

Local and Global Search

Parts adapted from:

- Chapter 4 of AI 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) that takes a complete assignment of the variables as parameters and returns a real number;

find a complete assignment so that the value of the objective function is optimised (maximised or minimised).

Example

Variables: a, b $\text{dom}(a) = \text{dom}(b) = \{-1, 0, 1\}$

Objective function: $f(a, b) = ab - a$

Maximise f .

Solving an optimisation instance

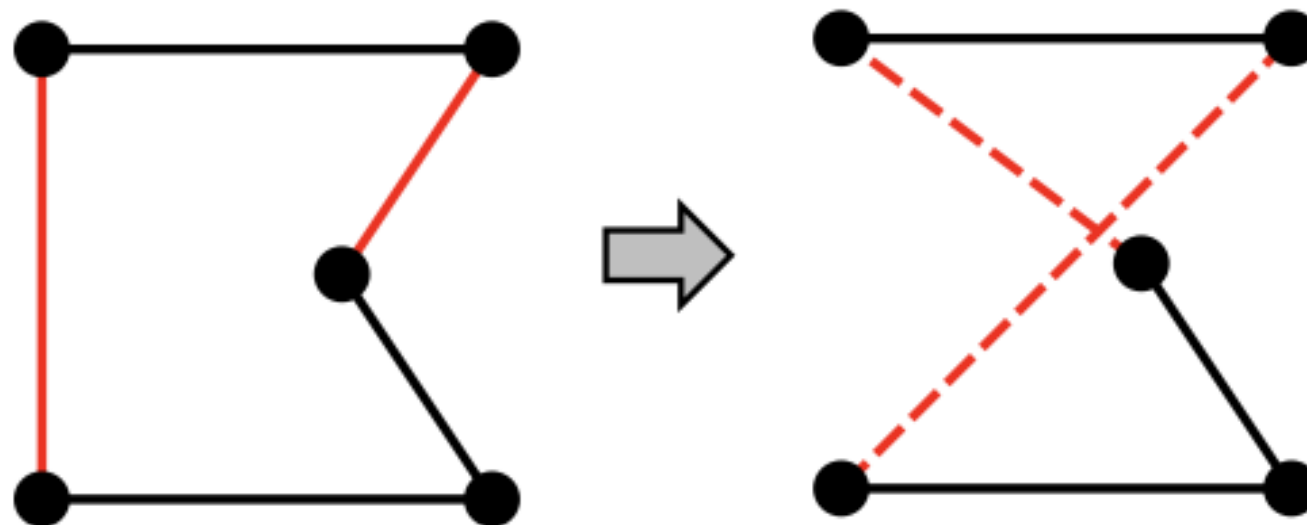
- A straightforward algorithm is the **exhaustive search** (generate and evaluate).
 - Good: guarantees to find an optimal solution
 - Bad: for many problems it is intractable
- In this lecture we look at two families of algorithms: **local search** and **global search**.
 - Good: can find optimal or near-optimal solutions in reasonable time
 - Bad: do not guarantee optimality (in most cases)

Local search for optimisation

- A **local search** algorithm is an iterative algorithm that keeps a single **current state** (complete assignment) and in each iteration tries to improve it by **moving** to one of its **neighbouring states**.
- Two key aspects to define:
 - **Neighbourhood**: which states are the neighbours of a given state
 - **Movement**: which neighbouring state should the algorithm go to
- A search algorithm is considered to be **greedy** if it always moves to the best neighbour. Two variants:
 - **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.

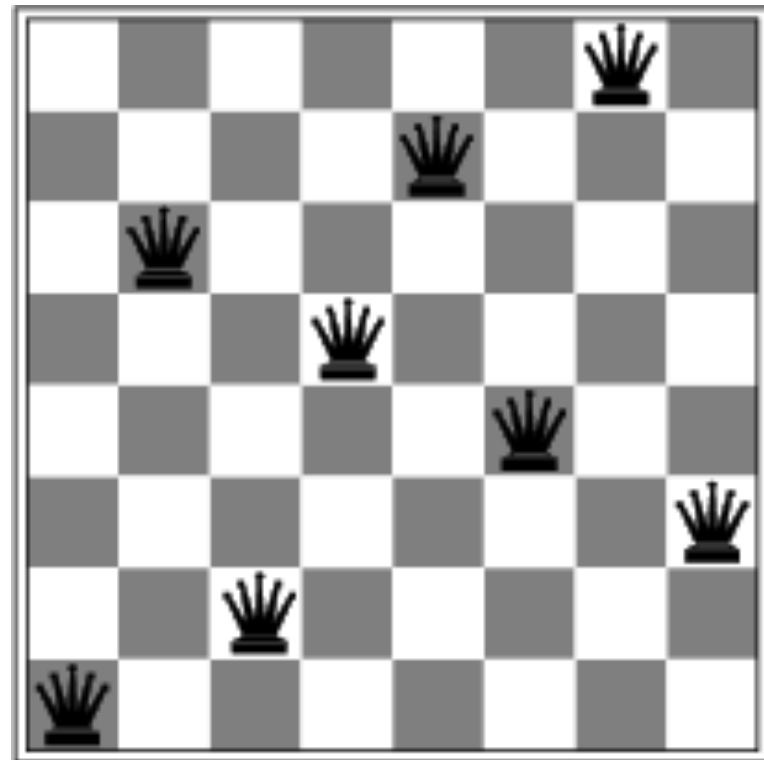
Local Search for CSP: Neighbourhood

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

- All possible assignments except the current one (poor design - why?)
- Select a variable. Neighbours are assignments in which that variable takes a different value from its domain.
- 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

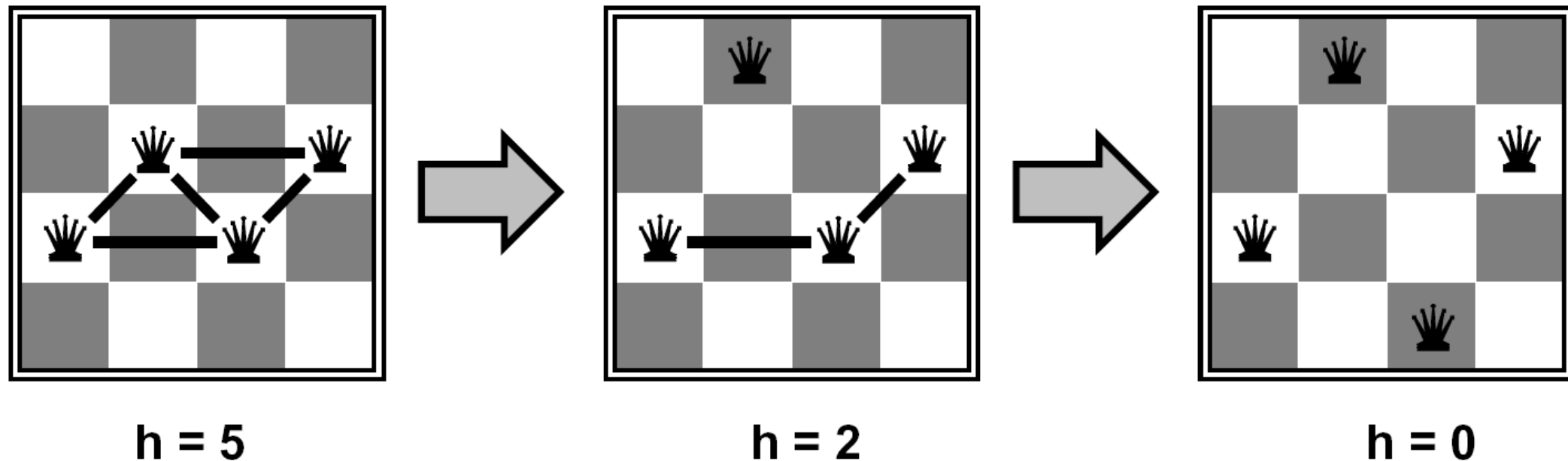
- Aim: Put n queens on an $n \times n$ board with no two queens attacking each other.
- The objective (heuristic) function to minimise: number of conflicts.



$$h = 1$$

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: $h(\text{board}) = \text{number of pairs of queens that are attacking each other (number of conflicts)}$



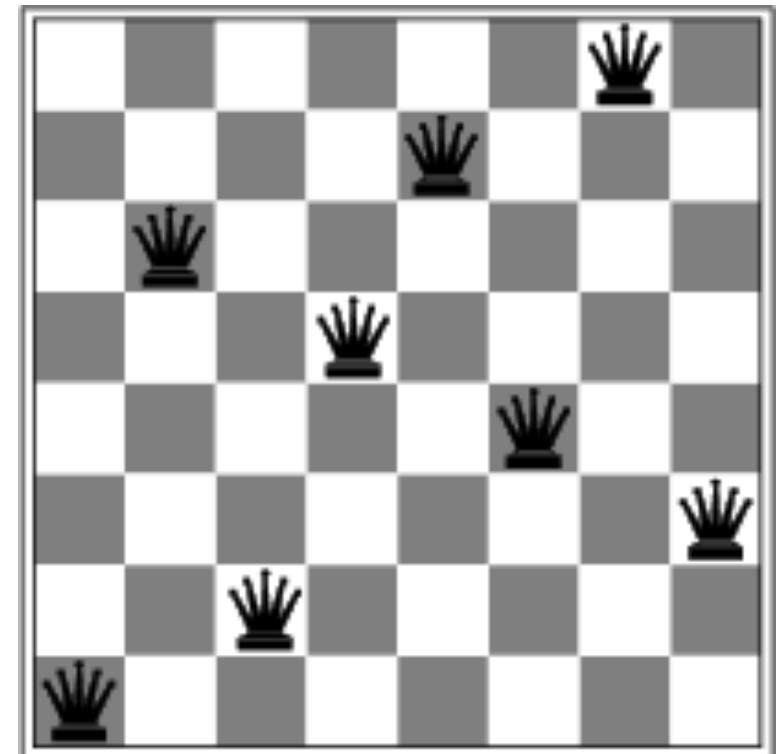
Example: neighbours

- Objective function (conflict count): number of pairs of queens that are attacking each other.
- Number of conflicts in the current state: 17

18	12	14	13	13	12	14	14
14	16	13	15	12	14	12	16
14	12	18	13	15	12	14	14
15	14	14	♚	13	16	13	16
♚	14	17	15	♚	14	16	16
17	♚	16	18	15	♚	15	♚
18	14	♚	15	15	14	♚	16
14	14	13	17	12	14	12	18

Local Search Issues

- Local (greedy) search can get stuck in local optima or flat areas 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 so called **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.

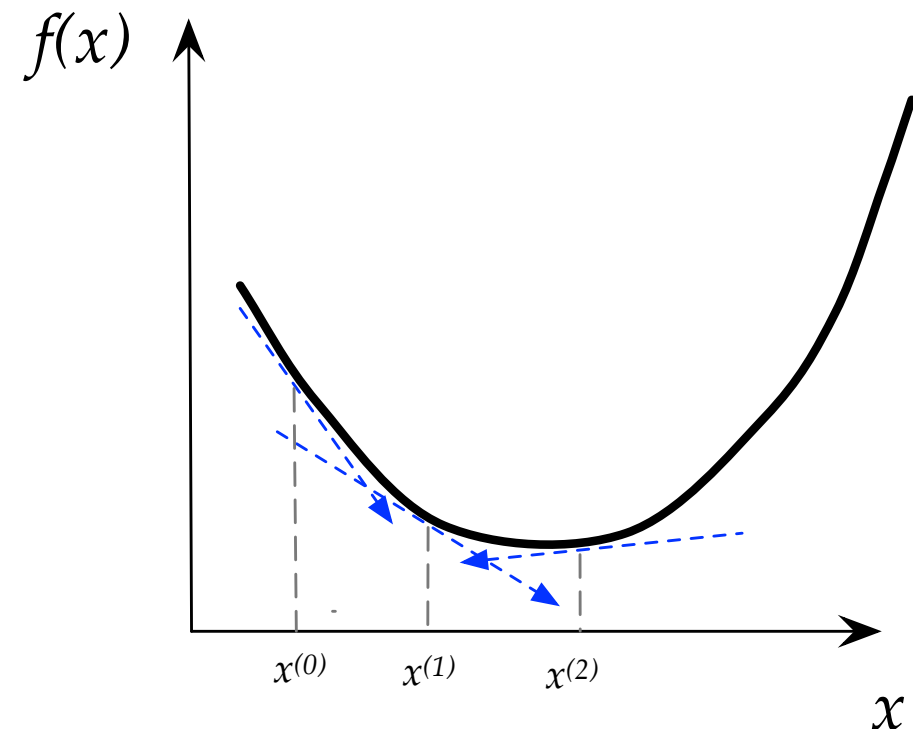
Probability of accepting a change:

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).

```
1: Guess  $\mathbf{x}^{(0)}$ , set  $k \leftarrow 0$   
2: while  $\|\nabla f(\mathbf{x}^{(k)})\| \geq \epsilon$  do  
3:    $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - t_k \nabla f(\mathbf{x}^{(k)})$   
4:    $k \leftarrow k + 1$   
5: end while  
6: 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

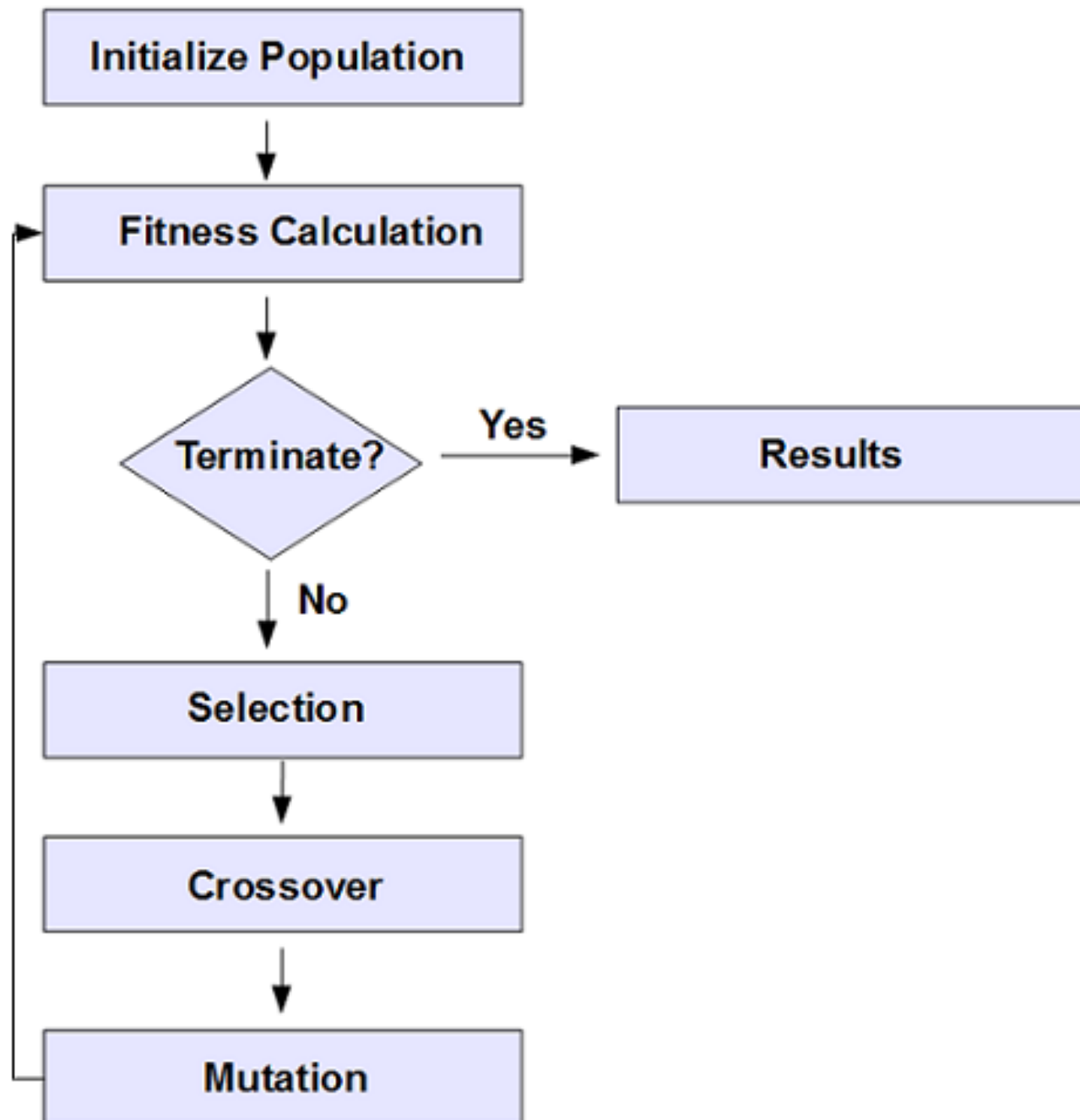
J. C. Spall
*Introduction to Stochastic Search
and Optimization*, John Wiley and
Sons



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

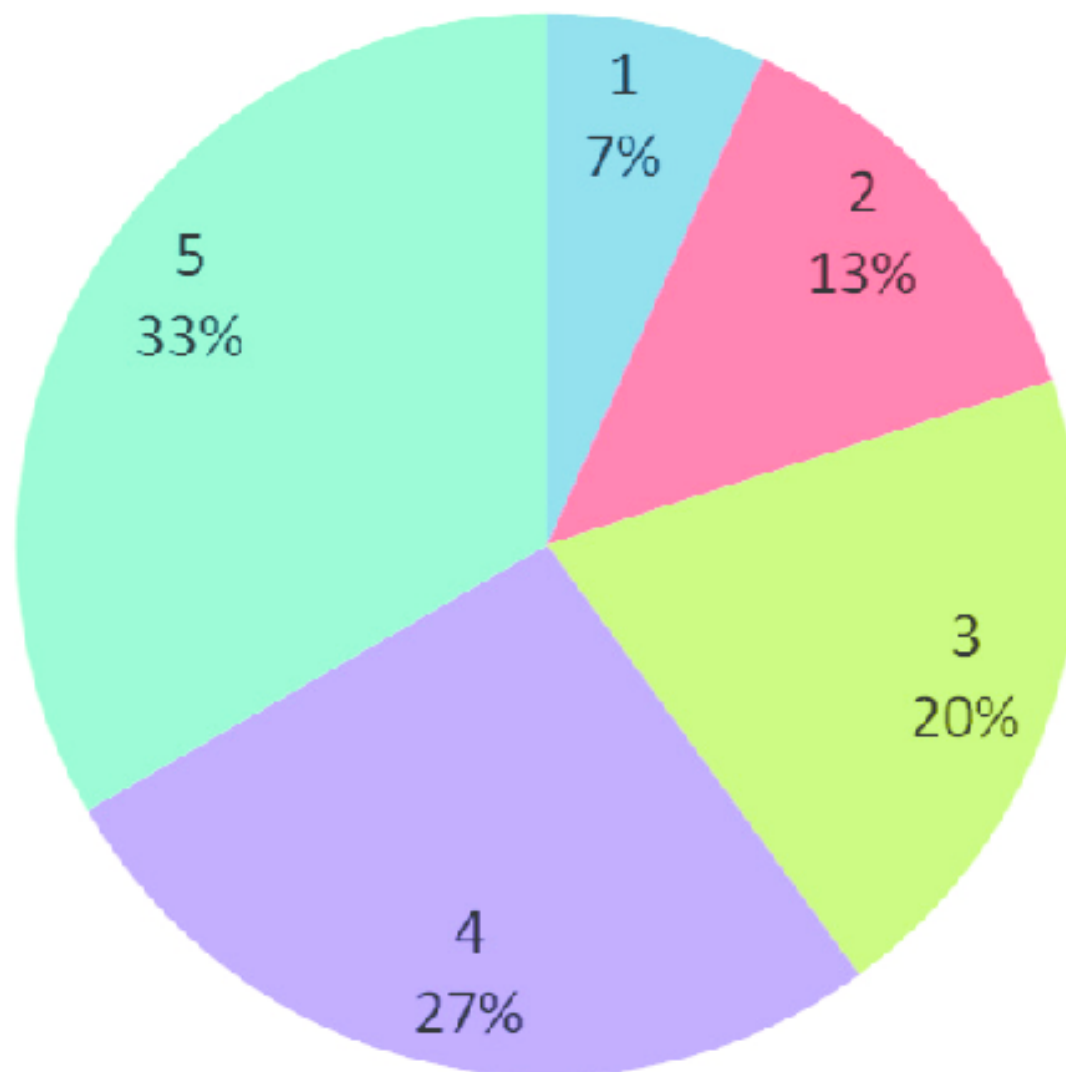
Main idea: better individuals should have higher chance of surviving and breeding.

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

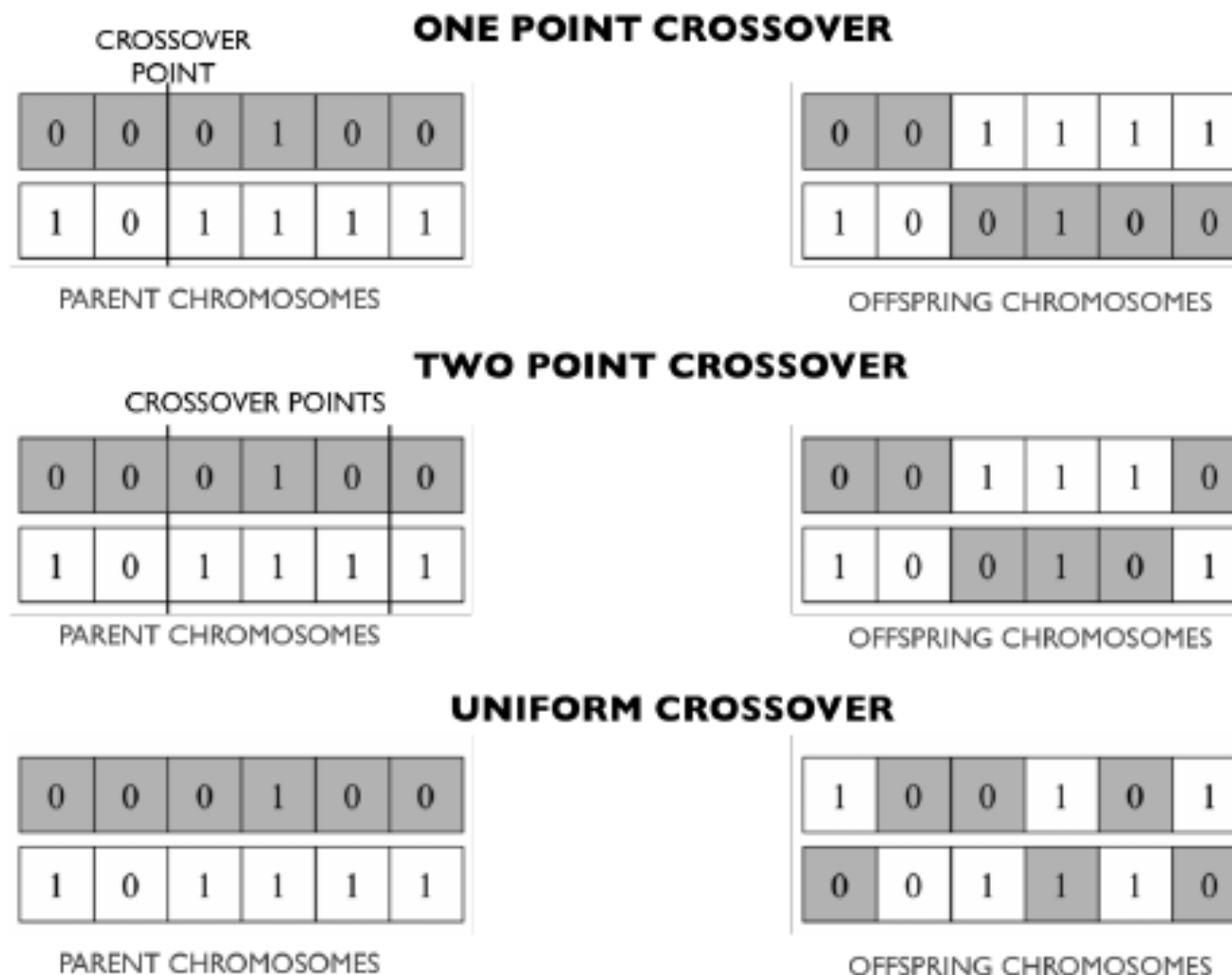
Mutation

- 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

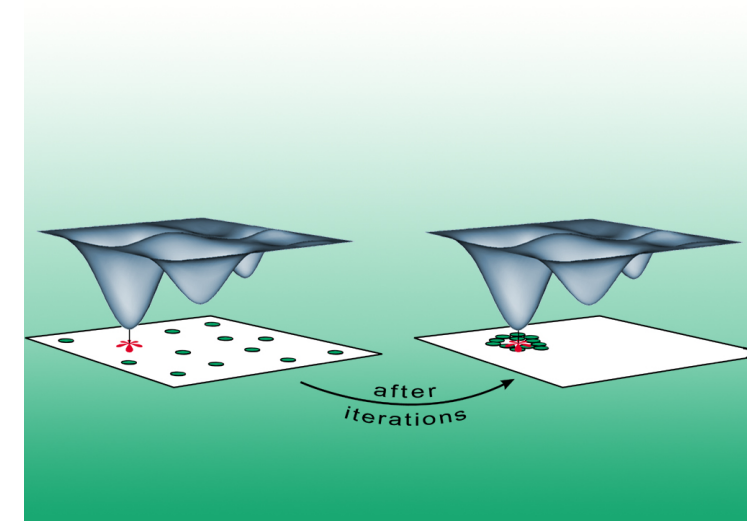
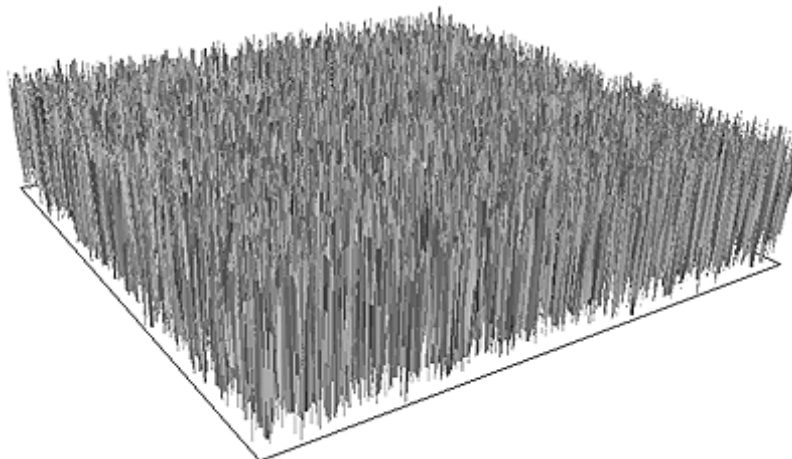
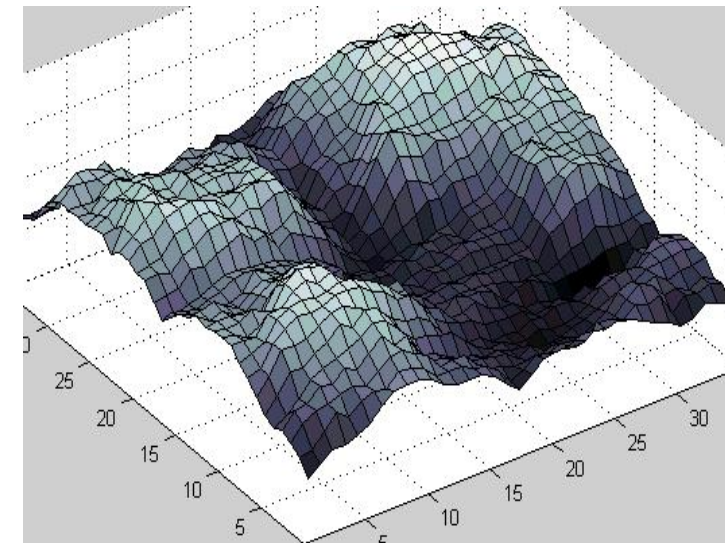
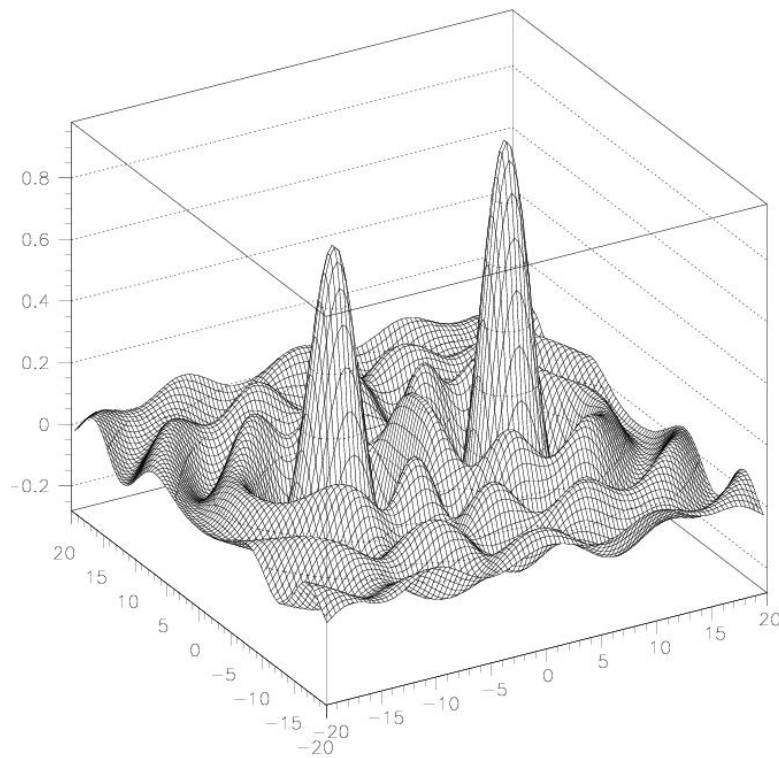
With sequential representation (e.g. tuples), mutation is performed by selecting 1 or more random locations (indices) and changing the values at those locations to some random value (from the domain).

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.

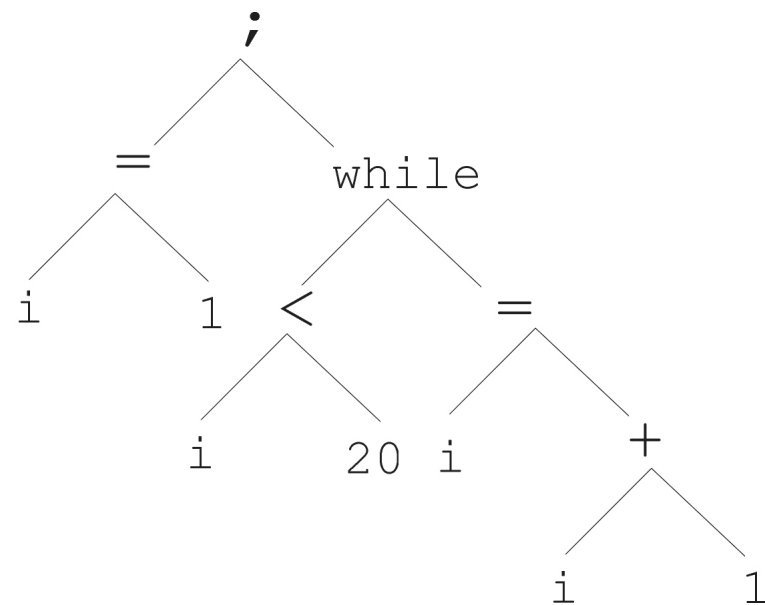
Fitness landscapes

- 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.

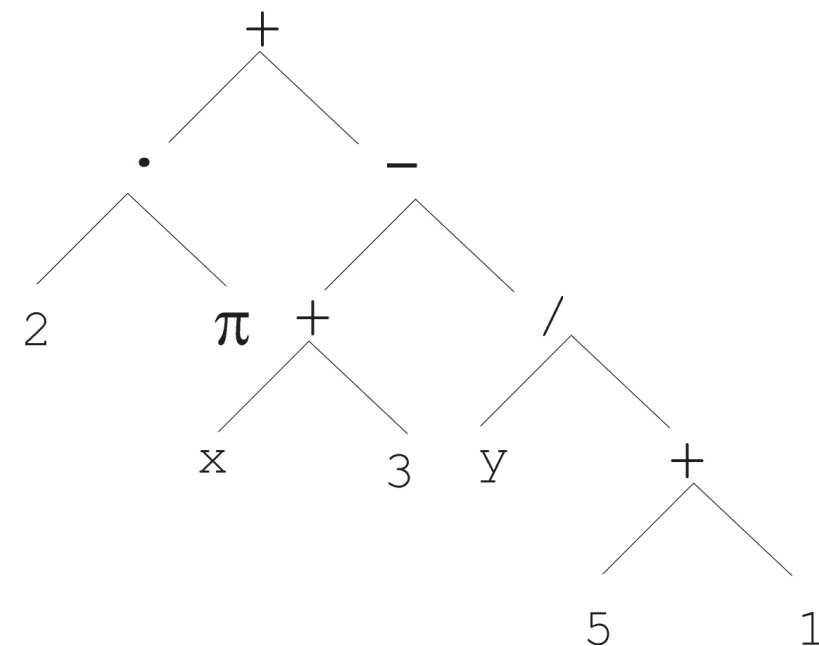


Tree representation

- 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.



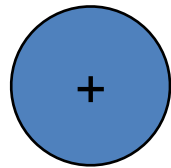
```
i = 1;
while (i < 20)
{
    i = i + 1
}
```



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

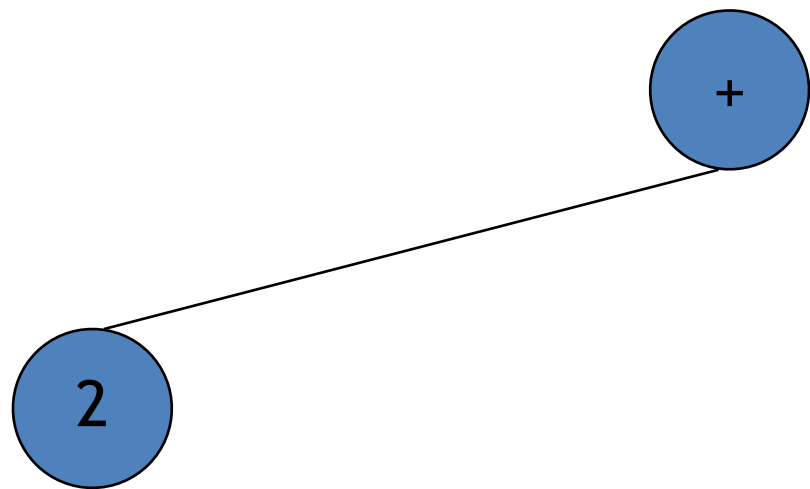
Randomly Generating Programs

(+ ...)



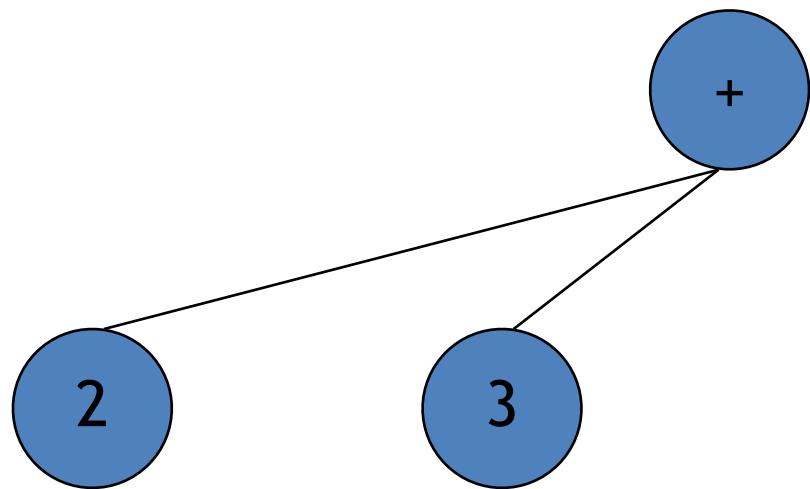
Randomly Generating Programs

(+ 2 ...)



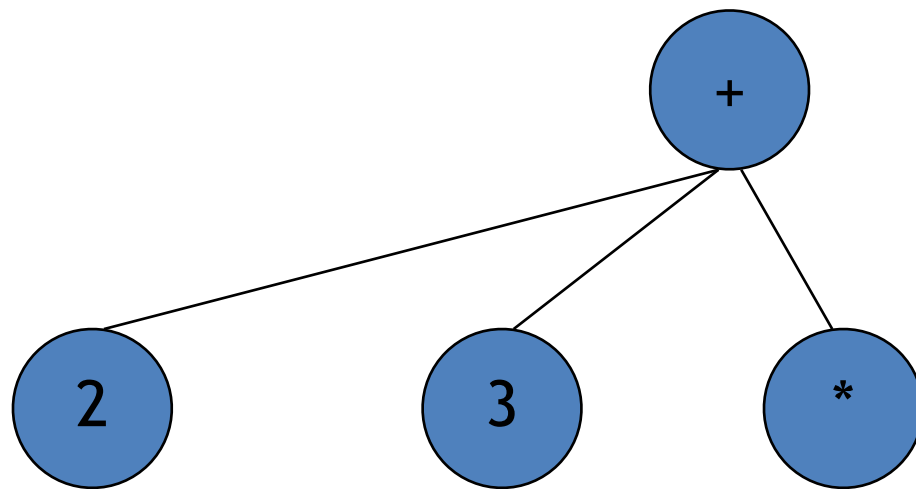
Randomly Generating Programs

(+ 2 3 ...)



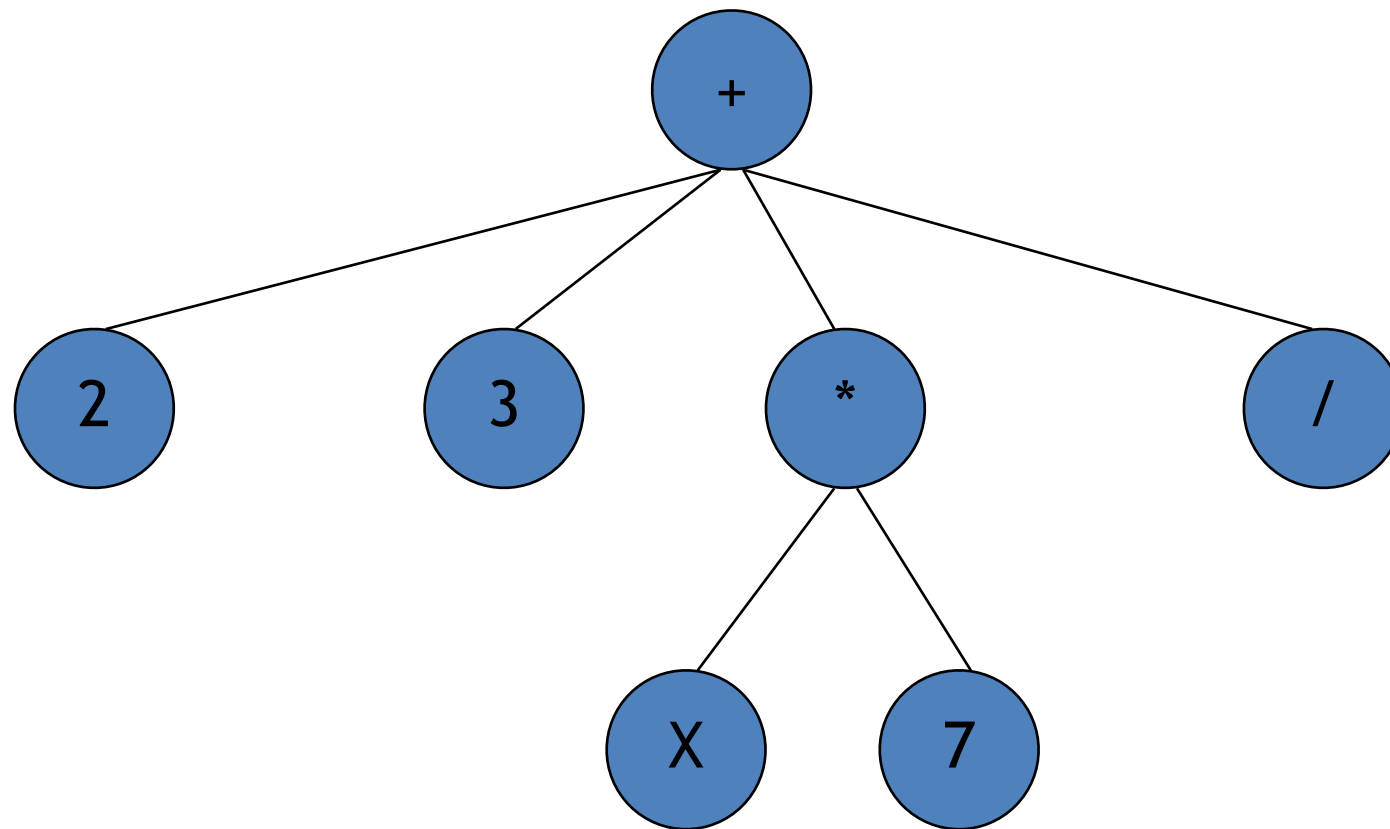
Randomly Generating Programs

(+ 2 3 (* ...) ...)



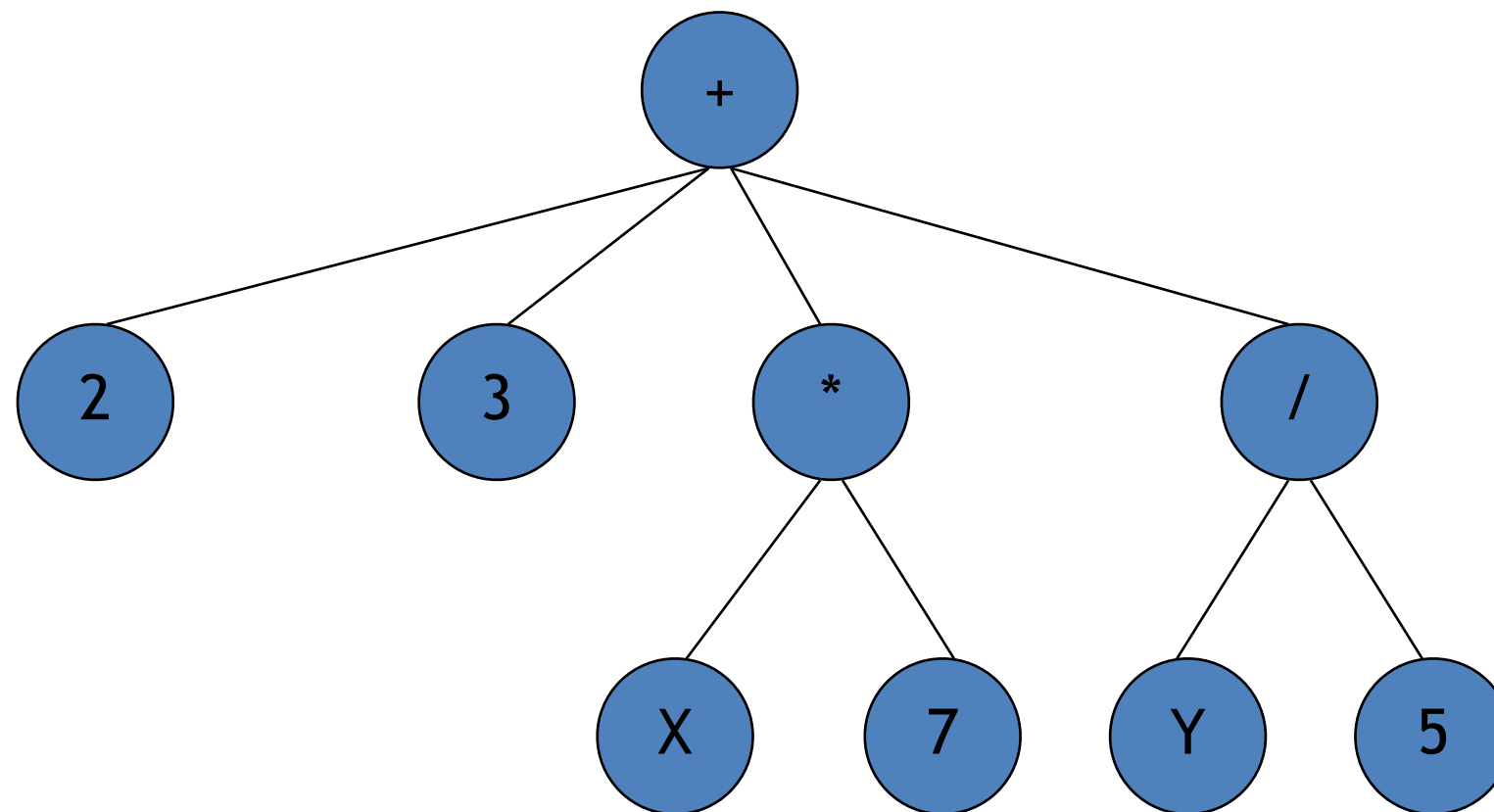
Randomly Generating Programs

`(+ 2 3 (* X 7) (/ ...))`



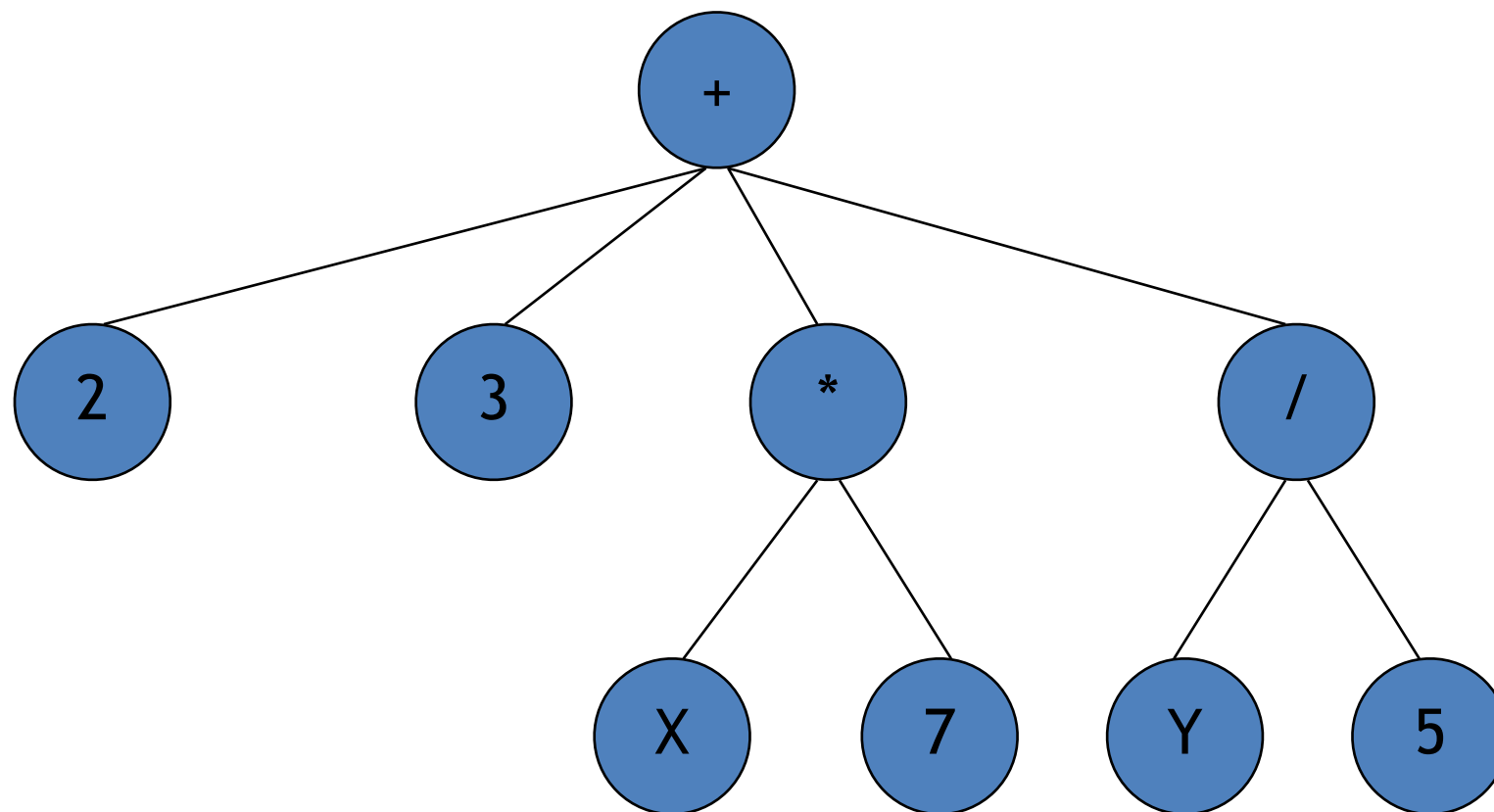
Randomly Generating Programs

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



Mutation

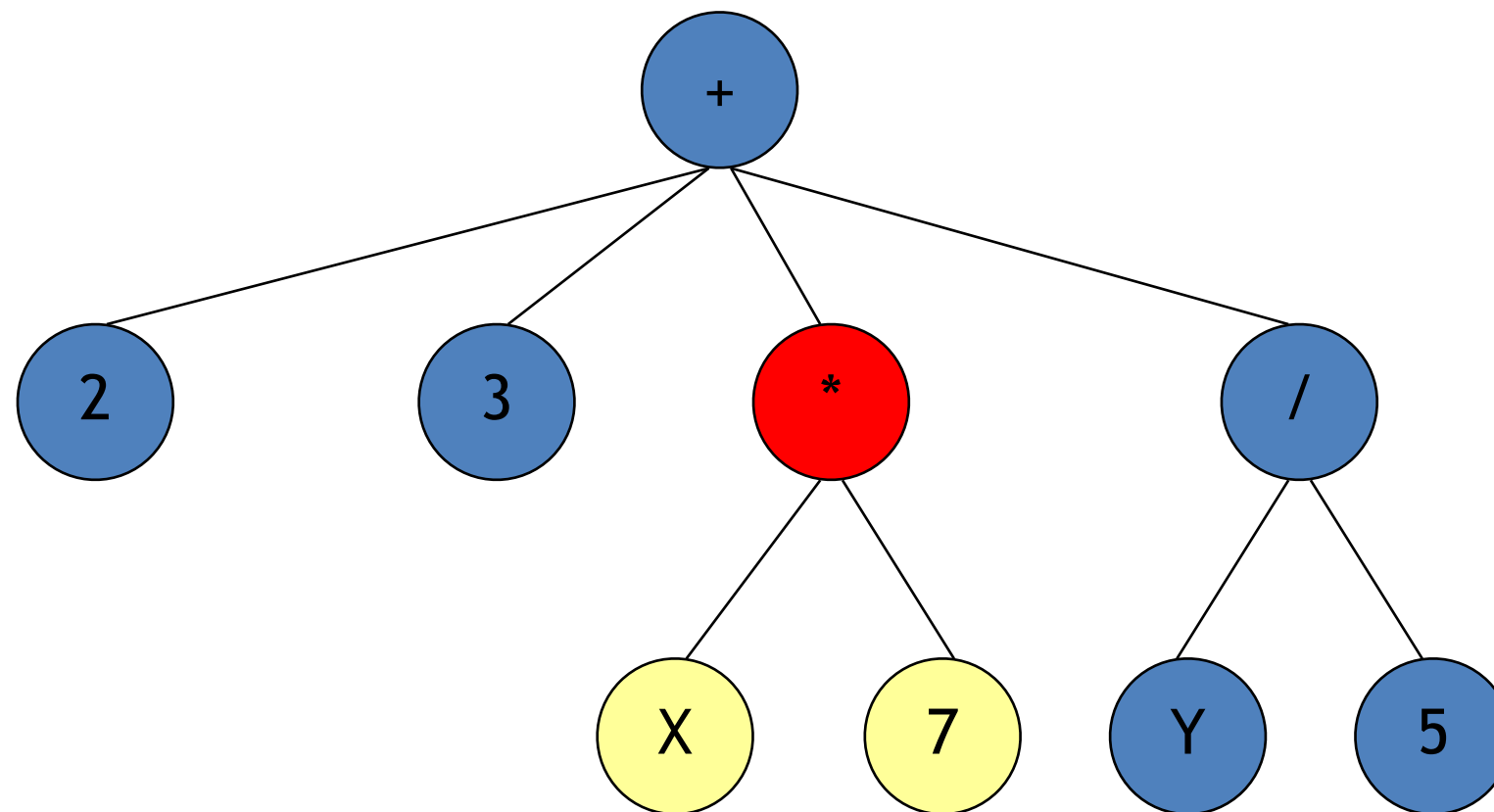
(+ 2 3 (* X 7) (/ Y 5))



Mutation

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

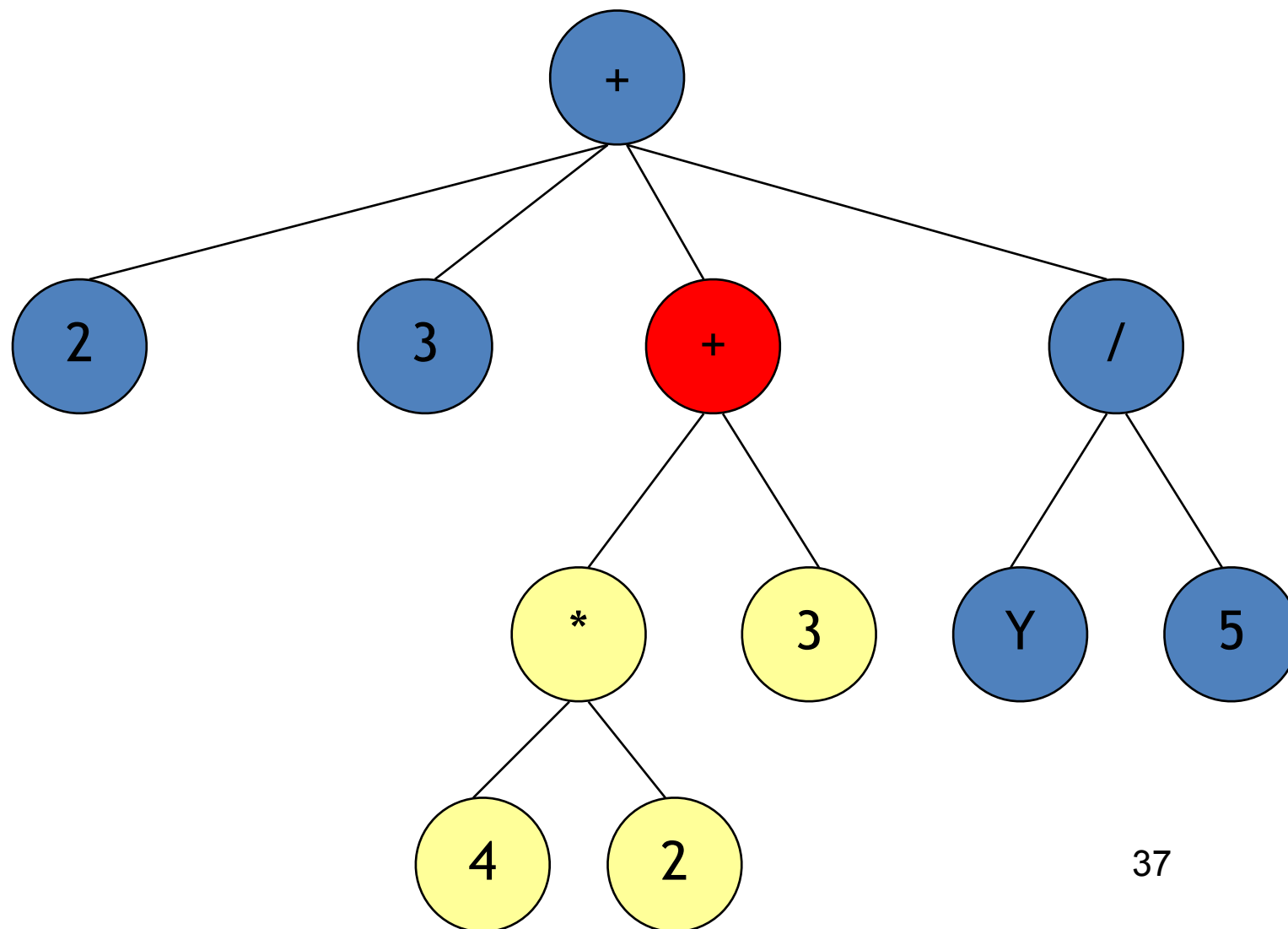
First pick a random point (node)



Mutation

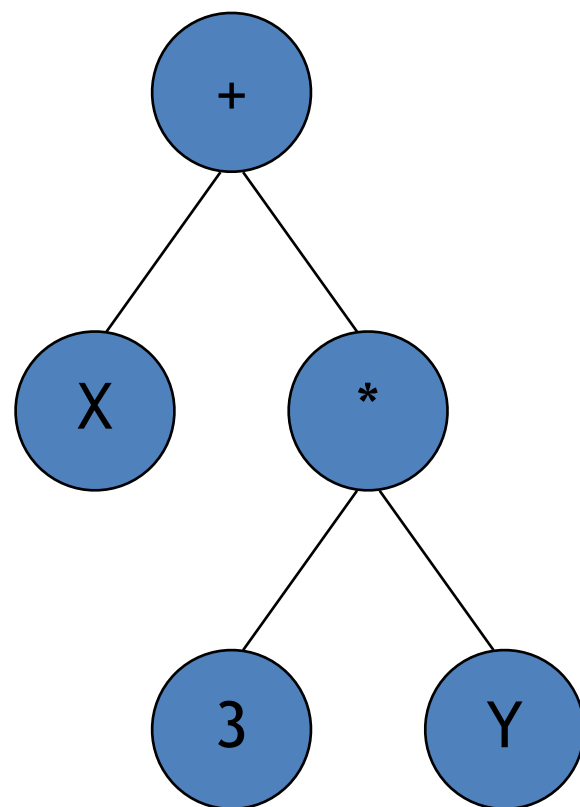
(+ 2 3 (+ (* 4 2) 3) (/ Y 5))

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

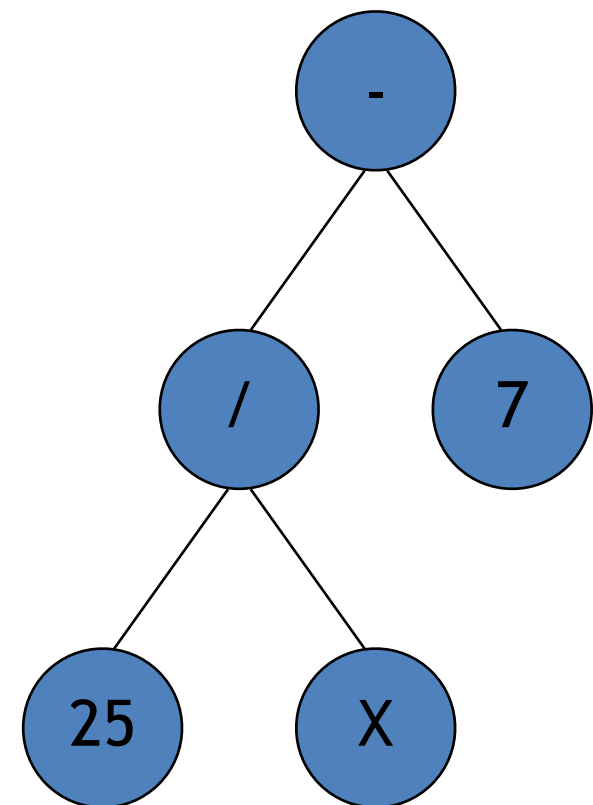


Crossover

$(+ X (* 3 Y))$

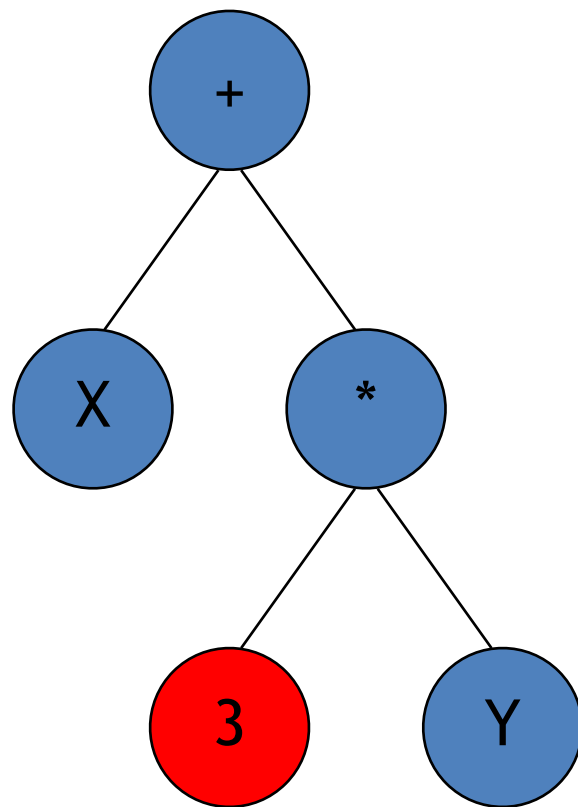


$(- (/ 25 X) 7)$



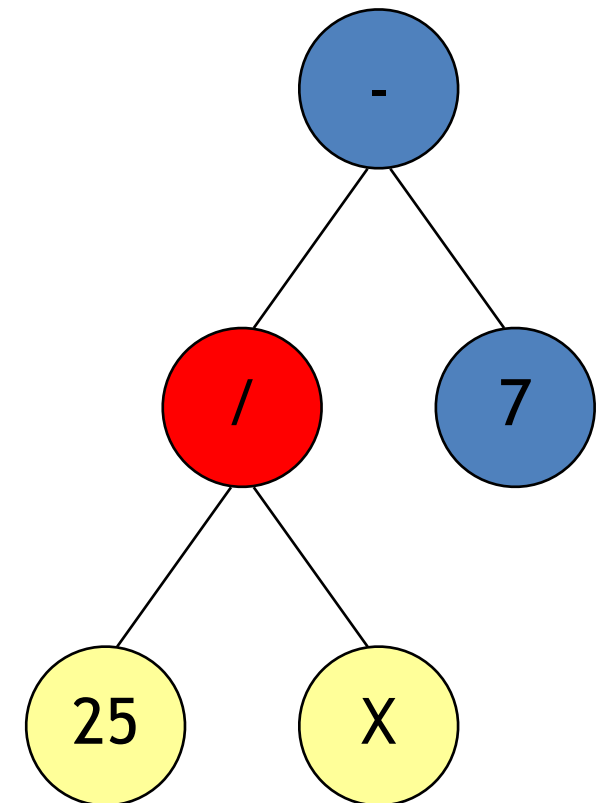
Crossover

(+ X (* 3 Y))



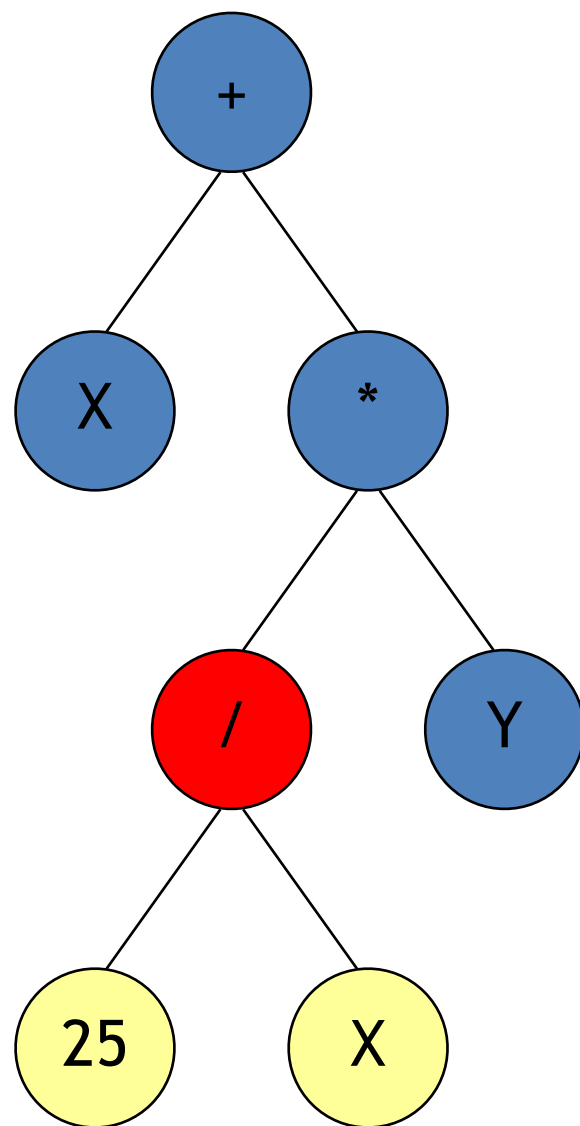
Pick crossover points (a random node in each tree)

(- (/ 25 X) 7)



Crossover

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



Swap the two nodes

(- 3 7)

