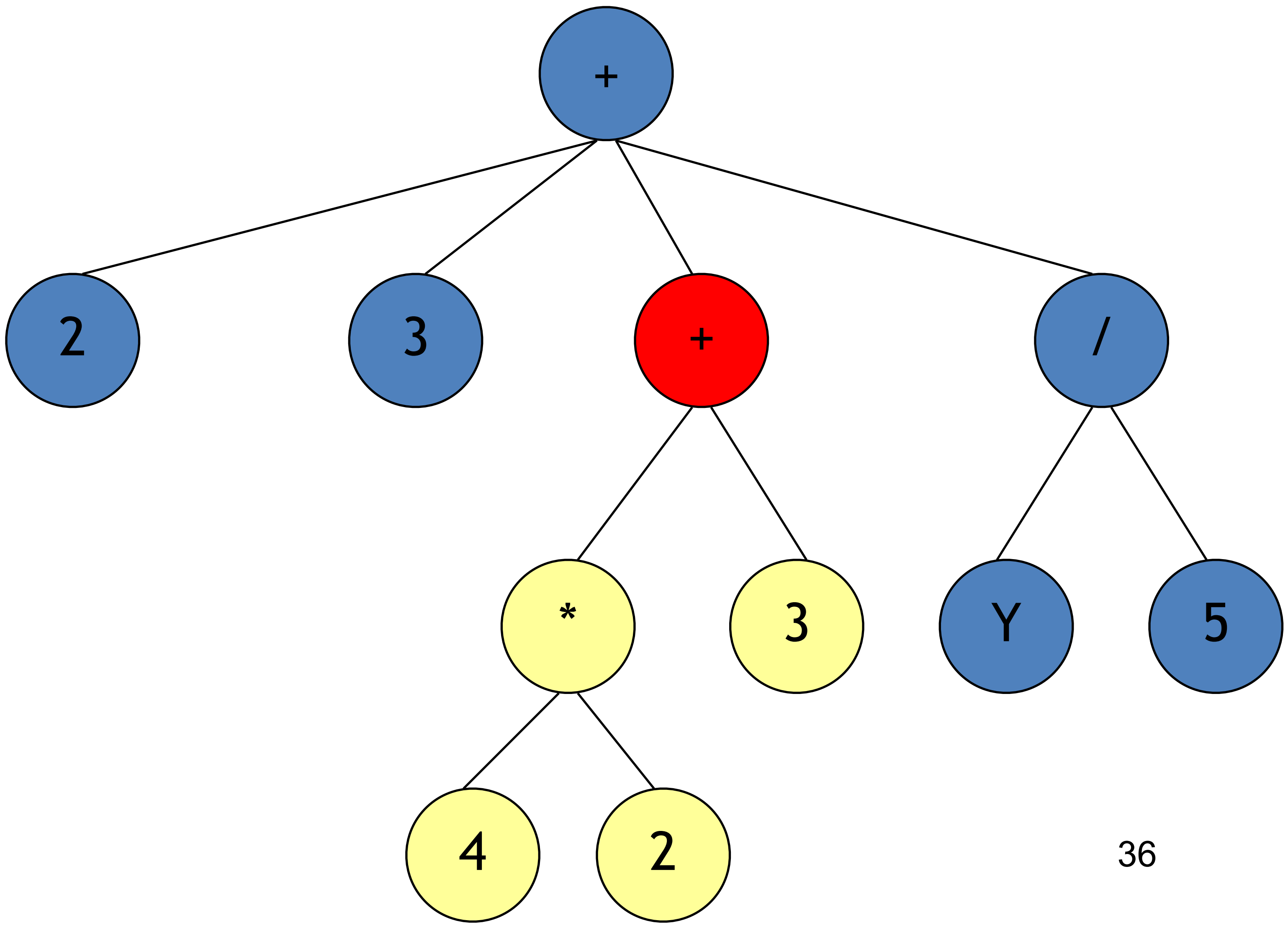
(+ 2 3 (* X 7) (/ Y 5))



Mutation

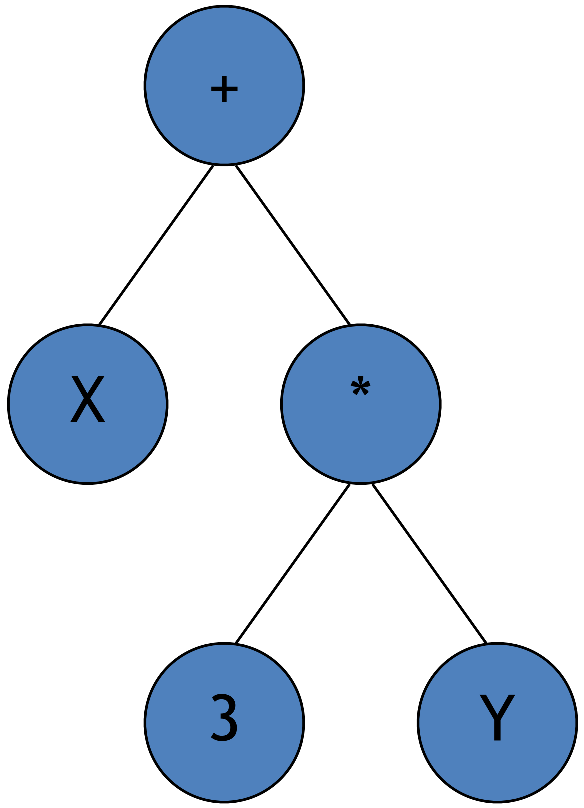
(+ 2 3 (+ (* 4 2) 3) (/ Y 5))

Delete the node and its children, and replace with a randomly generated tree

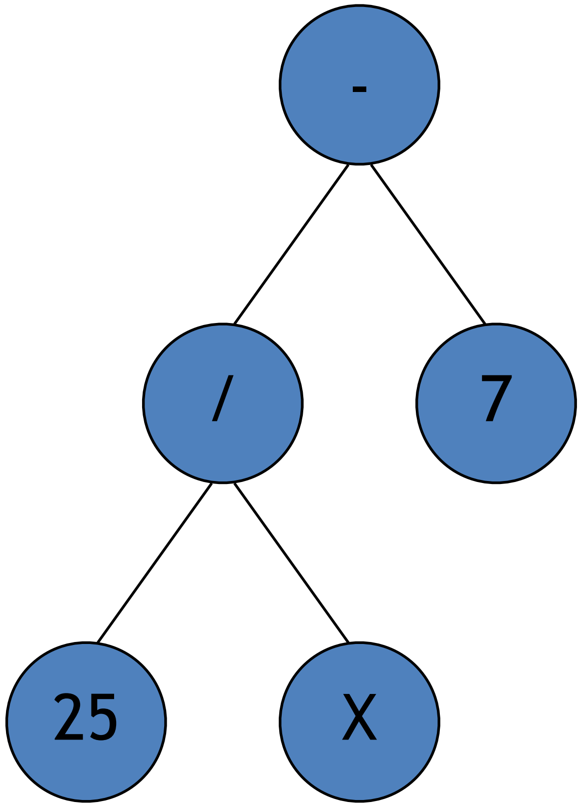


Crossover

(+ X (* 3 Y))

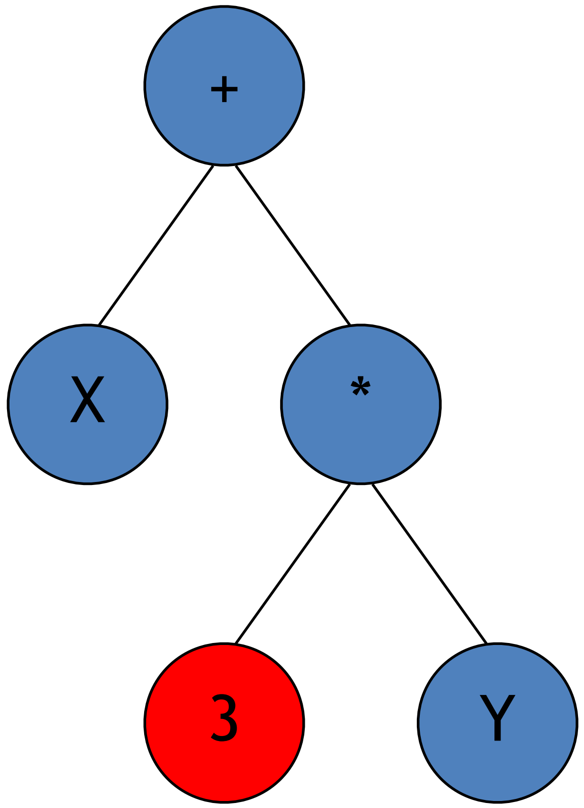


(- (/ 25 X) 7)



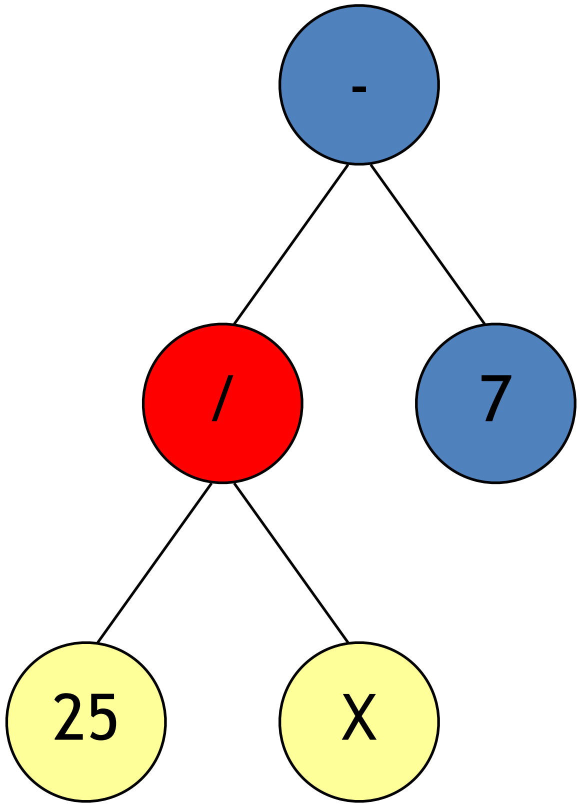
Crossover

(+ X (* 3 Y))



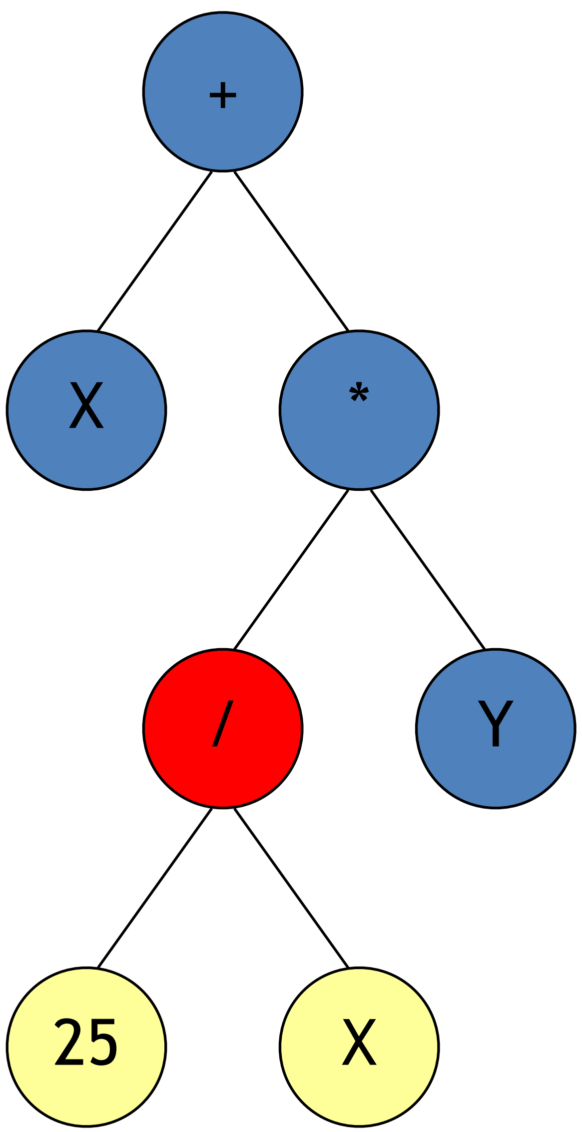
Pick crossover points (a random node in each tree)

(- (/ 25 X) 7)



Crossover

(+ X (* (/ 25 X) Y))



Swap the two nodes

(- 3 7)