OPTIMIZATION FOR AI

GLOBAL AND MULTI-OBJECTIVE OPTIMIZATION

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TEAM OF THE COURSE

Code:

bpplxhk

The slides and material of the lectures will be uploaded on the Teams of the course

EXAM STRUCTURE

- **Project** + **oral exam**
- Project should be sent about a week before the oral exam
- For December and January there will be some fixed dates for the exam…
- …but after that all exams can be “by appointment”, so take the time that you need

EXAM STRUCTURE

- Kinds of projects:
  - Implement an existing paper and reproduce the results
  - Apply evolutionary algorithms / swarm intelligence algorithms to an existing problem
  - Literature review on a specific topic
- A set of projects will be presented later in the course, but we can discuss personalized project

EXAM STRUCTURE

- Oral exam:
  - First part: presentation (15-20 minutes max) of your project
  - Second part: questions about all topics of the course
- Both parts are essential!

EXAM CHECKLIST

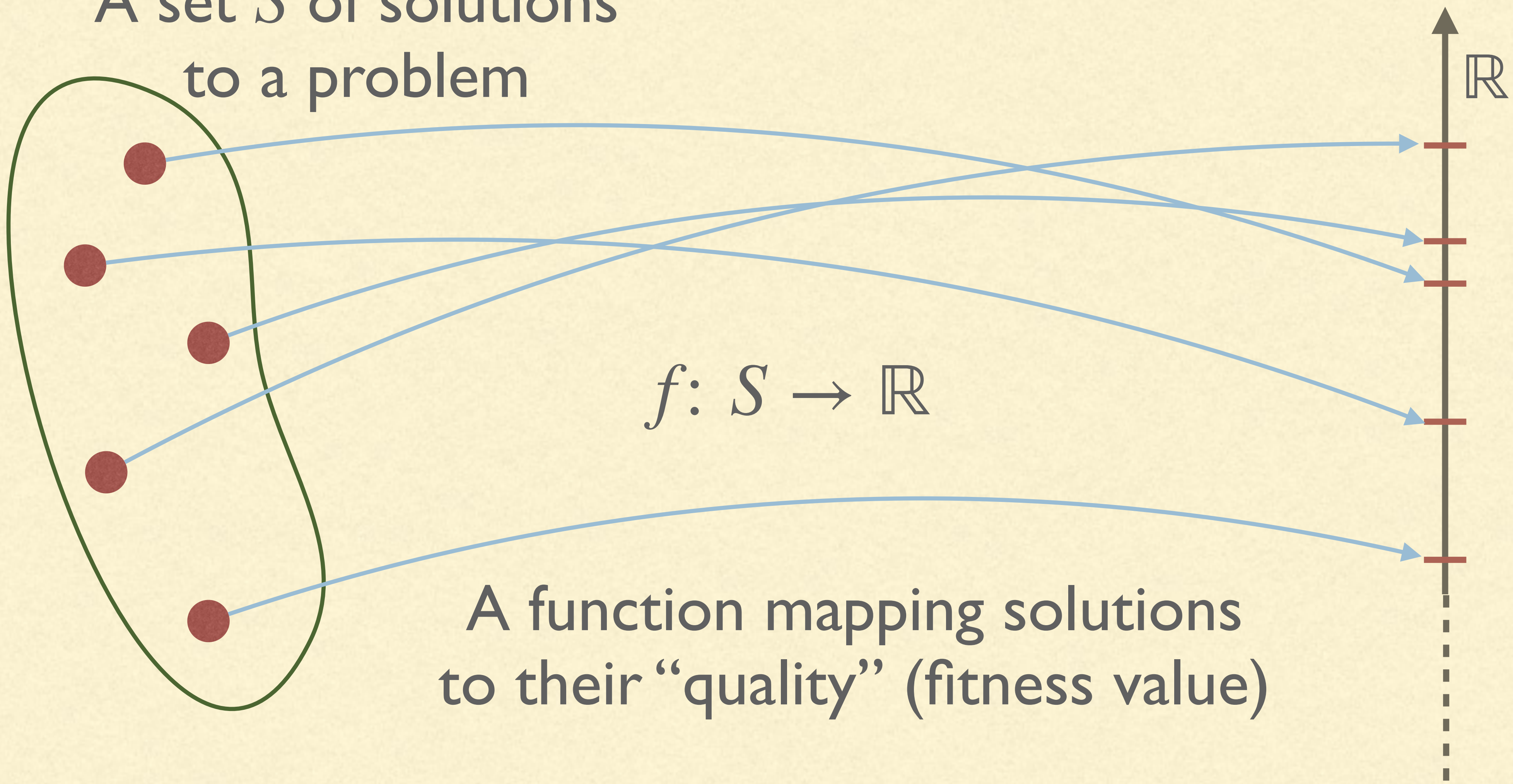
- **Project**
  - Select your project
  - Do your project
  - Fix a date for the oral exam
  - Send the project for evaluation one week before the oral exam
- **Oral Exam**
  - Present your project
  - Answer questions on all the topics of the course

OUTLINE

- What are population-based optimization methods
- Outline of the course
- Reference material
- Genetic Algorithms
- Evolution Strategies

WHAT ARE WE TALKING ABOUT?

A set S of solutions to a problem



A function mapping solutions to their "quality" (fitness value)

We want to find $\mathrm{argmax}_{x \in S} f(x)$ or $\mathrm{argmin}_{x \in S} f(x)$

HOW CAN WE FIND THE OPTIMUM?

- We might be unable to solve the problem analytically
- S might be too large to perform an exhaustive search
- We might have very few assumption on f, i.e., f is a "black box"
- It might be OK to return "good enough" solutions

A TRIVIAL PROBLEM: ONEMAX

- Let $S = \{0,1\}^n$, hence the size of the space is 2^n
- Let $f(x) = \#$ of ones in x
- We want to maximise f
- Clearly, the optimum is 1^n with fitness value n

APPROACH #1: RANDOM SEARCH

- Select a solution b from S (it is not important how)
- Repeat the following until some termination criteria is met
  - Let x be a solution selected uniformly at random from S
  - If $f(x) \geq f(b)$ substitute b with x
- Return b

APPROACH #1: RANDOM SEARCH

- Even if we avoid sampling the same solution more than once, we will still need to explore a significant fraction of the search space
- Without repetitions, it is like exhaustive search for some choice of the order of enumeration of the solutions
- Generally unfeasible
- In **some** search spaces this is better than other kinds of search…
- …but hopefully this is not something that happens for real problems

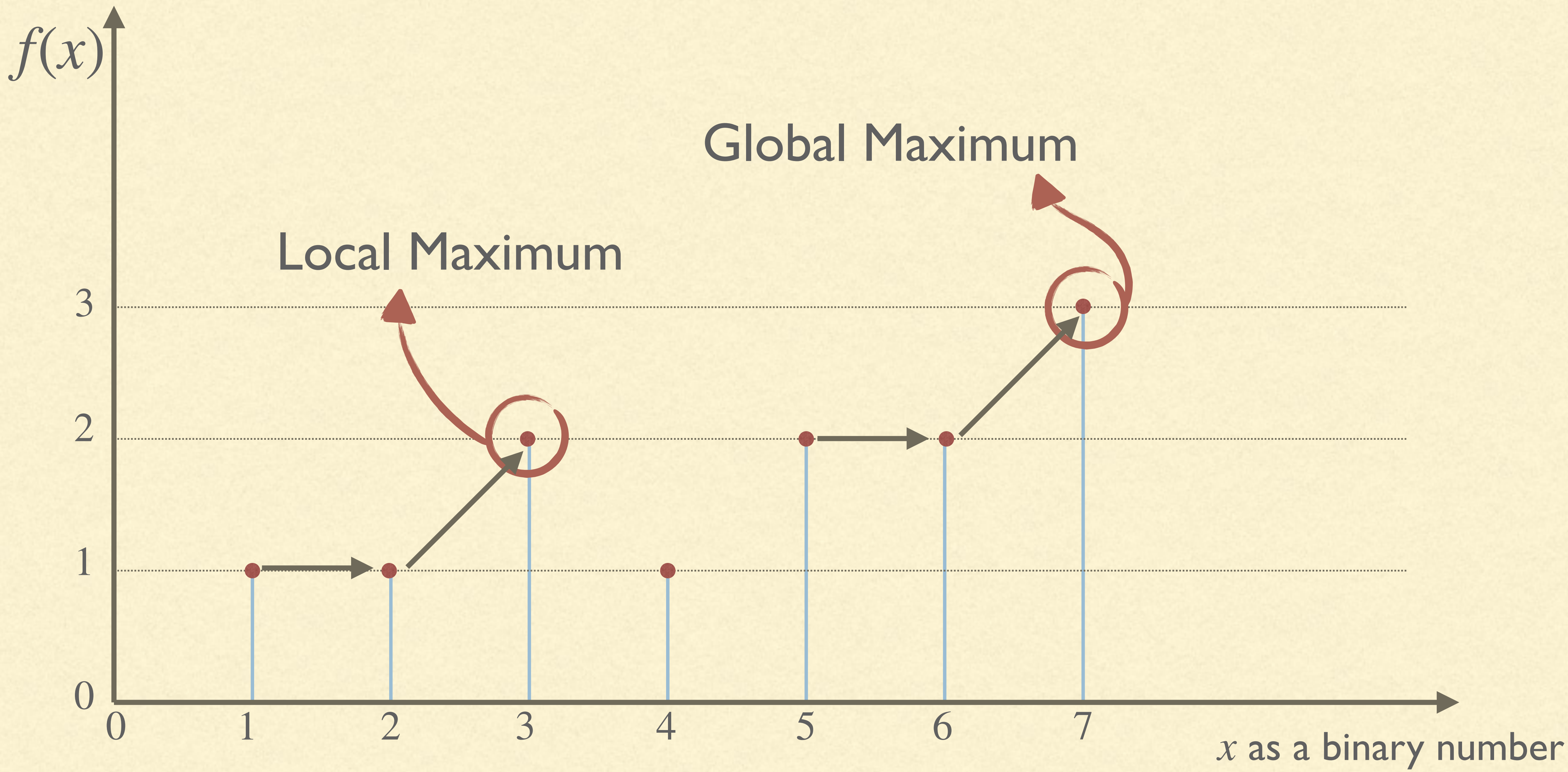
APPROACH #2: HILL CLIMBING

- Let b be an initial solution from S
- Repeat the following until some termination criteria is met
  - Let x be a **neighbor** of b
  - If $f(x) \geq f(b)$ then replace b with x
- Return b

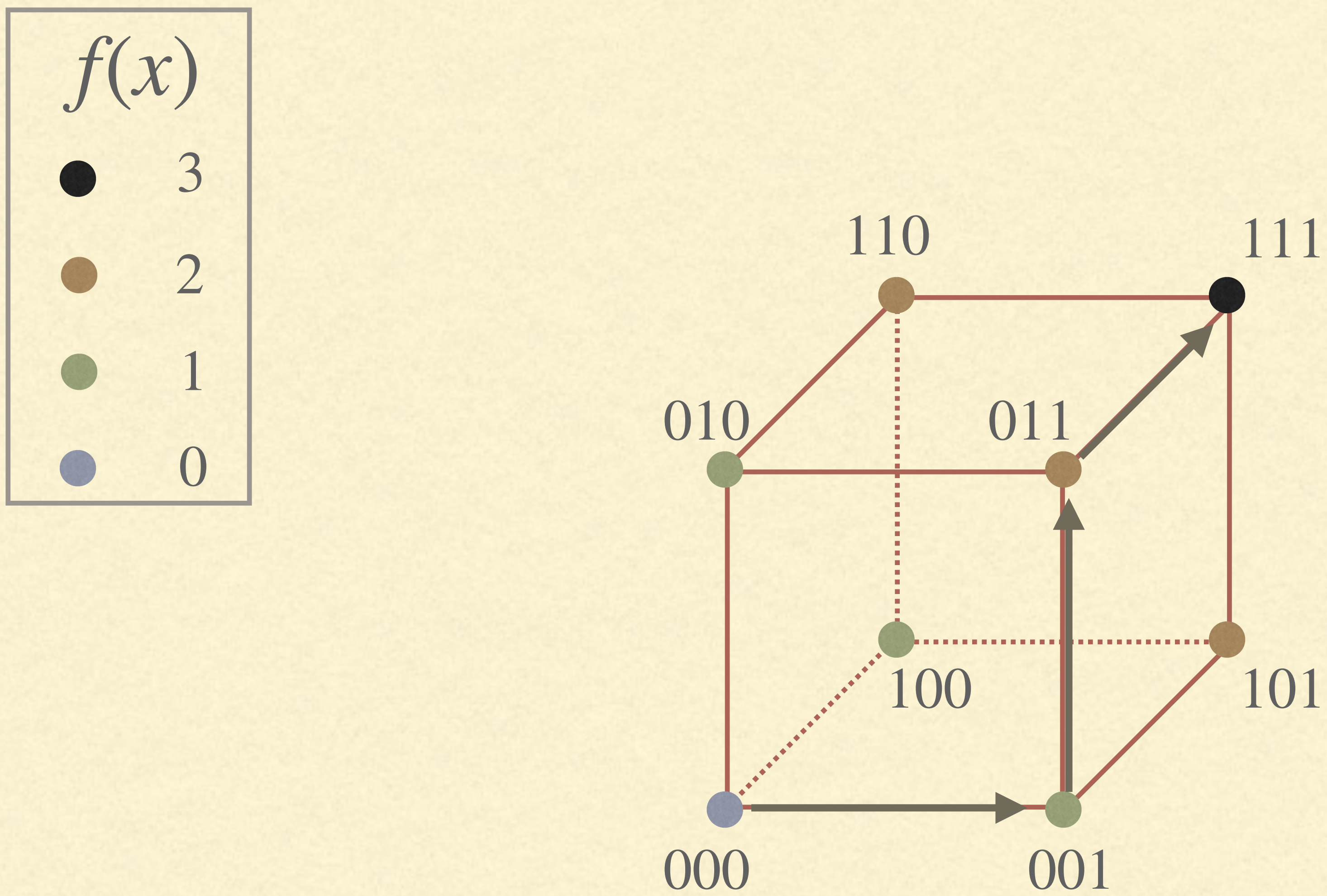
APPROACH #2: HILL CLIMBING

- We are defining a neighborhood structure on S
- The ability to find a global optimum depends on this structure:
  - OneMax with neighborhood of x given by $x + 1$ and $x - 1$
  - OneMax with neighborhood of x given by all binary strings at Hamming distance one.

LOCAL AND GLOBAL MAXIMA



LOCAL AND GLOBAL MAXIMA



Notice that there are no local optima

APPROACH #3: SIMULATED ANNEALING

- Let b be an initial solution from S and T the "temperature"
- Repeat the following until some termination criteria is met
  - Let x be a **neighbor** of b
  - If $f(x) \geq f(b)$ then replace b with x
  - Otherwise replace b with x with probability $e^{\frac{f(x) - f(b)}{T}}$
  - Update T (by decreasing it) according to some schedule
- Return b

APPROACH #3: SIMULATED ANNEALING

- The idea is to allow the selection of less fit solutions with some probability that depends from the time and the difference in fitness
- This allows to reduce the risk of getting stuck in a local optimum
- The choice of the schedule is important!

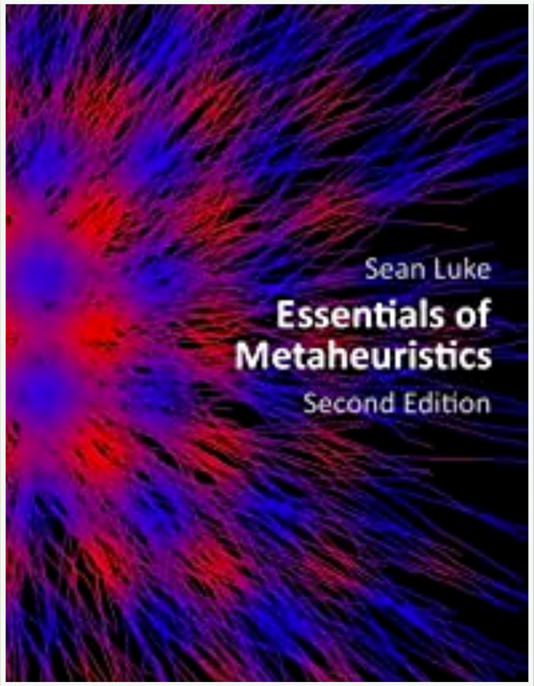
MULTIPLE RESTARTS

- For Hill Climbing and Simulated Annealing we can reduce the risk of getting stuck on a local optimum by repeating the process several times
- Each repetition is independent…
- …can we do better?
- The idea is to use a multiset of solutions instead of working with one solution at a time
- This time the different solutions “interact” in some way

OUTLINE OF THE COURSE

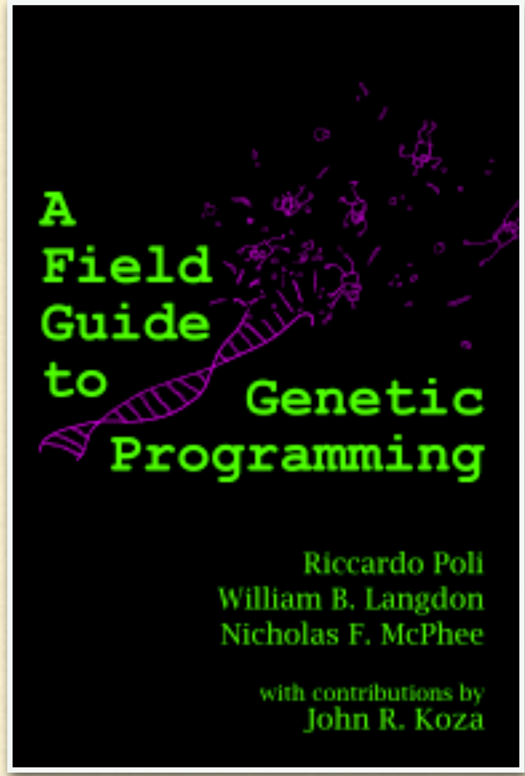
- Genetic Algorithms
- Evolution Strategies
- Genetic Programming
- Particle Swarm Optimization and Ant-Colony Optimization
- Differential Evolution
- Neuroevolution
- EDA and CMA-ES
- Parallel implementations
- Multi-objective optimization
- Coevolution
- Policy Optimization
- Theory of Evolutionary Computation

REFERENCE MATERIAL

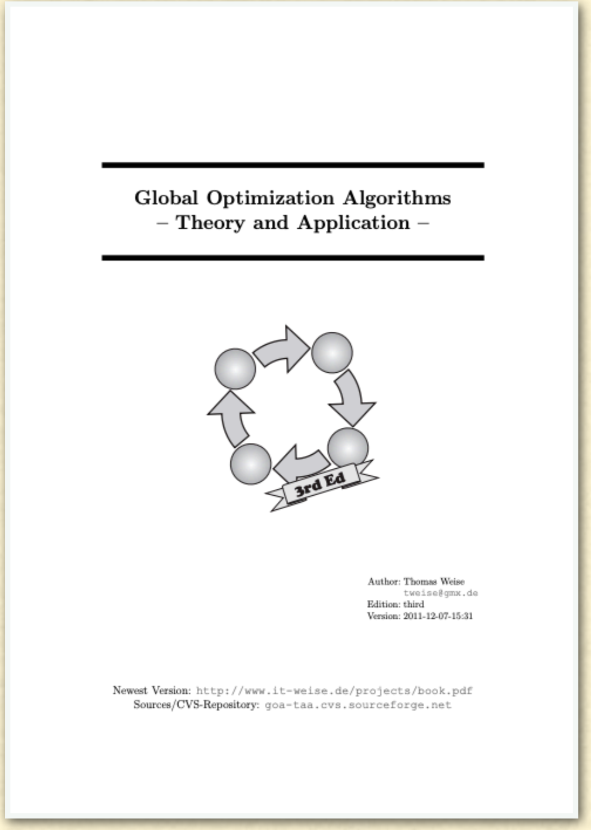


S. Luke
Essentials of Metaheuristics, 2nd Edition
https://cs.gmu.edu/~sean/book/metaheuristics/

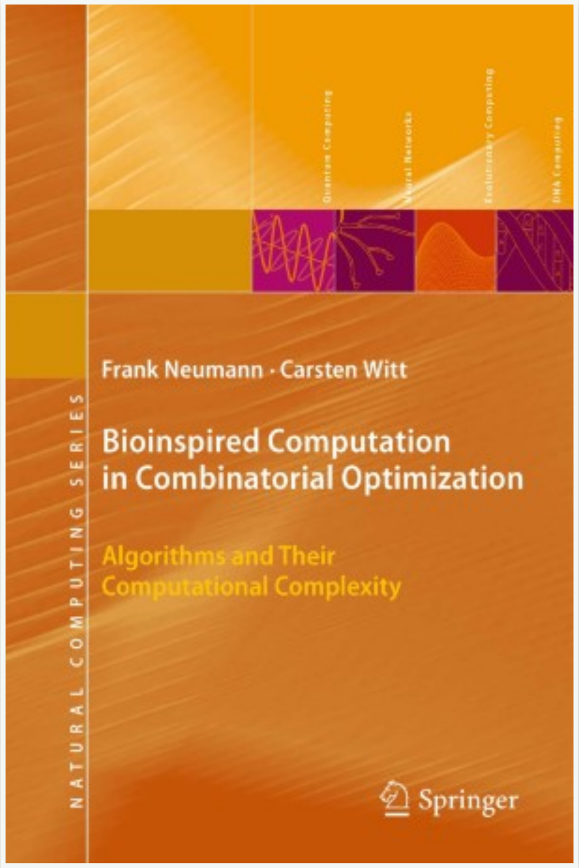
R. Poli, W. R. Langdon, N. F. McPhee
A Field Guide to Genetic Programming
http://www.gp-field-guide.org.uk



REFERENCE MATERIAL



T. Weise
Global Optimization Algorithms – Theory and Application, 3rd Edition
(Search for it online)



F. Neumann and C. Witt
Bioinspired Computation in Combinatorial Optimization
Algorithms and Their Computational Complexity
http://www.bioinspiredcomputation.com/self-archived-bookNeumannWitt.pdf

GENETIC ALGORITHMS

GENETIC ALGORITHMS

- Invented by John Holland in the Seventies:
  John Holland, *Adaptation in Natural and Artificial Systems*, University of Michigan Press, 1975

- Inspired by the Darwinian theory of evolution

- A multiset of solutions (called *population*, each solution is an *individual*) is iteratively evolved, with each iteration consisting of

  - Selection

  - Crossover and mutation

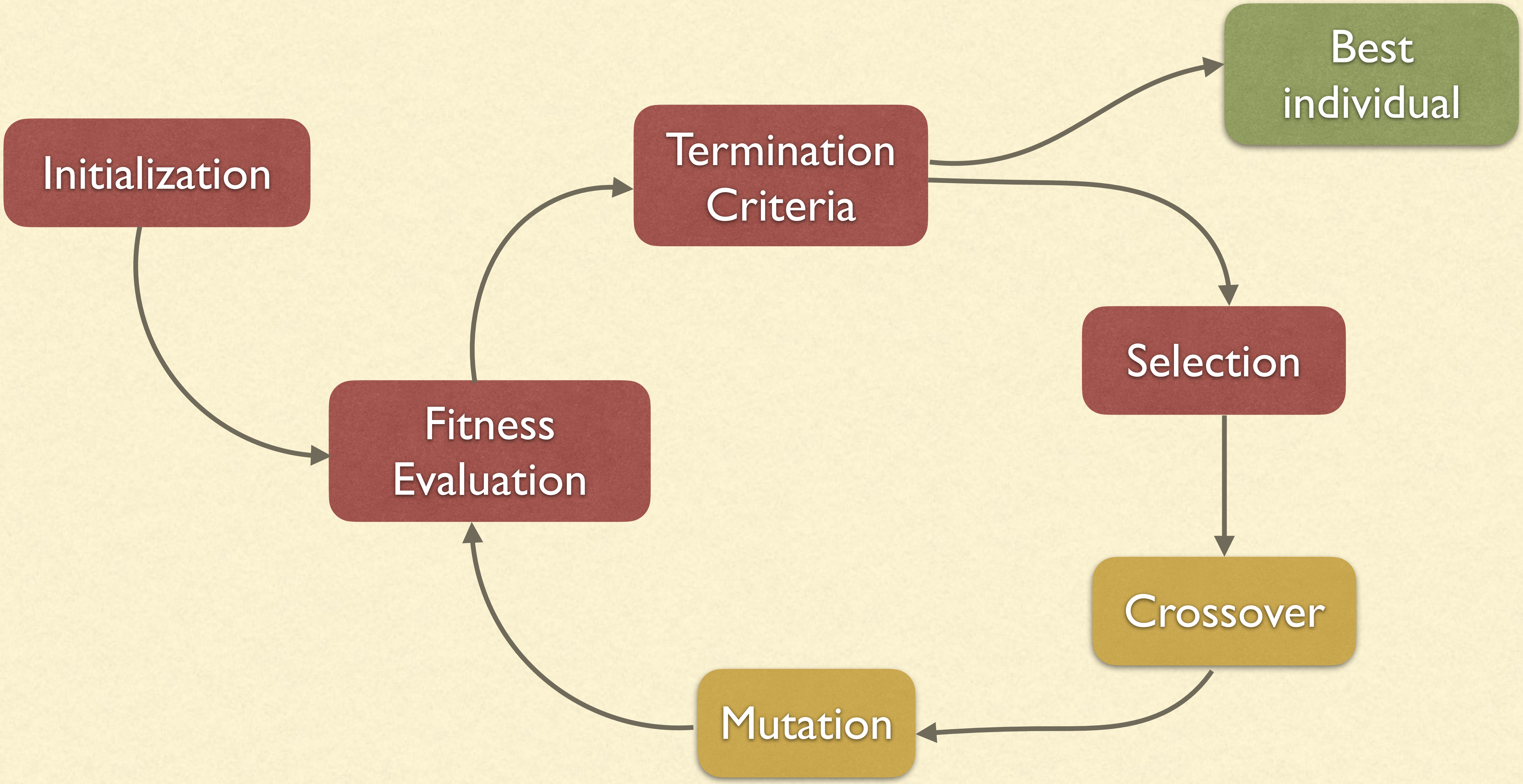
GENETIC ALGORITHMS

- Solutions are usually represented as binary strings of fixed length
- This is not a requirement, as we will see in one of the next lectures
- We must now distinguish between the **genotype** and the **phenotype** of a solution, since some operators works on the genotype and some on the phenotype

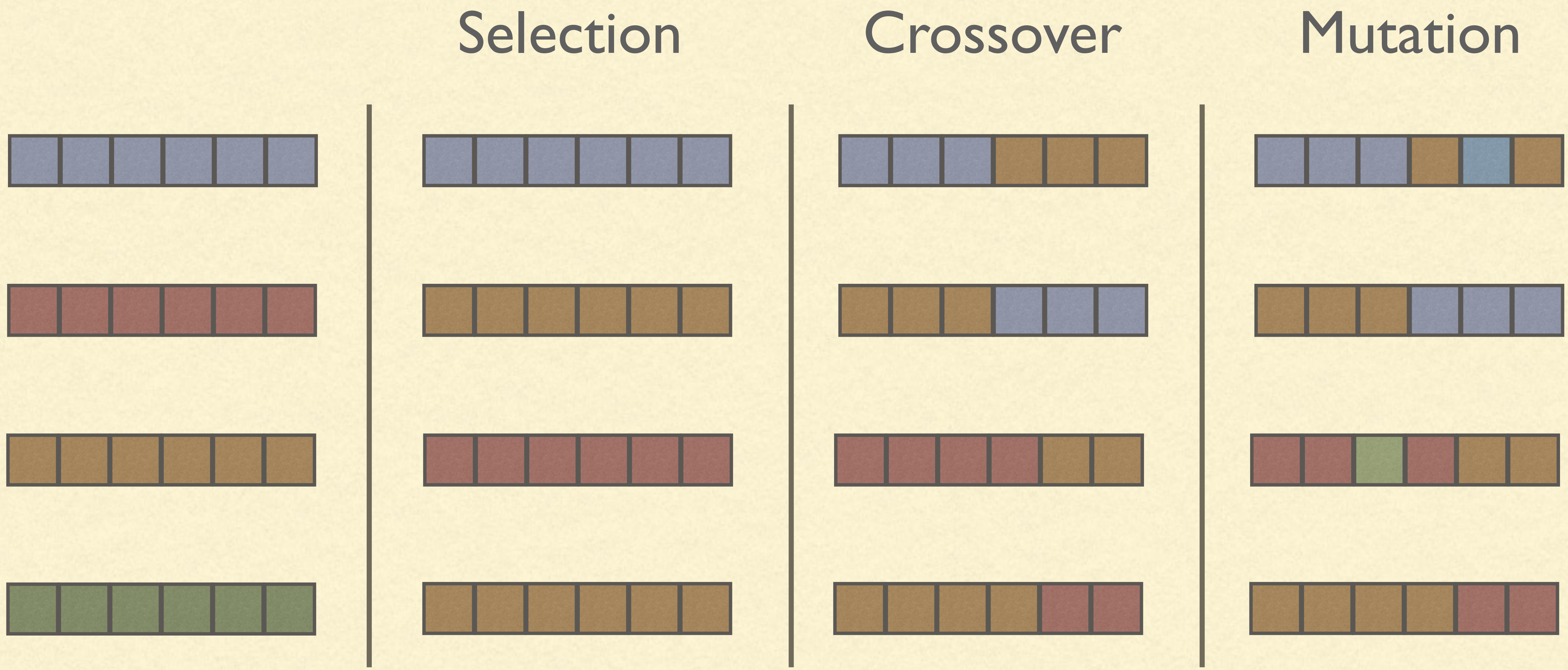
PHENOTYPE AND GENOTYPE

- The **genotype** is how a solution is represented.
  E.g., a string of bits.
  - Crossover and mutation works on the genotype of a solution
- The **phenotype** is the actual solution. E.g., the number of ones, the number represented by a string of bits, etc.
  - The fitness computes how good the phenotype of a solution is, without considering the genotype
  - Selection operates only on the phenotype ignoring the genotype

EVOLUTION CYCLE



A GA GENERATION



GA PARAMETERS

- Population size N
- Type of selection
- Type of crossover
- Crossover probability p_{cross}, usually near one
- Type of mutation
- Mutation probability p_{mut}, usually small
- Elitism or others additional modifications

SELECTION METHODS

- There are multiple ways to decide which individuals are selected:
  - Roulette wheel selection
  - Ranked selection
  - Tournament selection

ROULETTE WHEEL SELECTION

The probability of an individual to be selected is proportional to its fitness

$$p_{x,P} = \frac{f(x)}{\sum_{y \in P} f(y)}$$

Probability of x getting selected given that the current population is P.

ROULETTE WHEEL SELECTION

- **Pro**: easy to implement
- **Cons**: if an individual has a very large fitness w.r.t. the others in the population then we may reduce the diversity in the population by continuously selecting it
- We may want something that depends on the *ranking* of the fitnesses, not on their raw value

RANKED SELECTION

- We compute the fitness of all individuals in the population
- The individuals are ranked w.r.t. their fitness values
- Each rank has a fixed probability of being selected
  - E.g., the individual with the i^{th} best fitness will be selected with probability $\dfrac{N-i+1}{r_{\text{sum}}}$ where r_{sum} is a normalisation factor

TOURNAMENT SELECTION

- Tournament selection is the most used kind of selection in GA
- Let $t \in \mathbb{N}^+$ be the *tournament size*
- Extract t individuals from the current population (with reinsertion)
- Select the one with the best fitness

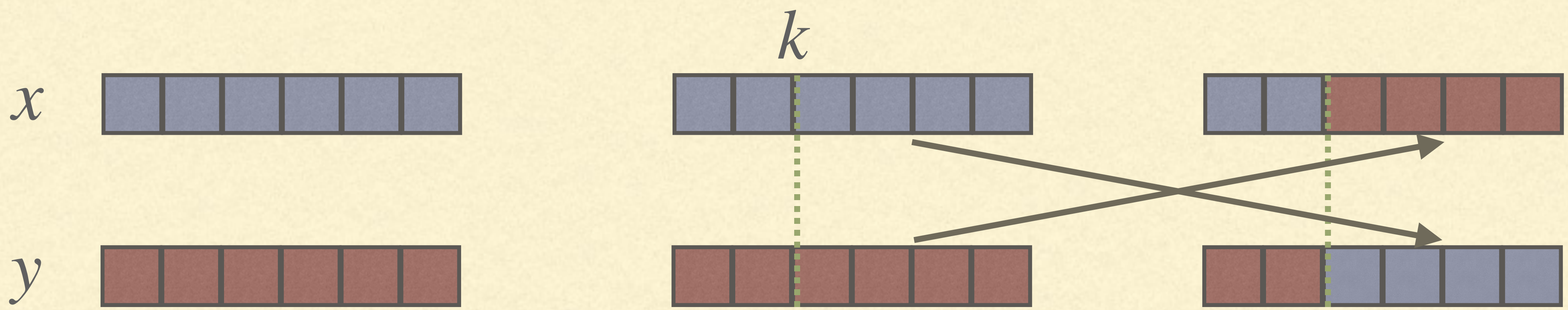
TOURNAMENT SELECTION

- Has the advantage of providing a "ranked" selection without specifying the function to assign the probabilities
- The "selection pressure" (how difficult it is for a non-fit individual to be selected) can easily be tuned via the tournament size
  - Large tournament size → high selection pressure
  - Low tournament size → low selection pressure

CROSSOVERS

- Some common crossovers:
  - One-point crossover
  - m-points crossover
  - Uniform crossover

ONE-POINT CROSSOVER



- Given the two parent $x = x_1 x_2 \cdots x_n$ and $y = y_1 y_2 \cdots y_n$
- A crossover point $k \in \{1, \ldots, n\}$ is selected uniformly at random
- The two offsprings are $x_1 \cdots x_k y_{k+1} \cdots y_n$ and $y_1 \cdots y_k x_{k+1} \cdots x_n$

m-POINTS CROSSOVER

- A direct generalization of one-point crossover where more than one point is selected
- $k_1 \ldots k_m \in \{1, \ldots, n\}$ crossover points are selected (with $k_i \leq k_{i+1}$ for all $i \in \{1, \ldots, m-1\}$)
- The elements of the two parents are swapped between each pair of consecutive crossover points

UNIFORM CROSSOVER

On average half of the bits will be exchanged

- Given the two parent $x = x_1 x_2 \cdots x_n$ and $y = y_1 y_2 \cdots y_n$
- For each $i \in \{1, \ldots, n\}$ with probability $1/2$ the i^{th} element in the first (resp., second) offspring will be x_i (resp., y_i) and otherwise y_i (resp., x_i)

BIT-FLIP MUTATION

x 

- Given an individual $x = x_1 x_2 \cdots x_n$
- For each $i \in \{1, \ldots, n\}$ flip the bit x_i with probability p_{mut}
- Usually $p_{\text{mut}} = \dfrac{1}{n}$ to mutate (on average) one bit per individual

CROSSOVER AND MUTATION

- Crossover is **not** “global” mutation
- That is, given two Boolean vectors x and y it is not possible to obtain every possible vector from them. Why?
- If $x_i = y_i = 1$ then the result of crossover will never have $x_i = 0$
- This will be important for the definition of the topological properties of crossover and mutation

EXPLOITATIVE VARIANTS

- **Elitism**. A certain fraction of the individuals with the best fitness are preserved in the next generation unless better solutions are found
  - Keep only the best individual found so far
  - Keep the top k individuals
  - Keep the top $p\%$ of individual
- Elitism changes the selection pressure: new individuals have better "competitors" in the next selection phase

STEADY STATE GA

- Instead of creating a completely new population at each iteration we only replace some of the individuals in the existing population
- Which individuals to replace?
  - The worst ones
  - A random selection

HYBRID GA

- After each generation all individuals are improved with a local search algorithm (e.g., hill climbing)
- Called “Memetic Algorithms”, better names are "Lamarckian algorithms” or “Baldwin Effect Algorithms”
- Parameters:
  - How frequently the local search is performed
  - How many iterations of local search are performed each time

REPRESENTATION

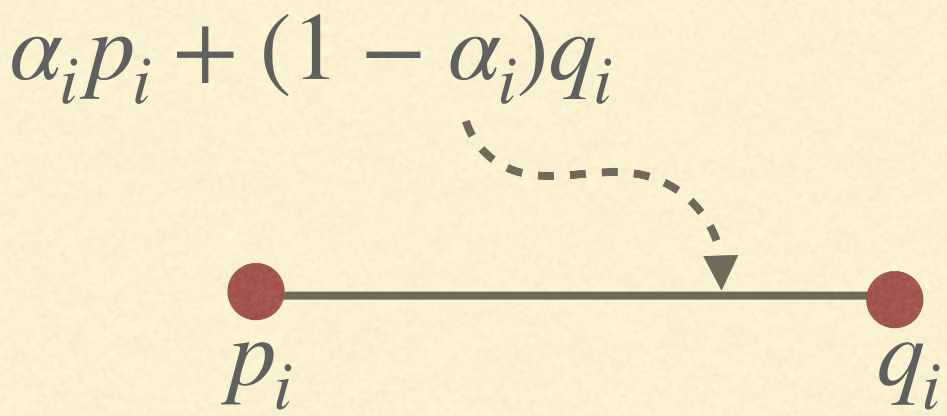
- **Beyond Binary**. It is possible to generalize GA to use symbols from a finite set/alphabet Σ instead of using only $\{0,1\}$
  - The only difference is that mutation will have to select (usually uniformly at random) between $|\Sigma| - 1$ symbols instead of simply flipping a bit
  - If there is an ordering between the elements of Σ (e.g., $\Sigma = \{0,1,2,3\}$) then mutation can be changed to be, for example "add or subtract one".

SPECIAL REPRESENTATIONS FOR GENETIC ALGORITHMS

REAL-VALUED GA

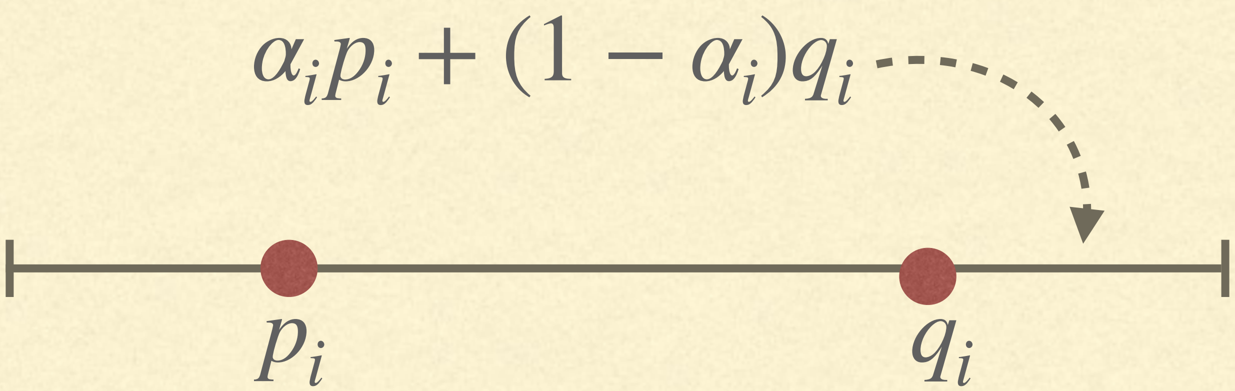
- Until now we have seen binary valued (or integer valued) GA
- We can represent each floating point numbers as 32/64 binary genes…
- …but this means that different bits have different impact on the encoded number
- If each gene is a floating point value then mutation and crossover should be adapted

CROSSOVER



Intermediate recombination

$\alpha_i \leftarrow$ random$(0,1)$

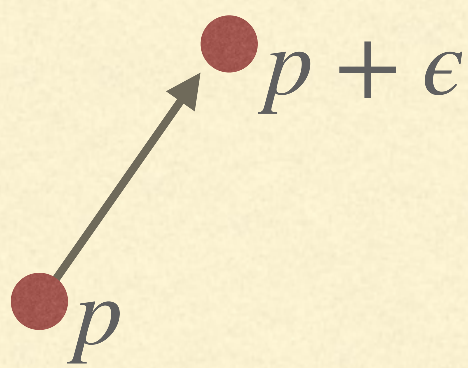


Line recombination

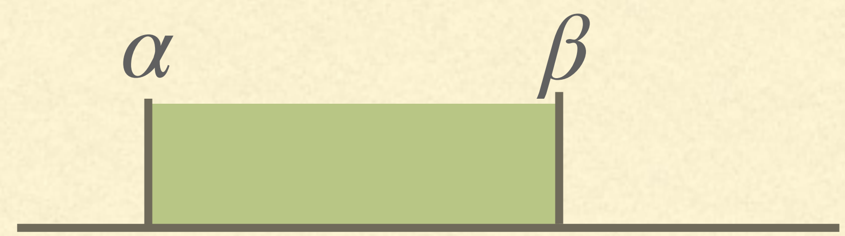
$\alpha_i \leftarrow$ random$(-k, 1 + k)$

MUTATION

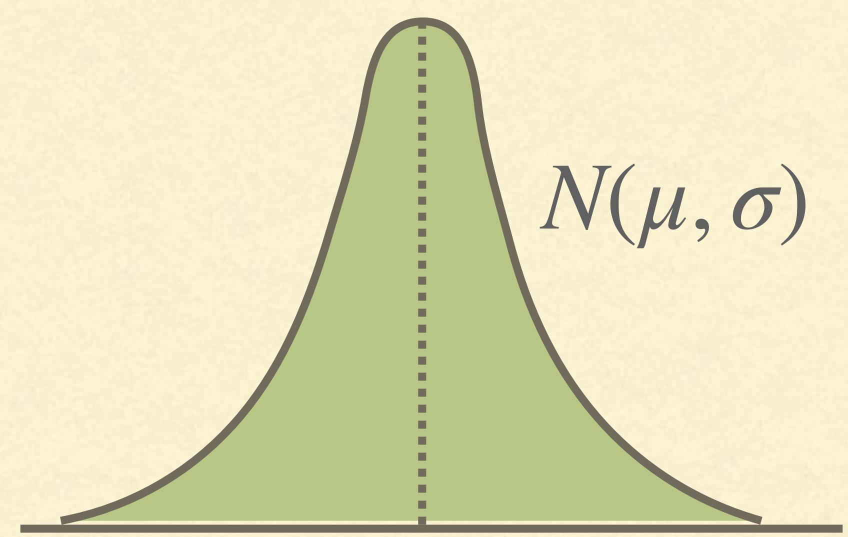
Add a small value
to each coordinate
of the individual



Uniform between two values



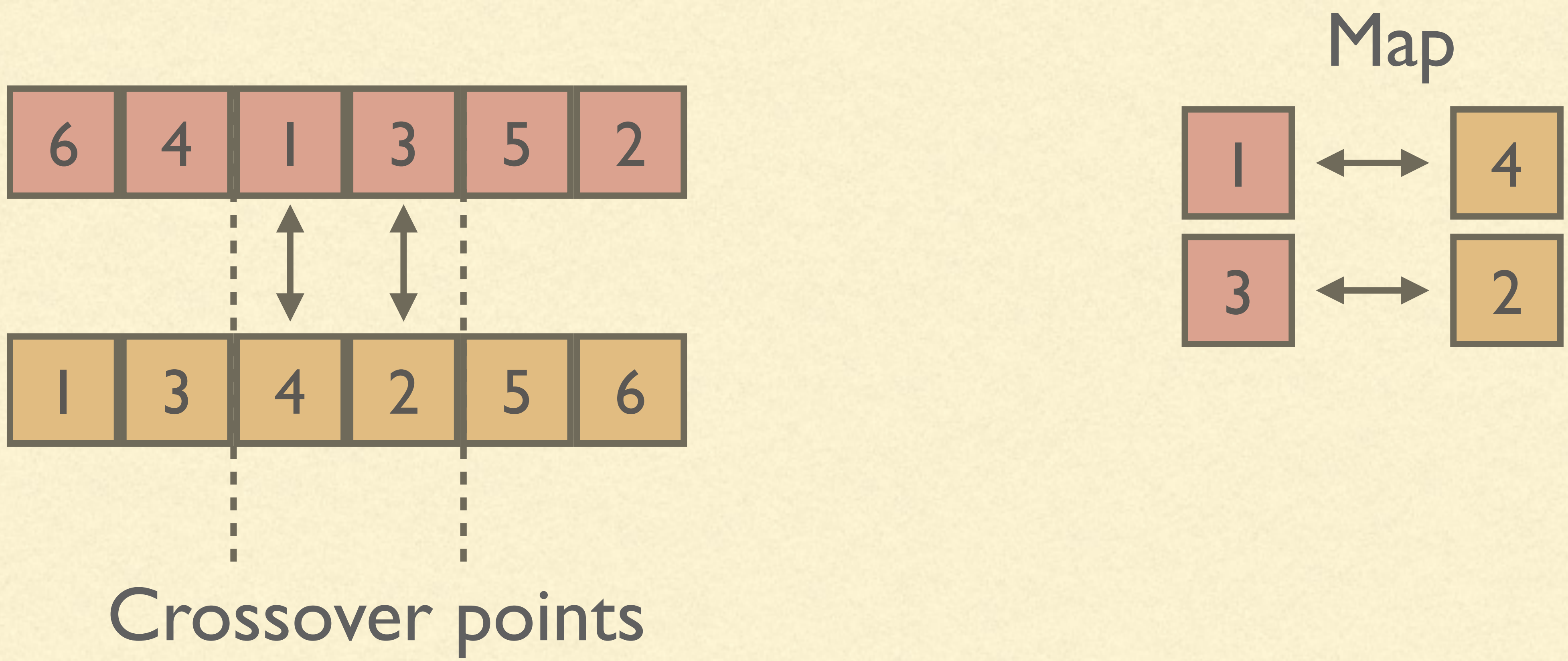
Gaussian



CYCLE AND PMX CROSSOVERS

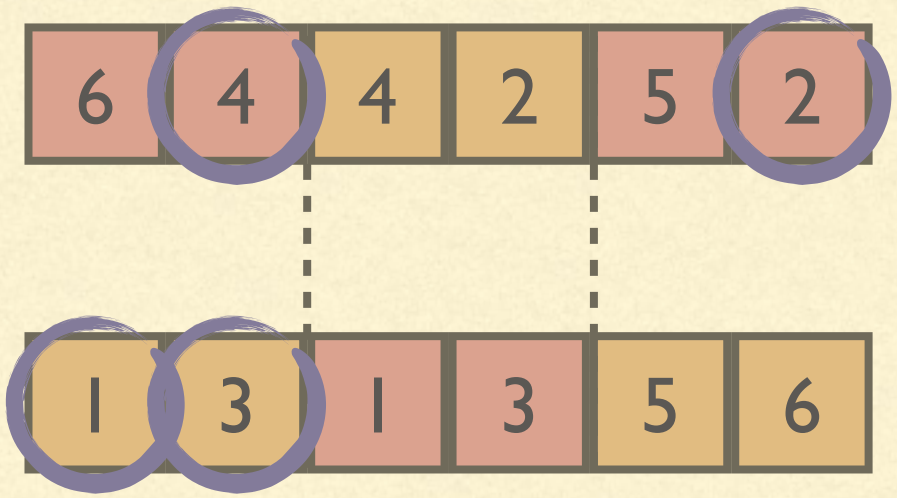
- Sometimes we need additional constraints in the representation of an individual by GA
- One usual constraint is that each individual must be a permutation of the numbers from 1 to n
- Mutation can be performed by swapping two positions
- Traditional crossover usually do not respect the constraints

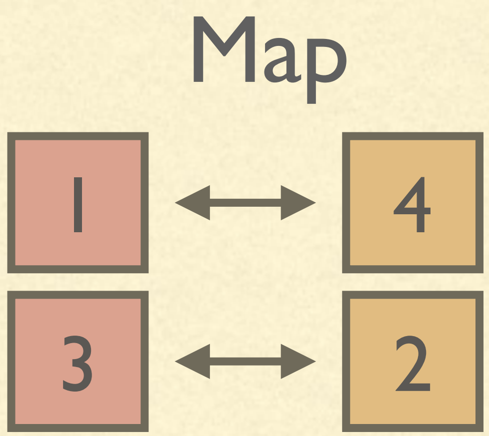
PARTIALLY MAPPED CROSSOVER (PMX)



We select two crossover point and we build a map

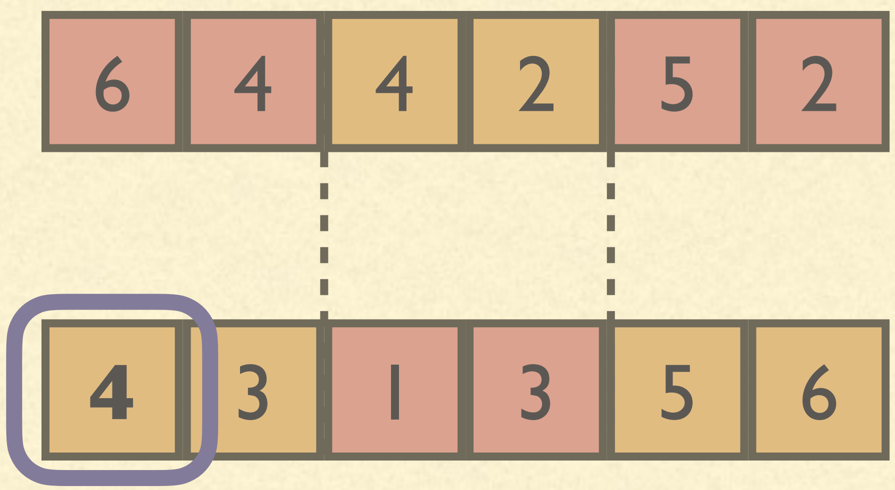
PARTIALLY MAPPED CROSSOVER (PMX)

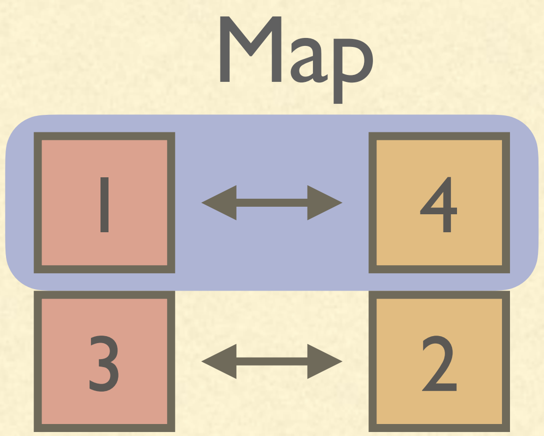




We perform the exchange but the offspring are not valid

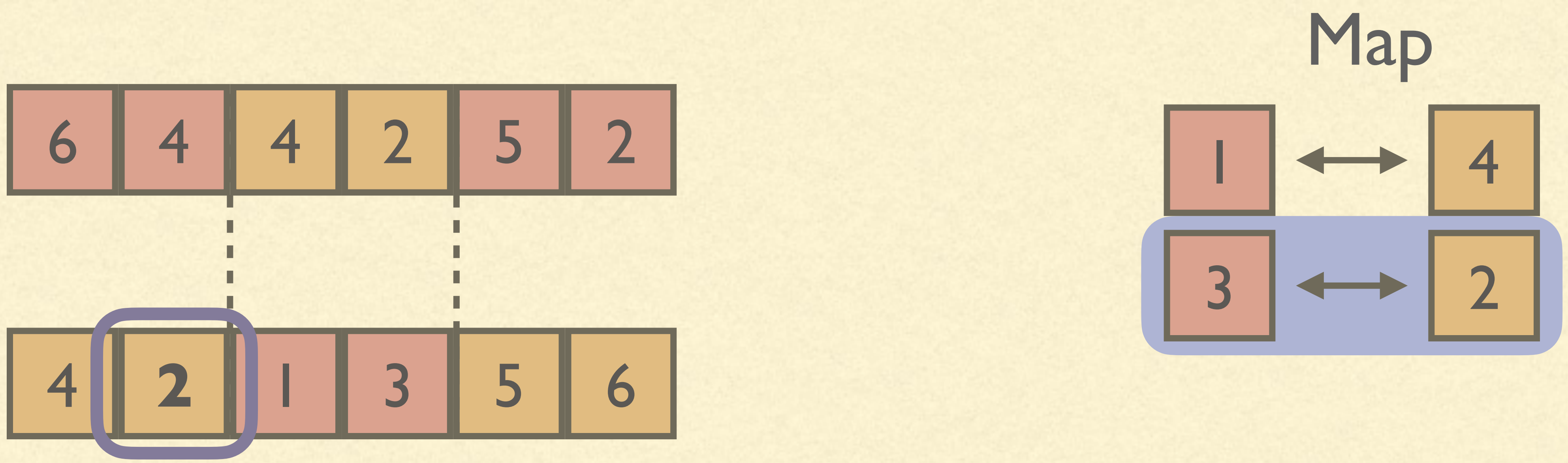
PARTIALLY MAPPED CROSSOVER (PMX)





We iterate the map until we have resolved the conflicts

PARTIALLY MAPPED CROSSOVER (PMX)



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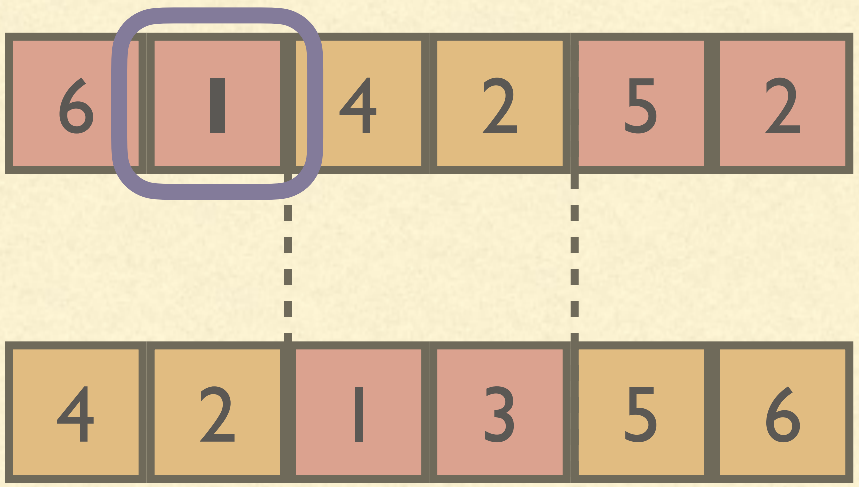

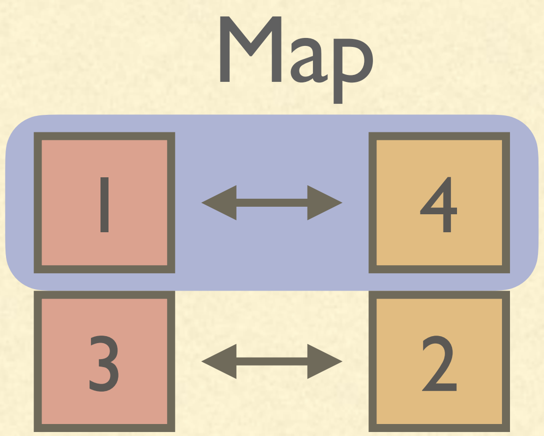

We iterate the map until we have resolved the conflicts

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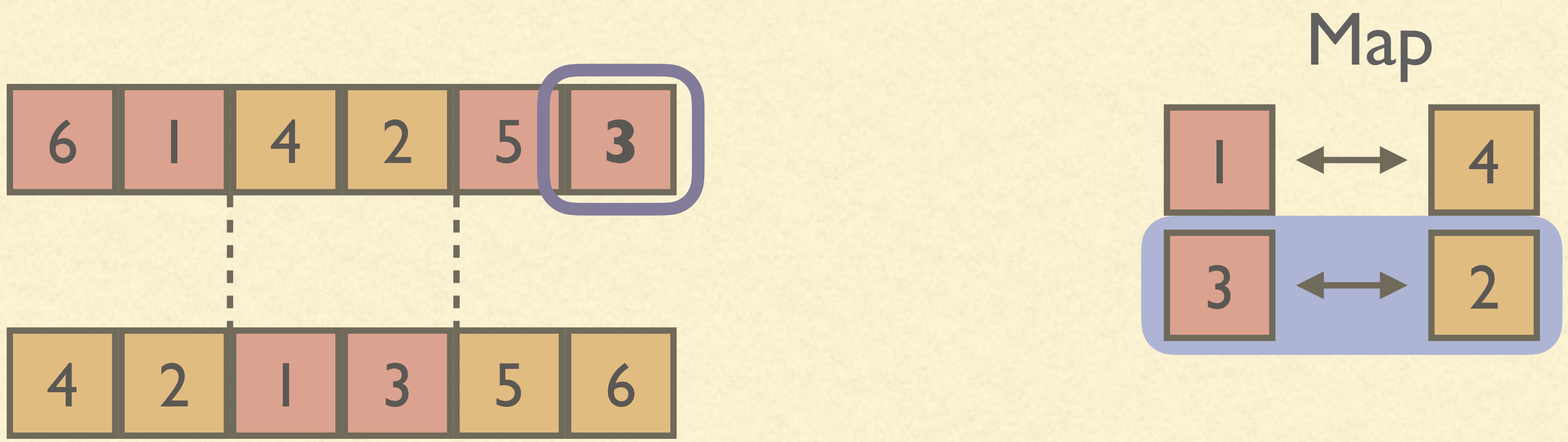
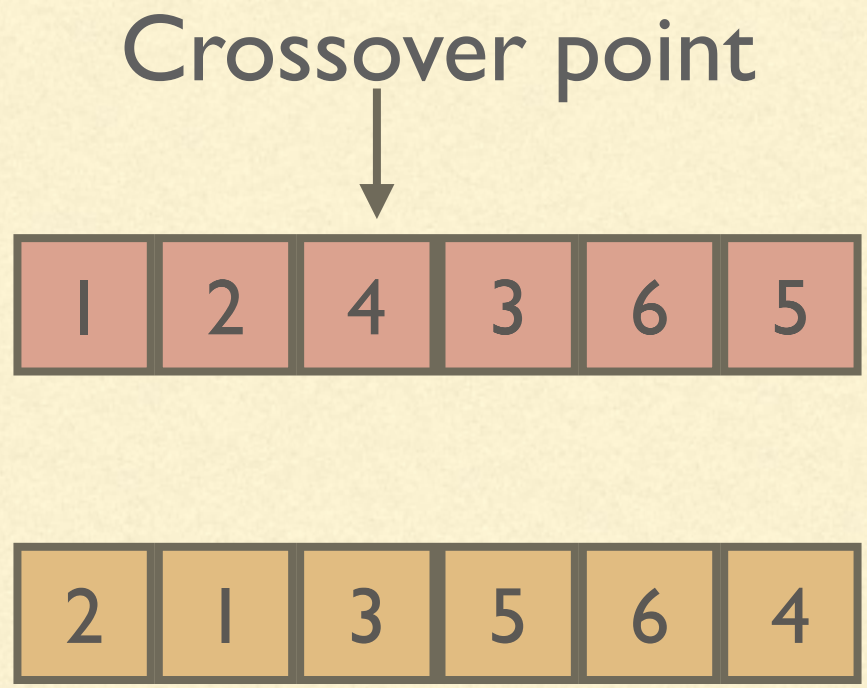


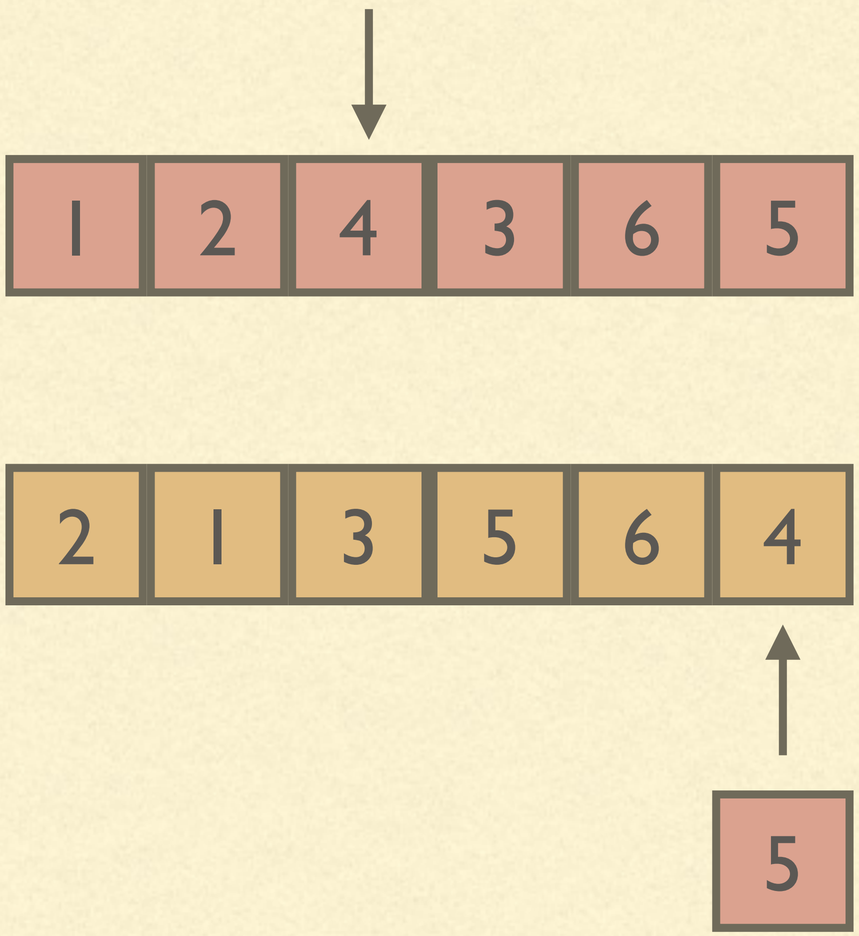
We iterate the map until we have resolved the conflicts

CYCLE CROSSOVER



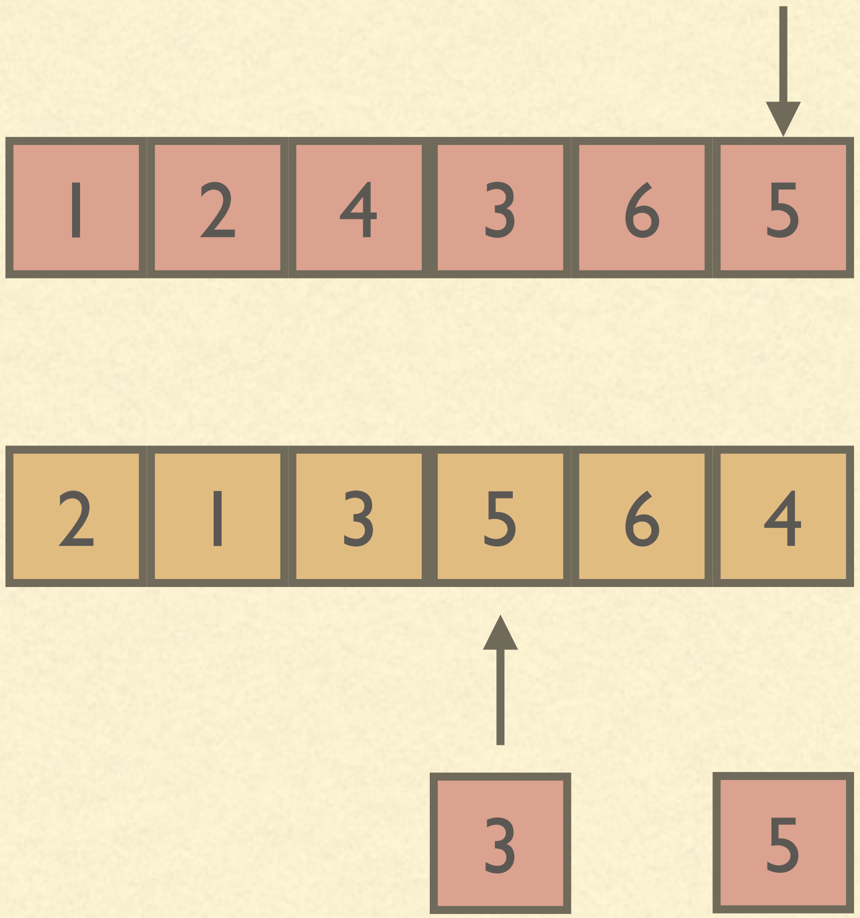
We select a single starting point
and we search che same value in the second parent

CYCLE CROSSOVER



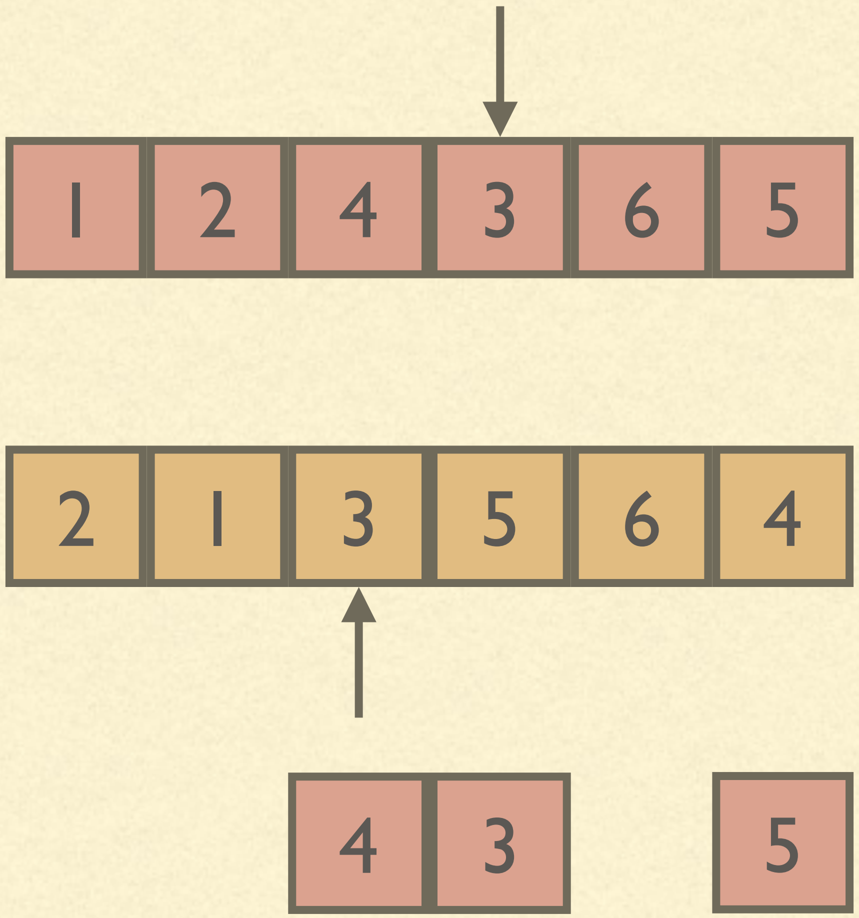
Once found we copy the value from the first parent.
Repeat until we return to the beginning

CYCLE CROSSOVER



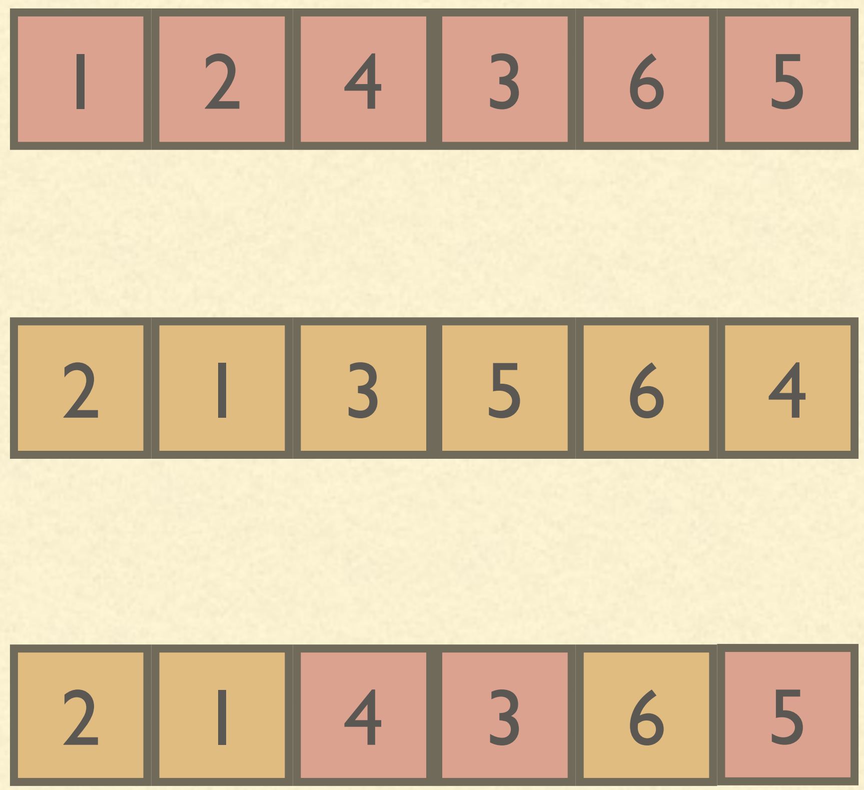
Once found we copy the value from the first parent.
Repeat until we return to the beginning

CYCLE CROSSOVER



Once found we copy the value from the first parent.
Repeat until we return to the beginning

CYCLE CROSSOVER



We copy the remaining elements from the second parent

REPRESENTING GRAPHS

- You might want to represent graphs. Possibly because the are ubiquitous in computer science.
- You can represent graph in two ways:
  - *Direct encoding*. By actually representing vertices and edges
  - *Indirect encoding*. By representing some "device" that builds a graph

ADJACENCY MATRIX

Side of the matrix = max number of nodes

$$\begin{bmatrix} 0.4 & \text{no edge} & 0.6 & -5.3 \\ \text{no edge} & 5.6 & 0.1 & 0.2 \\ 2.4 & 0.8 & 4.1 & 8.3 \\ -0.2 & \text{no edge} & 0.5 & \text{no edge} \end{bmatrix}$$

Special value to represent missing edges

LARGE GRAPHS

$V = \{a, b, c, d, e\}$ We evolve the sets of vertices and edges

$E = \{(a, b), (a, c), (d, a), (e, e)\}$

Possible mutations:

- Add an edge
- Add a node
- Remove an edge
- Remove a node and all its edges
- …

Each one can have
a different probability

Crossover is difficult
to define and you might
decide not to use it

PRODUCTION RULES

- There are terminal symbols and non-terminal symbols
- Production rules map a non-terminal symbol into a sequence/matrix of non-terminal and terminal symbols
- We continue the expansion until the configuration is composed only of terminal symbols
- By using adeguate production rules we can encode indirectly a graph (i.e., rules that build a graph)

PRODUCTION RULES

$$S \rightarrow \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

$$A \rightarrow \begin{bmatrix} c & p \\ a & c \end{bmatrix} \; B \rightarrow \begin{bmatrix} a & a \\ a & e \end{bmatrix} \; C \rightarrow \begin{bmatrix} a & a \\ a & a \end{bmatrix} \; D \rightarrow \begin{bmatrix} a & a \\ a & b \end{bmatrix}$$

$$a \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \; b \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \; c \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \; e \rightarrow \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} \; p \rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

Ruleset used in an example in:

Hiroaki Kitano, Designing neural networks using a genetic algorithm with a graph generation system

PRODUCTION RULES

Starting from an axiom [S] we can iterate the production rules

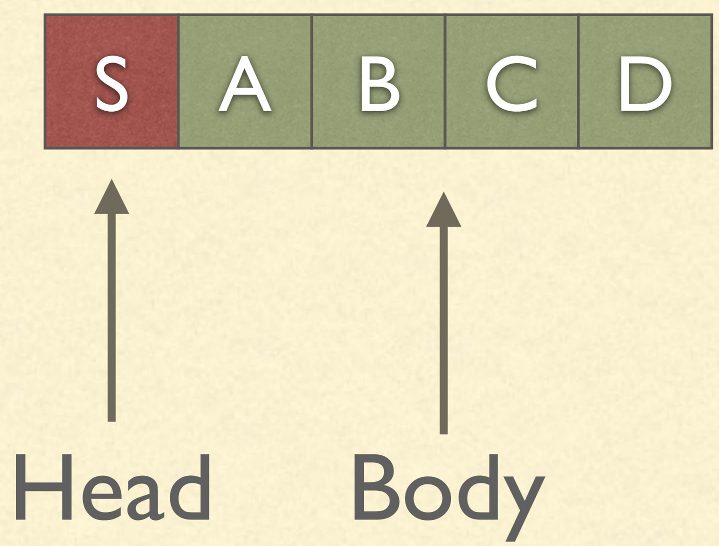
$$[S] \longrightarrow \begin{bmatrix} A & B \\ C & D \end{bmatrix} \longrightarrow \begin{bmatrix} c & p & a & a \\ a & c & a & e \\ a & a & a & a \\ a & a & a & b \end{bmatrix} \longrightarrow \cdots$$

PRODUCTION RULES

$$
\begin{bmatrix}
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
$$

A graph of 5 vertices
(8 encoded but 3 of them
are not connected to anything)

PRODUCTION RULE: ENCODING



encodes $S \rightarrow \begin{bmatrix} A & B \\ C & D \end{bmatrix}$

Since now we have a vector of fixed length,
to perform the evolution
we can apply traditional GA operators