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BASICS OF EVOLUTIONARY COMPUTING

Synopsis of lectures

Tutorial
for master's degree holders
according to the educational program "Software engineering of computer systems»
specialties 121 "Software engineering"
according to the educational program "Computer systems and networks»
specialty 123 "Computer engineering"
according to the educational program "Information management systems and technologies»
specialties 126 "Information systems and technologies»

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Основи еволюційних обчислень

-

Basics of Evolutional Algorithms

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Lecture 01. Introduction

Content

- Recommended Sources
- What are Genetic Algorithms (GAs)?
- GA Analogy with IT
- Components of GA
- Main Hypothesis behind GAs
- Differences between GAs and Traditional Algorithms
- Advantages of GAs
- Limitations of GAs
- When to use GAs

Recommended Sources - Books

(some of them are used here!)

Books (classic):

Holland, J. H. (1992). *Adaptation in natural and artificial systems: an introductory analysis with applications to biology, control, and artificial intelligence.* MIT press. **<- inventor of GA(!), the highest number of citations for GA-publication by Google Scholar!**

Mitchell, M. (1998). *An introduction to genetic algorithms.* MIT press. **<- classic textbook, the highest number of citations for GA-textbook by Google Scholar!**

Books (with codes at github):

Wirsansky, E. (2020). *Hands-On Genetic Algorithms with Python.* Packt Publishing

Sheppard, C. (2019). *Genetic Algorithms with Python* (self-published).

Recommended Sources - Papers

(some of them are used here!)

Holland, J. H. (1992). *Genetic algorithms*. Scientific American, 267(1), 66-73. <- inventor of GA(!) <- **Just for Fun! :)**

Katoch, S., Chauhan, S. S., & Kumar, V. (2020). *A review on genetic algorithm: past, present, and future*. Multimedia Tools and Applications, 1-36.

García-Martínez, C., Rodríguez, F. J., & Lozano, M. (2018). *Genetic Algorithms*, Handbook of Heuristics, 2018, p. 431-464.

Content

- Recommended Sources
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What are genetic algorithms?

Genetic algorithms (GA) are a family of search algorithms inspired by the principles of natural evolution.

Imitating the natural selection and reproduction, GAs can produce high-quality solutions for various **problems**:

- **search,**
- **optimization,**
- **learning.**

Analogy to natural evolution allows GAs **to overcome some problems that are hard for traditional algorithms**, especially for cases with:

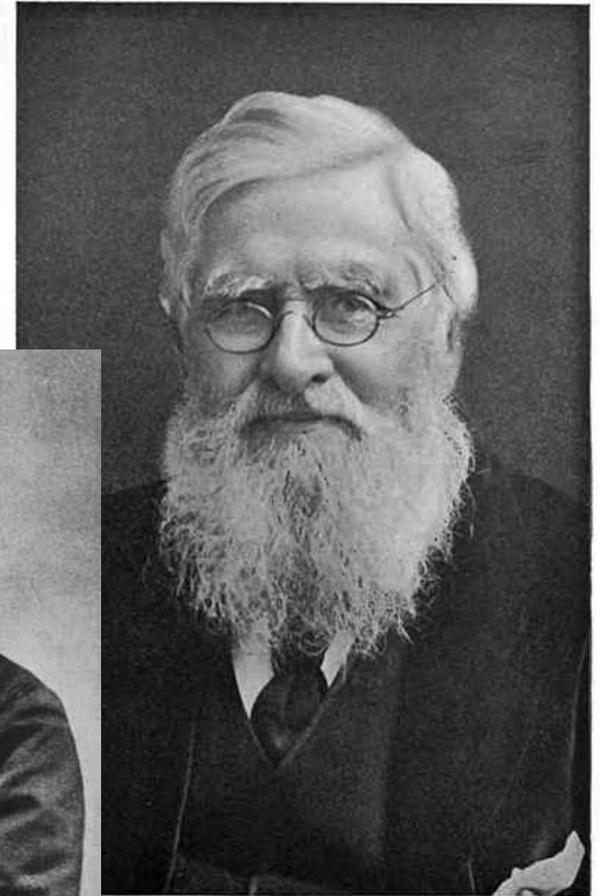
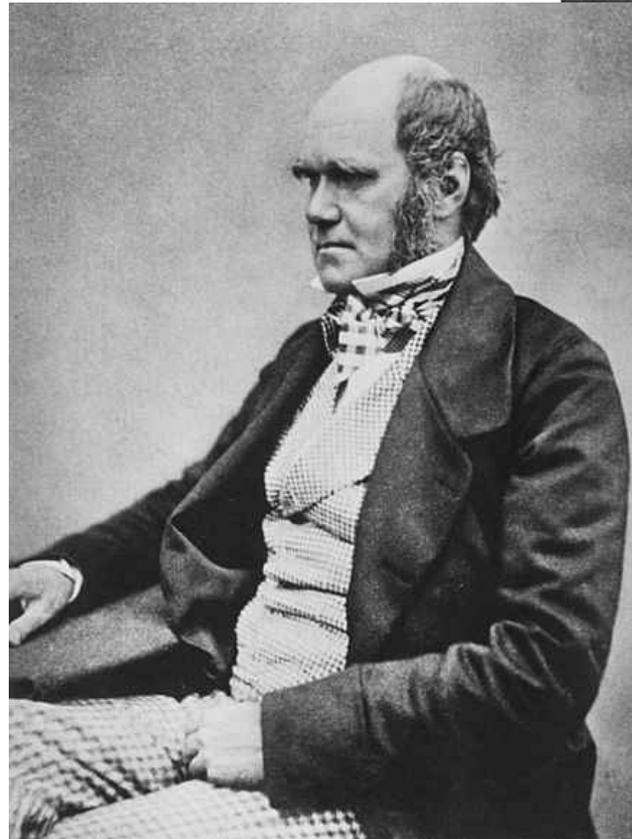
- **large number of parameters** and
- **complex mathematical representations.**

Theory behind GAs - Darwinian evolution

GAs implement a simplified version of the **Darwinian natural evolution.**

The principles of the Darwinian evolution:

- **Variation**
- **Inheritance**
- **Selection**



Alfred R. Wallace

Theory behind GAs - Darwinian evolution

Variation:

The **traits (attributes)** of individual specimens belonging to a population **may vary**.

As a result, the **specimens differ** from each other to some degree, for example, in:

- their **behavior** or
- their **appearance**.

Theory behind GAs - Darwinian evolution

Inheritance:

Some **traits** are consistently **passed** on from specimens **to their offspring**.

As a result, **offspring resemble their parents more than they resemble unrelated specimens**.

Theory behind GAs - Darwinian evolution

Selection:

Populations typically **struggle** for resources within their given environment.

The **specimens** with **traits** that are **better adapted** to the environment:

- **will be more successful** at surviving, and
- **will contribute more offspring** to the next generation.

Theory behind GAs - Darwinian evolution

Resume:

Evolution **maintains** a population of individual **specimens** that **vary** from each other.

Those who are **better adapted** to their environment have a **greater chance of surviving**, breeding, and **passing** their traits to **the next generation**.

This way, as generations go by, **species become more adapted** to their **environment** and to the **challenges** presented to them.

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GA analogy with IT

GAs should find the **optimal solution** for a problem.

Darwinian evolution maintains a population of **individual specimens,**

BUT(!) ... GAs maintain a population of **candidate solutions (individuals),** for that given problem.

The **individuals** are iteratively evaluated and used to create a new generation of **individuals.**

Those who are **better** at solving this problem have a **greater** chance of being selected and passing their qualities to the next generation of **individuals.**

This way ... with generations ... **individuals** get better at solving the problem at hand.

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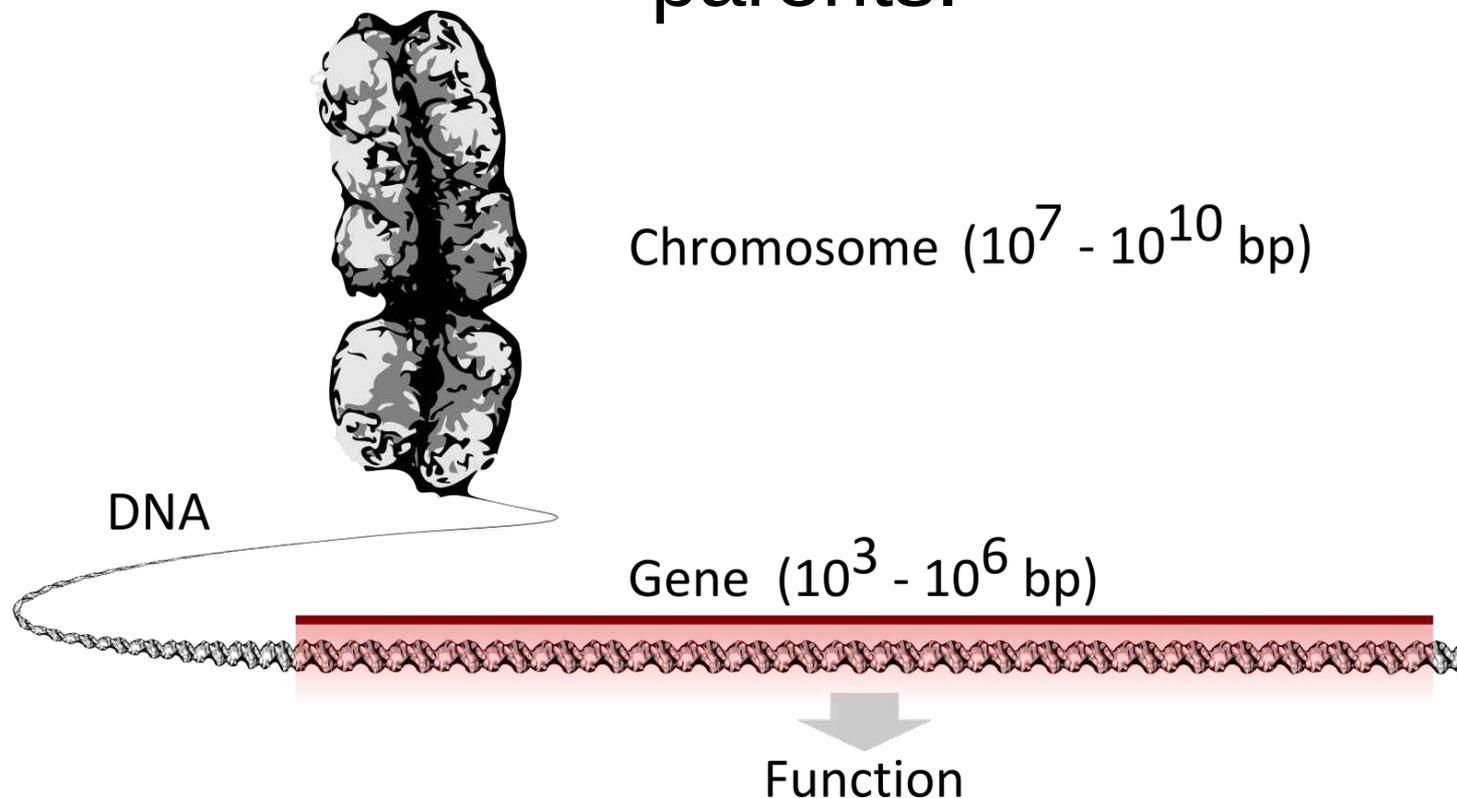
GA analogy with IT - Main Components

- Genotype
- Population
- Fitness function
- Selection
- Crossover
- Mutation

GA analogy with IT -

Main Components - **Genotype**

- **In biology:** **genotype** is a collection of **genes** that are grouped into **chromosomes**. If two specimens breed to create offspring, each **chromosome** of the offspring will **carry a mix of genes** from both parents.



GA analogy with IT -

Main Components - **Genotype**

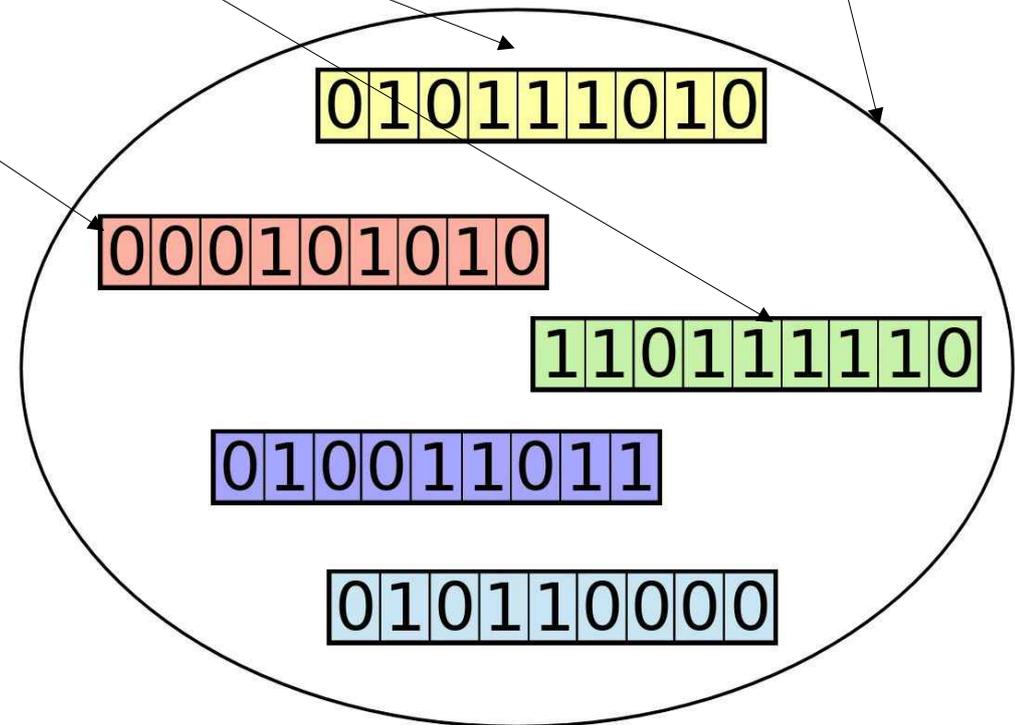
- In IT (GAs):
- each **individual** is represented by 'IT-chromosome' that can be expressed as a **binary string**, where **each bit** represents a single **gene**.

0 1 0 1 1 1 0 1 0

Main Components - Population

- GAs always maintain a **population** of individuals -> a **collection** of candidate solutions for the problem. Individual -> chromosome, population -> collection of chromosomes.

The population represents the **current generation** and **evolves over time** when the current generation is replaced by a new one.



Main Components - **Fitness function**

At each iteration of the GA, the individuals are **evaluated** by a **fitness function** (also called the *target function*). This is the function we seek to optimize or the problem we attempt to solve.

Individuals who achieve a **better** fitness score represent **better** solutions and are more likely to be **chosen to reproduce** and be **represented** in the next generation.

Over time, the **quality** of the solutions **improves**, the **fitness values increase**. The process **can stop** once a solution is **found** with a **satisfactory** fitness value.

Main Components - **Selection**

Selection process is used to **determine** which of the individuals in the population will get to **reproduce** and **create the offspring** that will form the next generation.

This is based on the fitness score of the individuals. Those with **higher** score values are **more likely** to be **chosen and pass** their genetic material to the next generation.

Individuals with **low fitness** values can still be chosen, but **with lower probability**. This way, their genetic material is not completely excluded.

Main Components - Crossover

To create a pair of new individuals, two parents are usually chosen from the current generation, and parts of their chromosomes are **interchanged (crossover or recombination)** to create two new chromosomes representing the offspring.

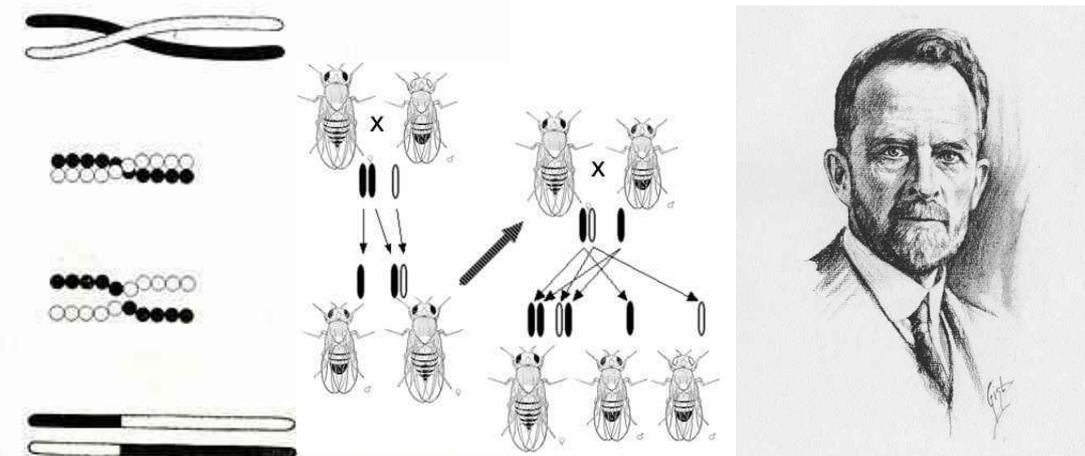
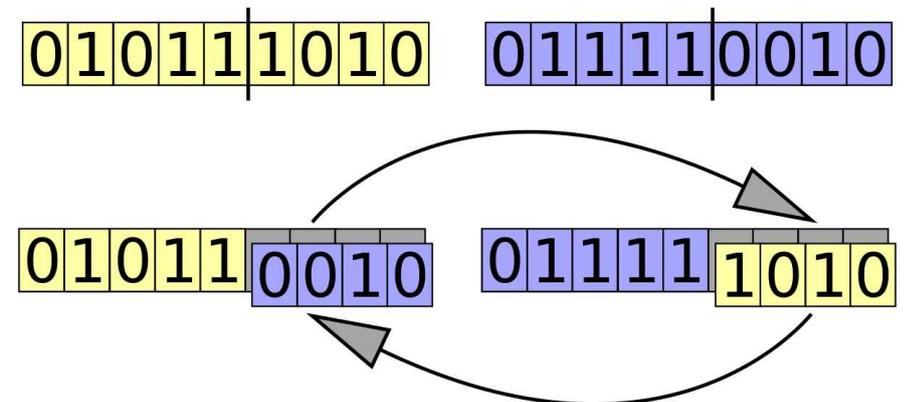


Diagram to illustrate a method of crossing over of chromosomes.

Thomas Hunt Morgan's (Nobel Prize - 1933) illustration of crossing over (1916)

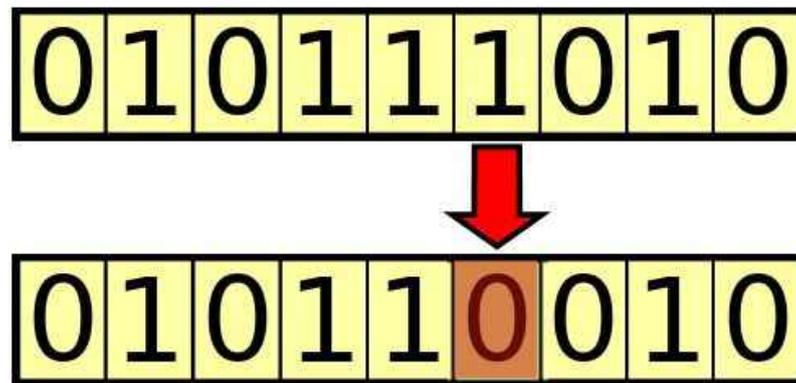


IT GA- version of crossover (recombination)

Main Components - Mutation

The aim of **mutation** (as an operator) is to periodically and randomly **refresh the population, introduce new patterns** into the chromosomes, and **encourage search** in uncharted areas of the solution space.

A **mutation** can be as a **random change** in a gene, for example, flipping a bit in a binary string.



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Main Hypothesis behind GAs

The **building-block hypothesis** -> the **optimal** solution to the problem is **assembled** of small building **blocks**, and as we bring **more** of these building blocks together, we get **closer** to this **optimal** solution.

Individuals in the population with the **desired building blocks** are identified by their **superior scores**.

The **repeated selection/crossover** result in the better individuals conveying these building blocks to the next generations, while possibly combining them with other successful building blocks.

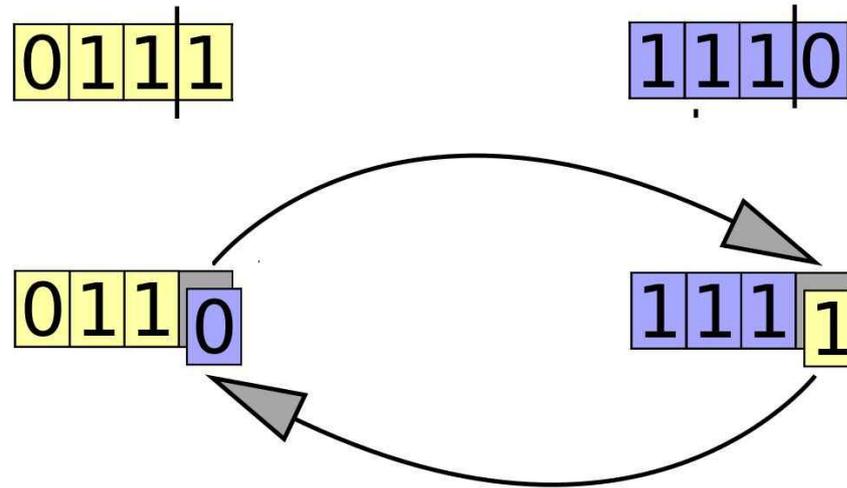
This creates **genetic pressure**, thus **guiding** the population **toward** having more individuals with the building blocks **that form the optimal** solution.

Main Hypothesis - Example

We have a population of 4-digit binary strings.

Aim: to find the string with the **largest** possible sum of digits.

Start: The digit 1 appearing at any of the 4 string positions will be a good building block.



The algorithm progresses will identify solutions that have these building blocks and bring them together. Each **new** generation will have **more** individuals with 1 values in various positions, ultimately resulting in the string 1111, which combines all the desired building blocks

Holland's Schema Theorem

Schema is a **pattern** (or template) that can be found within the chromosomes.

It represents (as a **regular expression** with wildcards) a subset of chromosomes that have a certain similarity among them.

Example: if the set of chromosomes is represented by binary strings of length 4, the schema $1*01$ represents all those chromosomes that have a 1 in the leftmost position, 01 in the rightmost two positions, and either a 1 or a 0 in the second from left position, since the * represents a wildcard value

John Henry Holland

(**February 2**, 1929 – August 9, 2015)

“He is a **founding father of the complex systems approach**. In particular, he developed genetic algorithms and learning classifier systems”.



SANTA FE INSTITUTE



He was a member of the Board of Trustees and Science Board of the Santa Fe Institute and a fellow of the **World Economic Forum**.



THE FRANKLIN INSTITUTE

He received the 1961 **Louis E. Levy Medal** from The Franklin Institute, and the **MacArthur Fellowship** (unofficially known as the "Genius Grant") in 1992.



Holland's Schema Theorem

For each schema, one can assign two metrics:

Order:

The number of digits that are fixed (not wildcards!)

The following table provides several examples of four-digit binary schemata and their measurements:

Schema	Order	Defining Length
1101	4	3
1*01	3	3
*101	3	2
*1*1	2	2
**01	2	1
1***	1	0
****	0	0

Each chromosome in the population corresponds to multiple schemata in the same way that a given string matches regular expressions. The chromosome **1101**, for example,

Holland's Schema Theorem

The fundamental theorem of GAs:

The frequency of schemata of **low order**, **short defining length**, and **above-average fitness** increases exponentially in successive generations.

In other words: the **smaller, simpler** building blocks that represent the attributes **that make a solution better** will become **increasingly present** in the population as the GA progresses.

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Differences GAs from Traditional Algorithms

The key characteristics of GAs distinguishing them from traditional algorithms are:

- Maintaining a **population** of solutions
- Using a **genetic representation** of the solutions
- Utilizing the outcome of a **fitness** function
 - Exhibiting a **probabilistic** behavior

Differences GAs

from Traditional Algorithms -

Maintaining a Population of Solutions

GA operates over a population of candidate solutions (individuals) rather than a single candidate.

GA works with a **set** of individuals that form the current generation. **Each iteration** of the GA creates the next generation of **set** of individuals.

In contrast, most other search algorithms **maintain a single solution** and iteratively modify it in search of the best solution.

Example: The ***gradient descent algorithm*** (widely used in ML/DL) iteratively **works with the current solution** (moves it in the direction of steepest descent, defined by the negative of the function's gradient).

Differences GAs from Traditional Algorithms - Genetic Representation of Solutions

Traditional algorithms: operate directly on candidate solutions,

GAs: operate on their representations (or coding), often referred to as **chromosomes**.

Example: a chromosome is a fixed binary string.

The **genetic operations** are used for chromosomes:

- **Crossover** is interchanging chromosome parts between two parents.
- **Mutation** is modifying parts of the chromosome.

A side effect: GAs are **not aware** of what the chromosomes represent and do **not interpret** them.

Differences GAs from Traditional Algorithms - Result of Fitness Function

Fitness function (FF) represents (estimate) the problem we would like to solve.

Aim of GAs: to find the individuals that yield the **highest score** when this FF is calculated for them.

Traditional algorithms: **use the derivatives** or any other information related to FF.

GAs: **only** consider the **value** obtained by the FF. This allows to use FFs that are hard or impossible to mathematically differentiate.

Differences GAs from Traditional Algorithms - **Probabilistic Behavior**

Traditional algorithms: are **deterministic**.

GAs: the rules are **probabilistic**.

Example: when selecting the individuals that will be used to create the next generation, the **probability** of selecting a given individual **increases with** the individual's **fitness**, but there is still a random element in making that choice.

Mutation is probability-driven, usually makes changes at random location(s) in the chromosome.

Crossover can have a probabilistic element as well.

Despite the probabilistic nature, **GA is not random**; instead, it **uses the random** aspect to direct the search toward areas in the search space where there is a better chance to improve the results.

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Advantages of GAs

- **Global** optimization capability
- Handling problems with a **complex** mathematical representation
- Handling problems that **lack** mathematical representation
 - **Resilience** to noise
- Support for **parallelism** and distributed processing
 - Suitability for **continuous learning**

Advantages of GAs - Global Optimization Capability

Traditional algorithms
(gradient-based):

may stuck in a local maximum rather than finding the global one

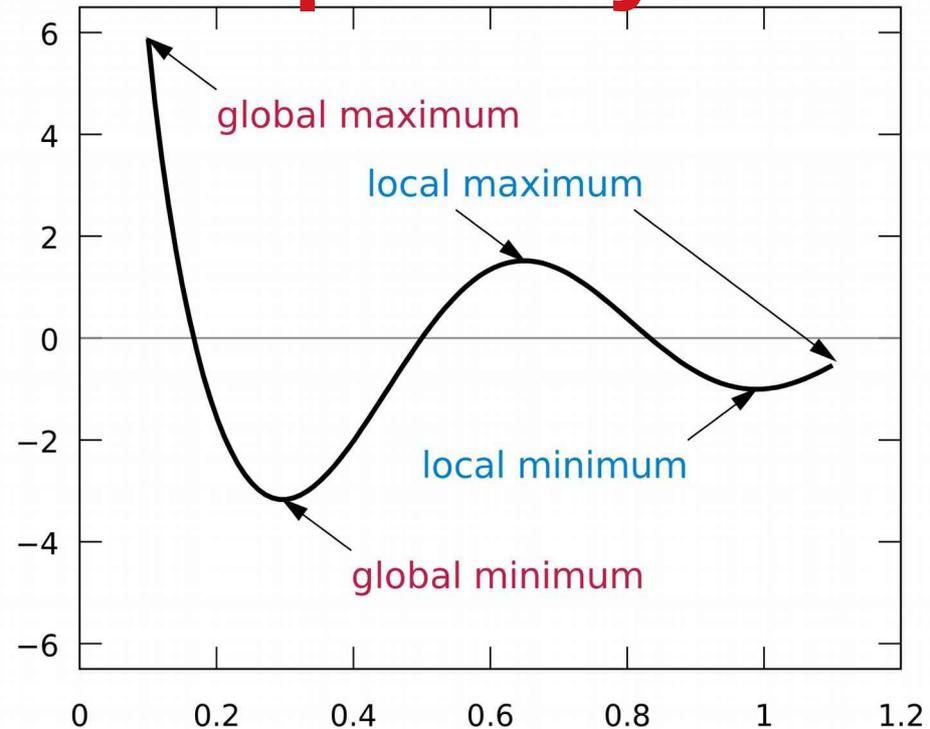
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because near a local maximum, any small change will degrade the score

GAs: are more likely to find the global maximum due to:

- 1 - the use of a **population** of candidate solutions,
- 2 - **crossover** and **mutation** that will, in many cases, result in candidate solutions that are **distant** from the previous ones.

This is **true** if we maintain the **diversity** of the population and **avoid premature convergence**.



Advantages of GAs - Complex Problems

GAs **need only the output** of FF for each individual and are not concerned with other aspects of the FF such as derivatives.

- That is why GAs **can be effective** for problems with
 - **complex mathematical representations** or
 - functions that are **hard** or impossible to **differentiate**,
- problems with a **large number of parameters**,
 - problems with a **mix of parameter types** (combination of continuous and discrete parameters).

Advantages of GAs - Problems without Mathematical Representation

Assume that the FF score is based on human opinion.

Example:

to find the most attractive color palette for a website.

Solution:

- to try **different color combinations** and ask users to rate the attractiveness of the site;
- to apply GAs to search for the **best scoring combination** while using this opinion-based score as the fitness function outcome.

GA will do it, **despite FF has NO mathematical representation** and there is **NO way to calculate the score** directly from a given color combination.

Advantages of GAs - Resilience to Noise

Some problems present **noisy behavior**:

- even for **similar input** parameter values, the **output** value may be **somewhat different** every time it's measured.

Examples:

- data go from sensor outputs, or
- FF score is based on human opinion.

Noisy behavior can **ruin** many **traditional** algorithms, but **GAs** are generally **resilient** to it, due to the **repetitive** operation of **reassembling** and **reevaluating** the individuals.

Advantages of GAs -

Parallelism

GAs by their definition are **ready to parallelization** and **distributed processing**.

- **FF is independently** calculated for **each** individual, which means **all the individuals** in the population can be **evaluated concurrently**.
- Genetic operations of **selection**, **crossover**, and **mutation** can each be performed **concurrently** on individuals and pairs of individuals in the population.

That is why **GAs are natural candidates** for **distributed and cloud-based implementation**

Advantages of GAs - Continuous Learning

In nature, **evolution never stops.**
But it is dubious ... :) ... look around.

As the environmental **conditions change**, the **population will adapt** to them.

Similarly, **GAs can operate continuously** in an ever-changing environment, and at any point in time, the **best current solution can be fetched and used.**

But what about time?

For GAs to be effective, the **changes** in the environment **need to be slow** in relation to the generation **turnaround rate** of the GA-based search.

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Limitations of GAs

- The need for special definitions
- The need for hyperparameter tuning
- Computationally-intensive operations
- The risk of premature convergence
 - No guaranteed solution

Limitations of GAs - **Special Definitions**

- To apply GAs to a given problem, we need to create a suitable representation for GAs and **define**:
 - **FF** and **chromosome** structure,
 - **genetic operators** (selection, crossover, and mutation) that will work for this problem.
- **This is challenging and time-consuming process!**
 - **BUT ... GAs have already been applied to countless different types of problems**, and many of these definitions have been standardized.
- In other lectures some types of real-life problems will be presented that can be solved using GAs.

Limitations of GAs -

Hyperparameter Tuning

The behavior of GAs is controlled by a set of **hyperparameters**, such as the **population size** and **mutation rate**, etc.

When applying GAs to the problem,
there are no exact rules (!)
for making these choices.

However, **this is true also for ... nearly all traditional search and optimization algorithms!**

After doing some experimentation of your own, you will be able to make sensible choices for these values.

Limitations of GAs - Computationally-Intensive Operations

Operating on (potentially **large and very large**) populations and the **repetitive** nature of GAs can be **computationally intensive**, as well as **time consuming** before a good result is reached.

These can be alleviated by:

- a **good choice** of hyperparameters,
- implementing **parallel processing**,
- and **caching** the intermediate results (in some cases).

Limitations of GAs - Risk of Premature Convergence

If the fitness of one individual is **much higher** than the rest of the population, it may be **duplicated enough** that it **takes over** the entire population.

This can lead to the GA getting **prematurely stuck** in a **local extremum, instead of** finding the **global one.**

To prevent this from occurring, it is important to **maintain the diversity** of the population.

Limitations of GAs - **No Guaranteed Solution**

- The use of GAs does **not guarantee** that the global extremum for the problem at hand **will be found**.
- However, this is almost **true for ... any traditional** search and optimization algorithm, unless it is an analytical solution for a particular type of problem.
 - Generally, GAs, when used appropriately, are known to **provide good solutions** within a **reasonable amount of time**.

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Use Cases of GAs

- GAs are **best suited** for the following types of problems:
 -
 - with **complex** mathematical representation
 - with **no** mathematical representation
 - involving a **noisy** environment
- involving an environment that **changes over time**

Lecture 1 - DEMO A - Introduction to Genetic Algorithms

(long version) based on (C) Eyal Wirsansky work

In this lecture we introduce **DEAP** – a **powerful and flexible evolutionary computation** framework capable of solving real-life problems using **genetic algorithms (GA)**.

Brief Content:

- introduction,
- installation,
- main modules: *creator* and *toolbox*,
- components needed for the GA workflow,
- the simplest example, *the OneMax problem*, so called the Hello World of genetic algorithms.

By the end of this lecture you will know:

- the DEAP framework and its modules,
- the concepts of creator and toolbox in the DEAP framework,
- the simplest example of GA,
- how to create a GA solution using the DEAP framework,
- how to use the DEAP framework's built-in algorithms to produce concise code
- how to solve the OneMax problem using a GA coded with the DEAP framework,
- how to experiment with various settings of the GA and interpret the differences in the results.

▼ Installation and import of libraries

In these and other lectures, we will use various Python packages:

- [NumPy](#)
- [Matplotlib](#)
- [Seaborn](#)

They are already pre-installed in Colab. Let's import them by the following code.

```
# Import all necessary standard libraries
import random
import numpy
```

```
import matplotlib.pyplot as plt
```

Install DEAP by *pip* with the following code:

```
# Install DEAP  
!pip install deap
```

```
Collecting deap  
  Downloading https://files.pythonhosted.org/packages/0a/eb/2bd0a32e3ce757fb2  
    |████████████████████████████████████████| 163kB 8.7MB/s  
Requirement already satisfied: numpy in /usr/local/lib/python3.6/dist-package  
Installing collected packages: deap  
Successfully installed deap-1.3.1
```

```
# Import DEAP  
from deap import base  
from deap import creator  
from deap import tools  
from deap import algorithms
```

▼ Example: OneMax problem

▼ Constants

```
# Let's declare constants that set the parameters for the problem and control the l  
  
# problem constants:  
ONE_MAX_LENGTH = 100 # length of bit string to be optimized  
  
# GA constants:  
POPULATION_SIZE = 200  
P_CROSSOVER = 0.9 # probability for crossover  
P_MUTATION = 0.1 # probability for mutating an individual  
MAX_GENERATIONS = 50
```

▼ Reproducibility of Results

One important aspect of the GA is the use of probability, which introduces a random element to the behavior of the algorithm.

However, **for reproducibility of results**, when experimenting with the code, we may want to be able to run the same experiment several times and get repeatable results.

To accomplish this, we set the random function seed to a constant number of some value, as shown in the following code:

```
# set the random seed:
RANDOM_SEED = 42
random.seed(RANDOM_SEED)
```

▼ Toolbox class

The **Toolbox** class is used as a container for functions (or operators), and enables us to create new operators by aliasing and customizing existing functions.

```
toolbox = base.Toolbox()
```

```
# For example, suppose we have a function, multiply() , defined as follows:
def multiply(a, b):
    return a*b
```

```
# Using toolbox, we can now create a new operator, incrementByFive(),
# which customizes the sumOfTwo() function as follows:
toolbox.register("MultiplyBy", multiply, b=5)
```

```
# examples:
A = toolbox.MultiplyBy(10)
print('toolbox.MultiplyBy(10) =', A)
B = multiply(10,5)
print('multiply(10,5) =', B)
```

```
    toolbox.MultiplyBy(10) = 50
    multiply(10,5) = 50
```

Let's create the *zeroOrOne* operator, which customizes the *random.randint(a, b)* function.

This function normally returns a random integer N such that $a \leq N \leq b$.

By fixing the two arguments, a and b , to the values 0 and 1 the *zeroOrOne* operator will randomly return either the value 0 or the value 1 when called later in the code.

```
# create an operator that randomly returns 0 or 1:
toolbox.register("zeroOrOne", random.randint, 0, 1)
```

```
# examples:
A = toolbox.zeroOrOne()
print('zeroOrOne =', A)
B = toolbox.zeroOrOne()
print('zeroOrOne =', B)
C = toolbox.zeroOrOne()
print('zeroOrOne =', C)
D = toolbox.zeroOrOne()
print('zeroOrOne =', D)
```

```
    zeroOrOne = 0
```

```
zeroOrOne = 0
zeroOrOne = 1
zeroOrOne = 0
```

▼ Fitness class

Next, we need to create the *Fitness* class. Since we only have one objective here—the sum of digits—and our goal is to maximize it, we choose the *FitnessMax* strategy, using a weights tuple with a single positive weight, as shown in the following code.

```
# define a single objective, maximizing fitness strategy:
creator.create("FitnessMax", base.Fitness, weights=(1.0,))
```

```
A = base.Fitness.weights
print(A)
```

```
None
```

In DEAP, the *Individual* class is used to represent each of the population's individuals. This class is created with the help of the creator tool. In our case, *list* serves as the base class, which is used as the individual's chromosome. The class is augmented with the fitness attribute, initialized to the *FitnessMax* class that we defined earlier

```
# create the Individual class based on list:
creator.create("Individual", list, fitness=creator.FitnessMax)
#creator.create("Individual", array.array, typecode='b', fitness=creator.FitnessMa
```

Next, register the *individualCreator* operator, which creates an instance of the *Individual* class, filled up with random values of either 0 or 1 . This is done by customizing the previously defined *zeroOrOne* operator.

Since the objects generated by the *zeroOrOne* operator are integers with random values of either 0 or 1 , the resulting *individualCreator* operator will fill an *Individual* instance with 100 randomly generated values of 0 or 1.

```
# create the individual operator to fill up an Individual instance:
toolbox.register("individualCreator", # Register the individualCreator operator,
                tools.initRepeat,    # The initRepeat operator is customized he
                creator.Individual,   # The container type (Individual) in which
                toolbox.zeroOrOne,     # The function used to generate objects (=
                ONE_MAX_LENGTH)       # The number of objects we want to generat
```

Register the *populationCreator* operator that creates a list of individuals.

```
# create the population operator to generate a list of individuals:
toolbox.register("populationCreator", # Register the populationCreator operator,
                tools.initRepeat,    # The initRepeat operator is customized here
                list,                 # The container type (list) in which the results are stored
                toolbox.individualCreator) # The function used to generate objects
```

Define the function *oneMaxFitness* that computes the number of 1s in the individual.

```
# fitness calculation:
# compute the number of '1's in the individual
def oneMaxFitness(individual):
    return sum(individual), # return a tuple,
                        # fitness values in DEAP are represented as tuples,
                        # and therefore a comma needs to follow when a single value is returned
```

Define the *evaluate* operator as an alias to the *oneMaxFitness()* function we defined earlier.

```
# create the evaluate alias for calculating the fitness (by a DEAP convention)
toolbox.register("evaluate", oneMaxFitness)
```

▼ Genetic operators

The genetic operators are typically created by aliasing existing functions from the tools module and setting the argument values as needed.

Note: The *mutFlipBit* function iterates over all the attributes of the individual, a list with values of 1s and 0s in our case, and for each attribute will use the argument value (*indpb* parameter) as the probability of flipping (applying the not operator to) the attribute value. This value is independent of the mutation probability, which is set by the *P_MUTATION* constant that we defined earlier and has not yet been used. The mutation probability serves to decide if the *mutFlipBit* function is called for a given individual in the population.

```
# genetic operators:

# Tournament selection with tournament size of 3:
toolbox.register("select", tools.selTournament, tournsize=3)

# Single-point crossover:
toolbox.register("mate", tools.cxOnePoint)

# Flip-bit mutation:
# indpb: Independent probability for each attribute to be flipped
toolbox.register("mutate", tools.mutFlipBit, indpb=1.0/ONE_MAX_LENGTH)
```

▼ GA workflow

```
# create initial population (generation 0):
population = toolbox.populationCreator(n=POPULATION_SIZE)
generationCounter = 0
```

▼ Long version

```
# calculate fitness tuple for each individual in the population:
fitnessValues = list(map(toolbox.evaluate, population)) # use map() to apply the e
for individual, fitnessValue in zip(population, fitnessValues):
    individual.fitness.values = fitnessValue
```

```
# extract the first value out of each fitness for gathering statistics:
fitnessValues = [individual.fitness.values[0] for individual in population]
```

```
# initialize statistics accumulators:
maxFitnessValues = []
meanFitnessValues = []
```

```
# main evolutionary loop:
# stop if max fitness value reached the known max value
# OR if number of generations exceeded the preset value:
while max(fitnessValues) < ONE_MAX_LENGTH and generationCounter < MAX_GENERATIONS:
    # update counter:
    generationCounter = generationCounter + 1

    # apply the selection operator, to select the next generation's individuals:
    offspring = toolbox.select(population, len(population))
    # clone the selected individuals:
    offspring = list(map(toolbox.clone, offspring))

    # apply the crossover operator to pairs of offspring:
    for child1, child2 in zip(offspring[::2], offspring[1::2]):
        if random.random() < P_CROSSOVER:
            toolbox.mate(child1, child2)
            del child1.fitness.values
            del child2.fitness.values

        for mutant in offspring:
            if random.random() < P_MUTATION:
                toolbox.mutate(mutant)
                del mutant.fitness.values

    # calculate fitness for the individuals with no previous calculated fitness value
    freshIndividuals = [ind for ind in offspring if not ind.fitness.valid]
    freshFitnessValues = list(map(toolbox.evaluate, freshIndividuals))
    for individual, fitnessValue in zip(freshIndividuals, freshFitnessValues):
        individual.fitness.values = fitnessValue
```

```

# replace the current population with the offspring:
population[:] = offspring

# collect fitnessValues into a list, update statistics and print:
fitnessValues = [ind.fitness.values[0] for ind in population]

maxFitness = max(fitnessValues)
meanFitness = sum(fitnessValues) / len(population)
maxFitnessValues.append(maxFitness)
meanFitnessValues.append(meanFitness)
print("- Generation {}: Max Fitness = {}, Avg Fitness = {}".format(generationCount, maxFitness, meanFitness))

# find and print best individual:
best_index = fitnessValues.index(max(fitnessValues))
print("Best Individual = ", *population[best_index], "\n")

```

```

- Generation 1: Max Fitness = 62.0, Avg Fitness = 52.59
Best Individual = 0 1 1 1 1 1 1 1 0 1 1 1 0 0 1 1 1 0 1 0 0 1 1 0 1 1 1 0

- Generation 2: Max Fitness = 64.0, Avg Fitness = 55.205
Best Individual = 0 1 1 1 0 0 0 1 1 1 0 1 0 0 1 1 0 1 0 0 1 1 1 1 1 0 0 1

- Generation 3: Max Fitness = 67.0, Avg Fitness = 56.88
Best Individual = 1 1 0 1 1 1 0 1 0 1 1 0 1 0 1 1 1 1 0 0 1 0 0 1 1 1 1 0

- Generation 4: Max Fitness = 71.0, Avg Fitness = 58.425
Best Individual = 1 1 1 0 1 1 0 0 1 1 0 0 1 0 1 1 1 1 0 0 1 1 0 1 1 1 1 1

- Generation 5: Max Fitness = 69.0, Avg Fitness = 59.77
Best Individual = 0 0 1 1 1 1 1 1 1 1 1 0 0 1 1 0 1 1 1 1 1 1 1 1 1 0 1 1

- Generation 6: Max Fitness = 73.0, Avg Fitness = 61.53
Best Individual = 1 1 1 1 1 1 1 1 1 1 1 0 0 1 1 0 1 1 1 1 1 1 1 1 0 1 1

- Generation 7: Max Fitness = 73.0, Avg Fitness = 62.525
Best Individual = 1 1 1 1 0 1 0 1 0 1 1 0 1 1 0 1 1 0 0 1 1 1 0 1 1 1 0 1

- Generation 8: Max Fitness = 74.0, Avg Fitness = 63.23
Best Individual = 1 1 0 1 0 0 1 1 1 1 1 1 0 0 1 1 0 1 1 1 1 1 1 1 1 0 1 1

- Generation 9: Max Fitness = 74.0, Avg Fitness = 63.76
Best Individual = 1 0 1 1 1 1 1 1 1 1 1 1 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1

- Generation 10: Max Fitness = 74.0, Avg Fitness = 64.165
Best Individual = 1 1 1 1 1 0 1 1 1 1 1 0 1 1 0 1 1 0 1 0 0 0 1 1 1 1 1 1

- Generation 11: Max Fitness = 75.0, Avg Fitness = 64.23
Best Individual = 1 0 1 0 1 1 1 1 1 1 1 1 0 1 1 0 1 0 1 1 1 1 1 1 1 1 1

- Generation 12: Max Fitness = 75.0, Avg Fitness = 64.83
Best Individual = 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 1 0 1 0 1 1 1 1 1 1 1 1

- Generation 13: Max Fitness = 78.0, Avg Fitness = 65.225
Best Individual = 1 0 1 1 1 1 1 1 1 1 0 1 0 1 1 0 1 1 1 1 1 1 1 1 0 0 1

- Generation 14: Max Fitness = 80.0, Avg Fitness = 65.355
Best Individual = 1 1 0 0 1 1 1 1 1 1 0 1 1 1 1 1 0 1 0 1 1 1 1 1 1 1 1

```

```

- Generation 15: Max Fitness = 75.0, Avg Fitness = 65.87
Best Individual = 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 1 1 1 1 1 1 1 1 1 1

- Generation 16: Max Fitness = 76.0, Avg Fitness = 65.705
Best Individual = 0 1 1 1 0 1 1 1 0 1 1 1 0 1 1 1 0 1 1 1 0 1 1 0 0 1 0 1

- Generation 17: Max Fitness = 75.0, Avg Fitness = 65.845
Best Individual = 1 1 1 1 1 1 1 0 0 1 1 1 1 0 0 0 0 1 1 1 1 1 1 1 1 0 1 1 1

- Generation 18: Max Fitness = 79.0, Avg Fitness = 66.02
Best Individual = 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1

- Generation 19: Max Fitness = 80.0, Avg Fitness = 66.44
Best Individual = 1 0 1 0 1 1 1 1 1 1 1 1 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1

```

You should get the following output:

```

-- Generation 1: Max Fitness = 62.0, Avg Fitness = 52.59 Best Individual = 0 1 1 1 1 1 1 1 1 0 1 1 1
0 0 1 1 1 0 1 0 0 1 1 0 1 1 1 1 0 0 1 1 0 1 0 1 0 0 0 1 0 1 0 0 0 1 1 0 1 1 1 1 0 0 1 1 1 0 1 0 1 1 0 1 1
0 1 0 1 1 1 1 1 0 1 0 0 1 1 0 1 0 1 1 1 0 1 0 1 0 0 1 1 1 1 1 0 1 0

...

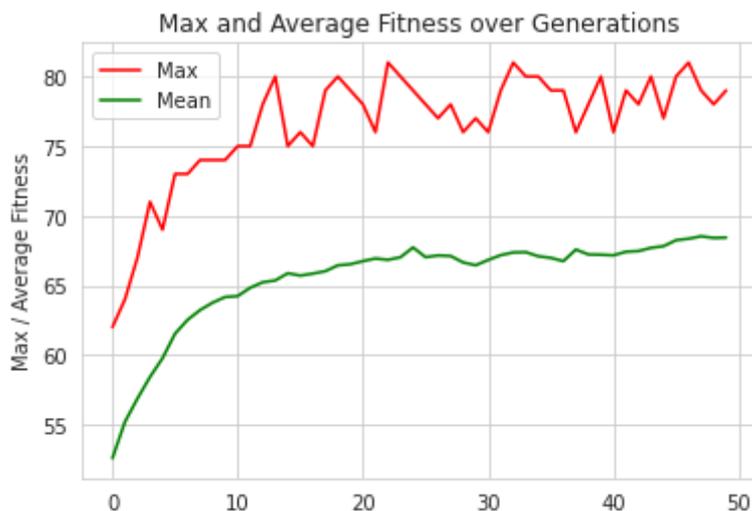
-- Generation 50: Max Fitness = 79.0, Avg Fitness = 68.43 Best Individual = 0 1 1 1 1 1 1 1 1 0 1 1 0
1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 0 1 1 1 1 1 1 1 0 1 1 1 1 1 1 0 1 0 1 1

```

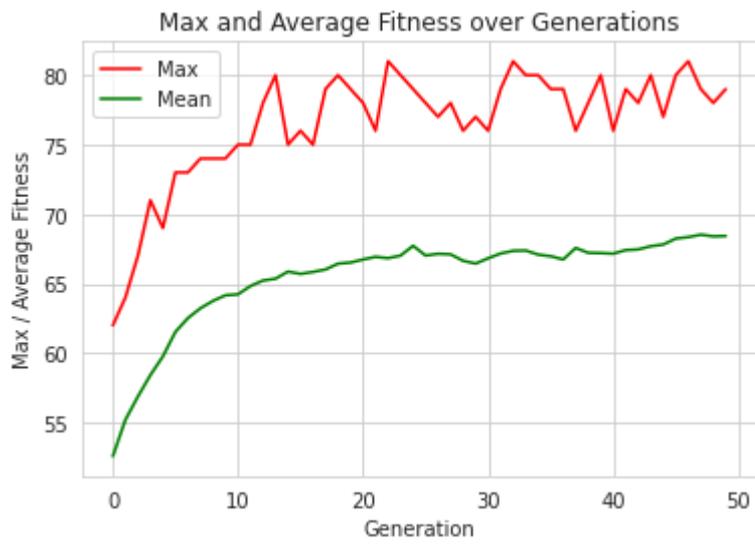
```

# Plot statistics:
sns.set_style("whitegrid")
plt.plot(maxFitnessValues, color='red', label='Max')
plt.plot(meanFitnessValues, color='green', label='Mean')
plt.xlabel('Generation')
plt.ylabel('Max / Average Fitness')
plt.title('Max and Average Fitness over Generations')
plt.legend()
plt.show()

```



You should get the following output:



Lecture 1 - DEMO B - Introduction to Genetic Algorithms

(short version of code implementation) based on (C) Eyal Wirsansky work

In this lecture we introduce **DEAP** – a powerful and flexible evolutionary computation framework capable of solving real-life problems using **genetic algorithms (GA)**.

Brief Content:

- introduction,
- installation,
- main modules: *creator* and *toolbox*,
- components needed for the GA workflow,
- the simplest example, *the OneMax problem*, so called the Hello World of genetic algorithms.

By the end of this lecture you will know:

- the DEAP framework and its modules,
- the concepts of creator and toolbox in the DEAP framework,
- the simplest example of GA,
- how to create a GA solution using the DEAP framework,
- how to use the DEAP framework's built-in algorithms to produce concise code
- how to solve the OneMax problem using a GA coded with the DEAP framework,
- how to experiment with various settings of the GA and interpret the differences in the results.

▼ Installation and import of libraries

In these and other lectures, we will use various Python packages:

- [NumPy](#)
- [Matplotlib](#)
- [Seaborn](#)

They are already pre-installed in Colab. Let's import them by the following code.

```
# Import all necessary standard libraries
import random
import numpy
```

```
import matplotlib.pyplot as plt
import seaborn as sns
```

Install DEAP by *pip* with the following code:

```
# Install DEAP
!pip install deap
```

```
Collecting deap
  Downloading https://files.pythonhosted.org/packages/0a/eb/2bd0a32e3ce757fb2
    |████████████████████████████████████████| 163kB 8.2MB/s
Requirement already satisfied: numpy in /usr/local/lib/python3.6/dist-package
Installing collected packages: deap
Successfully installed deap-1.3.1
```

```
# Import DEAP
from deap import base
from deap import creator
from deap import tools
from deap import algorithms
```

▼ Example: OneMax problem

▼ Constants

```
# Let's declare constants that set the parameters for the problem and control the |
# problem constants:
ONE_MAX_LENGTH = 100 # length of bit string to be optimized

# GA constants:
POPULATION_SIZE = 200
P_CROSSOVER = 0.9 # probability for crossover
P_MUTATION = 0.1 # probability for mutating an individual
MAX_GENERATIONS = 50
```

▼ Reproducibility of Results

One important aspect of the GA is the use of probability, which introduces a random element to the behavior of the algorithm.

However, **for reproducibility of results**, when experimenting with the code, we may want to be able to run the same experiment several times and get repeatable results.

To accomplish this, we set the random function seed to a constant number of some value, as shown in the following code:

```
# set the random seed:
RANDOM_SEED = 42
random.seed(RANDOM_SEED)
```

▼ **Toolbox** class

The **Toolbox** class is used as a container for functions (or operators), and enables us to create new operators by aliasing and customizing existing functions.

```
toolbox = base.Toolbox()
```

```
# For example, suppose we have a function, multiply() , defined as follows:
def multiply(a, b):
    return a*b
```

```
# Using toolbox, we can now create a new operator, incrementByFive(),
# which customizes the sumOfTwo() function as follows:
toolbox.register("MultiplyBy", multiply, b=5)
```

```
# examples:
A = toolbox.MultiplyBy(10)
print('toolbox.MultiplyBy(10) =', A)
B = multiply(10,5)
print('multiply(10,5) =', B)
```

```
    toolbox.MultiplyBy(10) = 50
    multiply(10,5) = 50
```

Let's create the *zeroOrOne* operator, which customizes the *random.randint(a, b)* function.

This function normally returns a random integer N such that $a \leq N \leq b$.

By fixing the two arguments, a and b , to the values 0 and 1 the *zeroOrOne* operator will randomly return either the value 0 or the value 1 when called later in the code.

```
# create an operator that randomly returns 0 or 1:
toolbox.register("zeroOrOne", random.randint, 0, 1)
```

```
# examples:
A = toolbox.zeroOrOne()
print('zeroOrOne =', A)
B = toolbox.zeroOrOne()
print('zeroOrOne =', B)
C = toolbox.zeroOrOne()
print('zeroOrOne =', C)
```

```
D = toolbox.zeroOrOne()
print('zeroOrOne =', D)
```

```
zeroOrOne = 0
zeroOrOne = 0
zeroOrOne = 1
zeroOrOne = 0
```

▼ Fitness class

Next, we need to create the *Fitness* class. Since we only have one objective here—the sum of digits—and our goal is to maximize it, we choose the *FitnessMax* strategy, using a weights tuple with a single positive weight, as shown in the following code.

```
# define a single objective, maximizing fitness strategy:
creator.create("FitnessMax", base.Fitness, weights=(1.0,))
```

```
A = base.Fitness.weights
print(A)
```

```
None
```

In DEAP, the *Individual* class is used to represent each of the population's individuals. This class is created with the help of the creator tool. In our case, *list* serves as the base class, which is used as the individual's chromosome. The class is augmented with the fitness attribute, initialized to the *FitnessMax* class that we defined earlier

```
# create the Individual class based on list:
creator.create("Individual", list, fitness=creator.FitnessMax)
#creator.create("Individual", array.array, typecode='b', fitness=creator.FitnessMa
```

Next, register the *individualCreator* operator, which creates an instance of the *Individual* class, filled up with random values of either 0 or 1 . This is done by customizing the previously defined *zeroOrOne* operator.

Since the objects generated by the *zeroOrOne* operator are integers with random values of either 0 or 1 , the resulting *individualCreator* operator will fill an *Individual* instance with 100 randomly generated values of 0 or 1.

```
# create the individual operator to fill up an Individual instance:
toolbox.register("individualCreator", # Register the individualCreator operator,
                tools.initRepeat,    # The initRepeat operator is customized he
                creator.Individual,  # The container type (Individual) in which
                toolbox.zeroOrOne,    # The function used to generate objects (=
                ONE_MAX_LENGTH)      # The number of objects we want to generat
```

Register the *populationCreator* operator that creates a list of individuals.

```
# create the population operator to generate a list of individuals:
toolbox.register("populationCreator", # Register the populationCreator operator,
                tools.initRepeat,    # The initRepeat operator is customized he
                list,                 # The container type (list) in which the re
                toolbox.individualCreator) # The function used to generate object:
```

Define the function *oneMaxFitness* that computes the number of 1s in the individual.

```
# fitness calculation:
# compute the number of '1's in the individual
def oneMaxFitness(individual):
    return sum(individual), # return a tuple,
                        # fitness values in DEAP are represented as tuples,
                        # and therefore a comma needs to follow when a single
```

Define the *evaluate* operator as an alias to the *oneMaxFitness()* function we defined earlier.

```
# create the evaluate alias for calculating the fitness (by a DEAP convention)
toolbox.register("evaluate", oneMaxFitness)
```

▼ Genetic operators

The genetic operators are typically created by aliasing existing functions from the tools module and setting the argument values as needed.

Note: The *mutFlipBit* function iterates over all the attributes of the individual, a list with values of 1s and 0s in our case, and for each attribute will use the argument value (*indpb* parameter) as the probability of flipping (applying the not operator to) the attribute value. This value is independent of the mutation probability, which is set by the *P_MUTATION* constant that we defined earlier and has not yet been used. The mutation probability serves to decide if the *mutFlipBit* function is called for a given individual in the population.

```
# genetic operators:

# Tournament selection with tournament size of 3:
toolbox.register("select", tools.selTournament, tournsize=3)

# Single-point crossover:
toolbox.register("mate", tools.cxOnePoint)

# Flip-bit mutation:
# indpb: Independent probability for each attribute to be flipped
toolbox.register("mutate", tools.mutFlipBit, indpb=1.0/ONE_MAX_LENGTH)
```

▼ GA workflow

```
# create initial population (generation 0):
population = toolbox.populationCreator(n=POPULATION_SIZE)
```

▼ Short version

```
# prepare the statistics object:
stats = tools.Statistics(lambda ind: ind.fitness.values)
stats.register("max", numpy.max)
stats.register("avg", numpy.mean)

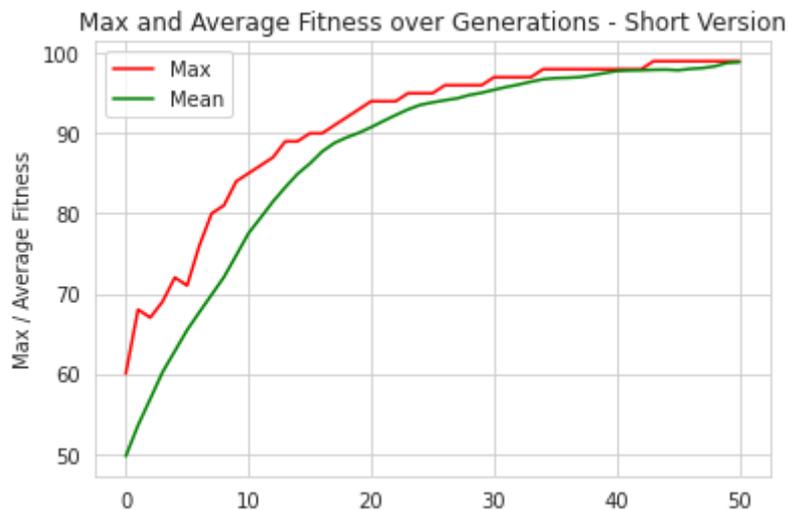
# perform the Genetic Algorithm flow:
population, logbook = algorithms.eaSimple(population, toolbox, cxpb=P_CROSSOVER, m
                                         stats=stats, verbose=True)

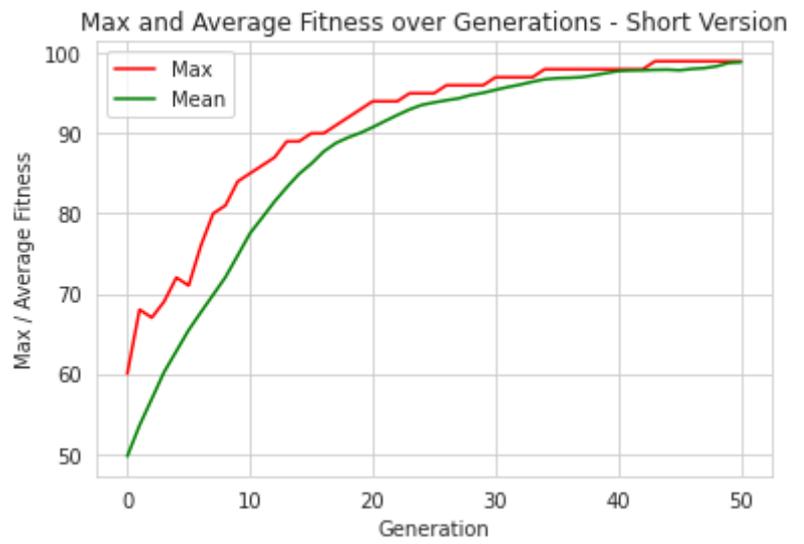
# Genetic Algorithm is done - extract statistics:
maxFitnessValues, meanFitnessValues = logbook.select("max", "avg")
```

gen	nevals	max	avg
0	200	60	49.705
1	190	68	53.56
2	175	67	56.87
3	179	69	60.21
4	175	72	62.825
5	184	71	65.45
6	178	76	67.68
7	187	80	69.865
8	189	81	72.055
9	184	84	74.765
10	185	85	77.515
11	181	86	79.485
12	190	87	81.49
13	181	89	83.27
14	184	89	84.94
15	189	90	86.22
16	176	90	87.725
17	176	91	88.79
18	182	92	89.485
19	185	93	90.065
20	182	94	90.765
21	170	94	91.535
22	179	94	92.28
23	178	95	92.985
24	181	95	93.545
25	189	95	93.855
26	174	96	94.125
27	179	96	94.36
28	186	96	94.78
29	185	96	95.055
30	185	97	95.43

31	186	97	95.775
32	187	97	96.075
33	179	97	96.435
34	176	98	96.745
35	187	98	96.885
36	186	98	96.93
37	190	98	97.015
38	175	98	97.245
39	171	98	97.515
40	179	98	97.78
41	188	98	97.845
42	188	98	97.87
43	178	99	97.925
44	174	99	97.95
45	176	99	97.87
46	185	99	98.04
47	184	99	98.14
48	184	99	98.37
49	187	99	98.79
50	185	99	98.885

```
# Plot statistics:
sns.set_style("whitegrid")
plt.plot(maxFitnessValues, color='red', label='Max')
plt.plot(meanFitnessValues, color='green', label='Mean')
plt.xlabel('Generation')
plt.ylabel('Max / Average Fitness')
plt.title('Max and Average Fitness over Generations - Short Version')
plt.legend()
plt.show()
```





You should get the following output:



Основи еволюційних обчислень

-

Evolutionary Computing Basics

-

Lecture 02. Overview

(based on Alan Turing, Holland, Khaled Rasheed, Ben Phillips, Eyal Wirsansky, and others works)

... in previous lecture ...

Content

- Recommended Sources
- What are Genetic Algorithms (GAs)?
- GA Analogy with IT
- Components of GA
- Main Hypothesis behind GAs
- Differences between GAs and Traditional Algorithms
- Advantages of GAs
- Limitations of GAs
- When to use GAs

Content — this lecture

- **Recommended Sources**
- What is Evolutionary Computing (EC)
- EC History
- Problem Types for EC
- What is Evolutionary Algorithm (EA)
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA

Recommended Sources - Books

(the same as for GA!)

Books (classic):

Holland, J. H. (1992). *Adaptation in natural and artificial systems: an introductory analysis with applications to biology, control, and artificial intelligence.* MIT press. **<- inventor of GA(!), the highest number of citations for GA-publication by Google Scholar!**

Mitchell, M. (1998). *An introduction to genetic algorithms.* MIT press. **<- classic textbook, the highest number of citations for GA-textbook by Google Scholar!**

Books (with codes at github):

Wirsansky, E. (2020). *Hands-On Genetic Algorithms with Python.* Packt Publishing

Sheppard, C. (2019). *Genetic Algorithms with Python* (self-published).

Recommended Sources - Papers

(the same as for GA!)

Holland, J. H. (1992). *Genetic algorithms*. Scientific American, 267(1), 66-73. **<- inventor of GA(!) <- Just for Fun! :)**

Katoch, S., Chauhan, S. S., & Kumar, V. (2020). *A review on genetic algorithm: past, present, and future*. Multimedia Tools and Applications, 1-36.

García-Martínez, C., Rodríguez, F. J., & Lozano, M. (2018). *Genetic Algorithms*, Handbook of Heuristics, 2018, p. 431-464.

Content

- Recommended Sources
- **What is Evolutionary Computing (EC)**
- EC History
- Problem Types for EC
- What is Evolutionary Algorithm (EA)
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA

What is Evolutionary Computing (EC)?

EVOLUTION

Environment

Individual

Fitness

**Fitness →
chances for
survival and
reproduction**



IT

-

Problem

Candidate Solution (Individual)

Quality

**Quality →
chance for
seeding
new solutions**

What is **EC** — Metaphor (nature-IT)

A **population of individuals** exists in an environment with **limited** resources.

Competition for those **resources** causes **selection** of those **fitter** individuals that are **better adapted** to the environment.

These **individuals** act as **seeds** for the **new generation** of individuals through some **variation operations** (for example, GA like recombination and mutation).

The new individuals have their **fitness evaluated** and compete (possibly also with parents) **for survival**.

Natural selection causes a **rise in the fitness** of the population.

Content

- Recommended Sources
- What is Evolutionary Computing (EC)
- **EC History**
- Problem Types for EC
- What is Evolutionary Algorithm (EA)
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA

EC — History — Founders

1948, Turing:

“genetical or evolutionary search”

1962, Bremermann

optimization through evolution and recombination

1964, Rechenberg

evolution strategies

1965, L. Fogel, Owens and Walsh

evolutionary programming

1975, Holland

genetic algorithms

1992, Koza

genetic programming

EC — History — Community

1985:

first international **conference** (ICGA)

1990:

first international **conference in Europe**
(PPSN)

1993:

first scientific EC **journal** (MIT Press)

1997:

launch of European EC **Research
Network** EvoNet

EC — History — NOW!

- 3 **major** EC conferences
+ 10 **small** related ones
- 3 scientific **core EC journals**
- **750-1000 papers** published in 2003
- numerous applications
- numerous consultancy and R&D firms

EC — History — Lessons

Nature has always served as a source of inspiration for engineers and scientists

The best problem solver known in nature is:

- **the (human) brain** that created “the wheel, New York, wars and so on” (after Douglas Adams’ Hitch-Hikers Guide)
- **the evolution mechanism** that created the human brain (after Darwin’s Origin of Species)

Answer 1 ☾ neurocomputing

Answer 2 ☾ evolutionary computing

EC — Current Needs

Developing, analyzing, applying
problem solving methods (algorithms)
is a central theme
in mathematics and computer science.

Why?

- **Time** for careful problem analysis **decreases**
- **Complexity** of the current problems **increases**

Resume:

Robust problem solving technology needed!

Content

- Recommended Sources
- What is Evolutionary Computing (EC)
- EC History
- **Problem Types for EC**
- What is Evolutionary Algorithm (EA)
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA

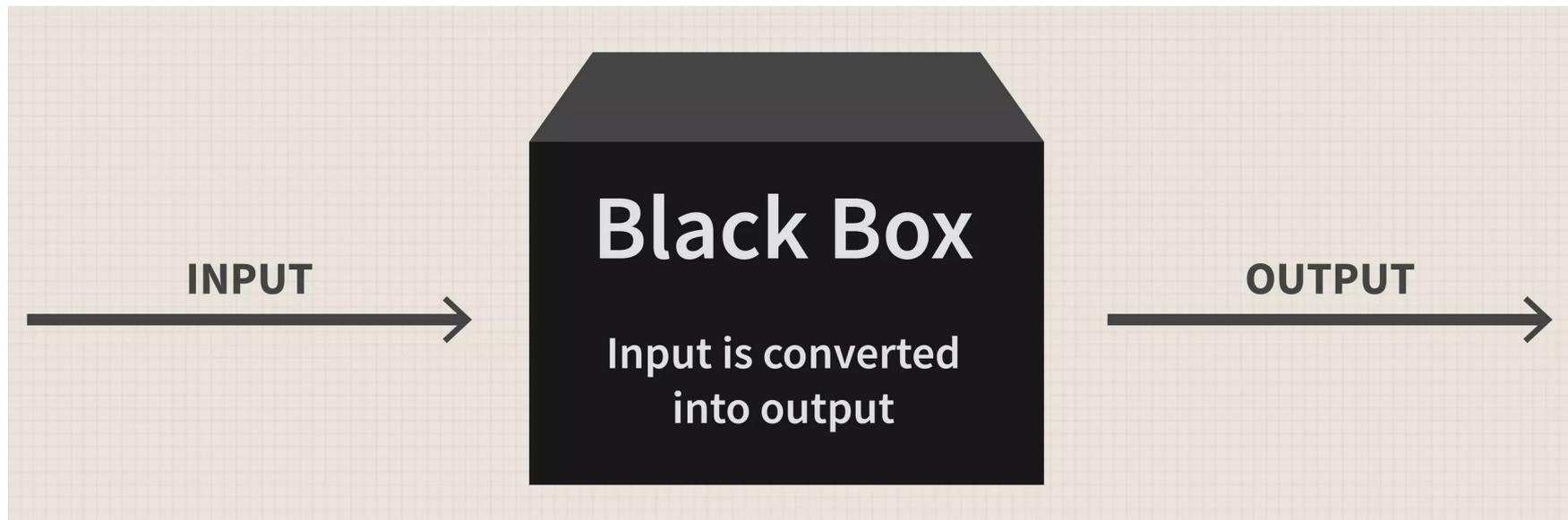
EC — Problem Types

We have
a model, inputs and outputs
of our system
and look for different entities:

- optimization,
- modeling,
- simulation.

Problem Types – Optimization

We have the model of our system and **seek inputs** that give us a specified goal:



Input?

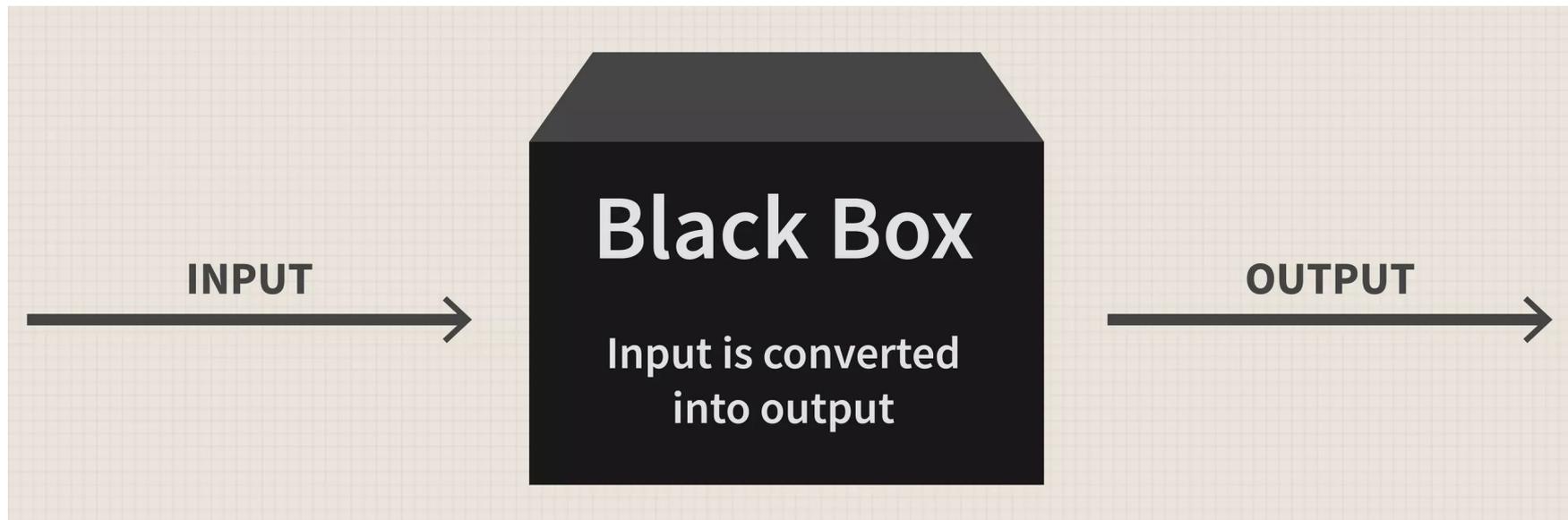
The model is known!

We **look for inputs** to reach the specified goal, for example:

- time table for KPI (rozklad.kpi.ua - fantastic!),
- software/hardware design specifications,
- etc.

Problem Types – Modeling

We have the corresponding input/output sets of our system and **seek model** that give us a specified goal:



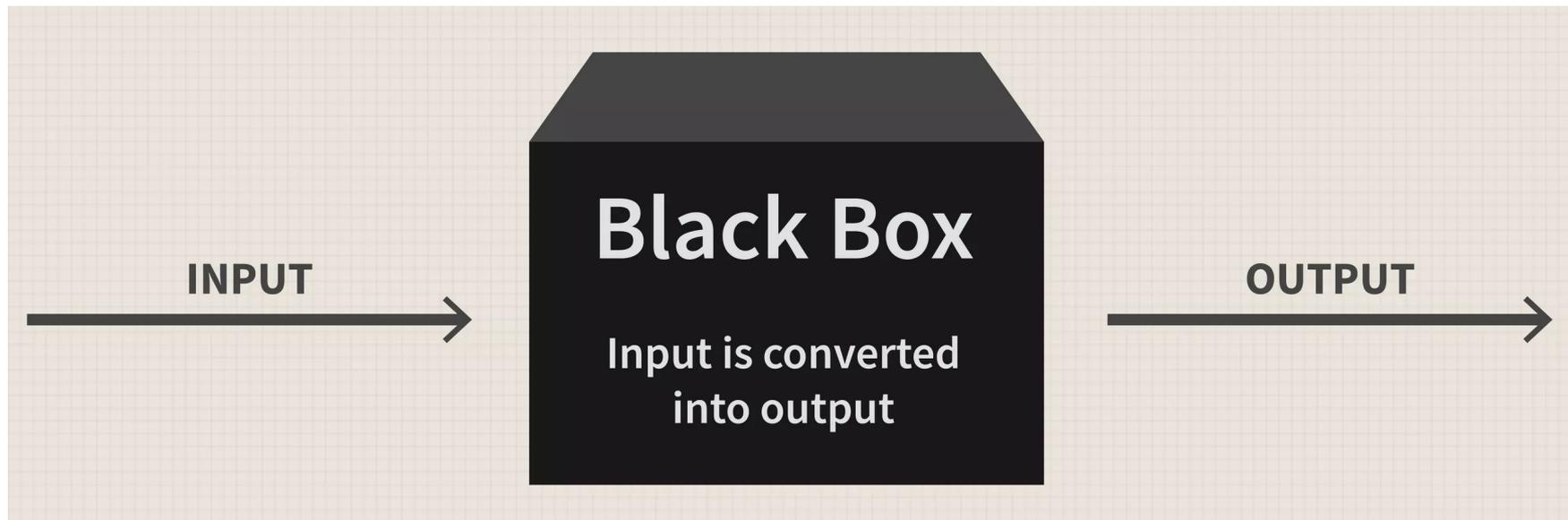
The input is known! **Model?** **The output is known!**

The model should deliver the correct output for every known input,
for example:

- machine learning models,
- deep learning models.

Problem Types – Simulation

We have the **model** of our system and look for the **outputs** that will appear under different **inputs**:



The input is known! The model is known! Output?

It is used to **investigate scenarios** the **evolving** dynamic environments:

- evolutionary economics,
- geo-politics,
- military planning,
- artificial life

Content

- Recommended Sources
- What is Evolutionary Computing (EC)
- EC History
- Problem Types for EC
- **What is Evolutionary Algorithm (EA)**
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA

Again:

What is **EC** — Metaphor (nature-IT)

EVOLUTION

Environment

Individual

Fitness

**Fitness →
chances for
survival and
reproduction**



IT

-

Problem

Candidate Solution (Individual)

Quality

**Quality →
chance for
seeding
new solutions**

What is **Evolutionary Algorithms (EA)** — **Metaphor (nature-IT)**

EAs is the category of “**generate and test**” algorithms.

They are stochastic, **population-based** algorithms.

Variation (genetic?) **operators** (recombination and mutation) **create** the necessary **diversity** and thereby facilitate **novelty**.

Selection **reduces(!) diversity**
and
acts as a force pushing quality.

EA — History and Types

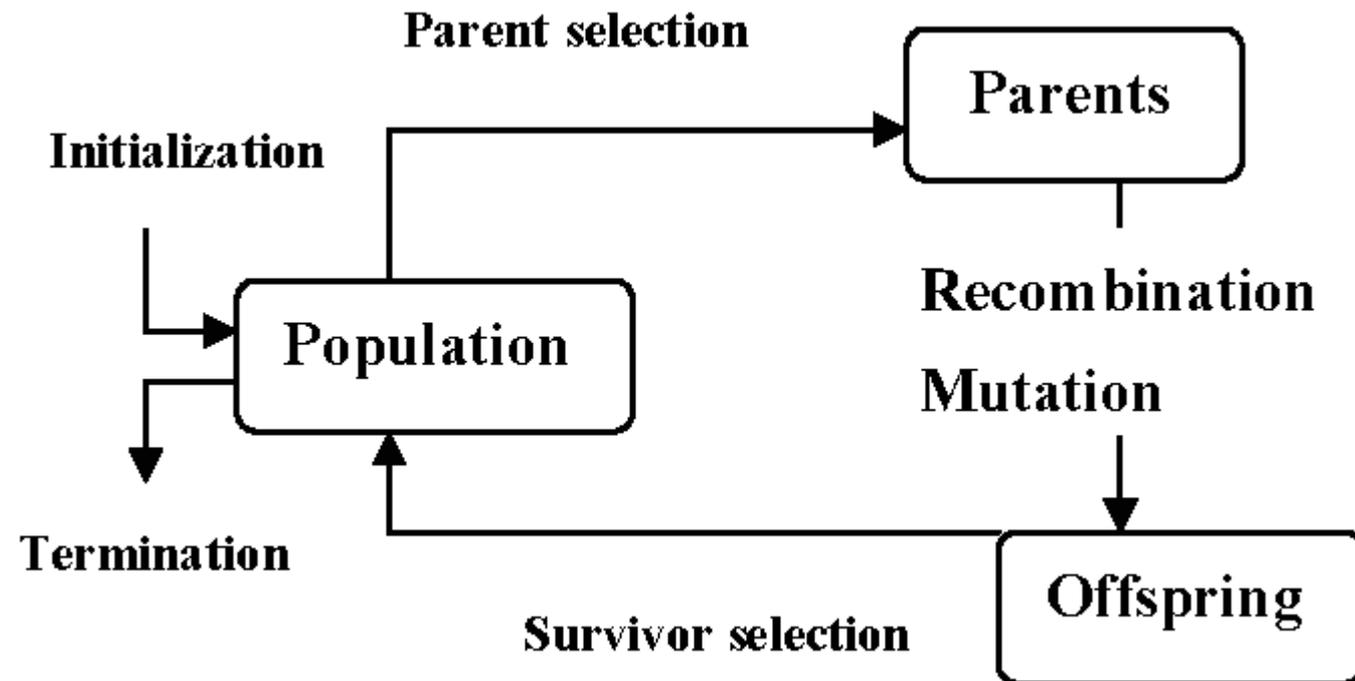
Different types of EAs have been associated with different representations:

- ◆ **Binary** strings : Genetic Algorithms (**GA**)
 - ◆ **Real-valued** vectors : Evolution Strategies (**ES**)
 - ◆ **Finite state** Machines: Evolutionary Programming (**EP**)
 - ◆ **LISP trees**: Genetic Programming (**GP**)
- These differences are largely irrelevant, best strategy
 - ◆ choose **representation** to suit **problem**
 - ◆ choose **variation operators** to suit **representation**
 - ◆ **Selection operators only use fitness**
 - ◆ and so
 - ◆ are **independent of representation**.

Content

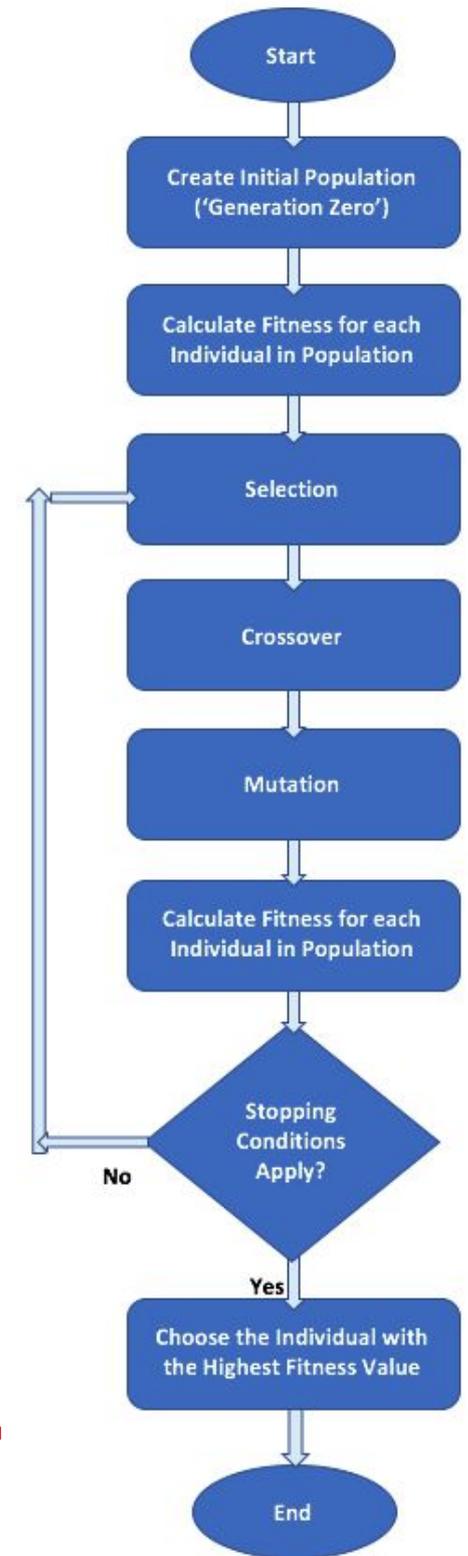
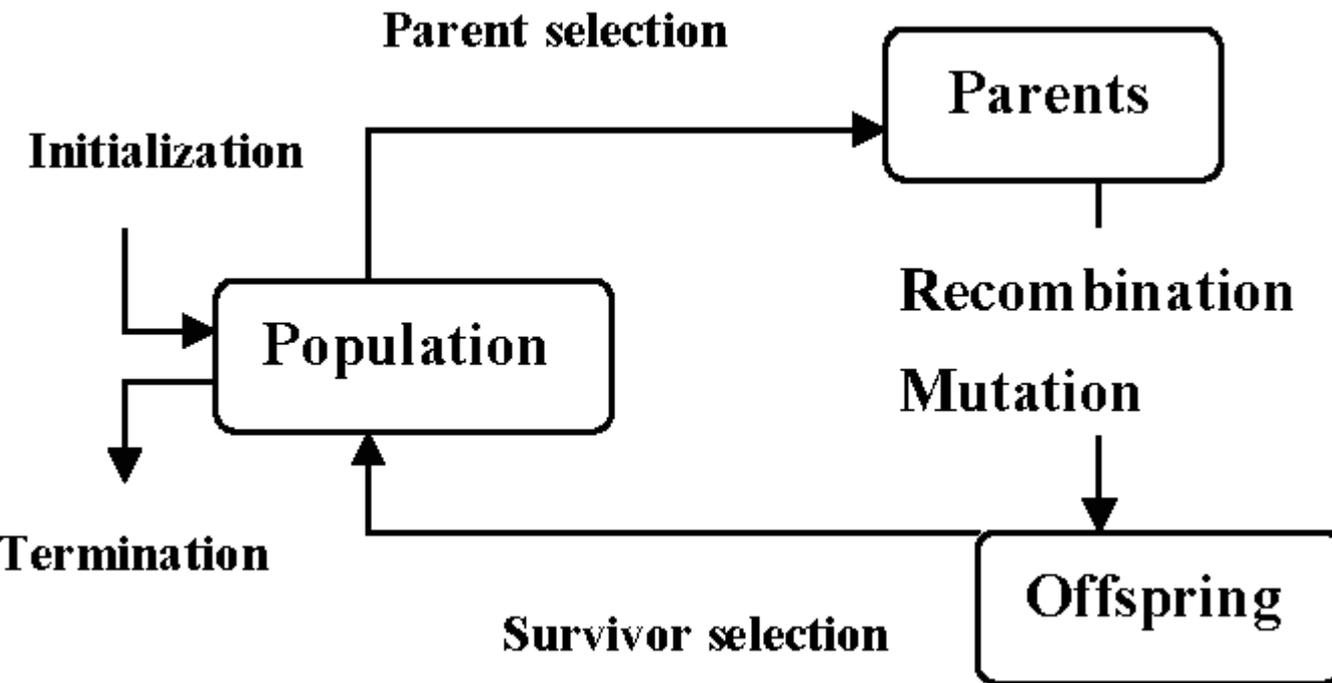
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EA — General Scheme ...



... and ...

EA — General Scheme ...



... and Workflow ----->

EA — Workflow — Terminology

Candidate solutions (**individuals**) exist in **phenotype space**.

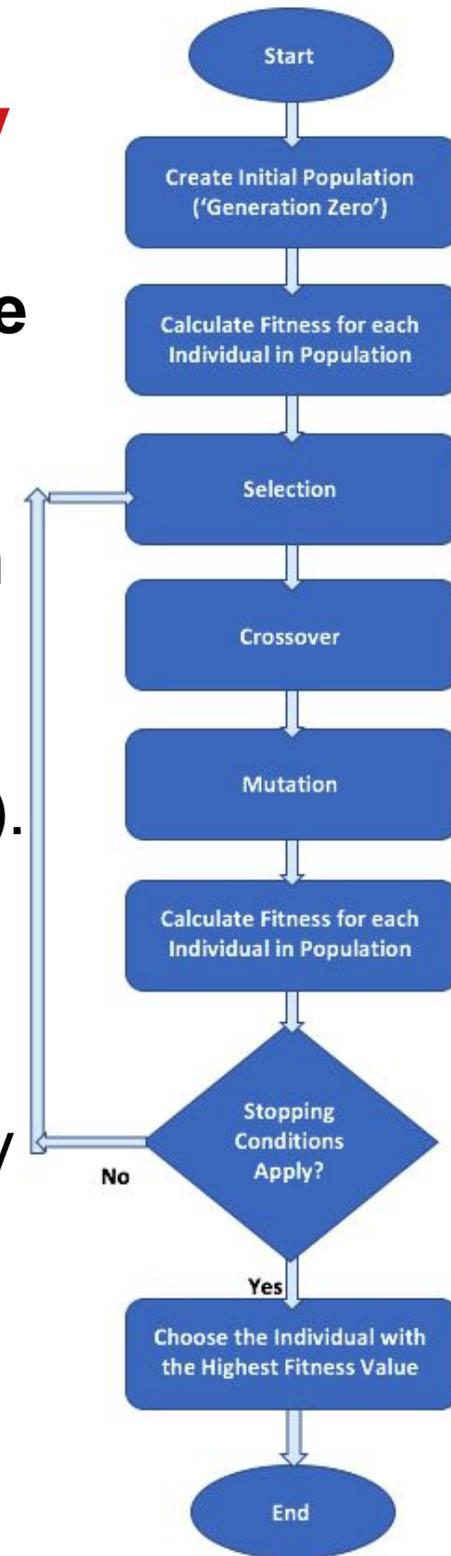
They are **encoded** in **chromosomes**, which exist in **genotype space**.

Encoding: phenotype->genotype (not always 1-to-1).

Decoding: genotype->phenotype (must be 1-to-1).

Chromosomes contain **genes**, which are in (usually fixed) positions called **loci** (sing. **locus**) and have a value (allele).

To find the **global optimum**, every feasible solution must be representable in genotype space!



EA — Workflow — Population

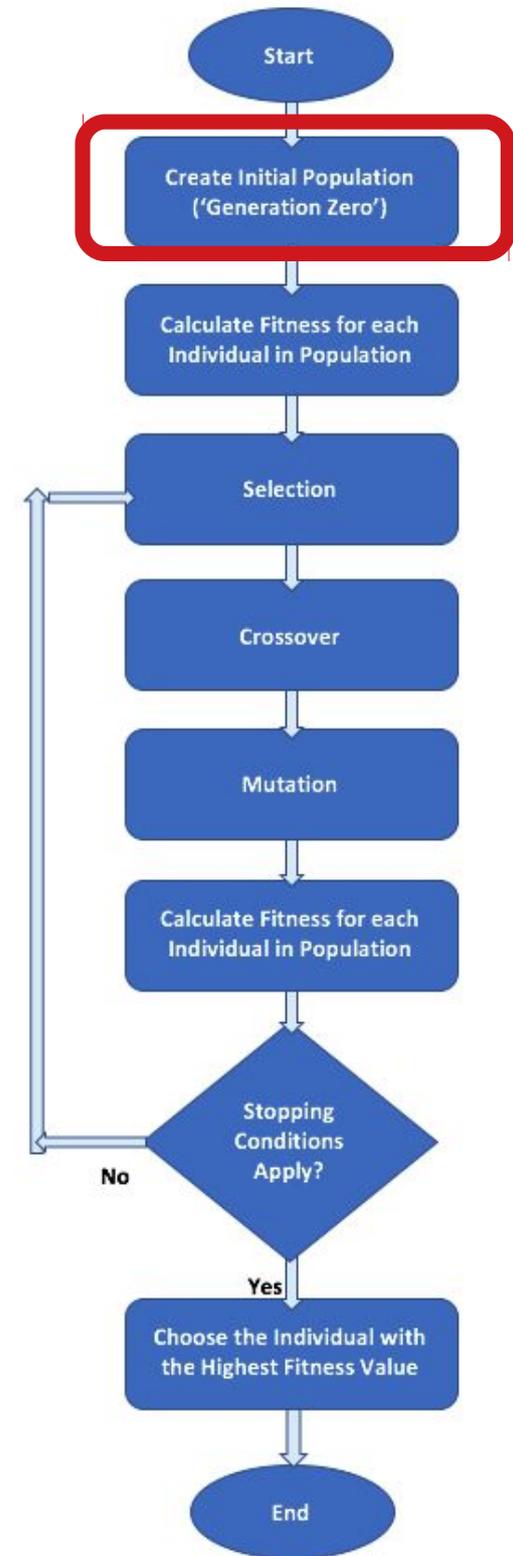
Has (representations of) **possible solutions**.

Usually has a **fixed size** and is a **multi-set of genotypes**.

Some sophisticated EAs also assert a **spatial structure** on the population e.g., a grid.

Selection operators work with **whole population** into account i.e., reproductive probabilities are relative to current generation.

Diversity of a population refers to the number of **different fitnesses / phenotypes / genotypes** present (note not the same thing).



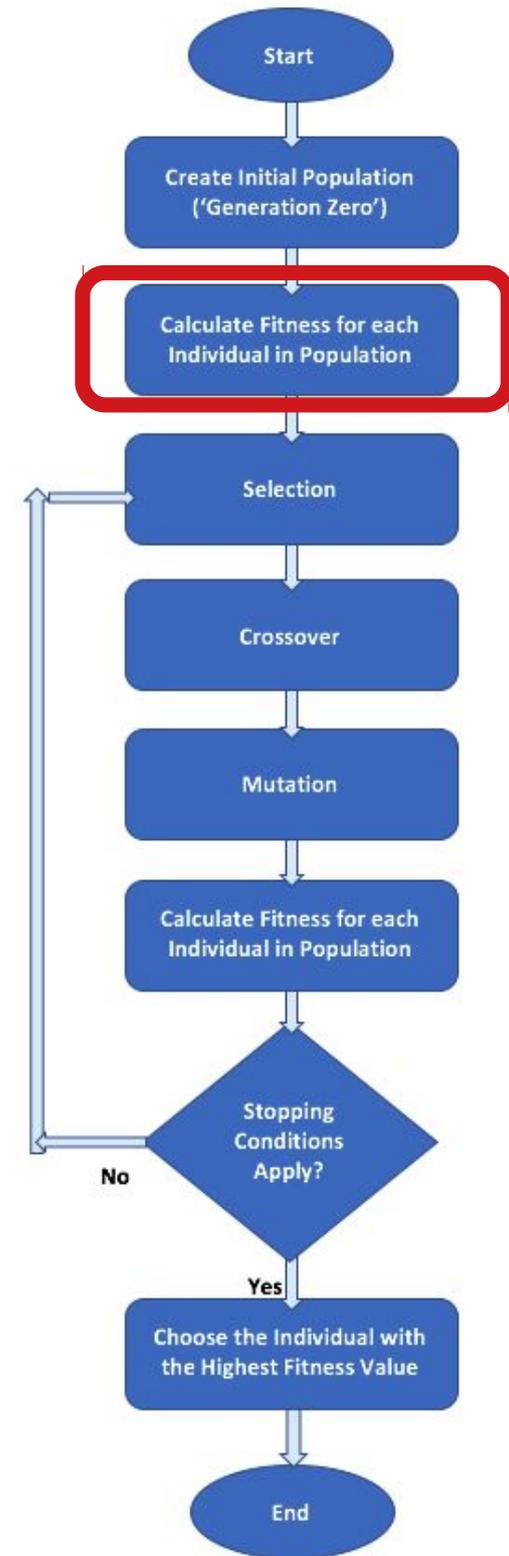
EA — Workflow — Fitness

Represents the requirements that the **population** should **adapt** to some **criteria** like **quality** function or **objective** function.

Assigns a single **real-valued** fitness to each **phenotype** which forms the **basis for selection**.

So the **more diversity** (different values) **the better**.

Typically **fitness** is assumed to be **maximized**, **but** ... some problems can be formulated as **minimization** problems.



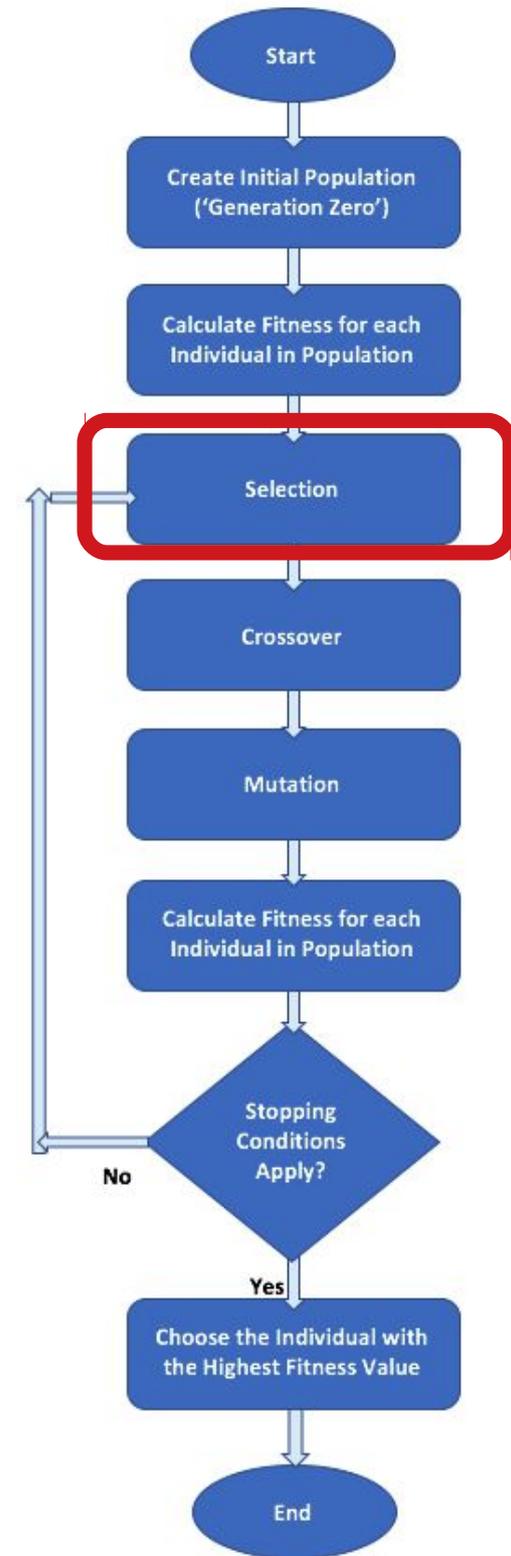
EA — Workflow — Selection

Assigns variable **probabilities** of individuals acting as parents depending on their fitnesses.

Usually **probabilistic**:
higher quality solutions **more** likely to become parents than **lower** quality, but ... not guaranteed.

Even **worst** in current population usually has **non-zero probability** of becoming a parent.

This **stochastic** nature can **aid** escape from **local optima!**



EA — Workflow — Variation Operators

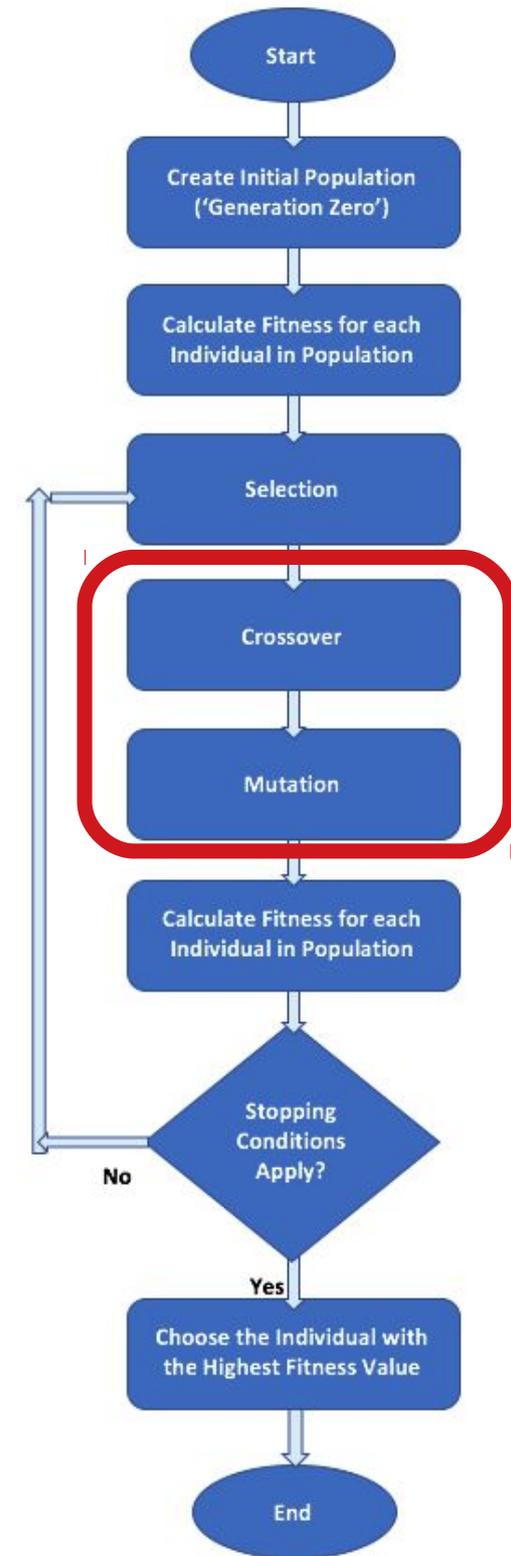
The main aim is to **generate** new **candidate solutions**.

Usually divided into types according to their *arity* (number of inputs):

- ♦ arity = 1 -> mutation operators
- ♦ arity > 1 -> recombination operators
- ♦ arity = 2 -> crossover operators

The relative importance of recombination and mutation is debated intensively now, but most EAs use both of them.

Choice of particular variation operators is representation dependant.



Workflow - Variation Operators - Crossover

Crossover or Recombination

Merges information from **parents** into **offspring**.

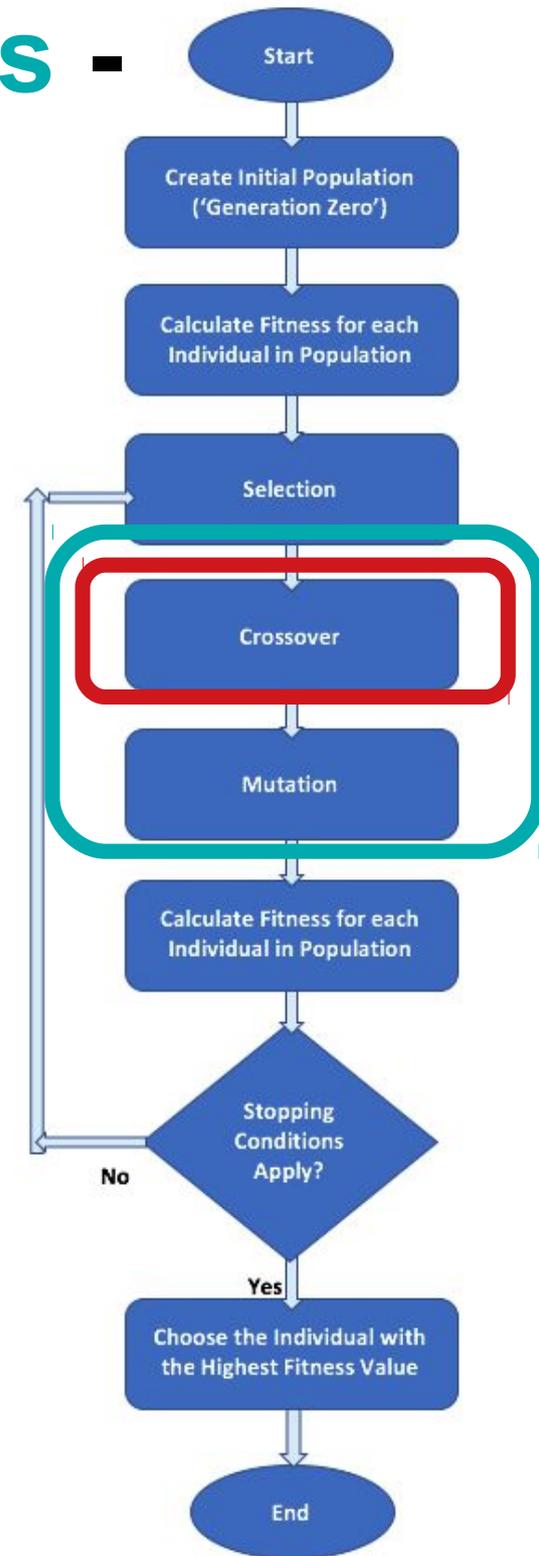
Choice of what information to merge is **stochastic**.

Most **offspring** may be **worse** or the **same** as the **parents**.

Hypothesis: some can be **better** by **combining elements** of genotypes that **lead to good traits**.

Metaphor from nature:

it has been **successfully used** by breeders of plants and livestock!



Workflow - Variation Operators - Mutation

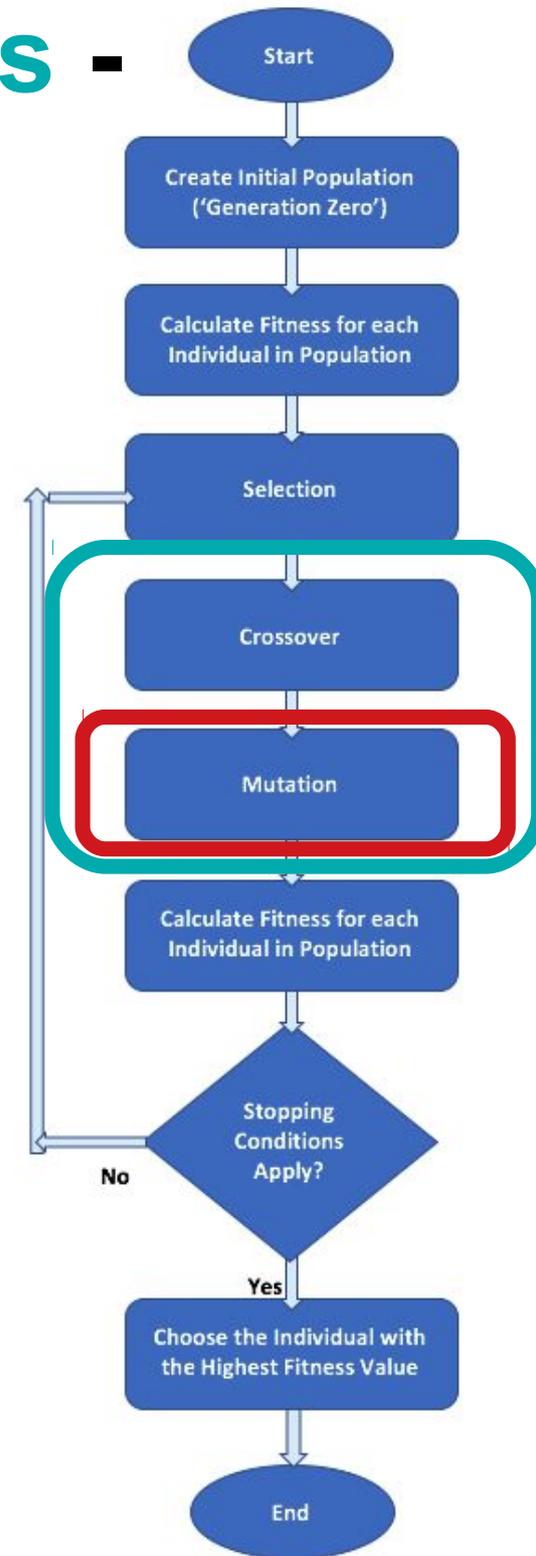
Operates on one genotype and **delivers another**.

Element of **randomness** is essential and differentiates it from other unary heuristic operators.

It depends on representation and dialect:

- ♦ **Binary GAs** – background operator responsible for preserving and introducing diversity,
- ♦ **EP** for FSM's/ continuous variables – only search operator,
- ♦ **GP** – hardly used.

May **guarantee** connectedness of search space and hence **convergence** proofs.



EA — Workflow — Start/Stop

Start

Initialization usually done at **random**.

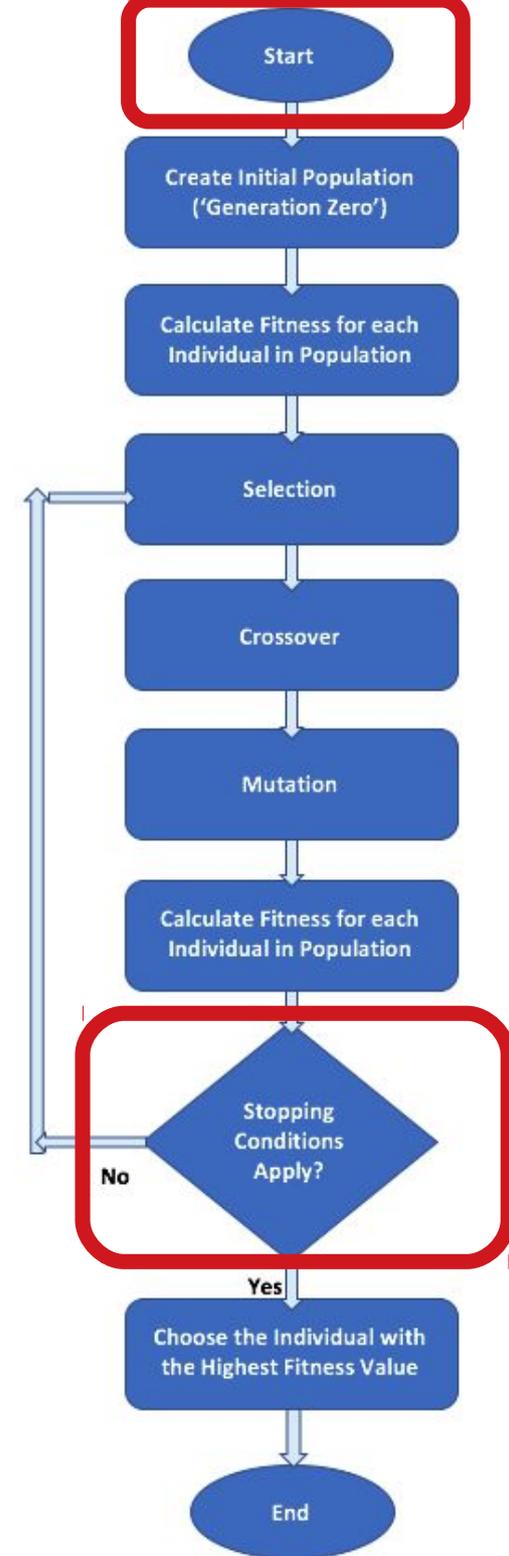
It should be even spread and mixture of possible allele values.

It can include **existing** solutions, or use problem-specific **heuristics**, to “**seed**” the population (care should be taken!)

Stop

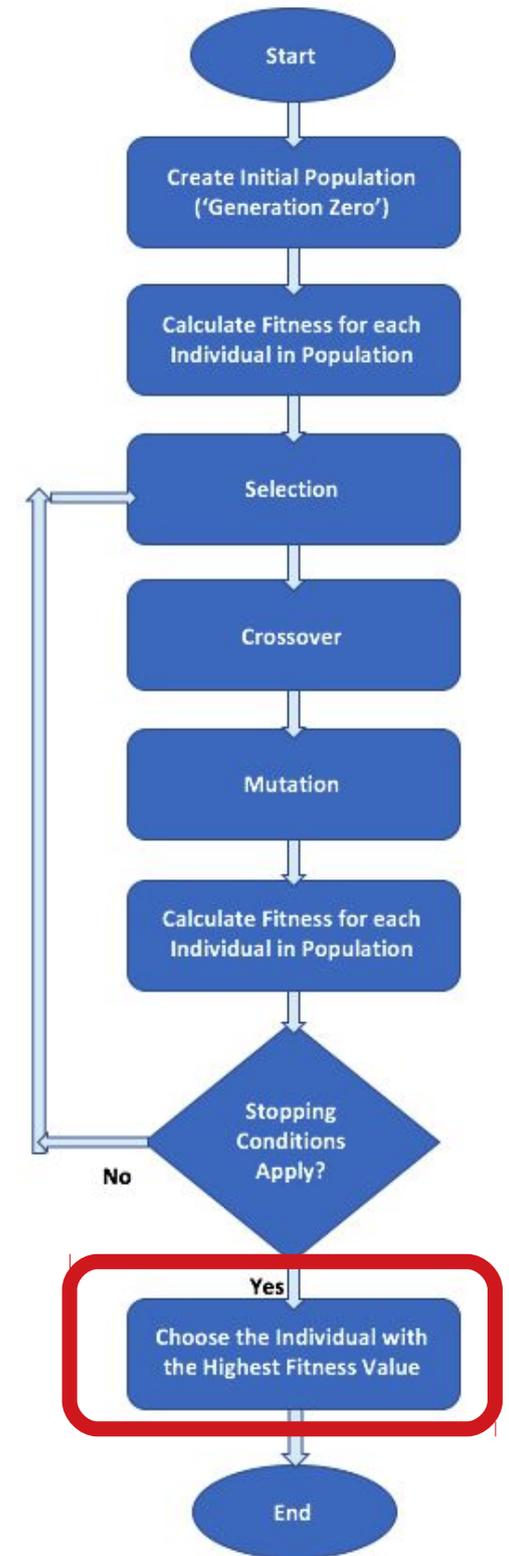
Termination condition checked every generation:

- ♦ some **planned** (known/assumed) **fitness**,
- ♦ some maximum allowed **number of generations**,
- ♦ some **minimum** level of **diversity**,
- ♦ some specified **number of generations without fitness improvement**.



EA — Workflow — End

Choose
the **individual**
with
the **highest fitness** value.

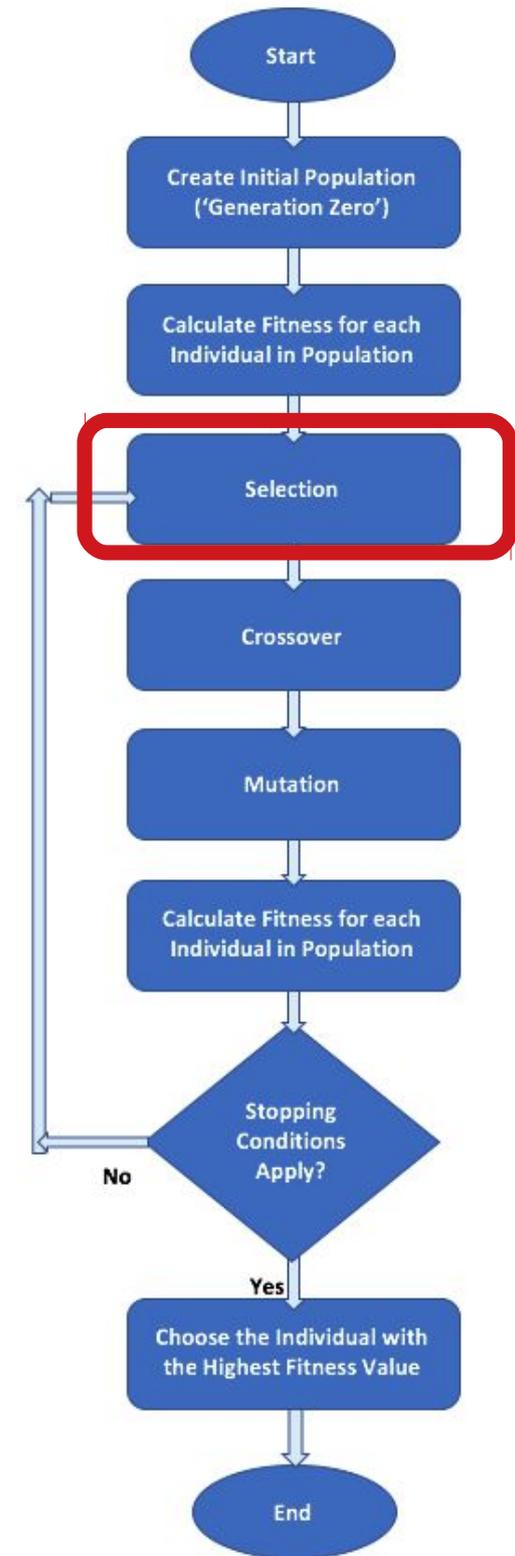


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EA — Workflow — Selection Methods

- ◆ Roulette wheel selection
(fitness proportionate selection — FPS)
- ◆ Stochastic universal sampling (SUS)
 - ◆ Rank-based selection
 - ◆ Tournament selection

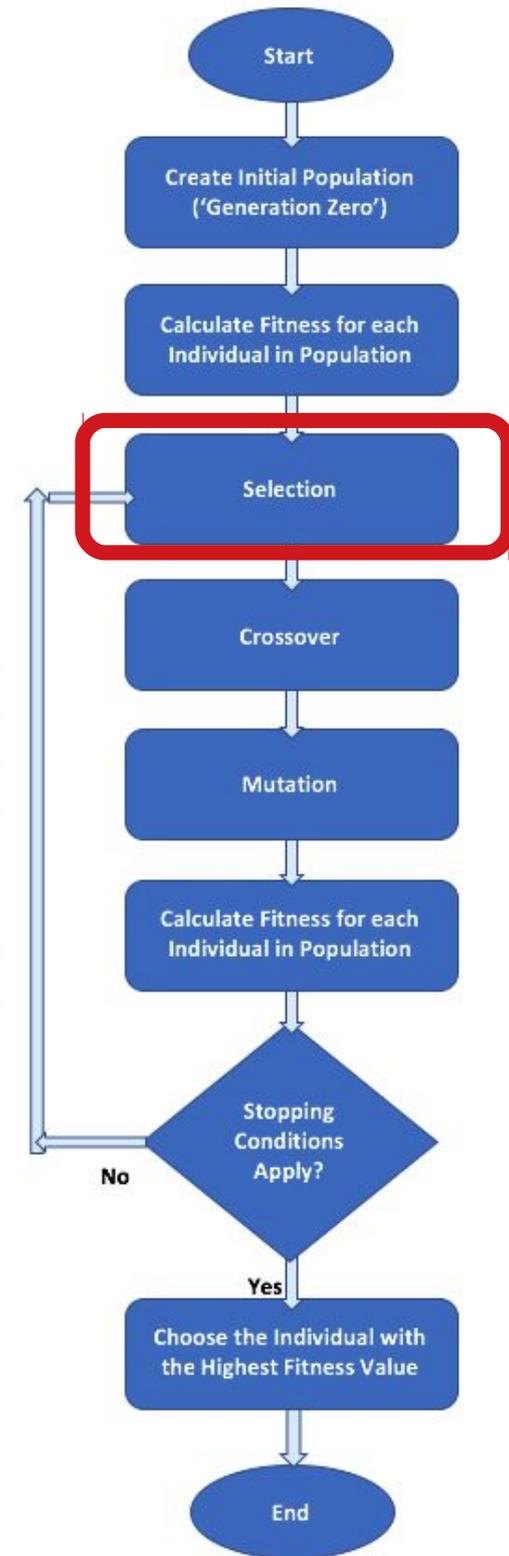
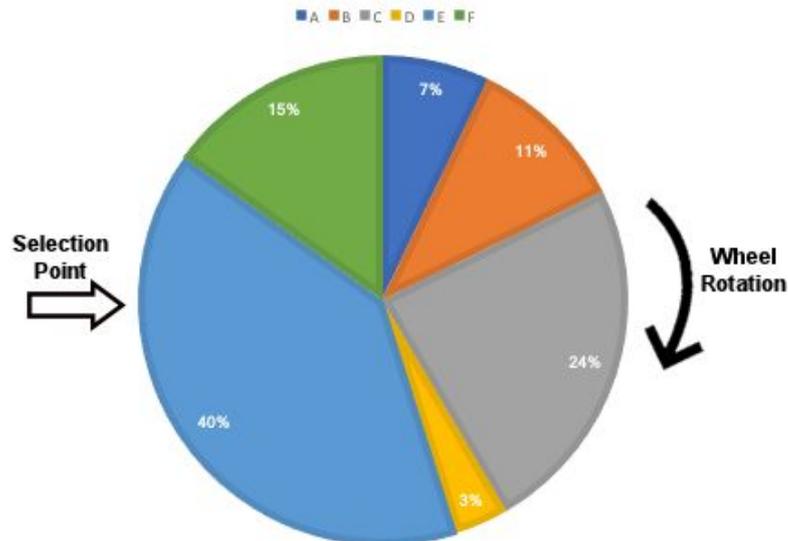


Workflow — Roulette Wheel Selection

Probability for selecting an individual is directly **proportionate** to its **fitness value**.

This is comparable to using a roulette wheel in a casino and assigning each individual a portion of the wheel proportional to its fitness value.

Individual	Fitness	Relative portion
A	8	7%
B	12	11%
C	27	24%
D	4	3%
E	45	40%
F	17	15%

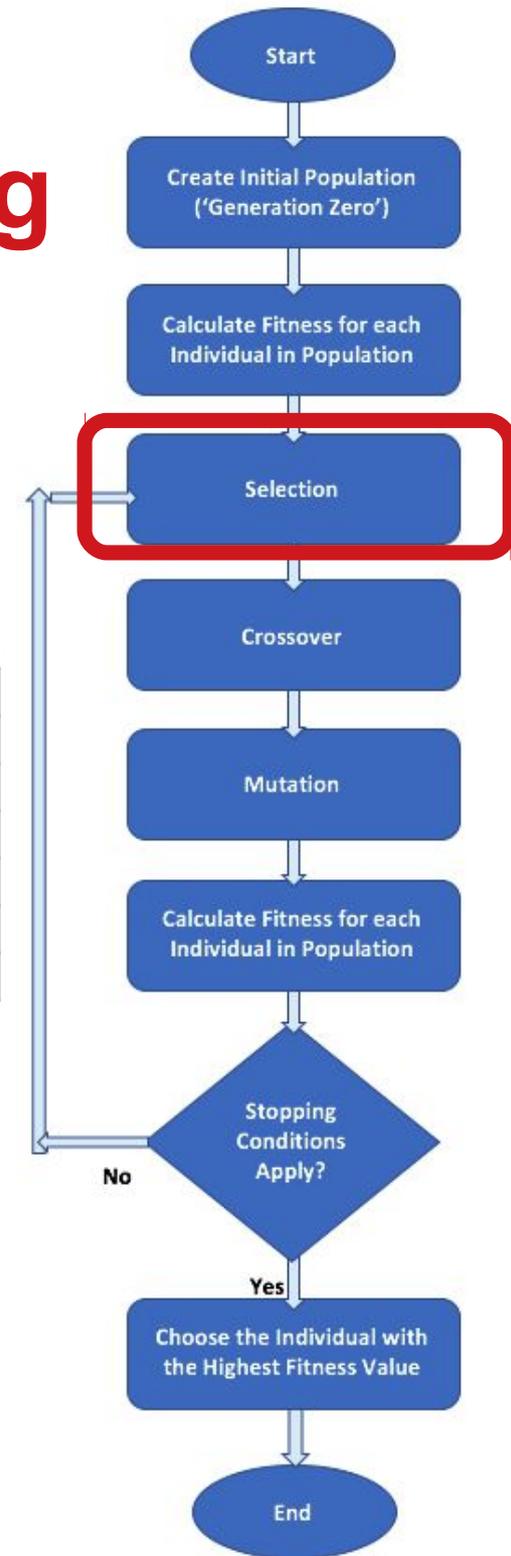
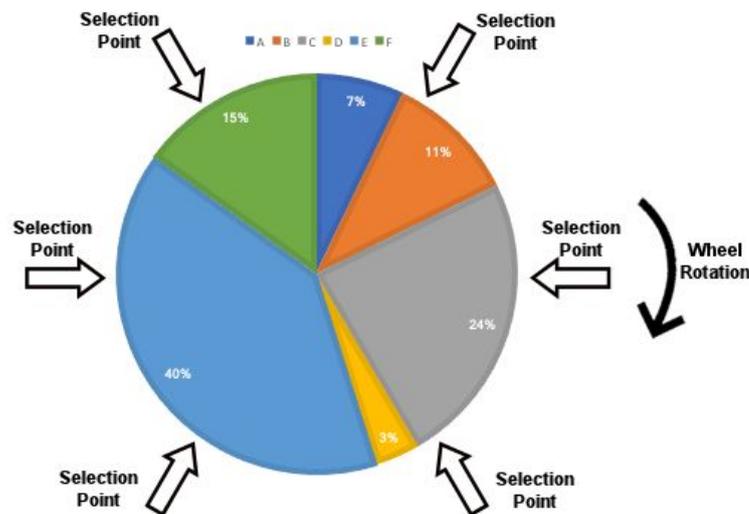


Workflow —

Stochastic Universal Sampling

Instead of a single selection point and turning the roulette wheel N times until all needed N individuals have been selected, we **turn the wheel only 1 time** and use **N selection points** that are equally spaced around the wheel

Individual	Fitness	Relative portion
A	8	7%
B	12	11%
C	27	24%
D	4	3%
E	45	40%
F	17	15%

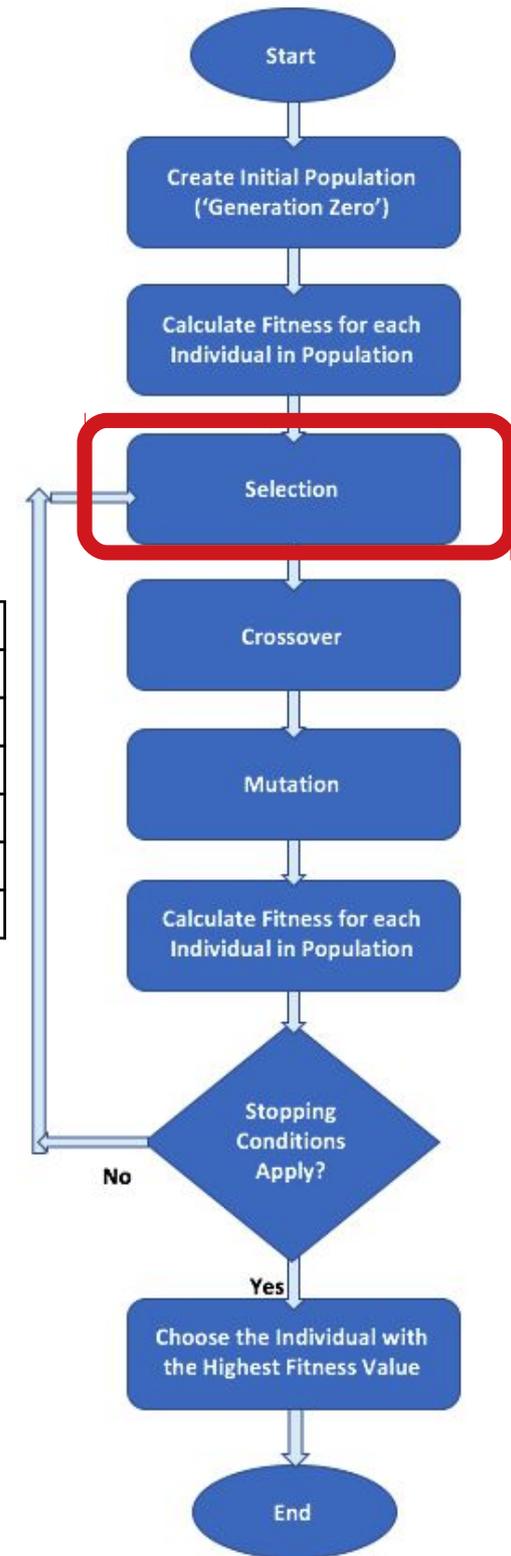
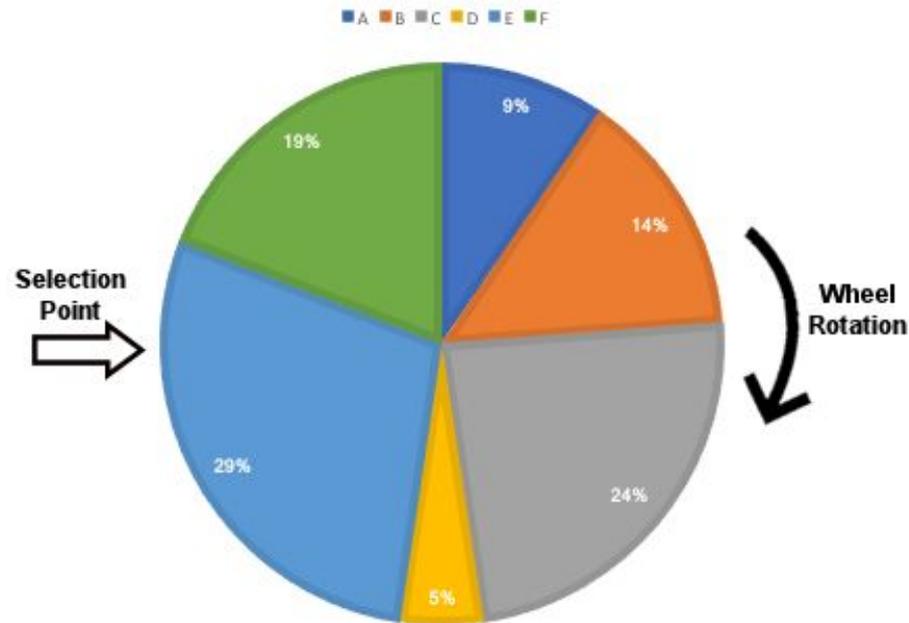


Workflow —

Rank-based Selection

The **fitness** is used to **sort** the individuals: each individual is given a **rank** for its **position** and **wheel-portion**, and the roulette probabilities are calculated based on these ranks.

Individual	Fitness	Rank	Relative portion
A	8	2	9%
B	12	3	14%
C	27	5	24%
D	4	1	5%
E	45	6	29%
F	17	4	19%

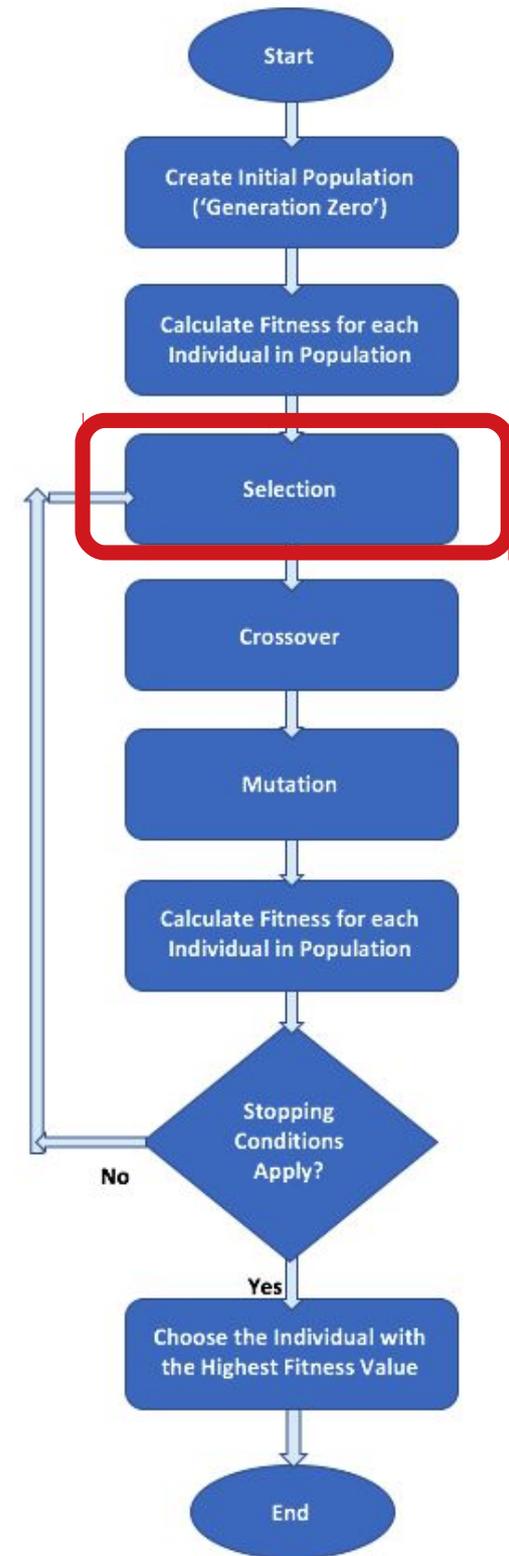
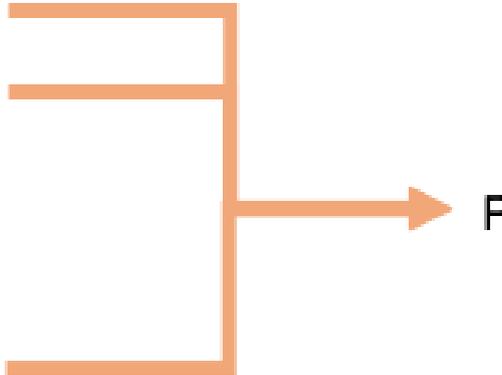


Workflow — Tournament Selection

In each round of the tournament selection method, two or more **individuals** are randomly **picked** from the population, and the **one** with the **highest** fitness score **wins** and gets **selected**.

The number of individuals participating at each tournament selection round (three in this figure) is suitably called ***tournament size***. The **larger** the tournament size, the **higher** the chances that the **best** individuals will **be selected**.

Individual	Fitness
A	8
B	12
C	27
D	4
E	45
F	17



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Workflow - Variation Operators - Crossover

Crossover or Recombination

Merges information from **parents** into **offspring**.

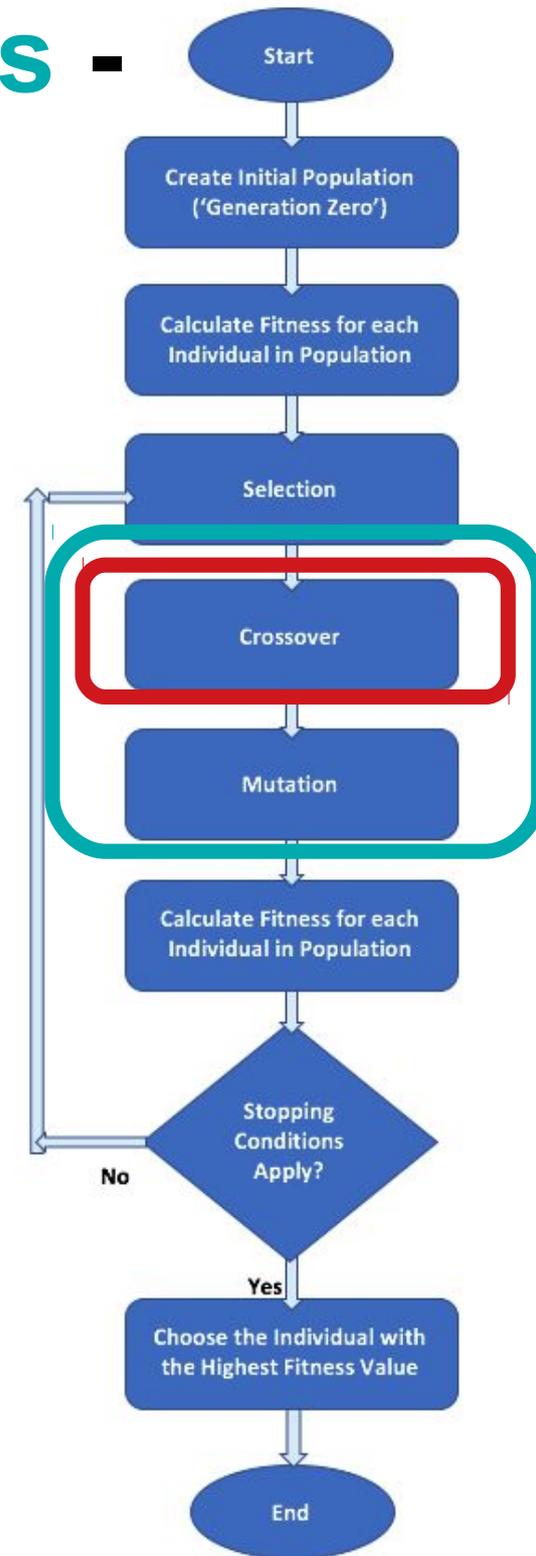
Choice of what information to merge is **stochastic**.

Most **offspring** may be **worse** or the **same** as the **parents**.

Hypothesis: some can be **better** by **combining elements** of genotypes that **lead to good traits**.

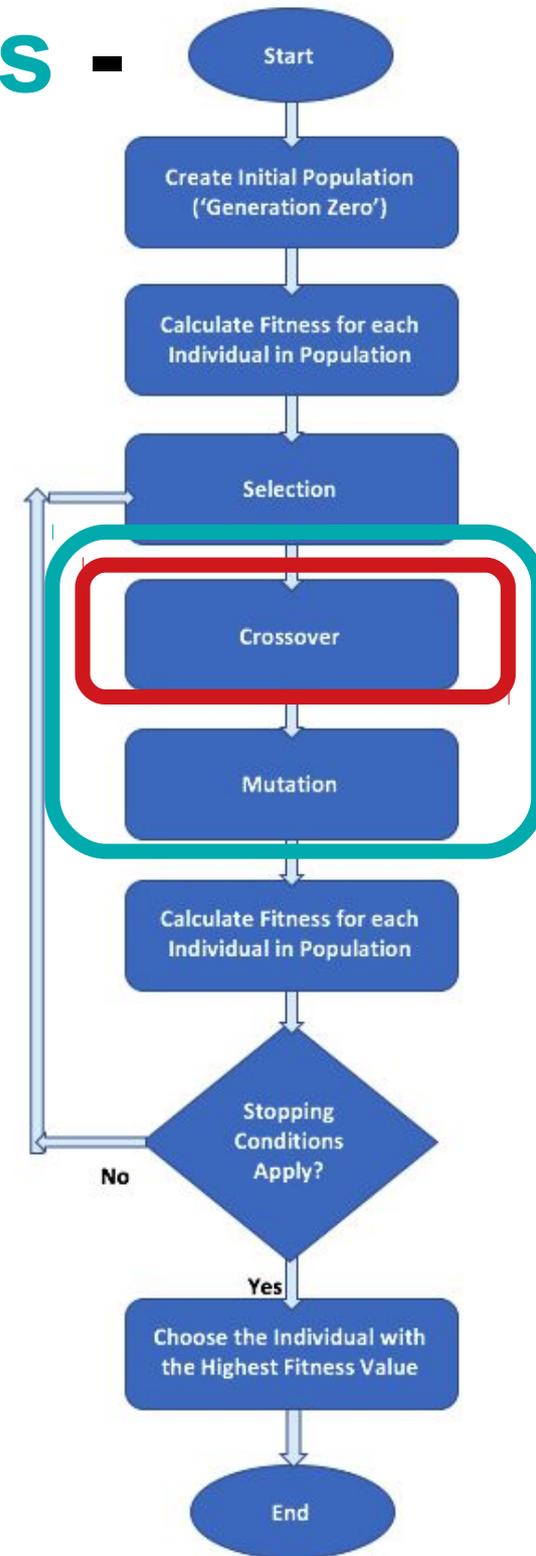
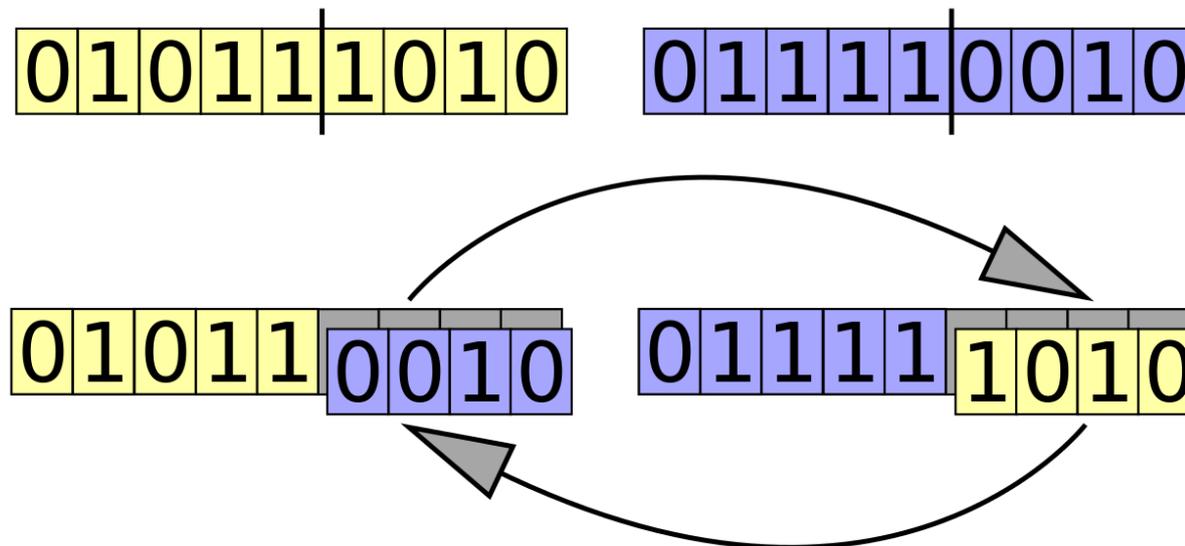
Metaphor from nature:

it has been **successfully used** by breeders of plants and livestock!



Workflow - Variation Operators - Crossover - Single-point

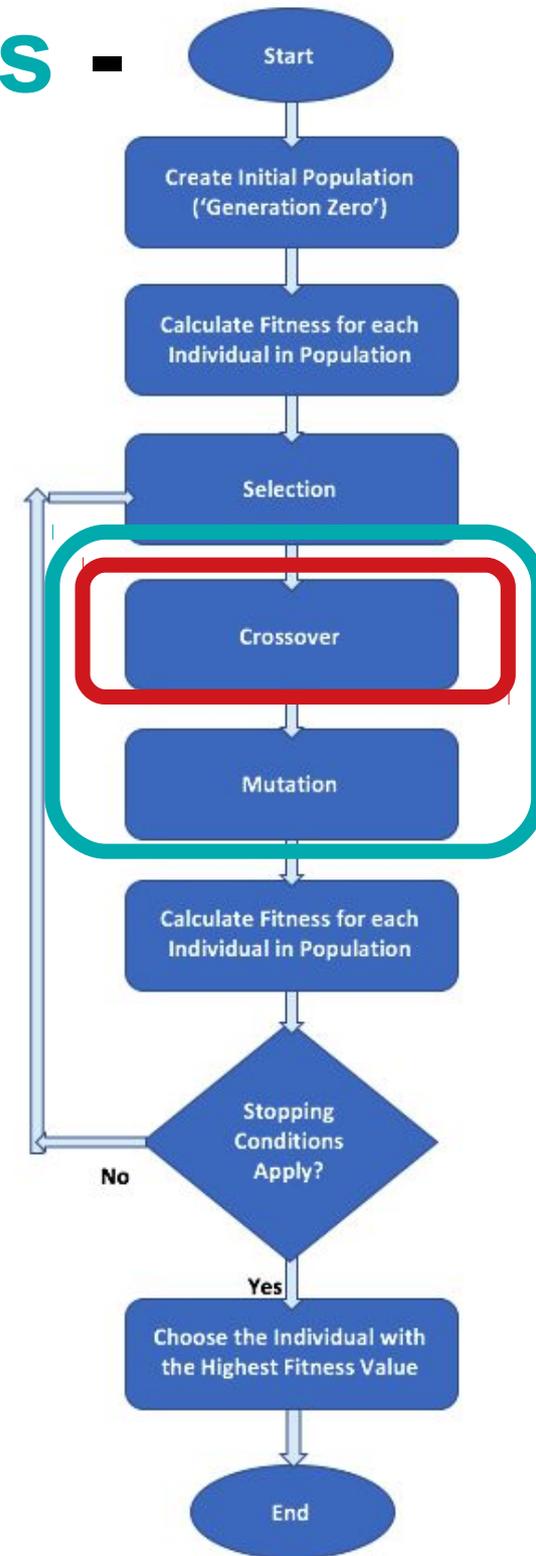
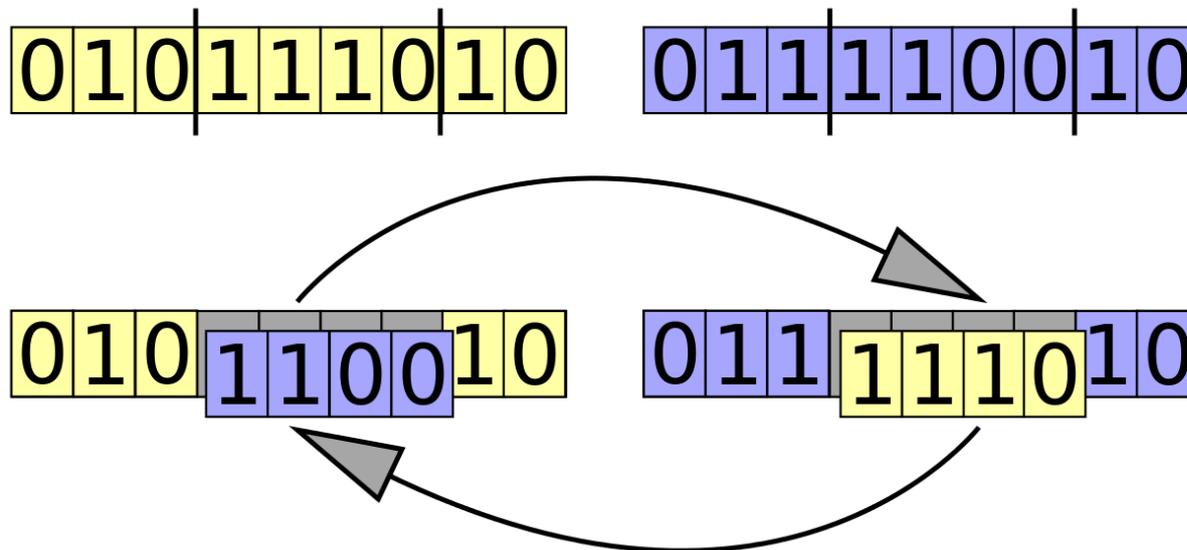
The **crossover point** (or **cut point**) on the chromosomes of both parents is **selected randomly**. Genes to the right of that point are swapped between the two parent chromosomes. As a result, we **get two offsprings**, where each of them **carry** some genetic information **from both** parents.



Workflow - Variation Operators - Crossover - K-point

For example, in 2-point crossover 2 points on the chromosomes of both parents are selected randomly. The genes residing between these points are swapped between the two parent chromosomes.

A generalization of this method is the **k-point crossover**, where **k** represents a positive



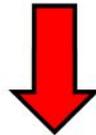
Workflow - Variation Operators - Crossover - Uniform

Each gene is **independently determined** by **randomly** choosing one of the parents. If the random distribution is 50%, each parent has the same chance of influencing the offspring.

NOTE: Below, **integer-based** chromosomes are shown, but it is **the same for binary** ones.

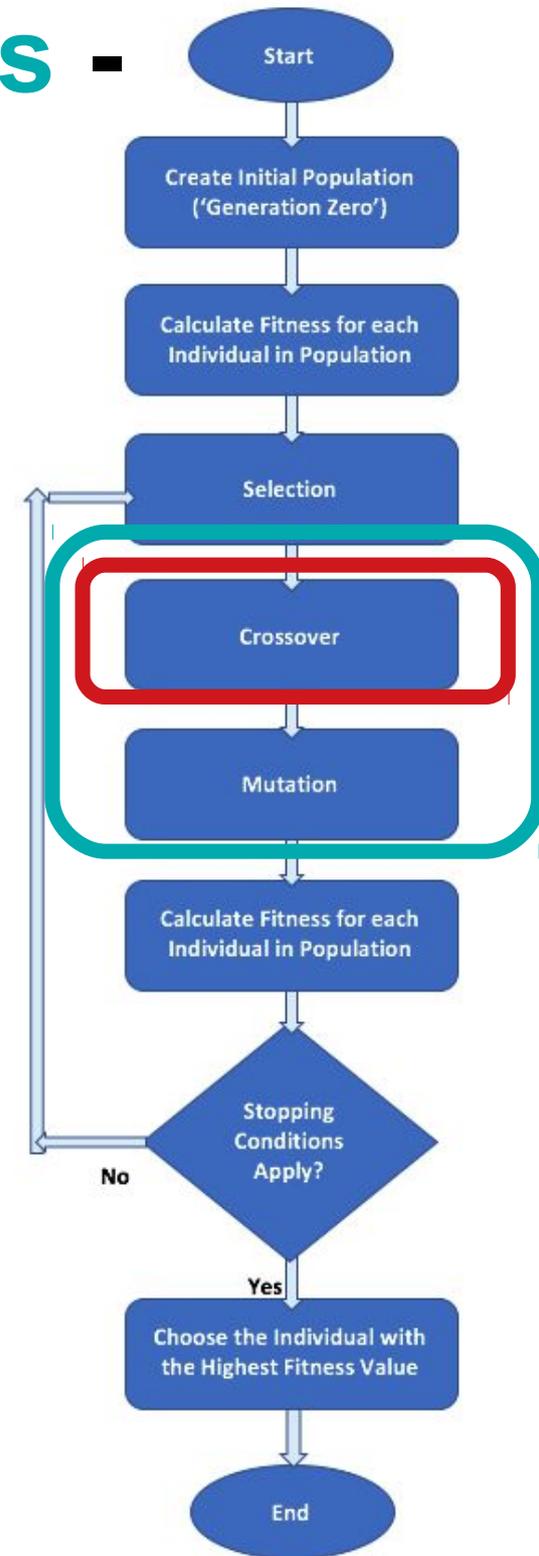
5	7	2	3	1	6	9	8	0
---	---	---	---	---	---	---	---	---

6	8	3	4	2	1	0	9	7
---	---	---	---	---	---	---	---	---



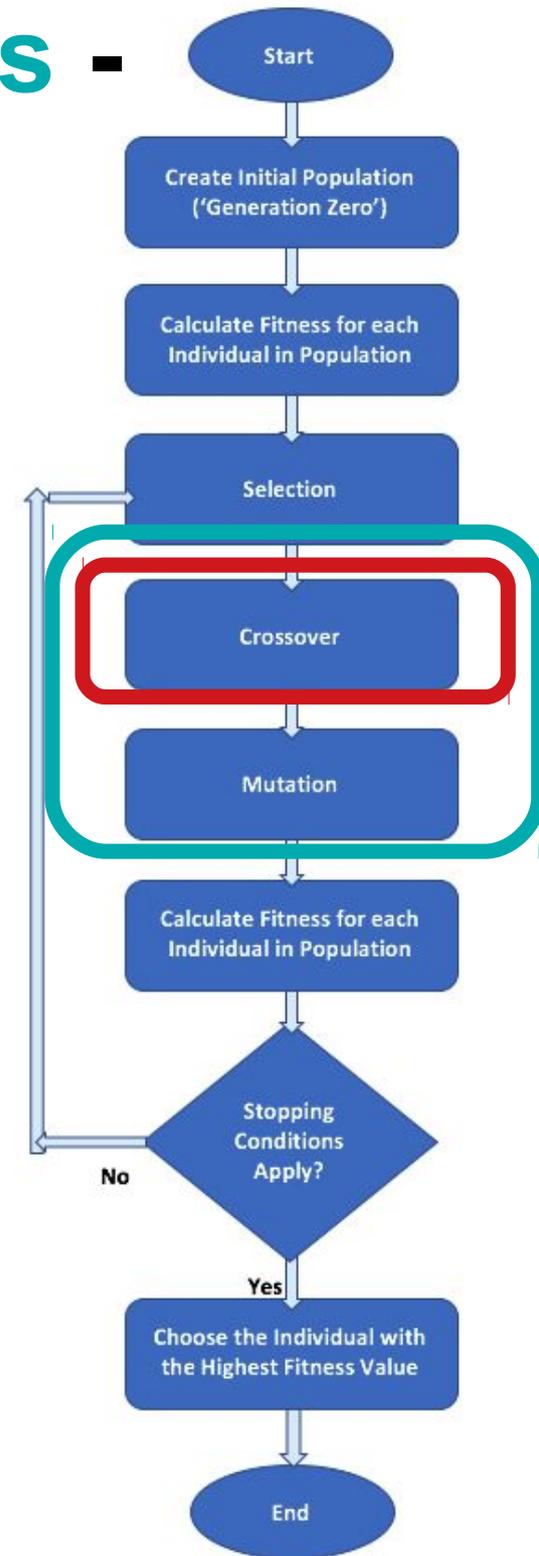
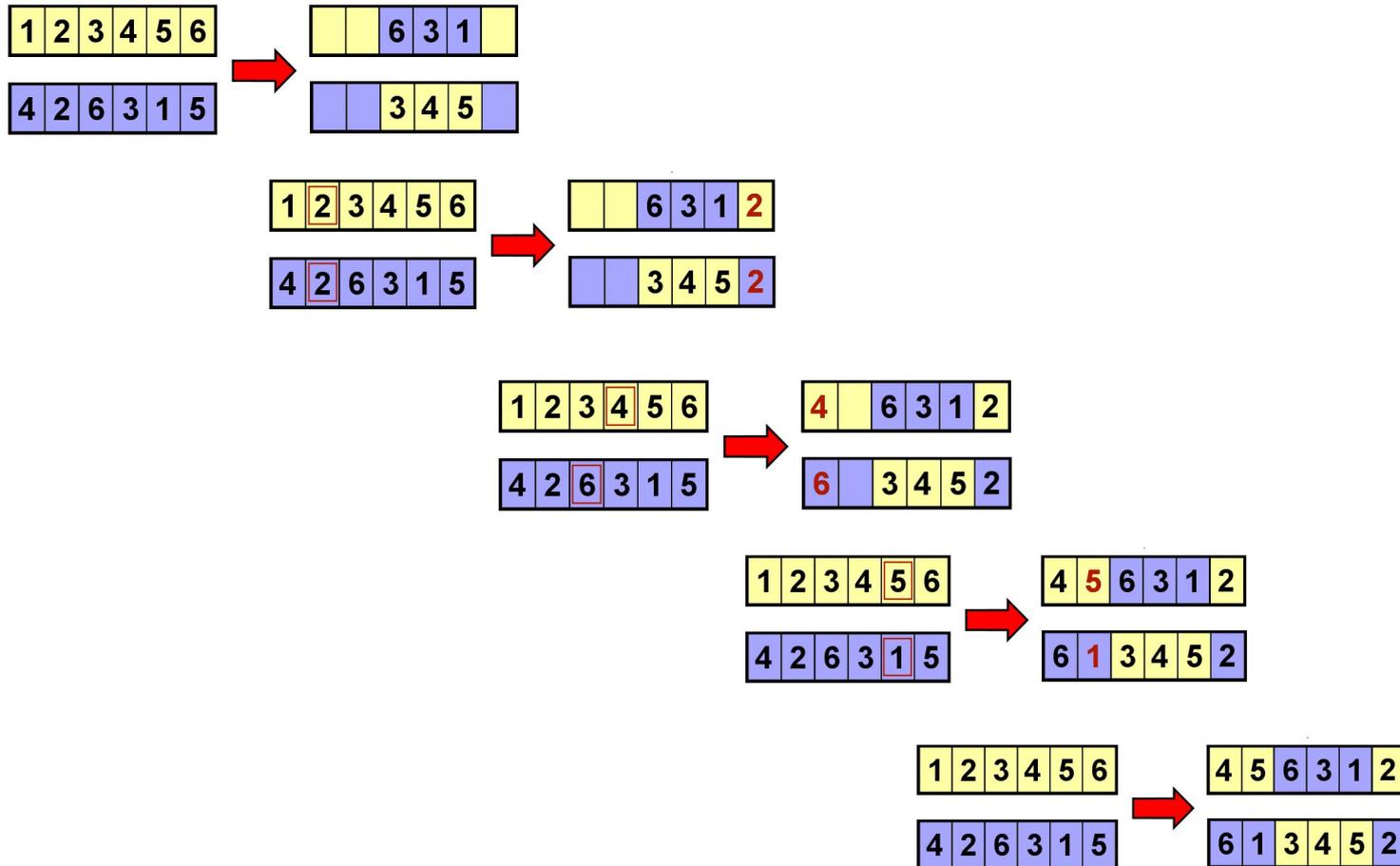
5	8	2	3	2	6	0	9	0
---	---	---	---	---	---	---	---	---

6	7	3	4	1	1	9	8	7
---	---	---	---	---	---	---	---	---



Workflow - Variation Operators - Crossover — Ordered Lists

The **ordered crossover** (OX1) method strives to preserve the relative ordering of the parent's genes as much as possible.



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Workflow - Variation Operators - Mutation

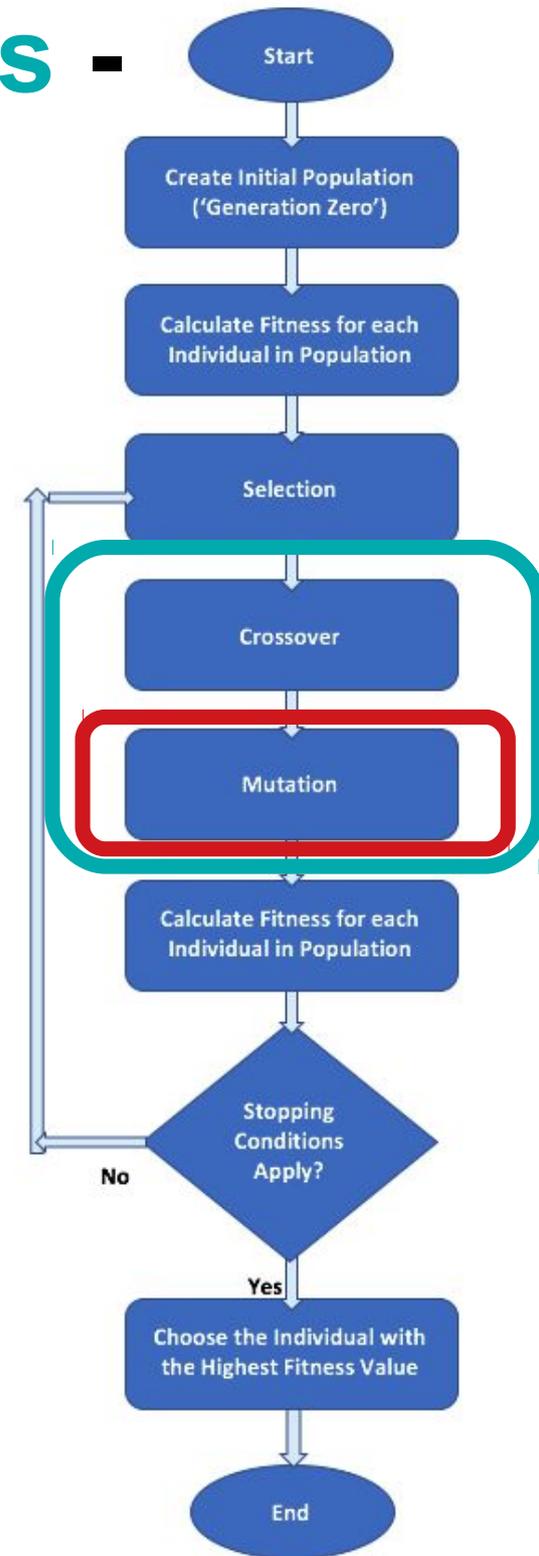
Operates on one genotype and **delivers another**.

Element of **randomness** is essential and differentiates it from other unary heuristic operators.

It depends on representation and dialect:

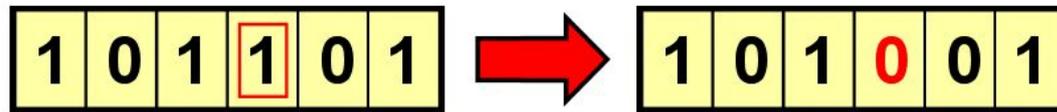
- ♦ **Binary GAs** – background operator responsible for preserving and introducing diversity,
- ♦ **EP** for FSM's/ continuous variables – only search operator,
- ♦ **GP** – hardly used.

May **guarantee** connectedness of search space and hence **convergence** proofs.

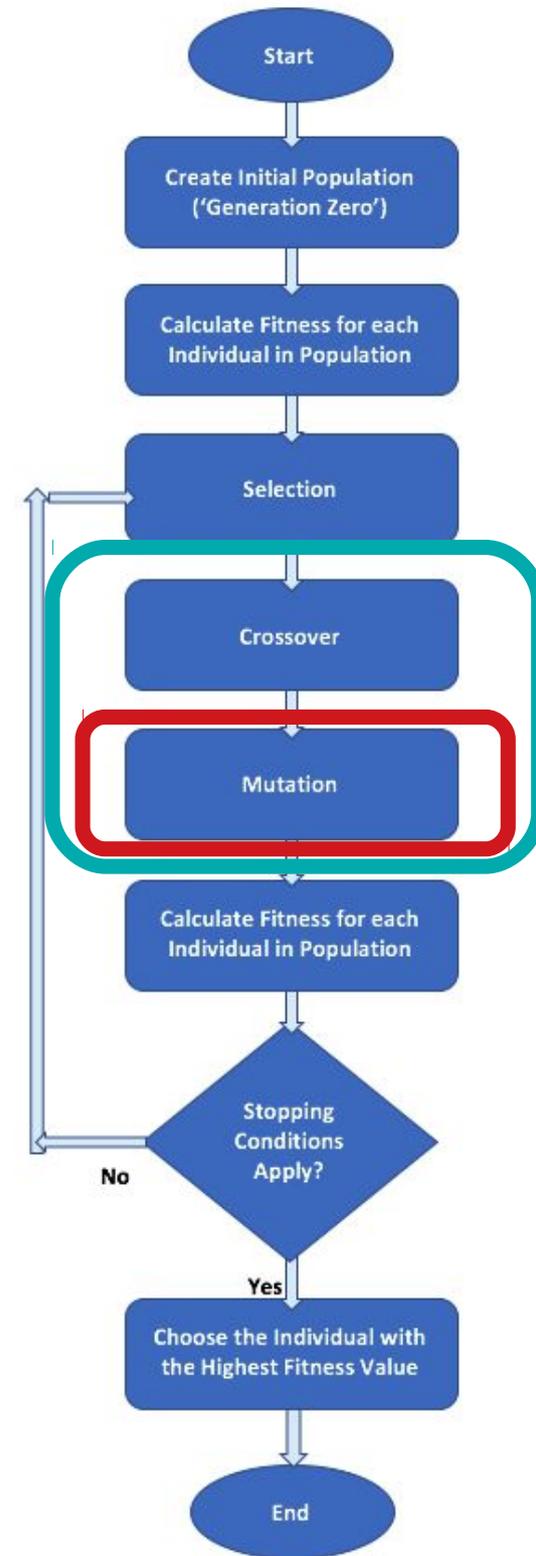


Workflow — Mutation - Flip bit

For a binary chromosome,
1 gene is randomly selected and its value is **flipped** (complemented).

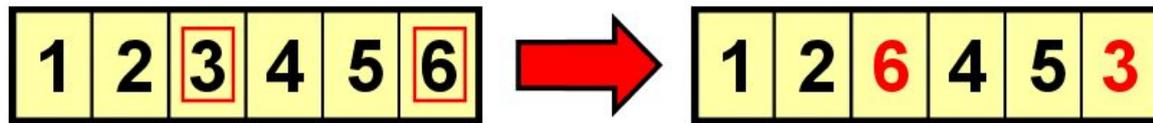


This can be extended to several random genes being flipped instead of just one.

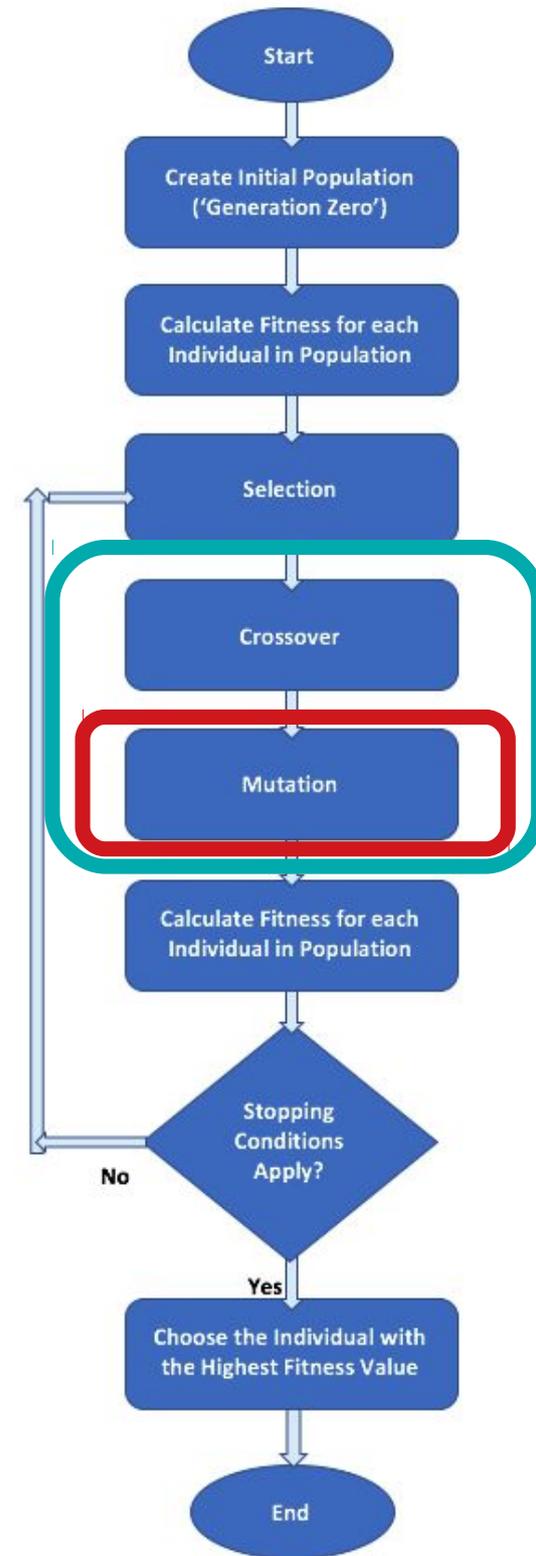


Workflow — Mutation - Swap

For a binary or integer-based chromosomes, **2 genes are randomly selected** and their values are **swapped**.

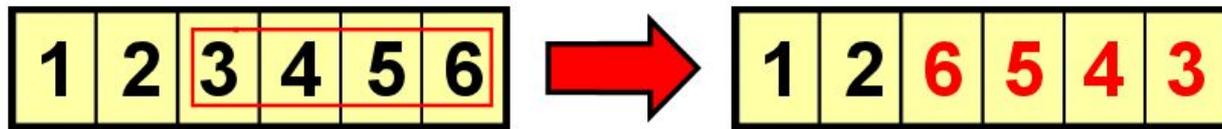


This mutation operation is **suitable** for the **chromosomes of ordered lists**, as the **new chromosome** still **carries the same genes** as the original one.

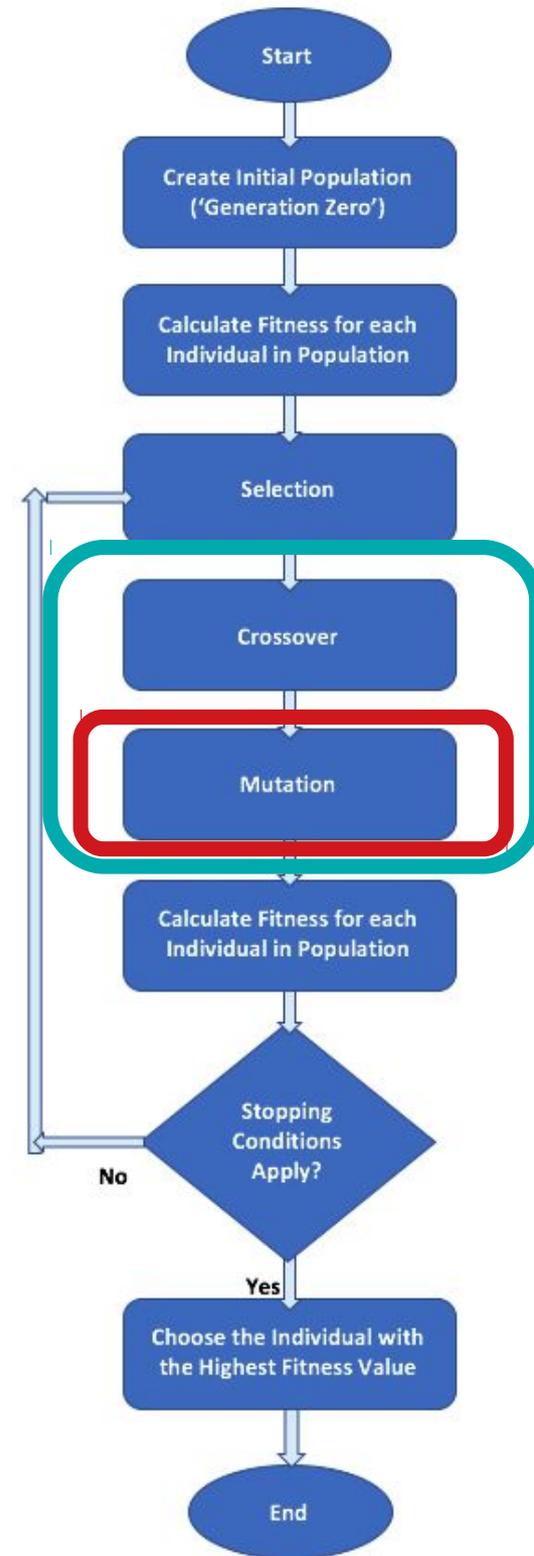


Workflow — Mutation - Inversion

For a **binary** or **integer-based** chromosomes, a **random sequence** of genes is selected and the **order** of the genes in that sequence is **reversed**.

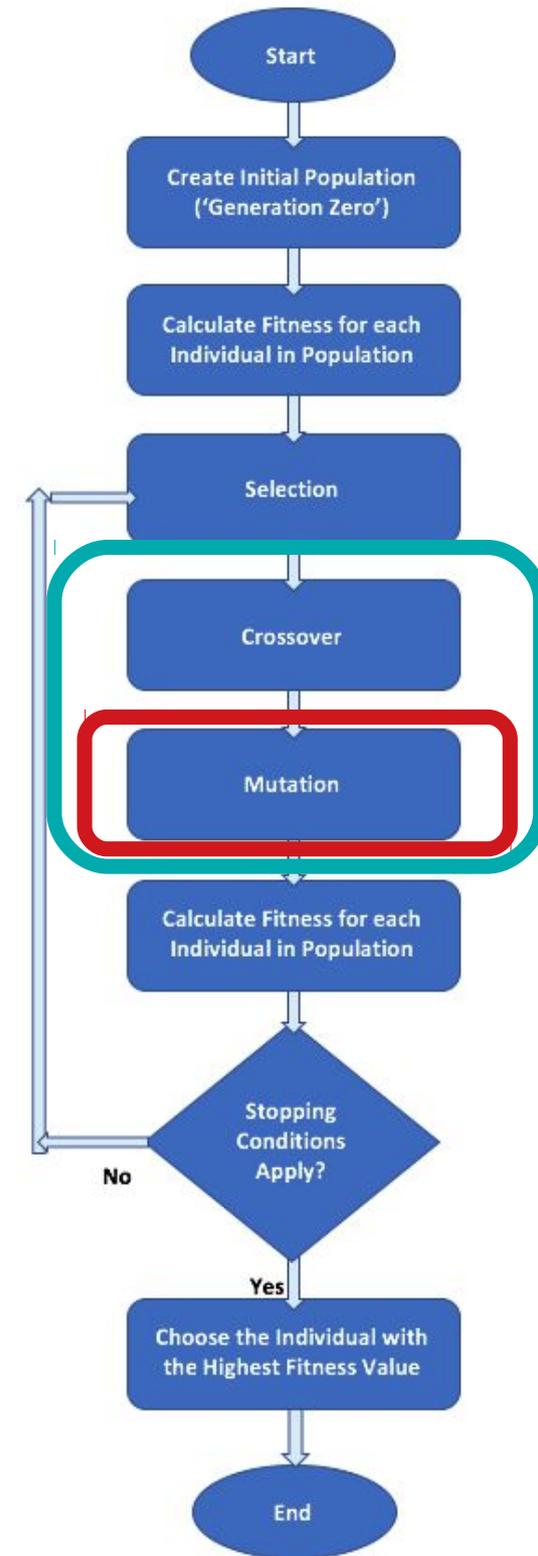
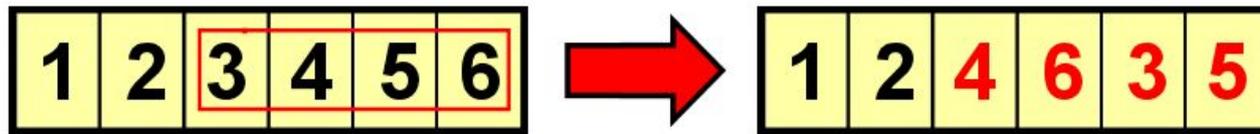


Similar to the **swap mutation**, the **inversion mutation** operation is **suitable** for the chromosomes of **ordered lists**.



Workflow — Mutation - Scramble

For a **binary** or **integer-based** chromosomes, a **random sequence** of genes is selected and the **order** of the genes in that sequence is **shuffled** (or **scrambled**).



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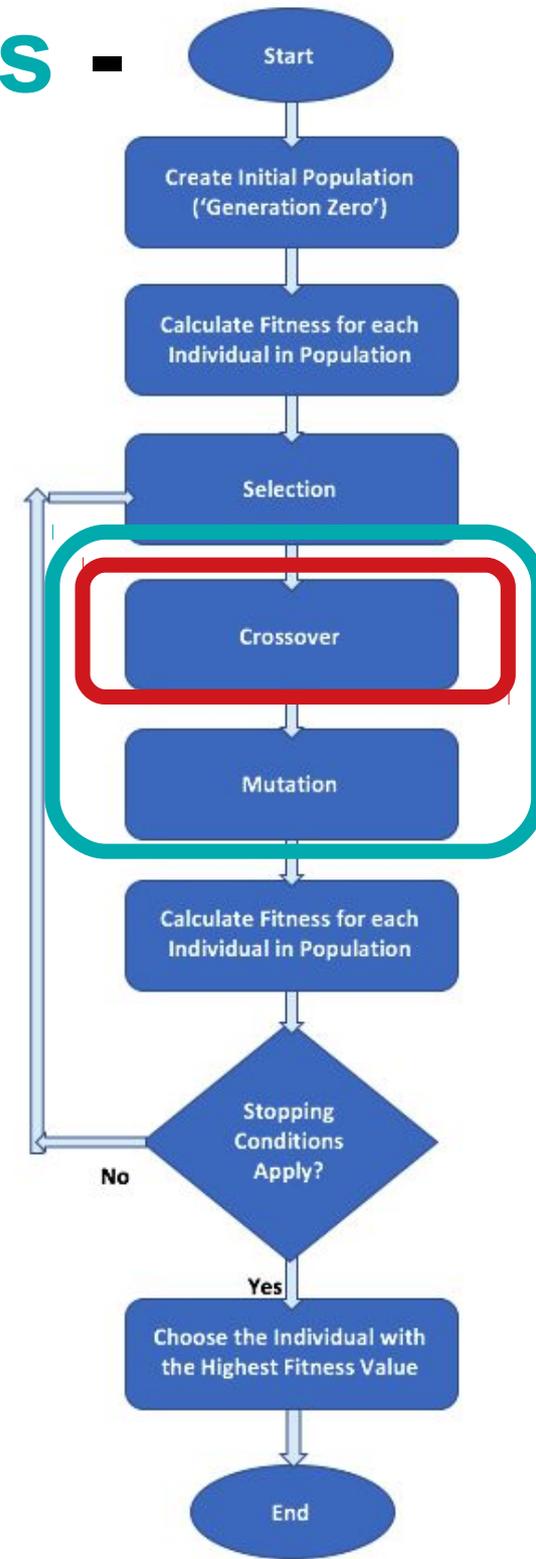
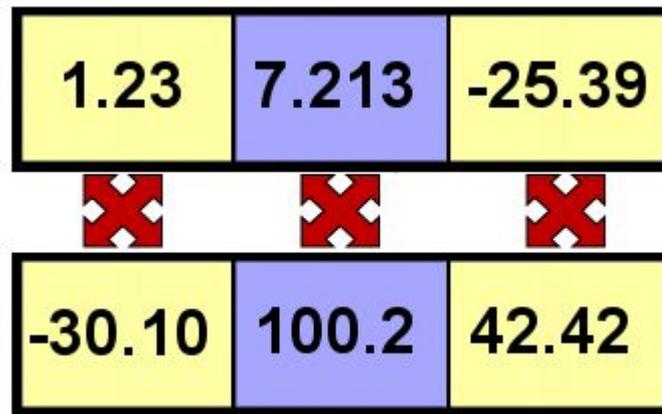
Workflow - Variation Operators -

Real-coded

The **selection** methods will work just the same as they only depend on the **fitness** of the individuals and not their representation.

But the **crossover** and **mutation** methods will not be suitable and so specialized ones need to be used.

They should be applied **separately** for each **dimension** of the array that forms the real-coded chromosome.

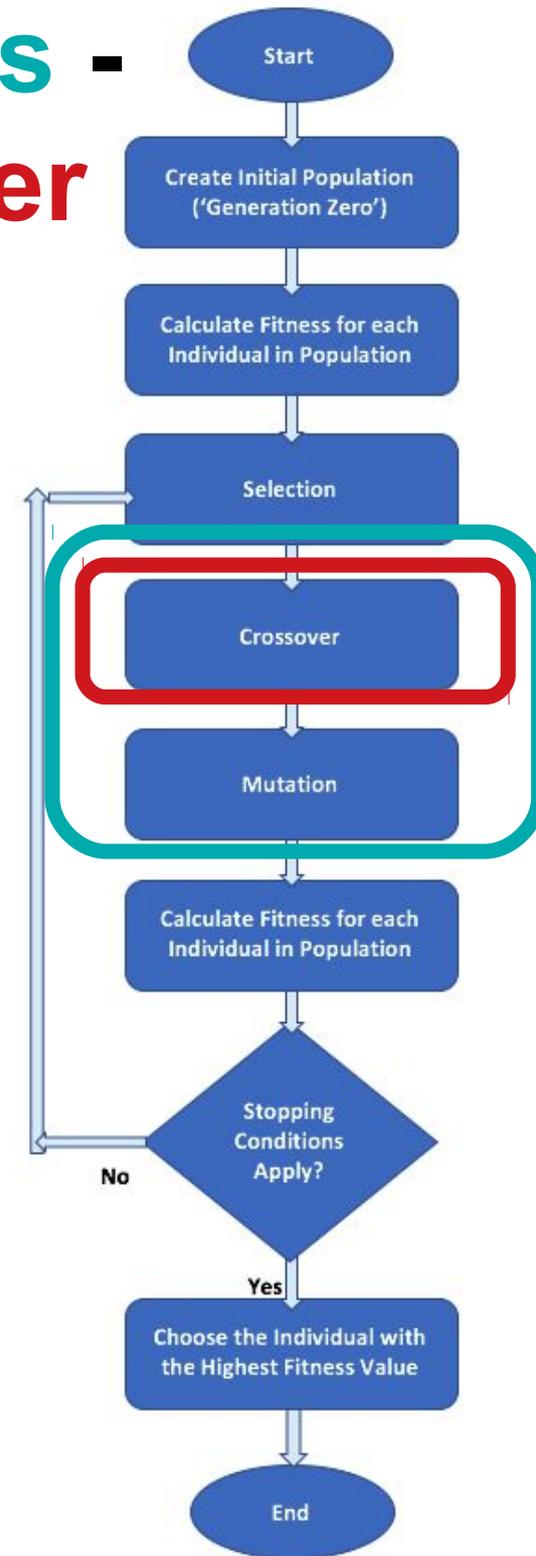
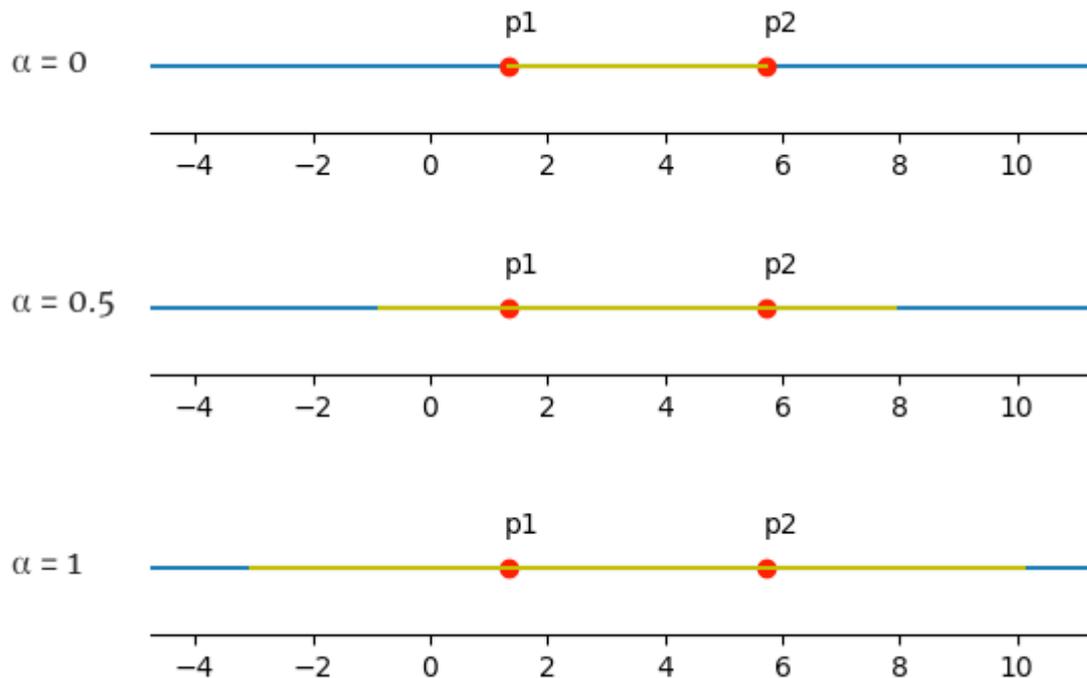


Workflow - Variation Operators - Real-coded — Blend Crossover

Blend crossover (BLX) - each offspring is randomly selected from the interval created by its parent values by some formulae:

$$[parent_1 - \alpha(parent_2 - parent_1), parent_2 + \alpha(parent_2 - parent_1)]$$

The parameter α is a constant, whose value lies between 0 and 1. With larger values of α , the

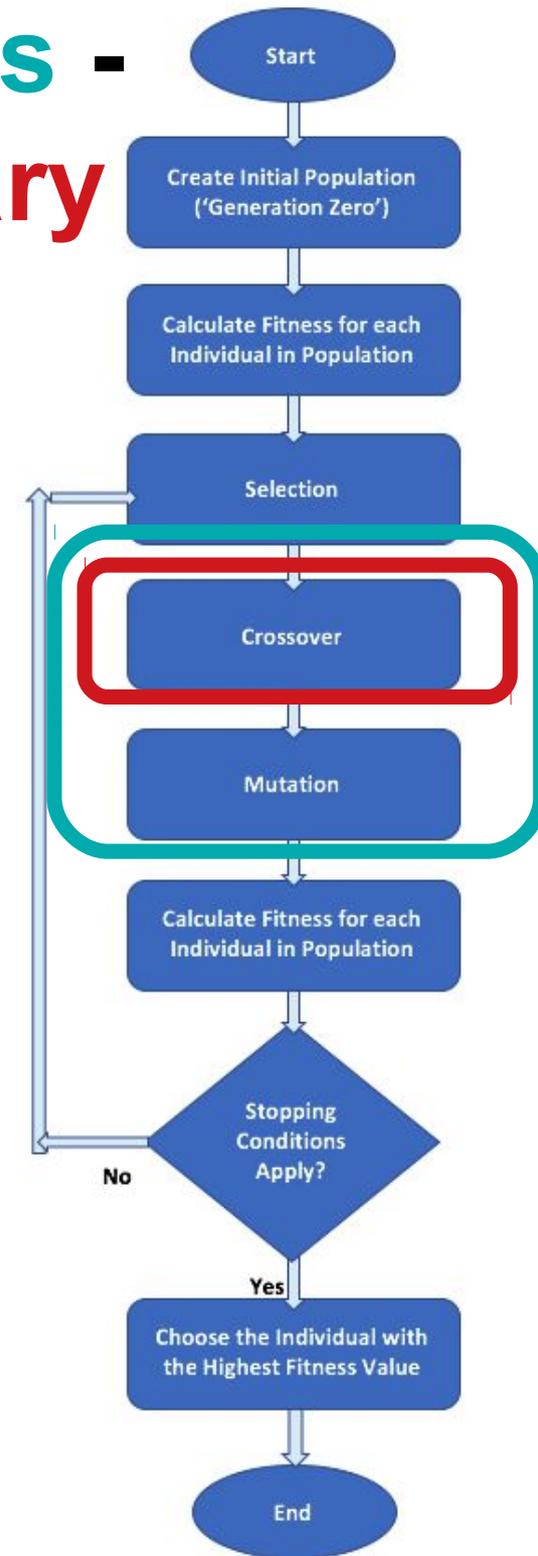
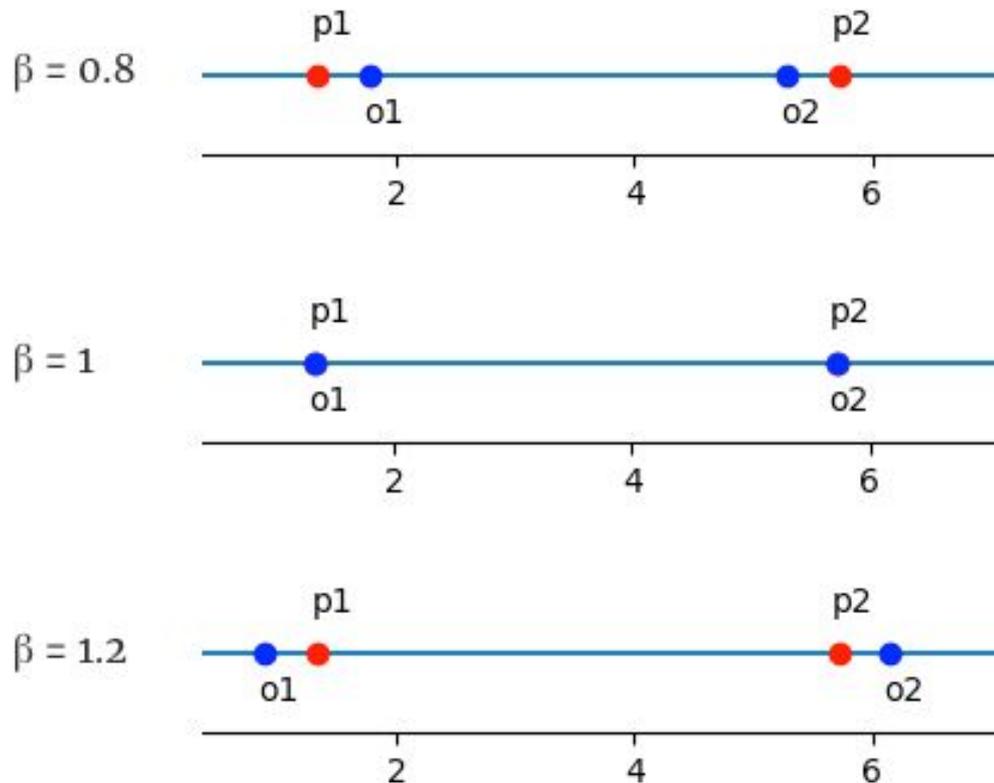


Workflow - Variation Operators - Real-coded — Simulated Binary

Simulated binary crossover (SBX) - each offspring is randomly selected from the interval created by its parent values by formula:

$$offspring_1 = \frac{1}{2} [(1 + \beta)parent_1 + (1 - \beta)parent_2]$$

$$offspring_2 = \frac{1}{2} [(1 - \beta)parent_1 + (1 + \beta)parent_2]$$



Workflow - Variation Operators - Real-coded — Simulated Binary

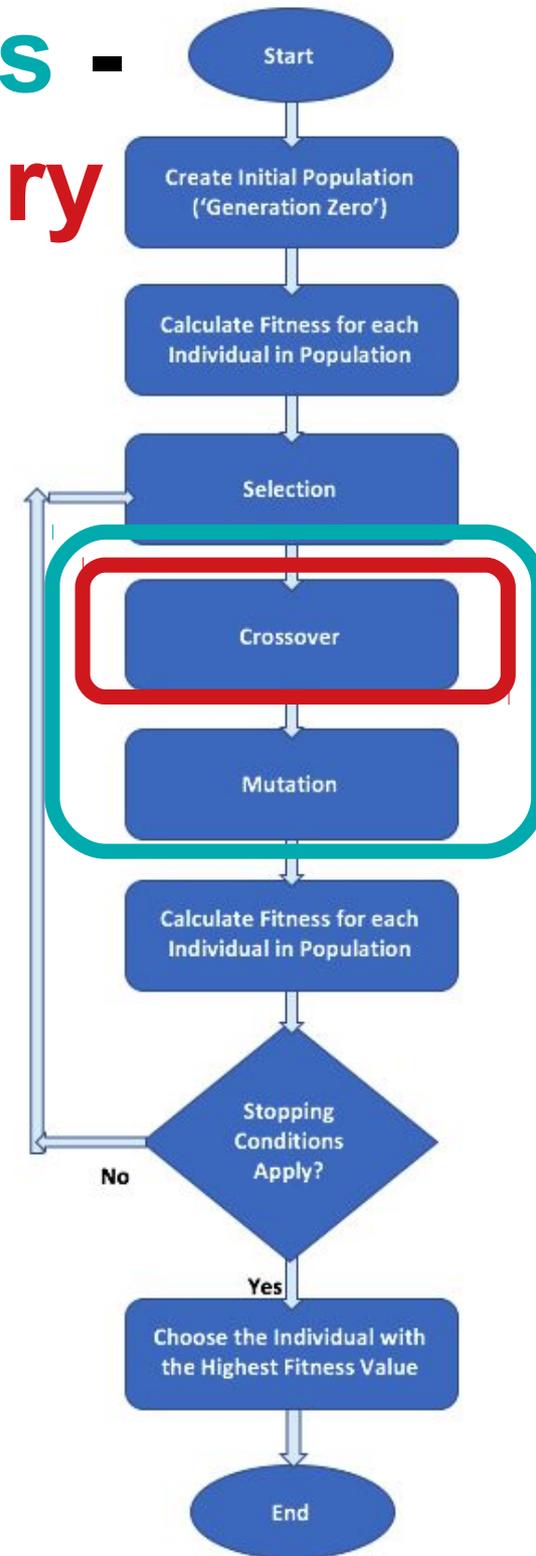
In the preceding cases, the **average** value of the two **offspring** is 3.525, which is **equal to the average** value of the two **parents**.

We need to preserve is the similarity between offspring and parents.

For this, the probability of β should be **much higher** for values **near 1**, where the offspring are **similar** to the parents.

That is why, the β value is calculated using **another random** value, denoted by u , that is uniformly distributed over the interval $[0, 1]$:

$$u \leq 0.5 \quad \beta = (2u)^{\frac{1}{\eta+1}}$$
$$u > 0.5 \quad \beta = \left[\frac{1}{2(1-u)} \right]^{\frac{1}{\eta+1}}$$

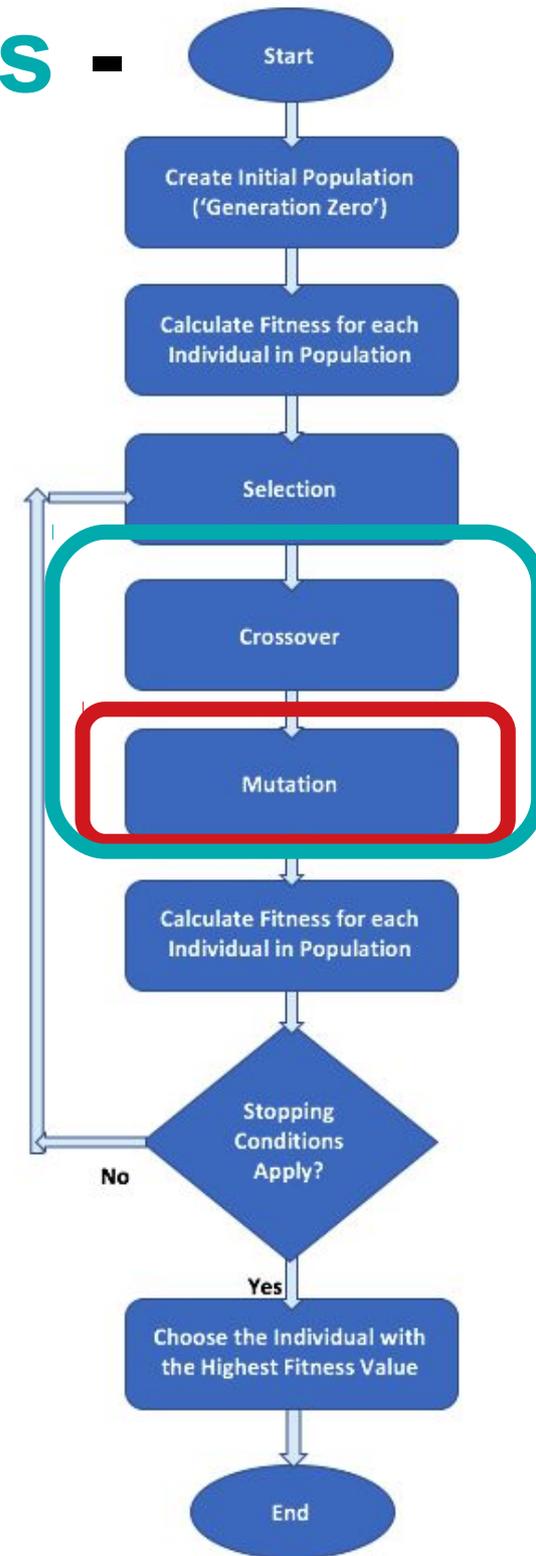
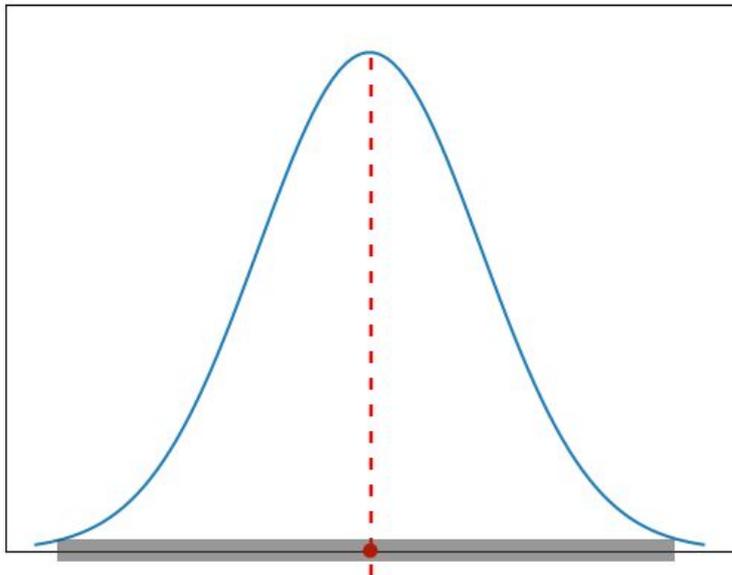


Workflow - Variation Operators -

Real-coded — Real Mutation

Another approach is to **generate a random real number that resides in the vicinity of the original individual.**

Example: the **normally distributed** (or Gaussian) **mutation** -> a random number is generated using a **normal distribution** with a **mean = 0** and some **predetermined standard deviation.**

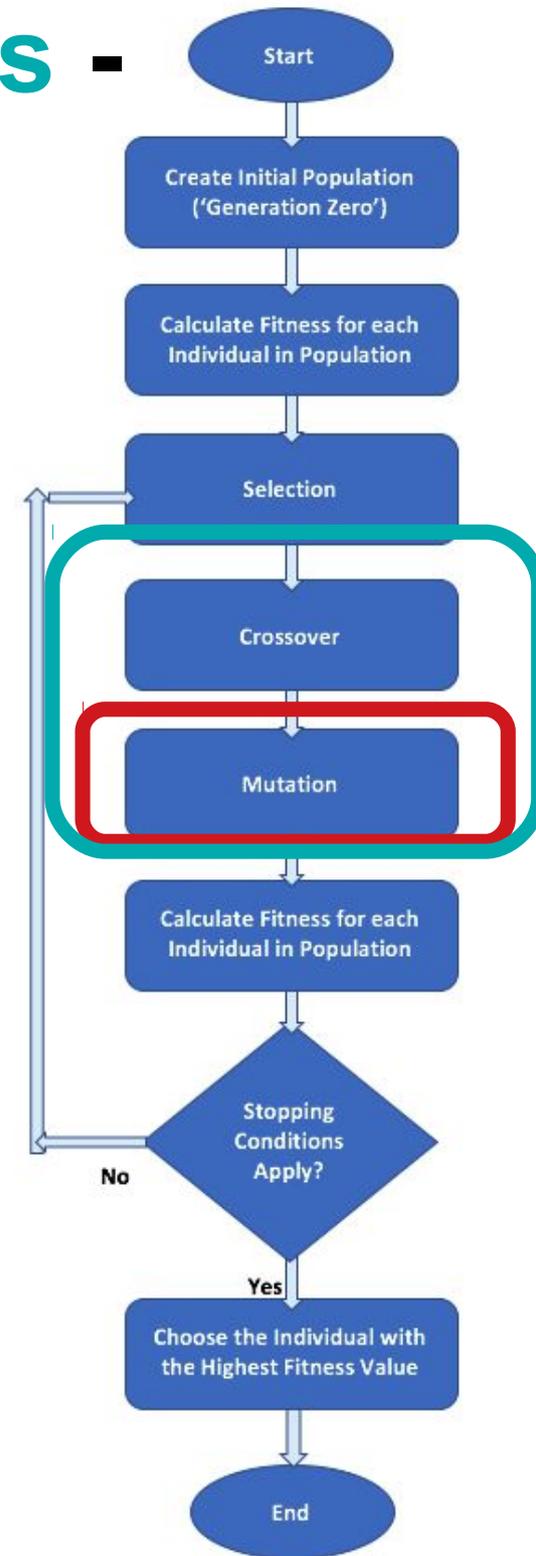
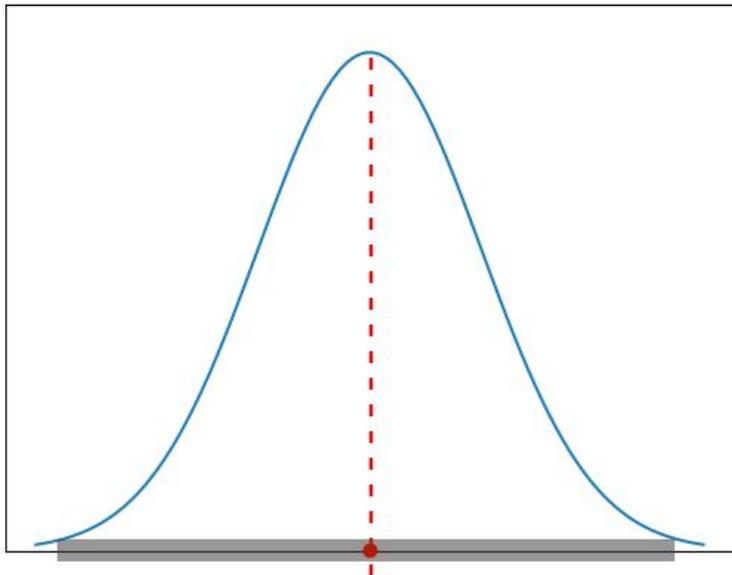


Workflow - Variation Operators -

Real-coded — Real Mutation

Another approach is to **generate a random real number that resides in the vicinity of the original individual.**

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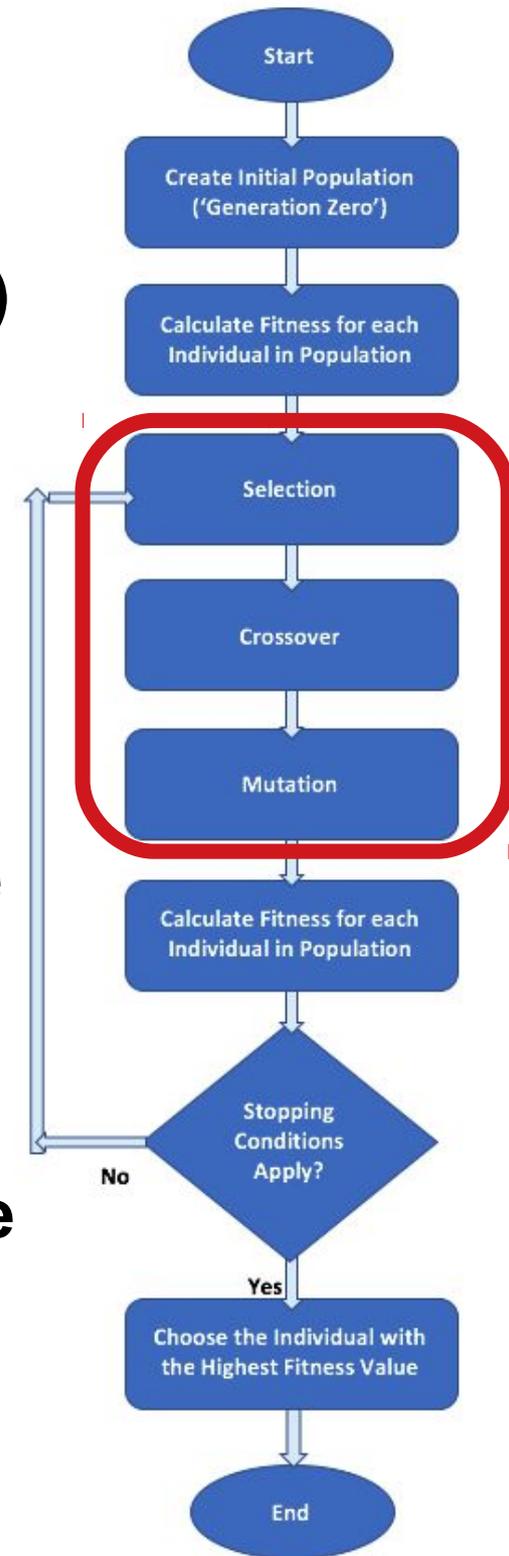
Content

- Recommended Sources
- What is Evolutionary Computing (EC)
- EC History
- Problem Types for EC
- What is Evolutionary Algorithm (EA)
- EA Workflow
- Selection
- Crossover
- Mutation
- Real-coded EA
- **Elitism, Niching, Sharing**

Workflow - Elitism Strategy

We want to guarantee that the **best individual(s)** always make it to the next generation, we can apply the **optional elitism strategy**.

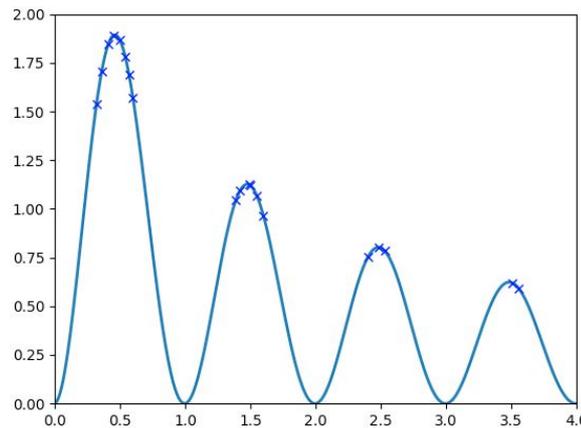
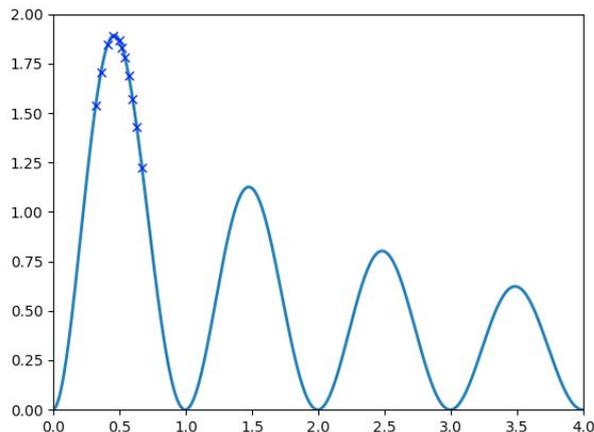
This means that the **top n individuals** (n is a predefined parameter) **are duplicated into the next generation** before we **fill the rest** of the available spots with **offspring** that are created **using selection, crossover, and mutation**. The **elite** individuals that were duplicated are still **eligible for the selection** process so they can still **be used as the parents** of new individuals. Elitism can sometimes have a significant **positive impact** on the algorithm's performance as it avoids the potential **time waste** needed for **re-discovering good solutions** that were lost.



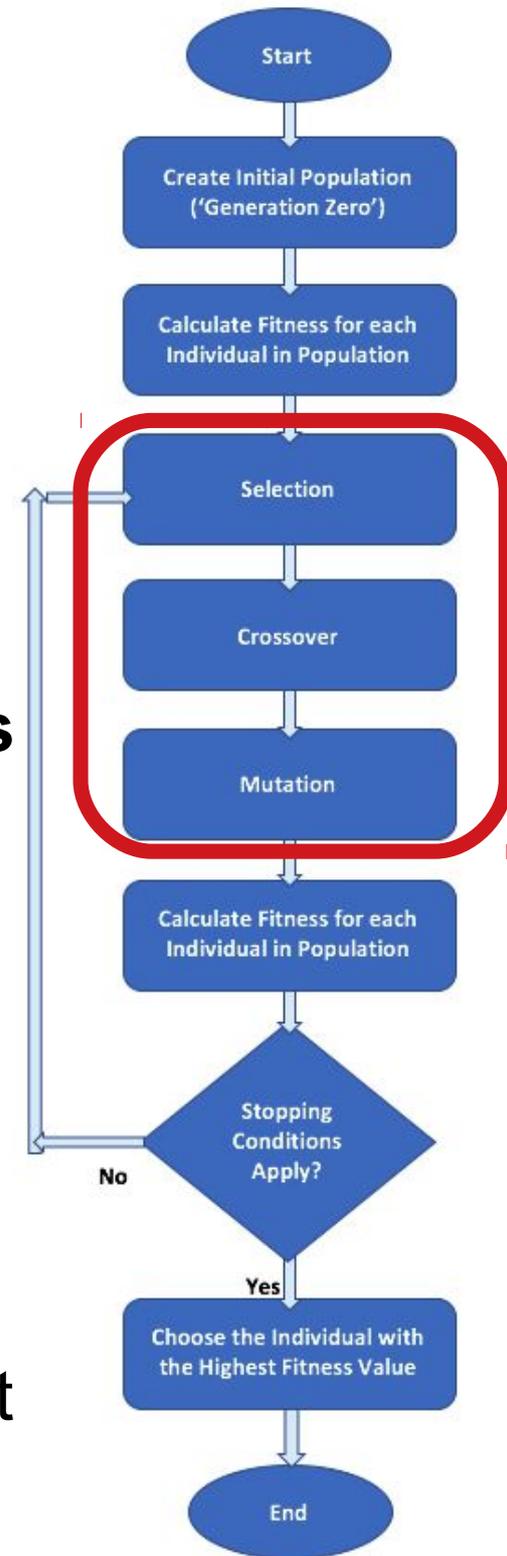
Workflow - Niching and Sharing

When several different species coexist in the same niche, they all compete over the same resources, and a **tendency** is to **search** for new, unpopulated **niches** and populate them.

This can be used to maintain the diversity of the population and to **find several optimal solutions**
-> **several niches.**



For this we should **offer resources** in the amount **proportional to a niche height** by **sharing fitness** depended on **distance to others.**



Основи еволюційних обчислень

-

Evolutionary Computing Basics

-

**Lecture 03. EC for Machine Learning
— Feature Selection**

(based on Alan Turing, Holland, Khaled Rasheed, Ben Phillips, Eyal Wirsansky, and others works)

Content

- **Recommended Sources**
- EA (GA) for Feature Selection — Why?
- Problem Types for Feature Selection:
- Regression: Friedman-1 Problem
 - Classic Solution
 - EA (GA) Solution
- Classification: Animals Problem
 - Classic Solution
 - EA (GA) Solution
- Resume

Recommended Sources

— Books

Books (scientific):

Guyon, I., Gunn, S., Nikravesh, M., & Zadeh, L. A. (Eds.). (2008). *Feature extraction: foundations and applications* (Vol. 207). Springer.

Dong, G., & Liu, H. (Eds.). (2018). *Feature engineering for machine learning and data analytics*. CRC Press.

Books (with codes at github):

Soledad Galli (2020). *Python Feature Engineering Cookbook*. Packt Publishing

Alice Zheng and Amanda Casari (2018). *Feature Engineering for Machine Learning* (O'Reilly)

Recommended Sources - Papers and Datasets

Regression Problem (F1RP):

Breiman, Leo (1996) Bagging predictors. Machine Learning 24, pages 123-140.

Friedman, Jerome H. (1991) Multivariate adaptive regression splines. The Annals of Statistics 19 (1), pages 1-67.

Classification Problem

UCI Zoo dataset (<http://archive.ics.uci.edu/ml/datasets/Zoo>)

Eibe Frank and Stefan Kramer. Ensembles of nested dichotomies for multi-class problems. ICML. 2004.

Huan Liu and Hiroshi Motoda and Lei Yu. Feature Selection with Selective Sampling. ICML. 2002.

Content

- Recommended Sources
- **EA (GA) for Feature Selection — Why?**
- Problem Types for Feature Selection:
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Evolutionary Computing (EC) — for Feature Selection — why?

Supervised learning:

Workflow: the **model** receives a set of **inputs**, called **features**, and maps them to a set of **outputs**.

Assumption: the information described by the **features** is **useful for** determining the value of the corresponding **outputs**.

Common sense: the **more** information we can use as input, the **better** our chances of predicting the output(s) correctly.

Reality: in many cases the **opposite is true** ... if some of the features we use are **irrelevant** or **redundant**, the consequence could be a (sometimes significant) **decrease in the accuracy** of the models.

That is why we need **feature selection**:
the **process** of **selecting** the most **beneficial set of features** out of the entire set of features to **reach the better** solution.

EC for Feature Selection — Benefits

- ◆ Decreasing the errors (the lost function) of the model
 - ◆ Increasing the accuracy of the model
 - ◆ Training times of the models are shorter.
 - ◆ Trained models are simpler and easier to interpret.
- ◆ Trained resulting models are likely to provide better **generalization**, that is, they perform better with new input data that is dissimilar to the data that was used for training.

Content

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- EA (GA) for Feature Selection — Why?
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EC for Feature Selection — Problem Types

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

- **regression** (use case of Friedman-1 Regression Problem)
and
- **classification** (use case of UCI-dataset animal classification)

for

– **feature selection**

or

– **dimensionality reduction**

with the purpose of:

– **decrease of MSE**

or

– **increase of mean accuracy.**

Content

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- EA (GA) for Feature Selection — Why?
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EC for Feature Selection — Example: Friedman-1 Regression Problem (F1RP)

F1RP was described by Friedman (1991) and Breiman (1996).

Inputs: *n_features* independent variables uniformly distributed on the interval $[0, 1]$, only 5 out of these *n_features* are actually used.

Outputs: are created according to the formula:

$$y(x_0, x_1, x_2, x_3, x_4) = 10 \cdot \sin(\pi \cdot x_0 \cdot x_1) + 20(x_2 - 0.5)^2 + 10x_3 + 5x_4 + \text{noise} \cdot N(0, 1)$$

The last component in the formula is the randomly generated noise. The noise is normally distributed and multiplied by the constant noise, which determines its level.

Various implementations in programming languages:

Python: `make_friedman1()` function in scikit-learn (**sklearn**) library

R: `friedman1()` function in **mlbench** library

Why F1RP is useful for us?

Breiman, Leo (1996) Bagging predictors. Machine Learning 24, pages 123-140.

Friedman, Jerome H. (1991) Multivariate adaptive regression splines. The Annals of

EC for Feature Selection — Example:

why F1RP is useful for us?

If **n_features = 15**, we will get a dataset with the original **5** input variables (or features) that were used to generate **y** values by the formula and **10** features that are completely irrelevant to the output.

Why: F1RP is used to **test** various **regression** models as to presence of **noise** and irrelevant features in the dataset.

Example:

Aim: test EC (GA) as a **feature selection** mechanism.

Workflow: use **make_friedman1()** function to create a dataset with 15 features and use GA to search for the **subset** of features that provides the **best** performance.

Hypothesis: EC (GA) will pick the first 5 features and drop the rest, assuming that the model's accuracy is better when only the relevant features are used as input.

EC (GA) role: The **fitness function (FF)** will use a **regression model** that, for each potential **solution** – a **subset of the feature** to use – will be **trained** using the dataset containing **only the selected** features.

EC for Feature Selection — Example: Individual Representation by EC (GA)

An **individual solution** (genotype) should indicate which **features are selected** and which are dropped:

- Each **individual solution** is a **list of binary** values
- Every **entry** in the list (0 or 1) is **one of the features** in the dataset:
 - ✓ 1 - the corresponding feature **WAS selected**,
 - ✓ 0 - the feature has **NOT** been **selected**.

This is very similar to the knapsack 0-1 problem from Lab01.

IMPORTANT:

Each 0 in the individual solution **means**

->

dropping the corresponding **feature's** data **column** from the dataset.

Content

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- Classification: Animals Problem
 - Classic Solution
 - EA (GA) Solution
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EC for Feature Selection — Example: F1RP — Classic Solution

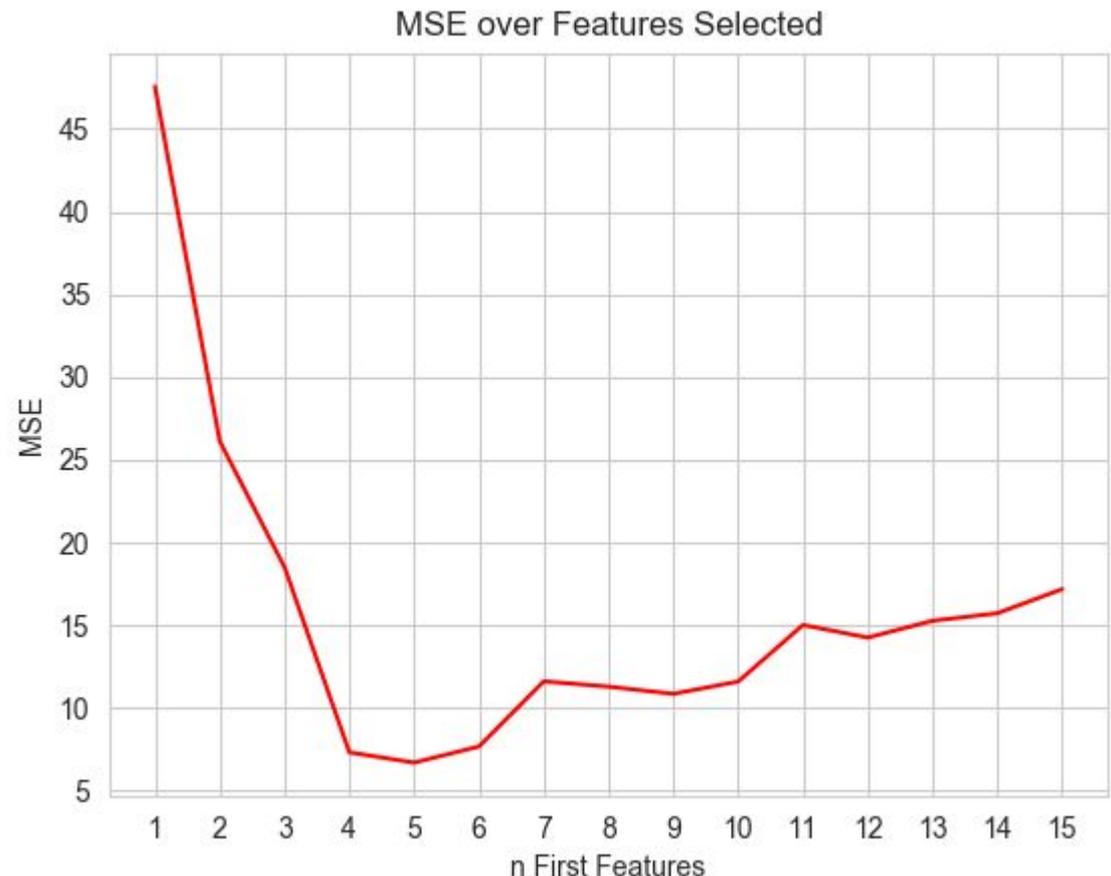
- 1) **Create** the **dataset** by Friedman formula using *make_friedman1()* function in scikit-learn (**sklearn**) library.
- 2) **Divide** the data into two subsets – a **training** set and a **validation** set – using *model_selection.train_test_split()* function in the scikit-learn.
- 3) **Create** the regression **model** ... various can be used ... **Gradient Boosting Regressor (GBR)** in this example.
- 4) **Determine the performance** of the used regression model for a set of selected features by *getMSE()* **function-metric***.
- 5) **Then** the **new training subset** (with the **selected features only!**) is used to train the model, while the new validation **subset** - to evaluate it.

*) **The mean square error (MSE)** = the average squared difference between the model's predicted values and the actual values. A **lower** value of this

EC for Feature Selection — Example: F1RP — Classic Solution — Results...

As far as we add the first 5 features one by one, the performance improves. However, later each additional feature degrades the performance of the model:

1 first features: score = 47.553993
2 first features: score = 26.121143
3 first features: score = 18.509415
4 first features: score = 7.322589
5 first features: score = 6.702669
6 first features: score = 7.677197
7 first features: score = 11.614536
8 first features: score = 11.294010
9 first features: score = 10.858028
10 first features: score = 11.602919
11 first features: score = 15.017591
12 first features: score = 14.258221
13 first features: score = 15.274851
14 first features: score = 15.726690
15 first features: score = 17.187479



EC for Feature Selection — Example: F1RP — Classic Solution — DEMO...

Try to reproduce these results:

1 first features: score = 47.553993
2 first features: score = 26.121143
3 first features: score = 18.509415
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EC for Feature Selection — Example: F1RP — EC (GA) Solution

The **differences** from **classic** solution:

1) **Chromosomes** - binary lists of selected features

2) **Fitness Function (FF)** - returns the regression model's **MSE**

3) **Selection**

- **tournament** selection with a tournament **size of 2**

- **elitism**, where the **hall of fame (HOF)** members – the current **best** individuals – are **always passed untouched** to the next generation

4) **Evolution (genetic) operators**

- **crossover**

and

- **mutation** operators

that are specialized for binary list chromosomes

EC for Feature Selection — Example: F1RP — EC (GA) Solution — Results

After 30 generations of EC (GA):

Best Ever Individual = [1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]

Best Ever Fitness = 6.702668910463287

What does it mean?

The best MSE (about 6.7) is provided by the first five features.

IMPORTANT:

EA (GA) makes **no assumptions** about the set of features.

EA (GA) does **not know** about the first or last n features.

EA (GA) simply searched for the **best possible subset** of features.

EC for Feature Selection — Example: F1RP — EC (GA) Solution — DEMO

Try to reproduce these results:

After 30 generations of EC (GA):

Best Ever Individual = [1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]

Best Ever Fitness = 6.702668910463287

What does it mean?

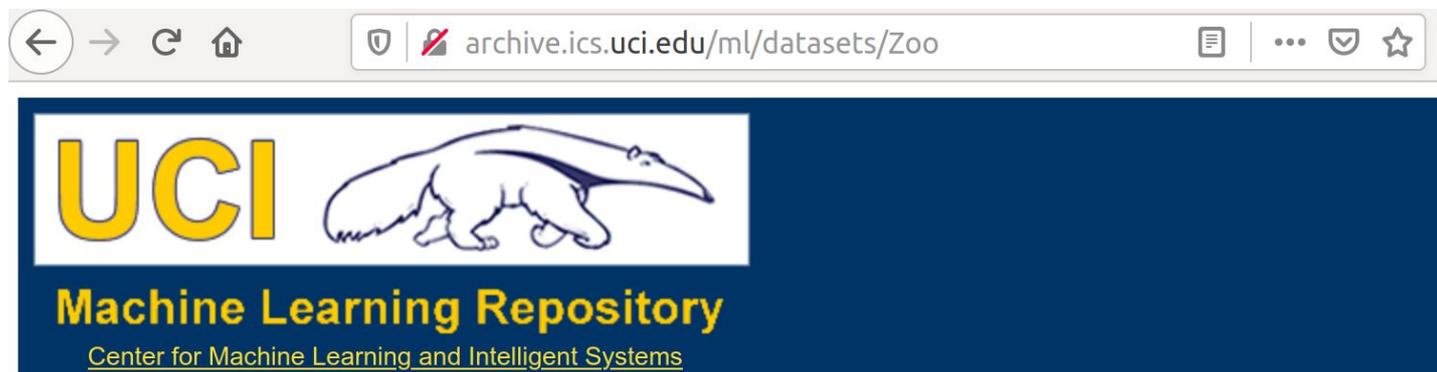
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- Resume

EC for Feature Selection — Example: Animals Classification Problem

It is the classic example of classification problem.



Zoo Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Artificial, 7 classes of animals



Data Set Characteristics:	Multivariate	Number of Instances:	101	Area:	Life
Attribute Characteristics:	Categorical, Integer	Number of Attributes:	17	Date Donated	1990-05-15
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	346207

UCI Zoo dataset (<http://archive.ics.uci.edu/ml/datasets/Zoo>).

EC for Feature Selection — Example: Animals Classification — Dataset

Dataset General Information:

A simple database containing **17 Boolean-valued attributes**.

The "**type**" attribute appears to be the **class** attribute. Here is a breakdown of which animals are in which type: (I find it unusual that there are **2 instances of "frog"** and **one of "girl"**!)

Class# -- Set of animals:

- 1 -- (41) aardvark, antelope, bear, boar, buffalo, calf, cavy, cheetah, deer, dolphin, elephant, fruitbat, giraffe, girl, goat, gorilla, hamster, hare, leopard, lion, lynx, mink, mole, mongoose, opossum, oryx, platypus, polecat, pony, porpoise, puma, pussycat, raccoon, reindeer, seal, sealion, squirrel, vampire, vole, wallaby, wolf
- 2 -- (20) chicken, crow, dove, duck, flamingo, gull, hawk, kiwi, lark, ostrich, parakeet, penguin, pheasant, rhea, skimmer, skua, sparrow, swan, vulture, wren
- 3 -- (5) pitviper, seasnake, slowworm, tortoise, tuatara
- 4 -- (13) bass, carp, catfish, chub, dogfish, haddock, herring, pike, piranha, seahorse, sole, stingray, tuna
- 5 -- (4) frog, frog, newt, toad
- 6 -- (8) flea, gnat, honeybee, housefly, ladybird, moth, termite, wasp
- 7 -- (10) clam, crab, crayfish, lobster, octopus, scorpion, seawasp, slug, starfish, worm

EC for Feature Selection — Example: Animals Classification — Dataset

Attribute (**Feature**) Information:

1. animal name: Unique for each instance
2. hair: Boolean
3. feathers: Boolean
4. eggs: Boolean
5. milk: Boolean
6. airborne: Boolean
7. aquatic: Boolean
8. predator: Boolean
9. toothed: Boolean
10. backbone: Boolean
11. breathes: Boolean
12. venomous: Boolean
13. fins: Boolean
14. legs: Numeric (set of values: {0,2,4,5,6,8})
15. tail: Boolean
16. domestic: Boolean
17. catsize: Boolean

EC for Feature Selection — Example: Animals Classification — **Problem**

Origin: it is the classic example of classification problem, where the input features need to be mapped into two or more categories/labels.

Inputs: features 2-17 (hair, feathers, fins, and so on), mostly features are Boolean (value of 1 or 0) meaning the presence or absence of a certain attribute, such as hair, fins, and so on.

Note: The 1st feature - **animal name** - is just to provide us with some information and **does not participate** in the learning.

Outputs: the last feature – **type** – represents 7 categories. For instance, type 5 represents a category with: frog, newt, and toad.

Aim: train a **classification model** on this dataset with **features 2-17** (hair, feathers, fins, and so on) to **predict** the value of **feature 18** (animal **type**).

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 - **Classic Solution**
 - EA (GA) Solution
- Resume

EC for Feature Selection — Example: Animals Classification — **Classic Way**

- 1) **Load** the UCI-Zoo **dataset** by the standard `read_csv` function.
- 2) **Divide** the data into **input** features (first remaining 16 columns) and the resulting **output** category (last column). Then instead of separating the data into **1 training** set and **1 test** set, like we did in the previous section, we're using ***k-fold cross-validation*** -> The data is split into ***k*** equal parts and the model is evaluated ***k*** times:
(k-1) parts for **training** and **1** remaining part for testing (or **validation**).
- 3) **Create** the classification **model** ... various models can be used ...
Decision Tree Classifier (DCT) in this example.
- 4) **Determine the performance** of the used regression model for a set of selected features by ***getMeanAccuracy()*** **function-metric***.

*) **Accuracy** – the portion of the cases that were classified correctly. A **higher** value of this measurement indicates **better performance** of the model.

EC for Feature Selection — Example: Classification — Classic Way — DEMO...

After training/testing:

the model - DTC-classifier
5-fold cross-validation
all 16 features

the classification accuracy was about **91%**.

Try to reproduce these results:

All features selected:

[1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]

Accuracy = 0.9099999999999999

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EC for Feature Selection — Example: Classification — **EC (GA) Solution**

The **differences** from **classic** solution:

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2) **Fitness Function (FF)** - returns the model's **mean accuracy**

3) **Selection**

- **tournament** selection with a tournament **size of 2**

- **elitism**, where the **hall of fame (HOF)** members – the current **best** individuals – are **always passed untouched** to the next generation

4) **Evolution (genetic) operators**

- **crossover**

and

- **mutation** operators

that are specialized for binary list chromosomes

EC for Feature Selection — Example: Classification — EC (GA) — Results

After 50 generations of EC (GA) and HOF size of 5:

Best solutions are:

0 : [0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0] fitness = 0.964 accuracy = 0.97 features = 6
1 : [0, 1, 0, 1, 1, 1, 0, 1, 1, 0, 0, 1, 0, 0, 0, 0] fitness = 0.963 accuracy = 0.97 features = 7
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4 : [0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 1] fitness = 0.963 accuracy = 0.97 features = 7

The **top solution** is the set of **6 features**, which are as follows:
feathers, milk, airborne, backbone, fins, tail

By selecting these particular features out of the 16 given in the dataset:

- 1 - we **reduced the dimensionality** of the problem,
- 2 - we also **improved** our model **accuracy** from 91% to 97%.

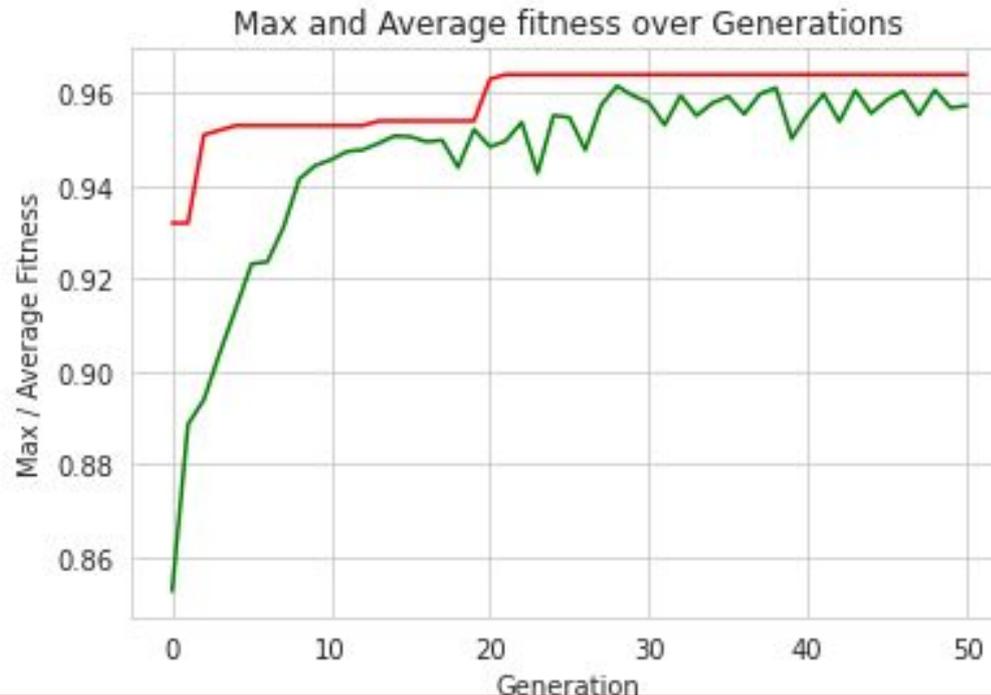
IMPORTANT: It is **not very large** increase of an absolute **accuracy**,
BUT a great (**TRIPLE!**) reduction of the **error rate** from 9% to 3% – a
very significant improvement in terms of classification performance

EC for Feature Selection — Example: Classification — EC (GA) — DEMO

Try to reproduce these results:

Best solutions are:

0 : [0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0] fitness = 0.964 accuracy = 0.97 features = 6
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EC for Feature Selection — **Resume**

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

- **regression** (use case of Friedman-1 Regression Problem)
and
- **classification** (use case of UCI-dataset animal classification)

for

– **feature selection**

or

– **dimensionality reduction**

with the purpose of:

– **decrease of MSE**

or

– **increase of mean accuracy.**

Основи еволюційних обчислень

-

Evolutionary Computing Basics

-

**Lecture 04. EC for Machine Learning
— Hyperparameter Tuning**

(based on Holland, Khaled Rasheed, Ben Phillips, Eyal
Wirsansky, and others works)

Content

- **Recommended Sources**
- EA (GA) for Hyperparameter Tuning — Why?
- Problem Types for Feature Selection
- Classification Problem Example
 - UCI Wine Dataset
 - Hyperparameter Tuning
- Classic Solutions
 - DEMO 1 - Default Values
 - DEMO 2 - Extensive Grid Search
- EA (GA) Solutions
 - DEMO 3 — GA-driven Grid Search
 - DEMO 4 — Direct GA
- Resume

Recommended Sources

— Books

Books (scientific):

Goodfellow, I., Bengio, Y., Courville, A., & Bengio, Y. (2016).
Deep learning. Cambridge: MIT press

Цитовано в 23692 джерелах.

Books (with codes at github):

Alan Fontaine (2018) *Mastering Predictive Analytics with scikit-learn and TensorFlow*. Packt Publishing.

Tanay Agrawal (2021). *Hyperparameter Optimization in Machine Learning: Make Your Machine Learning and Deep Learning Models More Efficient*, Apress

Recommended Sources - Papers and Datasets

Example Problem and Dataset

UCI Wine dataset (<https://archive.ics.uci.edu/ml/datasets/wine>)

S. Aeberhard, D. Coomans and O. de Vel,
Comparison of Classifiers in High Dimensional Settings,
Tech. Rep. no. 92-02, (1992), Dept. of Computer Science and Dept. of
Mathematics and Statistics, James Cook University of North Queensland.
The data was used for comparing various classifiers.
(RDA : 100%, QDA 99.4%, LDA 98.9%, 1NN 96.1% (z-transformed data))
(All results using the leave-one-out technique)

Mikhail Bilenko (**Head of AI and Research, Yandex**) and Sugato Basu and
Raymond J. Mooney. *Integrating constraints and metric learning in semi-
supervised clustering*. ICML. 2004.

Kamal Ali and Michael J. Pazzani. *Error Reduction through Learning Multiple
Descriptions*. Machine Learning, 24. 1996

Content

- Recommended Sources
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 - DEMO 3 — GA-driven Grid Search
 - DEMO 4 — Direct GA
- Resume

Evolutionary Computing (EC) — for Hyperparameter Tuning — why?

Supervised learning:

Workflow: the **model** receives a set of **inputs**, called **features**, and maps them to a set of **outputs**.

Assumption: the information described by the **features** is **useful for** determining the value of the corresponding **outputs**.

Model: learning is **adjusting** (or tuning) the **internal parameters** of a model to produce the **desired outputs** in response to **given inputs**.

For this, each type of supervised learning model is accompanied by a **learning algorithm** that **iteratively adjusts** its internal parameters during the learning (or training) phase.

Reality: **BUT** ... most models have another set of **hyperparameters** that are set **before** the learning and they affect the way the learning is done!

Usually: hyperparameters have some **default values** that will take effect if we don't specifically set them and **they are not optimal!**

That is why we need **hyperparameter tuning!**

EC for Hyperparameter Tuning — Benefits and Overheads

Benefits:

- ◆ Decreasing the errors (the lost function) of the model
 - ◆ Increasing the accuracy of the model
 - ◆ Training times of the models are shorter.

Overheads:

- ◆ The possible number of hyperparameter combinations can be very-very huge.
 - ◆ Search for the best hyperparameter combinations (hyperparameter tuning) takes significant amounts of time.

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EC for Hyperparameter Tuning — Problem Type - Classification

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

– **classification** (use case of UCI-dataset Wine classification)

for

– **hyperparameter tuning**

with the purpose of:

– **decrease of MSE**

or

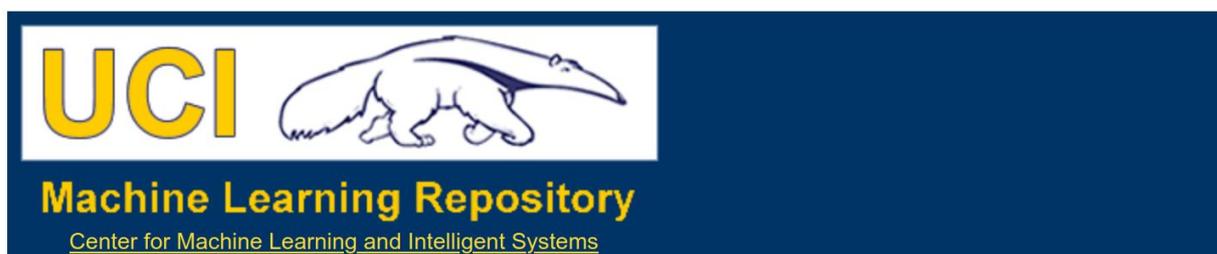
– **increase of mean accuracy.**

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EC for Hyperparameter Tuning — Example: Wine Classification Problem

It is the classic example of classification problem.



Wine Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Using chemical analysis determine the origin of wines



Data Set Characteristics:	Multivariate	Number of Instances:	178	Area:	Physical
Attribute Characteristics:	Integer, Real	Number of Attributes:	13	Date Donated	1991-07-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	1602802

Source:

Original Owners:

Forina, M. et al, PARVUS -
An Extendible Package for Data Exploration, Classification and Correlation.
Institute of Pharmaceutical and Food Analysis and Technologies, Via Brigata Salerno,
16147 Genoa, Italy.

UCI Wine dataset (<https://archive.ics.uci.edu/ml/datasets/wine>)

EC for Hyperparameter Tuning — Wine Classification — Dataset

Dataset General Information:

These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from **3 different cultivars**.

The analysis determined the quantities of **13 constituents** found in each of the 3 types of wines.

- ◆ In a classification context, this is a well posed problem with "well behaved" class structures.
- ◆ A good data set for first testing of a new classifier, but not very challenging.



EC for Hyperparameter Tuning — Wine Classification — Dataset

Attribute (Feature) Information:

- 1) Alcohol
- 2) Malic acid
- 3) Ash
- 4) Alcalinity of ash
- 5) Magnesium
- 6) Total phenols
- 7) Flavanoids
- 8) Nonflavanoid phenols
- 9) Proanthocyanins
- 10) Color intensity
- 11) Hue
- 12) OD280/OD315 of diluted wines
- 13) Proline

Class identifier: One (0th) attribute is class identifier (1,2,3)

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EC for Hyperparameter Tuning — Wine Classification — **Problem**

Origin: it is the **classic** example of **classification problem**, where the input features need to be mapped into **3 categories/labels**.

Inputs: all features (wine properties) are **continuous**.

Outputs: the one feature — **class** — represents 3 categories (**cultivars**).

Aim: train a **classification model** on this dataset with **13 features** to **predict** the value of **feature 0 (cultivar)**.

Wine Classification — Workflow

1) **Load** the UCI Wine **dataset** by the standard **read_csv** function (with `url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.data'`).

2) **Divide** the data into **input** features (first remaining 13 columns) and the resulting **output** category (the first column). Then instead of separating the data into **1 training** set and **1 test** set, like we did in the previous example, we're using ***k-fold cross-validation*** -> The data is split into ***k*** equal parts and the model is evaluated ***k*** times:

(***k-1***) parts for **training** and **1** remaining part for testing (or **validation**).

3) **Create** the classification **model** ... various models can be used ... **AdaBoostClassifier** in this example.

4) **Determine the performance** of the used regression model for a set of selected **hyperparameters** by ***accuracy* metric***.

*) **Accuracy** – the portion of the cases that were classified correctly. A **higher** value of this measurement indicates **better performance** of the model.

Wine Classification — Hyperparameter Tuning

Let's consider in details this stage:

- 3) **Create** the classification model ... various models can be used ...
AdaBoostClassifier in this example.

The *adaptive boosting algorithm (AdaBoost)*

is a powerful ML model that **combines** the **outputs** of multiple **instances** of a simple ML algorithm (weak learner) using a weighted sum. AdaBoost adds instances of the weak learner during the learning process, each of which is adjusted to improve previously misclassified inputs.

We'll use *sklearn* library's implementation of `AdaBoostClassifier` with some hyperparameters:

Name	Type	Description	Default Value
<code>n_estimators</code>	int	The maximum number of estimators	50
<code>learning_rate</code>	float	Can be used to shrink the contribution of each classifier	1
<code>algorithm</code>	{ 'SAMME', 'SAMME.R' }	'SAMME.R' – uses a real boosting algorithm, 'SAMME' – uses a discrete boosting algorithm	2

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Wine Classification — Classic Way

Let's start from 2 classic approaches:

◆ **default values** of model hyperparameters:
{**'algorithm'**: 'SAMME.R', **'learning_rate'**: 1.0, **'n_estimators'**: 50,
 'random_state': 42},

◆ **grid search** of the **best values** of model hyperparameters:

Algorithm — 2 possible values 'SAMME' and 'SAMME.R',

learning_rate - 10 values logarithmically spaced

 between 0.01 (10^{-2}) and 1 (10^0),

n_estimators -> 10 values linearly spaced between 10 and 100,

Total: 200 = (10×10×2) different combinations of the grid parameters.

Wine Classification — Classic Way — DEMO 1 and 2

Results:

DEMO 1 - Default values:

Default Classifier Hyperparameter values:

```
{'algorithm': 'SAMME.R', 'base_estimator': None, 'learning_rate': 1.0,  
  'n_estimators': 50, 'random_state': 42}
```

Score (with default values) = 0.6457142857142857

Time Elapsed = 0.4167492389678955

DEMO 2 - After gridSearch:

Best parameters: {'algorithm': 'SAMME.R', 'learning_rate':
0.3593813663804626, 'n_estimators': 70}

Score (after gridSearch): 0.9325842696629213

Time Elapsed = 74.51628732681274

Try to reproduce these results!

Wine Classification — Classic Way — DEMO 1 and 2

After training/testing - see `test.gridTest()` function in the DEMO code:

- ◆ the model is **AdaBoostClassifier**-classifier
- ◆ 5-fold cross-validation

Results:

DEMO 1 - Default values:

Model hyperparameter values:

```
{'algorithm': 'SAMME.R', 'learning_rate': 1.0, 'n_estimators': 50,  
  'random_state': 42}
```

Accuracy: **0.65%**

Time Elapsed = **0.42** seconds

DEMO 2 - After gridSearch:

Best hyperparameter values:

```
{'algorithm': 'SAMME.R', 'learning_rate': 0.359, 'n_estimators': 70}
```

Accuracy: **0.93%**

Time Elapsed = **74** seconds

Try to reproduce these results!

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Wine Classification — EC (GA) Ways

Difference from Classic Ways

The differences from classic solution:

1) **Chromosomes** — **heterogeneous** sets of selected **values of hyperparameters**:

- ◆ **n_estimators values** - a list of **10 integers**
- ◆ **learning_rate** - an ndarray of **10 floats**,
- ◆ **algorithm** - a list of **2 strings**

2) **Fitness Function (FF)** - returns the model's **mean accuracy**

3) **Selection**

- **tournament** selection with a tournament **size of 2**
- **elitism**, where the **hall of fame (HOF)** members – the current **best** individuals – are **always passed untouched** to the next generation

4) **Evolution (genetic) operators**

- **crossover** and
 - **mutation** operators
- that are specialized for chromosomes

Wine Classification — EC (GA) Ways — Grid and Direct

The possible EC-GA-based approaches:

- ◆ **GA-based grid search:**

to search among the **initially selected** 200 grid combinations **only**,

- ◆ **direct GA:**

to search directly the **entire parameter space**,
where each hyperparameter can be represented
as a variable participating in the search,

and the **chromosome** can be a **combination** of **all** these variables.

Wine Classification — EC (GA) Ways

3. GA-based Grid Search — DEMO 3

3) GA-based grid search:

--- Evolve in 200 possible combinations ---

	gen	nevals	avg	min	max	std
0	20	0.708427	0.117978	0.910112	0.265992	
1	13	0.865169	0.662921	0.926966	0.0717915	
2	15	0.887921	0.646067	0.926966	0.0571676	
3	12	0.896348	0.679775	0.926966	0.0526256	
4	16	0.918539	0.88764	0.926966	0.0110233	
5	9	0.911517	0.730337	0.926966	0.0425958	

Best individual is: {'n_estimators': 60, 'learning_rate': 0.5994842503189409,
'algorithm': 'SAMME.R'}

with fitness: 0.9269662921348315

Time Elapsed = 24.287983655929565

Try to reproduce these results!

Wine Classification — EC (GA) Ways

3. GA-based Grid Search — DEMO 3

3) GA-based grid search:

to search among the **initially selected** 200 grid combinations **only**

GA-parameters:

population_size=20,
gene_mutation_prob=0.30,
tournament_size=2,
generations_number=5

Results:

Model hyperparameter values:

```
{'algorithm': 'SAMME.R', 'learning_rate': 0.5995, 'n_estimators': 60,  
  'random_state': 42}
```

Accuracy: 0.93%

Time Elapsed = 24 secs for 6 generations (compare with **gridSearch: 74 sec, but it takes **only 2** generations - **8 secs!** - to reach Max Accuracy)**

Try to reproduce these results!

Wine Classification — EC (GA) Ways

3. GA-based Grid Search — DEMO 3

Conclusions:

GA-driven grid search can find the same best result (found by the classic search), but in a **6 times(!) faster** – about 12 seconds (2 generations).

BUT ... in real-life situations:

- ◆ **datasets** are much **larger**,
 - ◆ **models** are more **complex**, and
 - ◆ **hyperparameter grids** are **larger!**
- ◆ That is why **exhaustive classic grid search** can be **prohibitively lengthy**, while the **GA-driven grid search** can reach **good results** within a **reasonable time**.

BUT here ... GAs are limited to the subset of hyperparameter values that are defined by the grid.

Let's search outside the grid of a subset of predefined values?

Wine Classification — EC (GA) Ways

4. Direct GA — DEMO 4

4) Direct GA:

to search directly the **entire parameter space**,
where each hyperparameter can be represented
as a variable participating in the search,
and the **chromosome** can be a **combination** of **all** these variables.

We need to represent each hyperparameter as a floating-point number,
regardless of its actual type:

- ◆ **n_estimators** - originally an **integer** — it will be represented by a **float** value in the **range of [1, 100]**,
- ◆ **learning_rate** - already a **float**, so no conversion is needed — it will be bound to the **range of [0.01, 1.0]**,
- ◆ **algorithm** - have one of two **string** values, 'SAMME' or 'SAMME.R' — it and will be represented by a **float** number in the range of **[0, 1]**.

Wine Classification — EC (GA) Ways

4. Direct GA — DEMO 4

4) Direct GA - Results:

	gen	nevals	max	avg
0	20	0.92127	0.841024	
1	14	0.943651	0.900603	
2	13	0.943651	0.912841	
3	14	0.943651	0.922476	
4	15	0.949206	0.929468	
5	13	0.949206	0.938563	

Time Elapsed = 46.62226867675781

- Best solution is:

params = 'n_estimators'= 69, 'learning_rate'=0.628, 'algorithm'=SAMME.R

Accuracy = 0.94921

Try to reproduce these results!

Wine Classification — EC (GA) Ways

4. Direct GA — DEMO 4

4) Direct GA with GA-parameters:

population_size=20,
gene_mutation_prob=0.50,
probability for crossover = 0.90,
tournament_size=2,
generations_number=5
hall_of_fame_size=5

Results:

Model hyperparameter values:

{'algorithm': 'SAMME.R', 'learning_rate': 0.628, 'n_estimators': 69,
'random_state': 42}

Accuracy: 0.95%

Time Elapsed = 46 secs for 6 generations (compare with gridSearch: 74 sec, but it takes only 2 generations - 16 secs! - to > GA-grid Accuracy)

Try to reproduce these results!

Wine Classification — EC (GA) Ways

4. Direct GA — DEMO 4

Conclusions:

- ◆ Direct GA can find the **better accuracy 95%** than classic (65-93%) and GA-driven grid search (93%),
- ◆ and in **4-5 times(!) faster** (8 secs for 2 generations) than classic and the same time for GA-driven grid search.

NOTE: the **best** hyperparameter values (for `n_estimators` and `learning_rate`) were found **outside the grid** values!

BUT ... again! ... in real-life situations:

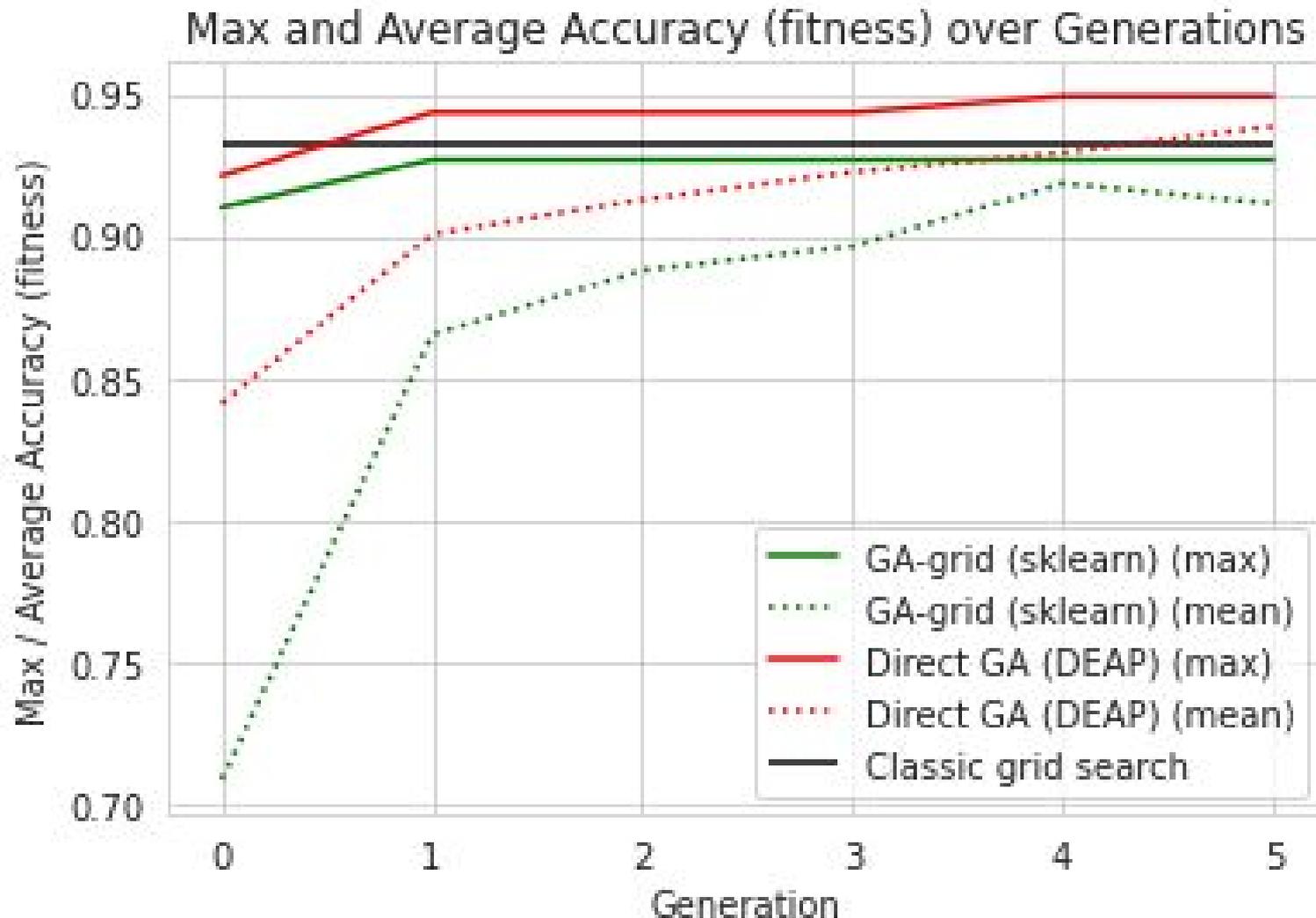
- ◆ **datasets** are much **larger**,
- ◆ **models** are more **complex**, and
- ◆ **hyperparameter grids** are **larger!**

- That is why **exhaustive classic grid search** can be **prohibitively lengthy**, while the **GA-driven grid search** can reach **good results** within a **reasonable time**.

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- **Resume**

EC for Feature Selection — Classification — Comparative Plot



Try to reproduce these results!

EC for Feature Selection — **Resume**

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

- **regression** (use case of Friedman-1 Regression Problem)
and
- **classification** (use case of UCI-dataset animal classification)

for

– **feature selection**

or

– **dimensionality reduction**

with the purpose of:

– **decrease of MSE**

or

– **increase of mean accuracy.**

Основи еволюційних обчислень

-

Evolutionary Computing Basics

-

**Lecture 05. EC for Neural Networks
— Architecture and Hyperparameter
Tuning**

(based on Varoquaux, Grobler, Rasheed, Phillips,
Wirsansky, and others works)

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 - Max NN Layer Number
- DEMO - Part 2: NN Hyperparameter Tuning Solution
- DEMO - Part 3: NN Architecture + Hyperparameter Tuning Solution
- Resume

Recommended Sources

— Books

Books (scientific):

Goodfellow, I., Bengio, Y., Courville, A., & Bengio, Y. (2016).
Deep learning. Cambridge: MIT press

Цитовано в 23692 джерелах.

Books (with codes at github):

Alan Fontaine (2018) *Mastering Predictive Analytics with scikit-learn and TensorFlow*. Packt Publishing.

Tanay Agrawal (2021). *Hyperparameter Optimization in Machine Learning: Make Your Machine Learning and Deep Learning Models More Efficient*, Apress

Recommended Sources - Papers and Datasets

Example Problem and Dataset

UCI Wine dataset (<https://archive.ics.uci.edu/ml/datasets/wine>)

S. Aeberhard, D. Coomans and O. de Vel,
Comparison of Classifiers in High Dimensional Settings,
Tech. Rep. no. 92-02, (1992), Dept. of Computer Science and Dept. of
Mathematics and Statistics, James Cook University of North Queensland.

UCI Iris dataset (<https://archive.ics.uci.edu/ml/datasets/iris>)

Fisher, R.A. *The use of multiple measurements in taxonomic problems*, Annual
Eugenics, 7, Part II, 179-188 (1936); also in "Contributions to Mathematical
Statistics" (John Wiley, NY, 1950).

UCI Breast Cancer dataset

([https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+\(Diagnostic\)](https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)))
W.N. Street, W.H. Wolberg and O.L. Mangasarian. *Nuclear feature extraction for
breast tumor diagnosis*. IS&T/SPIE 1993 International Symposium on Electronic
Imaging: Science and Technology, volume 1905, 861-870, San Jose, CA, 1993.

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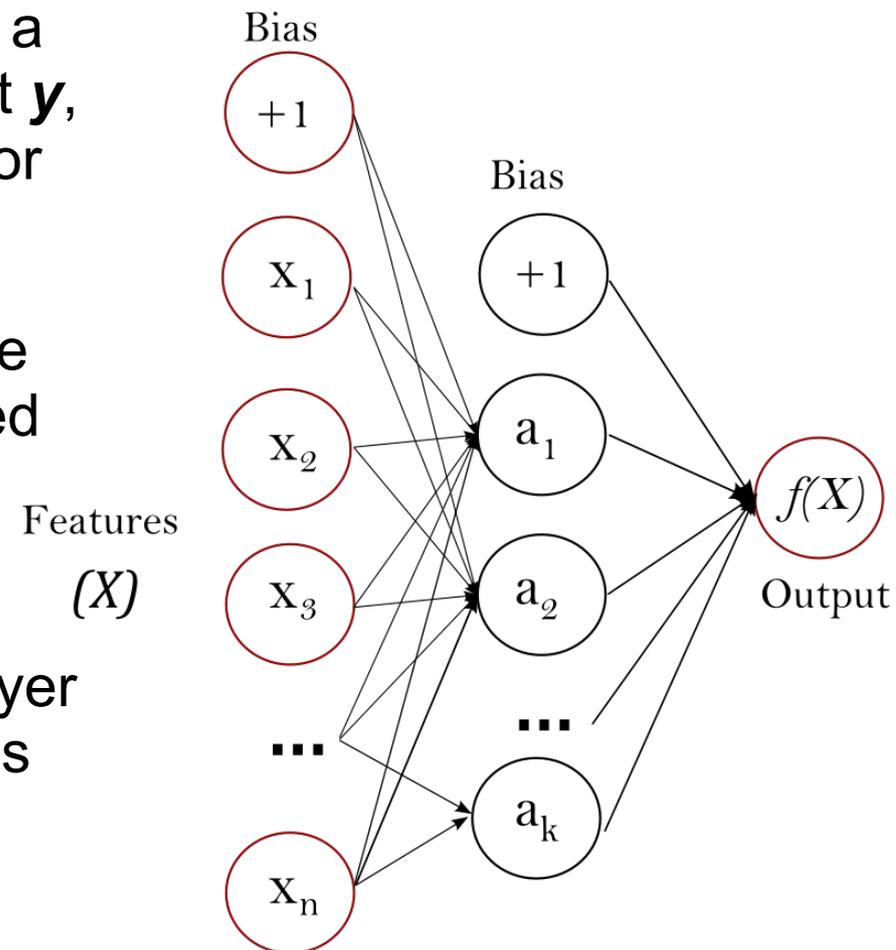
Evolutionary Computing (EC) — MLP/Neural Network (NN) — Intro

Multi-layer Perceptron (MLP) is a supervised learning algorithm (**artificial neural network - NN**) that learns a function $f(X)$ by training on a dataset. Given a set of features X and a target y , it can learn a non-linear function approximator for classification or regression.

Between the input and the output layer, there can be one or **more non-linear layers**, called **hidden layers**.

The weight matrix W_i at some index i represents the weights between layer i and layer $i+1$. The bias b_i at index i represents the bias values added to layer $i+1$.

MLP uses **backpropagation** for training. It can **distinguish not linearly** separable data.



NN Tuning —

What are Tuning Objects?

Supervised learning:

Workflow: the **model (NN here)** receives a set of **inputs**, called **features**, and maps them to a set of **outputs**.

Assumption: the information described by the **features** is **useful for** determining the value of the corresponding **outputs**.

Model: learning is **adjusting** (or tuning) the **internal parameters (weights in NN layers here)** of a model to produce the **desired outputs** in response to **given inputs**. Each type of supervised learning model is accompanied by a **learning algorithm** that **iteratively adjusts** its internal **parameters (weights in NN layers here)** during the learning.
AND ... most models (**NN here**) have structure (**NN architecture here: layers, blocks, and connections between them**) + **hyperparameters** (learning rate, ...) that are set **before** the learning and they affect it!

Usually: EC can be applied for search of optimal: a) **weights**, b) **hyperparameters** (like in the previous lecture for ML), c) **architecture**.

IMPORTANT: **Weights tuning by EC is NOT considered here**, because it is performed by gradient-based methods.

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NN Tuning —

What Types of Tuning?

Tuning Types ... for various parts of NN:

◆ **internal parameters:**

weights in NN - is **NOT considered** here, because it is performed by gradient-based methods;

◆ **external parameters:**

1) NN **architecture** (layers and nodes in layers here)

+ influence of various ...

- **RANDOM_SEEDs**,

- **datasets**,

- **MAX number of layers**.

2) NN **hyperparameters** (learning rate, activation function, optimization solver, and regularization, here),

3) NN **architecture + NN hyperparameters**.

EC for Hyperparameter Tuning — Benefits and Overheads

Benefits:

- ◆ Decreasing the errors (the lost function) of the model
 - ◆ Increasing the accuracy of the model
 - ◆ Training times of the models are shorter.

Overheads:

- ◆ The possible **number** of **NN architectures** and **NN hyperparameter** combinations can be very-very **huge**.
 - ◆ Search for the best **NN architectures** and **NN hyperparameter** combinations (hyperparameter tuning) takes **significant** amounts of **time**.

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EC for Hyperparameter Tuning — Problem Type - Classification

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

– **classification** (use case of UCI-dataset Wine classification)

for

– **NN tuning**

with the purpose of:

– **decrease of MSE**

or

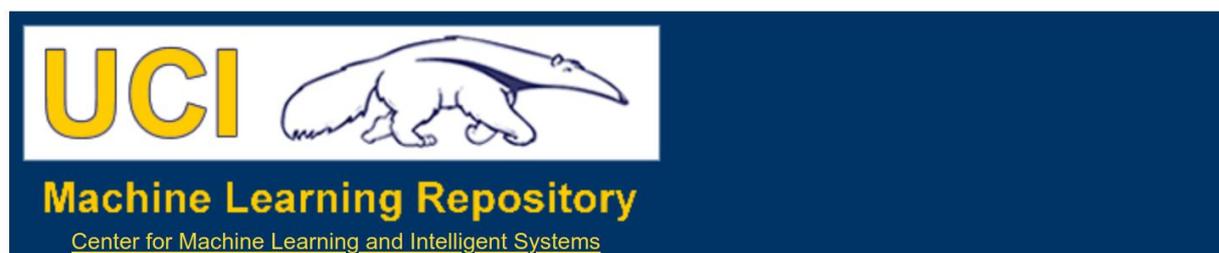
– **increase of mean accuracy.**

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EC for Hyperparameter Tuning — Example: Wine Classification Problem

It is the classic example of classification problem.



Wine Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Using chemical analysis determine the origin of wines



Data Set Characteristics:	Multivariate	Number of Instances:	178	Area:	Physical
Attribute Characteristics:	Integer, Real	Number of Attributes:	13	Date Donated	1991-07-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	1602802

Source:

Original Owners:

Forina, M. et al, PARVUS -
An Extendible Package for Data Exploration, Classification and Correlation.
Institute of Pharmaceutical and Food Analysis and Technologies, Via Brigata Salerno,
16147 Genoa, Italy.

UCI Wine dataset (<https://archive.ics.uci.edu/ml/datasets/wine>)

EC for Hyperparameter Tuning — Wine Classification — Dataset

Dataset General Information:

These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from **3 different cultivars**.

The analysis determined the quantities of **13 constituents** found in each of the 3 types of wines.

- ◆ In a classification context, this is a well posed problem with "well behaved" class structures.
- ◆ A good data set for first testing of a new classifier, but not very challenging.



EC for Hyperparameter Tuning — Wine Classification — Dataset

Attribute (Feature) Information:

- 1) Alcohol
- 2) Malic acid
- 3) Ash
- 4) Alcalinity of ash
- 5) Magnesium
- 6) Total phenols
- 7) Flavanoids
- 8) Nonflavanoid phenols
- 9) Proanthocyanins
- 10) Color intensity
- 11) Hue
- 12) OD280/OD315 of diluted wines
- 13) Proline

Class identifier: One (0th) attribute is class identifier (1,2,3)

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EC for Hyperparameter Tuning — Wine Classification — **Workflow**

Origin: it is the **classic** example of **classification problem**, where the input features need to be mapped into **3 categories/labels**.

Inputs: all features (wine properties) are **continuous**.

Outputs: the one feature — **class** — represents 3 categories (**cultivars**).

Aim: train a **classification model** on this dataset with **13 features** to **predict** the value of **feature 0 (cultivar)**.

NN Tuning — Wine Classification — **Workflow**

1) **Load** the UCI Wine **dataset** by the standard **read_csv** function (with `url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.data'`).

2) **Divide** the data into **input** features (first remaining 13 columns) and the resulting **output** category (the first column). Then instead of separating the data into **1 training** set and **1 test** set, like we did in the previous example, we're using ***k-fold cross-validation*** -> The data is split into ***k*** equal parts and the model is evaluated ***k*** times:

(***k-1***) parts for **training** and **1** remaining part for testing (or **validation**).

3) **Create** the classification **model** ... various models can be used ... **Multi-layer Perceptron (MLP)** in this example.

4) **Determine the performance** of the used regression model for a set of selected **hyperparameters** by ***accuracy* metric***.

*) **Accuracy** – the portion of the cases that were classified correctly. A **higher** value of this measurement indicates **better performance** of the model.

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- Classification Problem Example: Dataset + Workflow
- **DEMO - Part 1: NN Architecture Tuning Solution**
 - Random Seed
 - Dataset (Wine, Iris, Breast Cancer)
 - Max NN Layer Number
- DEMO - Part 2: NN Hyperparameter Tuning Solution
- DEMO - Part 3: NN Architecture + Hyperparameter Tuning Solution
- Resume

DEMO — Part1: NN Architecture Tuning

— Layers and Nodes

We limit NN to 4 hidden layers, the chromosome will be:

$$[n_1, n_2, n_3, n_4]$$

Here, n_i denotes the number of nodes in the layer i from 1 to 4. To control the number of hidden layers in NN, some of n_i may be 0 or <0 ... it means \rightarrow **no more layers** will be added to NN.

Example of some chromosomes:

[10, 20, **-5**, 15] \rightarrow tuple (10, 20) since **-5** ends the layer count.

[10, **0**, -5, 15] \rightarrow tuple (10,) since **0** ends the layer count.

[10, 20, 5, **-15**] \rightarrow tuple (10, 20, 5) since **-15** ends the count.

[10, 20, 5, 15] $>$ tuple (10, 20, 5, 15).

DEMO — Part1: NN Architecture Tuning

— Layers and Nodes

We limit NN to **4** hidden layers, the chromosome will be:

$$[n_1, n_2, n_3, n_4]$$

Here, n_i denotes the number of nodes in the layer i from 1 to 4. To control the number of hidden layers in NN, some of n_i may be 0 or <0 ... it means \rightarrow **no more layers** will be added to NN.

Example of some chromosomes:

[**10**, 20, -5, 15] \rightarrow tuple (10, 20) since -5 ends the layer count.

[**10**, 0, -5, 15] \rightarrow tuple (10,) since 0 ends the layer count.

[**10**, 20, 5, -15] \rightarrow tuple (10, 20, 5) since -15 ends the count.

[**10**, 20, 5, 15] $>$ tuple (10, 20, 5, 15).

To **guarantee** that there is **at least 1 hidden layer**, the **1st** parameter (**10** here) is **always >0** .

The **other layer parameters** can have **varying distributions** around 0 ... why ... to control their chances of being the terminating parameters.

DEMO - Part 1:

NN Architecture Tuning Solution

Results:

DEMO 1 - Default MLP Hyperparameter values.

gen	nevals	max	avg
0	20	0.769841	0.284063
1	17	0.769841	0.473413
2	15	0.769841	0.606905
3	16	0.769841	0.659238
4	17	0.769841	0.673444
5	14	0.769841	0.703746
6	17	0.769841	0.739619
7	14	0.769841	0.70954
8	16	0.769841	0.686921
9	17	0.769841	0.689833
10	15	0.769841	0.680286

Time Elapsed = 82.1906521320343

Best solution is: 'hidden_layer_sizes'=(13, 4, 7)

Accuracy = 0.76984

Try to reproduce these results!

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DEMO - Part 1: NN Architecture Tuning Solution

What is Influence of ...

- **Random Seed**
- Dataset (Wine, Iris, Breast Cancer)
- Max NN Layer Number

DEMO - Part 1: NN Architecture Tuning

Solution — Various Random Seeds?

Results for various RANDOM_SEEDs:

```
# dataset = 'wine'
# RANDOM_SEED = 42

gen nevals  max      avg
0   20      0.769841  0.284063
1   17      0.769841  0.473413
2   15      0.769841  0.606905
3   16      0.769841  0.659238
4   17      0.769841  0.673444
5   14      0.769841  0.703746
6   17      0.769841  0.739619
7   14      0.769841  0.70954
8   16      0.769841  0.686921
9   17      0.769841  0.689833
10  15      0.769841  0.680286

Best solution is:  'hidden_layer_sizes'=(13, 4, 7)
Accuracy = 0.76984
```

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning

Solution — Various Random Seeds?

Results for various RANDOM_SEEDs:

```
# dataset = 'wine'
# RANDOM_SEED = 42
```

gen	nevals	max	avg
0	20	0.769841	0.284063
1	17	0.769841	0.473413
2	15	0.769841	0.606905
3	16	0.769841	0.659238
4	17	0.769841	0.673444
5	14	0.769841	0.703746
6	17	0.769841	0.739619
7	14	0.769841	0.70954
8	16	0.769841	0.686921
9	17	0.769841	0.689833
10	15	0.769841	0.680286

```
Best solution is: 'hidden_layer_sizes'=(13, 4, 7)
Accuracy = 0.76984
```

```
# dataset = 'wine'
# RANDOM_SEED = 666
```

```
*****
```

gen	nevals	max	avg
0	20	0.647937	0.31354
1	17	0.647937	0.41869
2	15	0.647937	0.478095
3	16	0.647937	0.418651
4	17	0.647937	0.503325
5	12	0.647937	0.492421
6	17	0.647937	0.435524
7	16	0.647937	0.503032
8	16	0.647937	0.466016
9	16	0.647937	0.51246
10	17	0.647937	0.572524

```
Time Elapsed = 93.69340062141418
```

```
Best solution is: 'hidden_layer_sizes'=(14, 3, 4, 4)
```

```
Accuracy = 0.64794
```

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning

Solution — Various Random Seeds?

Results for various RANDOM_SEEDs:

```
# dataset = 'wine'
# RANDOM_SEED = 42
```

gen	nevals	max	avg
0	20	0.769841	0.284063
1	17	0.769841	0.473413
2	15	0.769841	0.606905
3	16	0.769841	0.659238
4	17	0.769841	0.673444
5	14	0.769841	0.703746
6	17	0.769841	0.739619
7	14	0.769841	0.70954
8	16	0.769841	0.686921
9	17	0.769841	0.689833
10	15	0.769841	0.680286

```
Best solution is: 'hidden_layer_sizes'=(13, 4, 7)
Accuracy = 0.76984
```

```
# dataset = 'wine'
# RANDOM_SEED = 666
```

```
*****
gen nevals  max      avg
0   20      0.647937 0.31354
1   17      0.647937 0.41869
2   15      0.647937 0.478095
3   16      0.647937 0.418651
4   17      0.647937 0.503325
5   12      0.647937 0.492421
6   17      0.647937 0.435524
7   16      0.647937 0.503032
8   16      0.647937 0.466016
9   16      0.647937 0.51246
10  17      0.647937 0.572524
```

```
Time Elapsed = 93.69340062141418
Best solution is: 'hidden_layer_sizes'=(14, 3, 4, 4)
Accuracy = 0.64794
```

```
# dataset = 'wine'
```

```
# RANDOM_SEED = 1042
```

```
*****
```

gen	nevals	max	avg
0	20	0.520159	0.289151
1	15	0.520159	0.322095
2	12	0.520159	0.42246
3	17	0.541587	0.419079
4	14	0.541587	0.41527
5	17	0.541587	0.471929
6	15	0.541587	0.457198
7	16	0.541587	0.472865
8	17	0.541587	0.493143
9	16	0.541587	0.45669
10	13	0.541587	0.488968

```
Time Elapsed = 84.34443235397339
```

```
Best solution is: 'hidden_layer_sizes'=(9, 9, 5)
```

```
Accuracy = 0.54159
```

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning

Solution — **Various Random Seeds - Resume**

Resume for various RANDOM_SEEDs:

For various RANDOM_SEED we can obtain NNs with the very different:

performance (accuracy),

- **the number of nodes in layers,**
- **the number of layers.**

The **possible reason** is the **stochastic** (so-called **non-gradient**) manner of **parameter change** during evolution.

There is some possibility that all these **models** for different RANDOM_SEEDs can **reach** the different **local** (**NOT** global) the **maximum** value of **fitness function** (**accuracy** here).

Try to reproduce these results!

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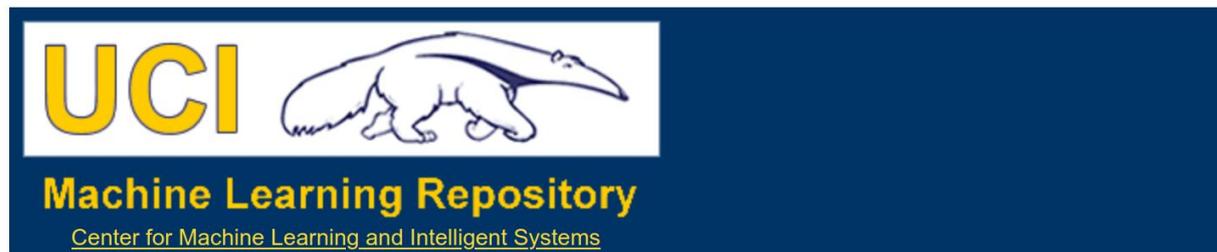
DEMO - Part 1: NN Architecture Tuning Solution

What is Influence of ...

- Random Seed
- **Dataset (Wine, Iris, Breast Cancer)**
- Max NN Layer Number

NN Tuning Example: Wine Dataset

It is the classic example of classification problem.



Wine Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Using chemical analysis determine the origin of wines



Data Set Characteristics:	Multivariate	Number of Instances:	178	Area:	Physical
Attribute Characteristics:	Integer, Real	Number of Attributes:	13	Date Donated	1991-07-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	1602802

Source:

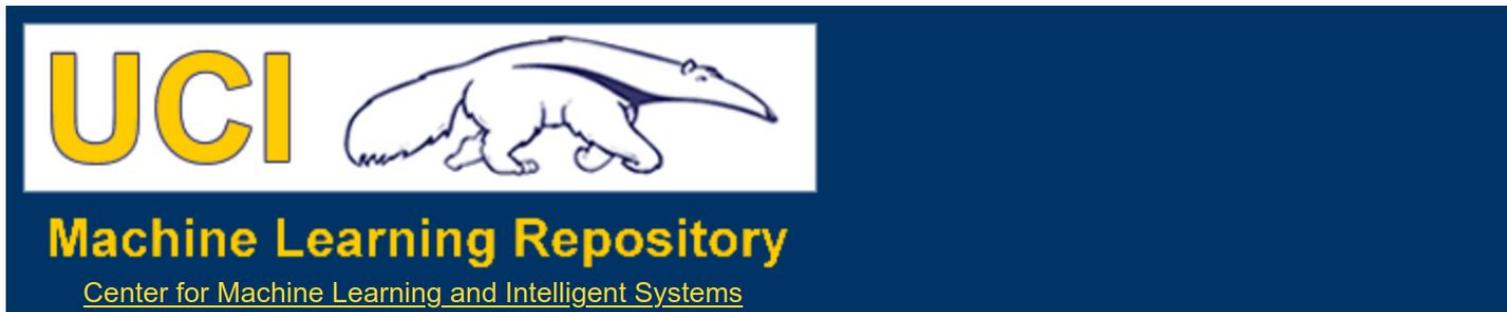
Original Owners:

Forina, M. et al, PARVUS -
An Extendible Package for Data Exploration, Classification and Correlation.
Institute of Pharmaceutical and Food Analysis and Technologies, Via Brigata Salerno,
16147 Genoa, Italy.

UCI Wine dataset (<https://archive.ics.uci.edu/ml/datasets/wine>)

NN Tuning Example: Iris Dataset

It is the classic example of classification problem.



Iris Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Famous database; from Fisher, 1936



Data Set Characteristics:	Multivariate	Number of Instances:	150	Area:	Life
Attribute Characteristics:	Real	Number of Attributes:	4	Date Donated	1988-07-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	3847949

UCI Iris dataset (<https://archive.ics.uci.edu/ml/datasets/iris>)

NN Tuning Example: Breast Cancer Dataset

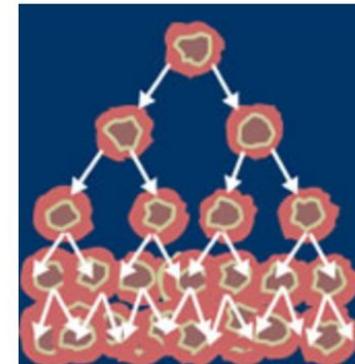
It is the classic example of classification problem.



Breast Cancer Wisconsin (Diagnostic) Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: Diagnostic Wisconsin Breast Cancer Database



Data Set Characteristics:	Multivariate	Number of Instances:	569	Area:	Life
Attribute Characteristics:	Real	Number of Attributes:	32	Date Donated	1995-11-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	1444676

UCI Breast Cancer dataset

([https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+\(Diagnostic\)](https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)))

DEMO - Part 1: NN Architecture Tuning

Solution — Various Datasets?

Results for various RANDOM_SEEDs:

```
### wine
# RANDOM_SEED = 42

gen nevals  max      avg
0   20      0.769841 0.284063
1   17      0.769841 0.473413
2   15      0.769841 0.606905
3   16      0.769841 0.659238
4   17      0.769841 0.673444
5   14      0.769841 0.703746
6   17      0.769841 0.739619
7   14      0.769841 0.70954
8   16      0.769841 0.686921
9   17      0.769841 0.689833
10  15      0.769841 0.680286

- Best solution is: 'hidden_layer_sizes'=(13, 4, 7) , accuracy = 0.7698412698412699
```

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning

Solution — Various Datasets?

Results for various RANDOM_SEEDs:

```
### wine
# RANDOM_SEED = 42

gen nevals  max      avg
0  20      0.769841  0.284063
1  17      0.769841  0.473413
2  15      0.769841  0.606905
3  16      0.769841  0.659238
4  17      0.769841  0.673444
5  14      0.769841  0.703746
6  17      0.769841  0.739619
7  14      0.769841  0.70954
8  16      0.769841  0.686921
9  17      0.769841  0.689833
10 15      0.769841  0.680286
- Best solution is: 'hidden_layer_sizes'=(13, 4, 7) , accuracy = 0.7698412698412699

### iris
# RANDOM_SEED = 42

gen nevals  max      avg
0  20      0.666667  0.416333
1  17      0.693333  0.487
2  15      0.76      0.537333
3  14      0.76      0.550667
4  17      0.76      0.568333
5  17      0.76      0.653667
6  14      0.76      0.589333
7  15      0.76      0.618
8  16      0.866667  0.616667
9  16      0.866667  0.666333
10 16      0.866667  0.722667
- Best solution is: 'hidden_layer_sizes'=(15, 5, 8) , accuracy = 0.8666
```

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning

Solution — Various Datasets?

Results for various RANDOM_SEEDs:

```
### wine
# RANDOM_SEED = 42
```

gen	nevals	max	avg
0	20	0.769841	0.284063
1	17	0.769841	0.473413
2	15	0.769841	0.606905
3	16	0.769841	0.659238
4	17	0.769841	0.673444
5	14	0.769841	0.703746
6	17	0.769841	0.739619
7	14	0.769841	0.70954
8	16	0.769841	0.686921
9	17	0.769841	0.689833
10	15	0.769841	0.680286

- Best solution is: 'hidden_layer_sizes'=(13, 4, 7) , accuracy = 0.7698412698412699

```
### iris
# RANDOM_SEED = 42
```

gen	nevals	max	avg
0	20	0.666667	0.416333
1	17	0.693333	0.487
2	15	0.76	0.537333
3	14	0.76	0.550667
4	17	0.76	0.568333
5	17	0.76	0.653667
6	14	0.76	0.589333
7	15	0.76	0.618
8	16	0.866667	0.616667
9	16	0.866667	0.666333
10	16	0.866667	0.722667

- Best solution is: 'hidden_layer_sizes'=(15, 5, 8) , accuracy = 0.8666

```
### breast_cancer
# RANDOM_SEED = 42
```

gen	nevals	max	avg
0	20	0.927946	0.808865
1	15	0.929669	0.889953
2	15	0.929669	0.893562
3	15	0.929669	0.893683
4	16	0.934932	0.839395
5	17	0.934932	0.912204
6	14	0.934932	0.895351
7	16	0.934932	0.908839
8	17	0.934932	0.900869
9	16	0.934932	0.845574
10	15	0.934932	0.900429

- Best solution is: 'hidden_layer_sizes'=(15, 8, 10, 4) , accuracy = 0.934932

Try to reproduce these results!

DEMO - Part 1: NN Architecture Tuning Solution — **Various Datasets - Resume**

Resume for various datasets:

Again ... for various datasets we can obtain NNs with the very different:

performance (accuracy),

- **the number of nodes in layers,**
- **the number of layers.**

The **possible reason** is

more evident here:

- **different features,**
- **different number** of features,
- their **different contribution**
to fitness function (accuracy).

Try to reproduce these results!

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DEMO - Part 1: NN Architecture Tuning Solution

What is Influence of ...

- Random Seed
- Dataset (Wine, Iris, Breast Cancer)
- **Max NN Layer Number**

DEMO - Part 1: NN Architecture Tuning Solution — **Various MAX Layer Number?**

Results for various MAX Layer Number:

BUT

...

try it as a self-guided learning

...

if you want! :)

Try to reproduce these results!

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DEMO - Part 2: NN Hyperparameter Tuning

For the previous 1) NN Architecture Tuning we used the default hyperparameters.

BUT ... from the previous lecture ... tuning the various hyperparameters can increase the classifier's performance.

Q: Can we use hyperparameter tuning here? **A:** Yes.

From *sklearn* implementation of MLP we can use numerous tunable hyperparameters:

Name	Type	Description	Default value
<code>activation</code>	<code>{'tanh', 'relu', 'logistic'}</code>	Activation function for the hidden layers	<code>'relu'</code>
<code>solver</code>	<code>{'sgd', 'adam', 'lbfgs'}</code>	The solver for weight optimization	<code>'adam'</code>
<code>alpha</code>	<code>float</code>	Regularization term parameter	<code>0.0001</code>
<code>learning_rate</code>	<code>{'constant', 'invscaling', 'adaptive'}</code>	Learning rate schedule for weight updates	<code>'constant'</code>

DEMO - Part 2: NN Hyperparameter Tuning

Like in the previous lecture demos, a floating point-based chromosome representation allows us to combine various types of hyperparameters into GA-based optimization process.

activation - one of three values: *tanh*, *relu*, or *logistic*.

This can be achieved by representing it as a float in the range of [0, 2.99] .

To transform the float into one of the aforementioned string values, we need to apply the *floor()* function to it, which will yield either 0, 1, or 2.

Then we replace 0 -> *tanh*, 1 -> *relu*, and 2 -> *logistic*.

solver - one of 3 values: *sgd*, *adam*, or *lbfgs*.

Like for **activation**: it can be represented using a float in [0, 2.99] range.

alpha - already a float, no conversion is needed.

It will be bound to the range of [0.0001, 2.0].

learning_rate - one of 3 values: *constant*, *invscaling*, *adaptive*.

Like for **activation**: it can be represented using a float in [0, 2.99] range.

DEMO - Part 2: NN Hyperparameter Tuning

Results:

DEMO 2 - The best NN Architecture from DEMO 1.
HIDDEN_LAYER_SIZES = [13, 4, 7]

gen	nevals	max	avg
0	20	0.946667	0.362
1	15	0.946667	0.599667
2	16	0.946667	0.864333
3	16	0.946667	0.927333
4	17	0.946667	0.944667
5	14	0.946667	0.887
6	15	0.946667	0.944667
7	14	0.946667	0.946
8	16	0.946667	0.907667
9	15	0.946667	0.945
10	17	0.946667	0.946

Time Elapsed = 92.3740484714508
Best solution is: 'activation'='logistic'
'solver'='lbfgs'
'alpha'=0.17139833879055075
'learning_rate'='invscaling'
Accuracy = 0.94667

Try to reproduce these results!

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- Resume

DEMO - Part 3: Hybrid: NN Architecture + NN Hyperparameter Tuning

The first 4 ranges for NN Architecture tuning
→ one for each hidden layer.

The next 4 ranges
→ represent the additional 4 hyperparameters.

```
# 'hidden_layer_sizes': first four values
# 'activation': 0..2.99
# 'solver': 0..2.99
# 'alpha': 0.0001..2.0
# 'learning_rate': 0..2.99
BOUNDS_LOW = [ 5, -5, -10, -20, 0, 0, 0.0001, 0 ]
BOUNDS_HIGH = [15, 10, 10, 10, 2.999, 2.999, 2.0, 2.999]
```

DEMO - Part 3: Hybrid: NN Architecture + NN Hyperparameter Tuning

Input Boundaries:

```
# boundaries for all parameters:  
# 'hidden_layer_sizes': first four values  
# 'activation': ['tanh', 'relu', 'logistic'] -> 0, 1, 2  
# 'solver': ['sgd', 'adam', 'lbfgs'] -> 0, 1, 2  
# 'alpha': float in the range of [0.0001, 2.0],  
# 'learning_rate': ['constant', 'invscaling', 'adaptive'] -> 0, 1, 2  
BOUNDS_LOW = [ 5, -5, -10, -20, 0, 0, 0.0001, 0 ]  
BOUNDS_HIGH = [15, 10, 10, 10, 2.999, 2.999, 2.0, 2.999]
```

DEMO - Part 3: Hybrid: NN Architecture + NN Hyperparameter Tuning

Results:

```
*****
gen      nevals  max      avg
0        20      0.94     0.448
1        16      0.94     0.633
2        15      0.94     0.737667
3        16      0.946667 0.842
4        17      0.946667 0.889667
5        15      0.946667 0.937667
6        16      0.946667 0.939
7        16      0.946667 0.875
8        16      0.946667 0.876333
9        14      0.946667 0.942333
10       16      0.946667 0.902667
Time Elapsed = 83.84976434707642
Best solution is: 'hidden_layer_sizes'=(8, 7)
'activation'='relu'
'solver'='lbfgs'
'alpha'=0.563775972907702
'learning_rate'='adaptive'
Accuracy = 0.94667
```

Try to reproduce these results!

DEMO - Part 3: Hybrid: NN Architecture + NN Hyperparameter Tuning

Results -> Compare with NN Hyper ONLY

```
*****
gen      nevals  max      avg
0        20      0.94     0.448
1        16      0.94     0.633
2        15      0.94     0.737667
3        16      0.946667 0.842
4        17      0.946667 0.889667
5        15      0.946667 0.937667
6        16      0.946667 0.939
7        16      0.946667 0.875
8        16      0.946667 0.876333
9        14      0.946667 0.942333
10       16      0.946667 0.902667
Time Elapsed = 83.84976434707642
Best solution is: 'hidden_layer_sizes'=(8, 7)
'activation'='relu'
'solver'='lbfgs'
'alpha'=0.563775972907702
'learning_rate'='adaptive'
Accuracy = 0.94667
```

```
*****
gen      nevals  max      avg
0        20      0.946667 0.362
1        15      0.946667 0.599667
2        16      0.946667 0.864333
3        16      0.946667 0.927333
4        17      0.946667 0.944667
5        14      0.946667 0.887
6        15      0.946667 0.944667
7        14      0.946667 0.946
8        16      0.946667 0.907667
9        15      0.946667 0.945
10       17      0.946667 0.946
Time Elapsed = 92.3740484714508
Best solution is: 'activation'='logistic'
'solver'='lbfgs'
'alpha'=0.17139833879055075
'learning_rate'='invscaling'
Accuracy = 0.94667
```

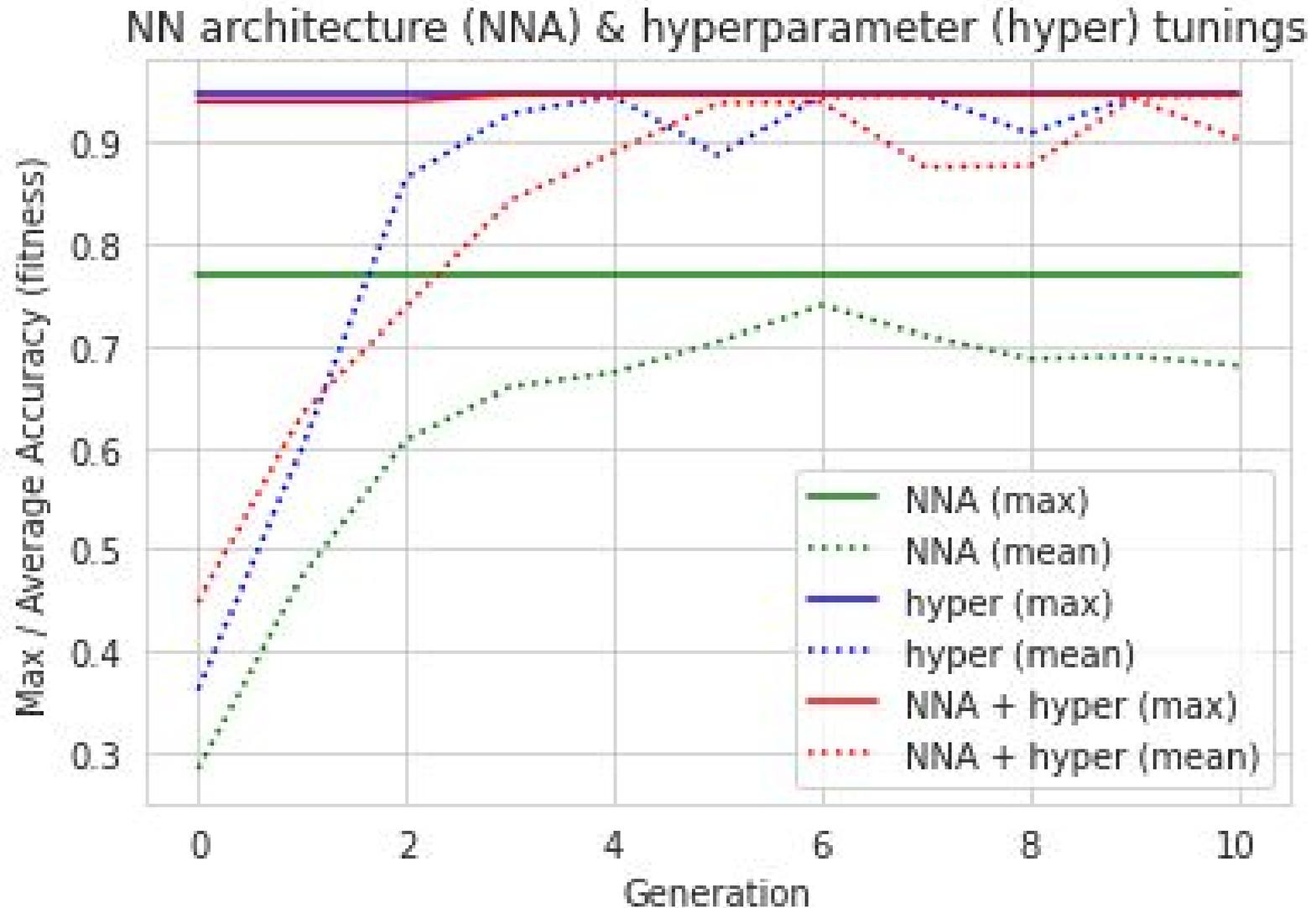
Funny Differences in Best Solution Parameters ... :)

Try to reproduce these results!

Content

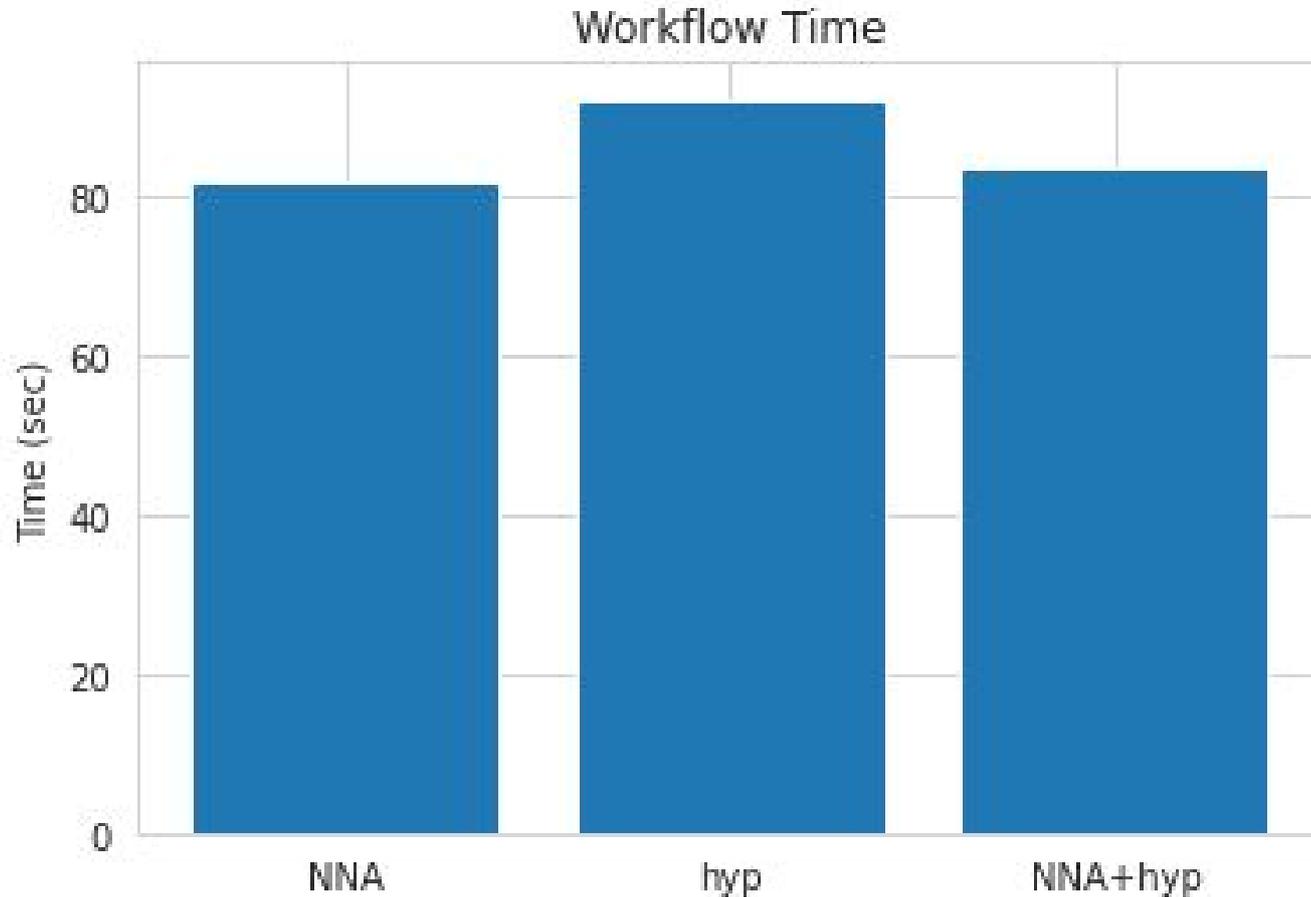
- Recommended Sources
- EA (GA) for Neural Network (NN) Tuning
- Types of NN Tuning
- Classification Problem Example: Dataset + Workflow
- DEMO - Part 1: NN Architecture Tuning Solution
 - Random Seed
 - Dataset (Wine, Iris, Breast Cancer)
 - Max NN Layer Number
- DEMO - Part 2: NN Hyperparameter Tuning Solution
- DEMO - Part 3: NN Architecture + Hyperparameter Tuning Solution
- **Resume**

EC for NN Architecture + NN Hyperparameter Tuning — Comparative Plot — Accuracy



Try to reproduce these results!

EC for NN Architecture + NN Hyperparameter Tuning — Comparative Plot — Time



It does not matter ... in such problem formulation ... but ...

Try to reproduce these results!

EC for Feature Selection — **Resume**

EC (GA) can be effectively applied to
the classic supervised machine learning problems:

- **regression** (use case of Friedman-1 Regression Problem)
and
- **classification** (use case of UCI-dataset animal classification)

for

– **feature selection**

or

– **dimensionality reduction**

with the purpose of:

– **decrease of MSE**

or

– **increase of mean accuracy.**

Evolutionary Algorithms (EA) Basics

Lecture 6 - DEMO A - OpenAI Gym platform

based on (C) OpenAI, Heaton, Moore, Varoquaux, Grobler, Wirsansky work

Brief Content:

- OpenAI Gym platform
- *Reinforcement Learning (RL) problems:*
 - MountainCar-v0,
 - MountainCarContinuous-v0,
 - CartPole-v1
 - ...
- Functions to visualize Gym-game-scenarios in Colab.

▼ Installation and import of libraries

▼ Library to support RL algorithms

Gym is a toolkit for developing and comparing reinforcement learning algorithms.

It supports teaching agents everything from walking to playing games like Pong or Pinball.

```
! pip install gym
```

```
Requirement already satisfied: gym in /usr/local/lib/python3.7/dist-packages  
Requirement already satisfied: pygame<=1.5.0,>=1.4.0 in /usr/local/lib/pythor  
Requirement already satisfied: numpy>=1.10.4 in /usr/local/lib/python3.7/dist  
Requirement already satisfied: cloudpickle<1.7.0,>=1.2.0 in /usr/local/lib/py  
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-package  
Requirement already satisfied: future in /usr/local/lib/python3.7/dist-packag
```

▼ Libraries to Render OpenAI Gym Environments in Colab

It is possible to visualize the activities performed in Gym (game your agent is playing), even on Colab. This section provides information on how to generate a video in Colab that shows you an

episode of the game your agent is playing.

```
%%time
!pip install gym pyvirtualdisplay > /dev/null 2>&1
!apt-get install -y xvfb python-opengl ffmpeg > /dev/null 2>&1
```

```
CPU times: user 28.9 ms, sys: 18.1 ms, total: 47 ms
Wall time: 11.6 s
```

```
%%time
!apt-get update > /dev/null 2>&1
!apt-get install cmake > /dev/null 2>&1
!pip install --upgrade setuptools > /dev/null 2>&1
!pip install ez_setup > /dev/null 2>&1
!pip install gym[atari] > /dev/null 2>&1
```

```
Collecting setuptools
  Downloading https://files.pythonhosted.org/packages/60/6a/dd9533a
|████████████████████████████████████████| 788kB 7.3MB/s
ERROR: datascience 0.10.6 has requirement folium==0.2.1, but you'll
Installing collected packages: setuptools
  Found existing installation: setuptools 54.0.0
  Uninstalling setuptools-54.0.0:
    Successfully uninstalled setuptools-54.0.0
  Successfully installed setuptools-54.1.1
CPU times: user 73.7 ms, sys: 44.5 ms, total: 118 ms
```

IMPORTANT: you should restart runtime!

▼ Part 1. Introduction to the OpenAI Gym

Gym - Advanages and Limitations

[OpenAI Gym](#) aims to provide an easy-to-setup general-intelligence benchmark with a wide variety of different environments. The goal is to standardize how environments are defined in AI research publications so that published research becomes more easily reproducible. The project claims to provide the user with a simple interface.

OpenAI gym is pip-installed onto your local machine. There are a few significant limitations to be aware of:

- developers can only use Gym with Python (as of June 2017).

- OpenAI Gym can not directly render animated games in Google CoLab.

Because OpenAI Gym requires a graphics display, the only way to display Gym in Google CoLab is an embedded video. The presentation of OpenAI Gym game animations in Google CoLab is discussed later in this module.

Gym - Leaderboard

The OpenAI Gym does have a leaderboard, similar to Kaggle; however, the OpenAI Gym's leaderboard is much more informal compared to Kaggle. The user's local machine performs all scoring. As a result, the OpenAI gym's leaderboard is strictly an "honor's system." The leaderboard is maintained the following GitHub repository:

- [OpenAI Gym Leaderboard](#)

If you submit a score, you are required to provide a writeup with sufficient instructions to reproduce your result. A video of your results is suggested, but not required.

Gym - Environments

The centerpiece of Gym is the environment, which defines the "game" in which your reinforcement algorithm will compete. An environment does not need to be a game; however, it describes the following game-like features:

- **action space**: What actions can we take on the environment, at each step/episode, to alter the environment.
- **observation space**: What is the current state of the portion of the environment that we can observe. Usually, we can see the entire environment.

Gym - Basic Termonology

- **Agent** - The machine learning program or model that controls the actions. Step - One round of issuing actions that affect the observation space.
- **Episode** - A collection of steps that terminates when the agent fails to meet the environment's objective, or the episode reaches the maximum number of allowed steps.
- **Render** - Gym can render one frame for display after each episode.
- **Reward** - A positive reinforcement that can occur at the end of each episode, after the agent acts.
- **Nondeterministic** - For some environments, randomness is a factor in deciding what effects actions have on reward and changes to the observation space.

It is important to note that many of the gym environments specify that they are not nondeterministic even though they make use of random numbers to process actions. It is

generally agreed upon (based on the gym GitHub issue tracker) that nondeterministic property means that a deterministic environment will still behave randomly even when given consistent seed value. The seed method of an environment can be used by the program to seed the random number generator for the environment.

▼ Environment - Attributes

The Gym library allows us to query some of these attributes from environments. I created the following function to query gym environments.

```
import gym

def query_environment(name):
    env = gym.make(name)
    spec = gym.spec(name)
    print(f"Action Space: {env.action_space}")
    print(f"Observation Space: {env.observation_space}")
    print(f"Max Episode Steps: {spec.max_episode_steps}")
    print(f"Nondeterministic: {spec.nondeterministic}")
    print(f"Reward Range: {env.reward_range}")
    print(f"Reward Threshold: {spec.reward_threshold}")
```

▼ Environment - Examples:

- MountainCar-v0,
- MountainCarContinuous-v0,
- CartPole-v1
- ...

▼ MountainCar-v0

We will begin by looking at the MountainCar-v0 environment, which challenges an underpowered car to escape the valley between two mountains. The following code describes the Mountain Car environment.

```
query_environment("MountainCar-v0")
```

```
Action Space: Discrete(3)
Observation Space: Box(-1.2000000476837158, 0.6000000238418579, (2,), float32)
Max Episode Steps: 200
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: -110.0
```

Actions

There are three distinct actions that can be taken:

- accelerate forward,
- decelerate,
- accelerate backwards.

Observation space

The observation space contains two continuous (floating point) values, as evident by the box object.

The observation space contains:

- the position and
- velocity of the car.

The car has 200 steps to escape for each episode.

Reward: The mountain car receives NO incremental reward. The only reward for the car is given when it escapes the valley.

▼ MountainCarContinuous-v0

There is also a continuous variant of the mountain car. This version does not simply have the motor on or off. For the continuous car the action space is a single floating point number that specifies how much forward or backward force is being applied.

```
query_environment("MountainCarContinuous-v0")
```

```
Action Space: Box(-1.0, 1.0, (1,), float32)
Observation Space: Box(-1.20000000476837158, 0.60000000238418579, (2,), float32)
Max Episode Steps: 999
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: 90.0
```

Note: ignore the warning above, it is a relatively inconsequential bug in OpenAI Gym.

▼ CartPole-v1

The CartPole-v1 environment challenges the agent to move a cart while keeping a pole balanced.

Observation space

The environment has an observation space of 4 continuous numbers:

- Cart Position
- Cart Velocity
- Pole Angle
- Pole Velocity At Tip

Actions

To achieve this goal, the agent can take the following actions:

- Push cart to the left
- Push cart to the right

```
query_environment("CartPole-v1")
```

```
Action Space: Discrete(2)
Observation Space: Box(-3.4028234663852886e+38, 3.4028234663852886e+38, (4,)),
Max Episode Steps: 500
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: 475.0
```

▼ Breakout-v0

Atari games, like breakout can use an observation space that is either equal to the size of the Atari screen (210x160) or even use the RAM memory of the Atari (128 bytes) to determine the state of the game. Yes thats bytes, not kilobytes!

```
query_environment("Breakout-v0")
```

```
Action Space: Discrete(4)
Observation Space: Box(0, 255, (210, 160, 3), uint8)
Max Episode Steps: 10000
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: None
```

▼ Breakout-ram-v0

```
query_environment("Breakout-ram-v0")
```

```
Action Space: Discrete(4)
Observation Space: Box(0, 255, (128,), uint8)
Max Episode Steps: 10000
Nondeterministic: False
```

Reward Range: (-inf, inf)
Reward Threshold: None

▼ Atlantis-v0

```
query_environment("Atlantis-v0")
```

```
Action Space: Discrete(4)  
Observation Space: Box(0, 255, (210, 160, 3), uint8)  
Max Episode Steps: 10000  
Nondeterministic: False  
Reward Range: (-inf, inf)  
Reward Threshold: None
```

▼ Part 2.Functions to visualize Gym-game-scenarios in Colab

Next we define functions used to show the video by adding it to the Colab notebook.

```
import gym  
from gym.wrappers import Monitor  
import glob  
import io  
import base64  
from IPython.display import HTML  
from pyvirtualdisplay import Display  
from IPython import display as ipythondisplay  
  
display = Display(visible=0, size=(1400, 900))  
display.start()  
  
"""  
Utility functions to enable video recording of gym environment  
and displaying it.  
To enable video, just do "env = wrap_env(env)"  
"""  
  
def show_video():  
    mp4list = glob.glob('video/*.mp4')  
    if len(mp4list) > 0:  
        mp4 = mp4list[0]  
        video = io.open(mp4, 'r+b').read()  
        encoded = base64.b64encode(video)  
        ipythondisplay.display(HTML(data='''<video alt="test" autoplay  
            loop controls style="height: 400px;">  
                <source src="data:video/mp4;base64,{0}" type="video/mp4" />  
            </video>'''.format(encoded.decode('ascii'))))  
    else:  
        print("Could not find video")  
  
def wrap_env(env):
```

```
env = Monitor(env, './video', force=True)
return env
```

Now we are ready to play the game. We use a simple random agent.

▼ MountainCar-v0

```
env = wrap_env(gym.make("MountainCar-v0"))

observation = env.reset()

while True:

    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:
        break;

env.close()
show_video()
```



▼ MountainCarContinuous-v0

```
env = wrap_env(gym.make("MountainCarContinuous-v0"))

observation = env.reset()

while True:

    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:
        break;

env.close()
show_video()
```



▼ CartPole-v1

```
env = wrap_env(gym.make("CartPole-v1"))

observation = env.reset()

while True:

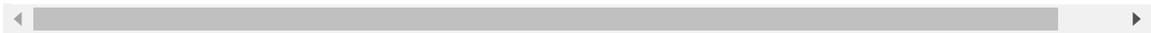
    env.render()
```

```
#your agent goes here
action = env.action_space.sample()

observation, reward, done, info = env.step(action)

if done:
    break;

env.close()
show_video()
```



▼ Breakout-v0

```
env = wrap_env(gym.make("Breakout-v0"))

observation = env.reset()

while True:

    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:
```

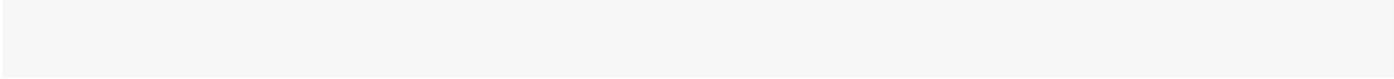
```
        break;
env.close()
show_video()
```

▼ Breakout-ram-v0

```
env = wrap_env(gym.make("Breakout-ram-v0"))
observation = env.reset()
while True:
    env.render()
    #your agent goes here
    action = env.action_space.sample()
    observation, reward, done, info = env.step(action)
    if done:
        break;
env.close()
show_video()
```

▼ Atlantis-v0

```
env = wrap_env(gym.make("Atlantis-v0"))  
  
observation = env.reset()  
  
while True:  
    env.render()  
  
    #your agent goes here  
    action = env.action_space.sample()  
  
    observation, reward, done, info = env.step(action)  
  
    if done:  
        break;  
  
env.close()  
show_video()
```



Colab paid products - Cancel contracts here



▼ Lecture 7 - Applications of EA for Reinforcement Learning

based on (C) OpenAI, Heaton, Moore, Varoquaux, Grobler, Wirsansky work

Brief Content:

- DEAP installation (**every time after start of Colab VM!**),
- components needed for the GA workflow,
- *Reinforcement Learning (RL) problems*:
 - MountainCar-v0,
 - MountainCarContinuous-v0,
 - CartPole-v1
 - ...
- performance comparison (accuracy and run time).

By the end of this lecture you will know:

- again, how to use the DEAP framework's built-in algorithms to produce concise code
- how to solve the *Reinforcement Learning* problem using a GA-based solutions for search of solutions,
- how to experiment with various settings of the GA and interpret the differences in the results.

▼ Get Figures for Text Description

```
from google.colab import drive
drive.mount('/content/drive')
```

Mounted at /content/drive

```
! cp -r /content/drive/MyDrive/COLAB_EV0/EV0_Lecture07_CartPole/figures .
! ls figures
```

MLPRegressor.png

▼ Installation and import of libraries


```
Collecting setuptools
  Downloading https://files.pythonhosted.org/packages/60/6a/dd9533ae9367a1f35
|████████████████████████████████████████| 788kB 4.2MB/s
ERROR: datascience 0.10.6 has requirement folium==0.2.1, but you'll have foli
Installing collected packages: setuptools
  Found existing installation: setuptools 54.0.0
  Uninstalling setuptools-54.0.0:
    Successfully uninstalled setuptools-54.0.0
  Successfully installed setuptools-54.1.1
CPU times: user 94.1 ms. svs: 46.3 ms. total: 140 ms
```

IMPORTANT: you should restart runtime!

▼ Part 1. Introduction to the OpenAI Gym

Gym - Advanages and Limitations

[OpenAI Gym](#) aims to provide an easy-to-setup general-intelligence benchmark with a wide variety of different environments. The goal is to standardize how environments are defined in AI research publications so that published research becomes more easily reproducible. The project claims to provide the user with a simple interface.

OpenAI gym is pip-installed onto your local machine. There are a few significant limitations to be aware of:

- developers can only use Gym with Python (as of June 2017).
- OpenAI Gym can not directly render animated games in Google CoLab.

Because OpenAI Gym requires a graphics display, the only way to display Gym in Google CoLab is an embedded video. The presentation of OpenAI Gym game animations in Google CoLab is discussed later in this module.

Gym - Leaderboard

The OpenAI Gym does have a leaderboard, similar to Kaggle; however, the OpenAI Gym's leaderboard is much more informal compared to Kaggle. The user's local machine performs all scoring. As a result, the OpenAI gym's leaderboard is strictly an "honor's system." The leaderboard is maintained the following GitHub repository:

- [OpenAI Gym Leaderboard](#)

If you submit a score, you are required to provide a writeup with sufficient instructions to reproduce your result. A video of your results is suggested, but not required.

Gym - Environments

The centerpiece of Gym is the environment, which defines the "game" in which your reinforcement algorithm will compete. An environment does not need to be a game; however, it describes the following game-like features:

- **action space**: What actions can we take on the environment, at each step/episode, to alter the environment.
- **observation space**: What is the current state of the portion of the environment that we can observe. Usually, we can see the entire environment.

Gym - Basic Terminology

- **Agent** - The machine learning program or model that controls the actions. Step - One round of issuing actions that affect the observation space.
- **Episode** - A collection of steps that terminates when the agent fails to meet the environment's objective, or the episode reaches the maximum number of allowed steps.
- **Render** - Gym can render one frame for display after each episode.
- **Reward** - A positive reinforcement that can occur at the end of each episode, after the agent acts.
- **Nondeterministic** - For some environments, randomness is a factor in deciding what effects actions have on reward and changes to the observation space.

It is important to note that many of the gym environments specify that they are not nondeterministic even though they make use of random numbers to process actions. It is generally agreed upon (based on the gym GitHub issue tracker) that nondeterministic property means that a deterministic environment will still behave randomly even when given consistent seed value. The seed method of an environment can be used by the program to seed the random number generator for the environment.

▼ Environment - Attributes

The Gym library allows us to query some of these attributes from environments. I created the following function to query gym environments.

```
import gym

def query_environment(name):
    env = gym.make(name)
    spec = gym.spec(name)
    print(f"Action Space: {env.action_space}")
    print(f"Observation Space: {env.observation_space}")
    print(f"Max Episode Steps: {spec.max_episode_steps}")
    print(f"Nondeterministic: {spec.nondeterministic}")
```

```
print(f"Reward Range: {env.reward_range}")
```

▼ Environment - Examples:

- MountainCar-v0,
- MountainCarContinuous-v0,
- CartPole-v1
- ...

▼ MountainCar-v0

We will begin by looking at the MountainCar-v0 environment, which challenges an underpowered car to escape the valley between two mountains. The following code describes the Mountain Car environment.

```
query_environment("MountainCar-v0")
```

```
Action Space: Discrete(3)
Observation Space: Box(-1.2000000476837158, 0.6000000238418579, (2,)), float32
Max Episode Steps: 200
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: -110.0
```

Actions

There are three distinct actions that can be taken:

- accelerate forward,
- decelerate,
- accelerate backwards.

Observation space

The observation space contains two continuous (floating point) values, as evident by the box object.

The observation space contains:

- the position and
- velocity of the car.

The car has 200 steps to escape for each episode.

Reward: The mountain car receives NO incremental reward. The only reward for the car is given when it escapes the valley.

▼ MountainCarContinuous-v0

There is also a continuous variant of the mountain car. This version does not simply have the motor on or off. For the continuous car the action space is a single floating point number that specifies how much forward or backward force is being applied.

```
query_environment("MountainCarContinuous-v0")
```

```
Action Space: Box(-1.0, 1.0, (1,)), float32)
Observation Space: Box(-1.20000000476837158, 0.60000000238418579, (2,)), float32)
Max Episode Steps: 999
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: 90.0
```

Note: ignore the warning above, it is a relatively inconsequential bug in OpenAI Gym.

▼ CartPole-v1

The CartPole-v1 environment challenges the agent to move a cart while keeping a pole balanced.

Observation space

The environment has an observation space of 4 continuous numbers:

- Cart Position
- Cart Velocity
- Pole Angle
- Pole Velocity At Tip

Actions

To achieve this goal, the agent can take the following actions:

- Push cart to the left
- Push cart to the right

```
query_environment("CartPole-v1")
```

```
Action Space: Discrete(2)
Observation Space: Box(-3.4028234663852886e+38, 3.4028234663852886e+38, (4,)), float32)
Max Episode Steps: 500
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: 475.0
```

▼ Breakout-v0

Atari games, like breakout can use an observation space that is either equal to the size of the Atari screen (210x160) or even use the RAM memory of the Atari (128 bytes) to determine the state of the game. Yes thats bytes, not kilobytes!

```
query_environment("Breakout-v0")
```

```
Action Space: Discrete(4)
Observation Space: Box(0, 255, (210, 160, 3), uint8)
Max Episode Steps: 10000
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: None
```

▼ Breakout-ram-v0

```
query_environment("Breakout-ram-v0")
```

```
Action Space: Discrete(4)
Observation Space: Box(0, 255, (128,), uint8)
Max Episode Steps: 10000
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: None
```

▼ Atlantis-v0

```
query_environment("Atlantis-v0")
```

```
Action Space: Discrete(4)
Observation Space: Box(0, 255, (210, 160, 3), uint8)
Max Episode Steps: 10000
Nondeterministic: False
Reward Range: (-inf, inf)
Reward Threshold: None
```

▼ Functions to visualize game-scenarios in Colab

Next we define functions used to show the video by adding it to the Colab notebook.

```
import gym
from gym.wrappers import Monitor
import glob
import io
```

```

import base64
from IPython.display import HTML
from pyvirtualdisplay import Display
from IPython import display as ipythondisplay

display = Display(visible=0, size=(1400, 900))
display.start()

"""
Utility functions to enable video recording of gym environment
and displaying it.
To enable video, just do "env = wrap_env(env)"
"""

def show_video():
    mp4list = glob.glob('video/*.mp4')
    if len(mp4list) > 0:
        mp4 = mp4list[0]
        video = io.open(mp4, 'r+b').read()
        encoded = base64.b64encode(video)
        ipythondisplay.display(HTML(data='''<video alt="test" autoplay
            loop controls style="height: 400px;">
                <source src="data:video/mp4;base64,{0}" type="video/mp4" />
            </video>'''.format(encoded.decode('ascii'))))
    else:
        print("Could not find video")

def wrap_env(env):
    env = Monitor(env, './video', force=True)
    return env

```

Now we are ready to play the game. We use a simple random agent.

▼ MountainCar-v0

```

env = wrap_env(gym.make("MountainCar-v0"))

observation = env.reset()

while True:

    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:

```

```
        break;
env.close()
show_video()
```

0:00 / 0:06



▼ MountainCarContinuous-v0

```
env = wrap_env(gym.make("MountainCarContinuous-v0"))
observation = env.reset()
while True:
    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:
        break;

env.close()
show_video()
```

0:00 / 0:33

▼ CartPole-v1

```
env = wrap_env(gym.make("CartPole-v1"))  
  
observation = env.reset()  
  
while True:  
    env.render()  
  
    #your agent goes here  
    action = env.action_space.sample()  
  
    observation, reward, done, info = env.step(action)  
  
    if done:  
        break;  
  
env.close()  
show_video()
```

▼ Breakout-v0

```
env = wrap_env(gym.make("Breakout-v0"))  
  
observation = env.reset()  
  
while True:  
    env.render()  
  
    #your agent goes here  
    action = env.action_space.sample()  
  
    observation, reward, done, info = env.step(action)  
  
    if done:  
        break;  
  
env.close()  
show_video()
```

▼ Breakout-ram-v0

```
env = wrap_env(gym.make("Breakout-ram-v0"))  
  
observation = env.reset()  
  
while True:  
    env.render()  
  
    #your agent goes here  
    action = env.action_space.sample()  
  
    observation, reward, done, info = env.step(action)  
  
    if done:  
        break;  
  
env.close()  
show_video()
```

0:00 / 0:08



▼ Atlantis-v0

```
env = wrap_env(gym.make("Atlantis-v0"))
```

```
observation = env.reset()

while True:

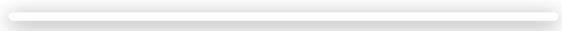
    env.render()

    #your agent goes here
    action = env.action_space.sample()

    observation, reward, done, info = env.step(action)

    if done:
        break;

env.close()
show_video()
```



▼ Part 3. GA Solution for RL problem - CartPole-v1

▼ CartPole-v1 - Problem Description

A pole is attached by an un-actuated joint to a cart, which moves along a frictionless track. The system is controlled by applying a force of +1 or -1 to the cart. The pendulum starts upright, and the goal is to prevent it from falling over.

Reward A reward of +1 is provided for every timestep that the pole remains upright. The episode ends when the pole is more than 15 degrees from vertical, or the cart moves more than 2.4 units from the center.

This environment corresponds to the version of the cart-pole problem described by Barto, Sutton, and Anderson:

AG Barto, RS Sutton and CW Anderson, *Neuronlike Adaptive Elements That Can Solve Difficult Learning Control Problem*, IEEE Transactions on Systems, Man, and Cybernetics, 1983.

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Let's try it as a self-guided learning!

Use the following CartPole-v1 resources:

- description at [Gym](#),
- Python-codes at [github](#)

▼ Import Python libraries

In these and other lectures, we will use various Python packages:

- [NumPy](#)
- [Matplotlib](#)
- [Seaborn](#)

They are already pre-installed in Colab. Let's import them by the following code.

```
import gym
import time
import pickle
import random
import numpy

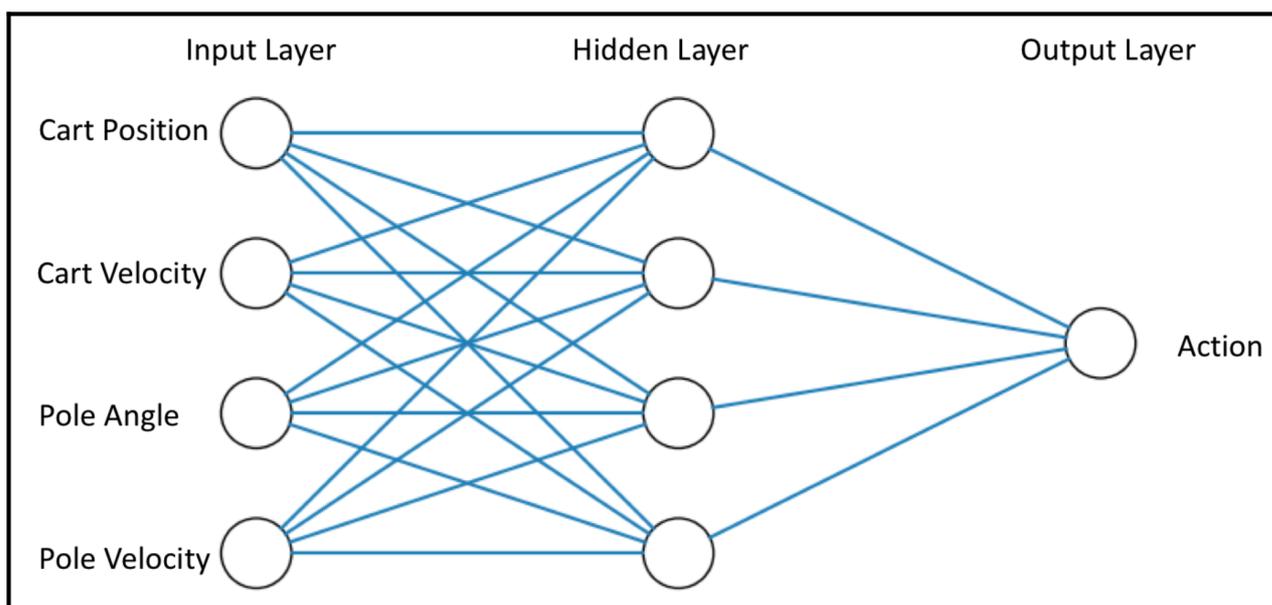
# for plotting
import matplotlib.pyplot as plt
import seaborn as sns
```

```
! rm -r ./video
! rm ./pickle
```

```
rm: cannot remove './video': No such file or directory
rm: cannot remove './pickle': No such file or directory
```

▼ Actors - CartPole

```
from IPython.display import Image
Image('./figures/MLPRegressor.png')
```



```
import gym
import time

import numpy as np
import pickle

from sklearn.neural_network import MLPRegressor
```

```

from sklearn.exceptions import ConvergenceWarning
from sklearn.utils.testing import ignore_warnings

INPUTS = 4
HIDDEN_LAYER = 4
OUTPUTS = 1

class CartPole:

    def __init__(self, randomSeed=None):

        #self.env = gym.make('CartPole-v1')
        self.env = wrap_env(gym.make('CartPole-v1'))
        self.env.seed(randomSeed)

        if randomSeed is not None:
            self.env.seed(randomSeed)

    def __len__(self):
        return INPUTS * HIDDEN_LAYER + HIDDEN_LAYER * OUTPUTS + HIDDEN_LAYER + OUT

@ignore_warnings(category=ConvergenceWarning)
def initMlp(self, netParams):
    """
    initializes a MultiLayer Perceptron (MLP) Regressor with the desired network
    and network parameters (weights and biases).
    :param netParams: a list of floats representing the network parameters (weights and biases)
    :return: initialized MLP Regressor
    """

    # create the initial MLP:
    mlp = MLPRegressor(hidden_layer_sizes=(HIDDEN_LAYER,), max_iter=1)

    # This will initialize input and output layers, and nodes weights and bias
    # we are not otherwise interested in training the MLP here, hence the settings
    mlp.fit(np.random.uniform(low=-1, high=1, size=INPUTS).reshape(1, -1), np.zeros(1))

    # weights are represented as a list of 2 ndarrays:
    # - hidden layer weights: INPUTS x HIDDEN_LAYER
    # - output layer weights: HIDDEN_LAYER x OUTPUTS
    numWeights = INPUTS * HIDDEN_LAYER + HIDDEN_LAYER * OUTPUTS
    weights = np.array(netParams[:numWeights])
    mlp.coefs_ = [
        weights[0:INPUTS * HIDDEN_LAYER].reshape((INPUTS, HIDDEN_LAYER)),
        weights[INPUTS * HIDDEN_LAYER:].reshape((HIDDEN_LAYER, OUTPUTS))
    ]

    # biases are represented as a list of 2 ndarrays:
    # - hidden layer biases: HIDDEN_LAYER x 1
    # - output layer biases: OUTPUTS x 1
    biases = np.array(netParams[numWeights:])
    mlp.intercepts_ = [biases[:HIDDEN_LAYER], biases[HIDDEN_LAYER:]]

    return mlp

```

```

def getScore(self, netParams):
    """
    calculates the score of a given solution, represented by the list of float
    by creating a corresponding MLP Regressor, initiating an episode of the Ca
    running it with the MLP controlling the actions, while using the observati
    Higher score is better.
    :param netParams: a list of floats representing the network parameters (we
    :return: the calculated score value
    """

    mlp = self.initMlp(netParams)

    self.env.reset()

    actionCounter = 0
    totalReward = 0
    observation = self.env.reset()
    action = int(mlp.predict(observation.reshape(1, -1)) > 0)

    while True:
        actionCounter += 1
        observation, reward, done, info = self.env.step(action)
        totalReward += reward

        if done:
            break
        else:
            action = int(mlp.predict(observation.reshape(1, -1)) > 0)
            #print(action)

    return totalReward

def saveParams(self, netParams):
    """
    serializes and saves a list of network parameters using pickle
    :param netParams: a list of floats representing the network parameters (we
    """
    savedParams = []
    for param in netParams:
        savedParams.append(param)

    pickle.dump(savedParams, open("cart-pole-data.pickle", "wb"))

def replayWithSavedParams(self):
    """
    deserializes a saved list of network parameters and uses it to replay an e
    """
    savedParams = pickle.load(open("cart-pole-data.pickle", "rb"))
    self.replay(savedParams)

def replay(self, netParams):
    """
    renders the environment and uses the given network parameters to replay an
    :param netParams: a list of floats representing the network parameters (we
    """

```

```

mlp = self.initMlp(netParams)

self.env.render()

actionCounter = 0
totalReward = 0
observation = self.env.reset()
action = int(mlp.predict(observation.reshape(1, -1)) > 0)

while True:
    actionCounter += 1
    self.env.render()
    observation, reward, done, info = self.env.step(action)
    totalReward += reward

    print(actionCounter, ": -----")
    print("action = ", action)
    print("observation = ", observation)
    print("reward = ", reward)
    print("totalReward = ", totalReward)
    print("done = ", done)
    print()

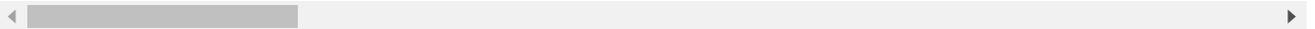
    if done:
        break
    else:
        time.sleep(0.03)
        action = int(mlp.predict(observation.reshape(1, -1)) > 0)

self.env.close()

def replayVideo(self):
    #self.env.close()
    show_video()

```

/usr/local/lib/python3.7/dist-packages/sklearn/utils/deprecation.py:144: FutureWarning



```

# Set the random seed
# for reproducibility of results:
RANDOM_SEED = 42
random.seed(RANDOM_SEED)

# Create the instance of the MountainCar class:
cartPole = CartPole(RANDOM_SEED)

NUM_OF_PARAMS = len(cartPole)
# boundaries for layer size parameters:

# weight and bias values are bound between -1 and 1:
BOUNDS_LOW, BOUNDS_HIGH = -1.0, 1.0 # boundaries for all dimensions

```

▼ GA Solution

```
from deap import base
from deap import creator
from deap import tools
from deap import algorithms
```

```
# Genetic Algorithm constants:
POPULATION_SIZE = 100
P_CROSSOVER = 0.9 # probability for crossover
P_MUTATION = 0.5 # probability for mutating an individual
MAX_GENERATIONS = 40
HALL_OF_FAME_SIZE = 3
CROWDING_FACTOR = 10.0 # crowding factor for crossover and mutation
```

▼ Genetic Tools

```
toolbox = base.Toolbox()

# define a single objective, maximizing fitness strategy:
creator.create("FitnessMax", base.Fitness, weights=(1.0,))

# create the Individual class based on list:
creator.create("Individual", list, fitness=creator.FitnessMax)

# helper function for creating random real numbers uniformly distributed within a
# it assumes that the range is the same for every dimension
def randomFloat(low, up):
    return [random.uniform(l, u) for l, u in zip([low] * NUM_OF_PARAMS, [up] * NUM_OF_PARAMS)]

# create an operator that randomly returns a float in the desired range:
toolbox.register("attrFloat", randomFloat, BOUNDS_LOW, BOUNDS_HIGH)

# create an operator that fills up an Individual instance:
toolbox.register("individualCreator",
                tools.initIterate,
                creator.Individual,
                toolbox.attrFloat)

# create an operator that generates a list of individuals:
toolbox.register("populationCreator",
                tools.initRepeat,
                list,
                toolbox.individualCreator)

# fitness calculation using the CrtPole class:
def score(individual):
    return cartPole.getScore(individual),
```

```

toolbox.register("evaluate", score)

# genetic operators:
toolbox.register("select", tools.selTournament, tournsize=2)

toolbox.register("mate",
                 tools.cxSimulatedBinaryBounded,
                 low=BOUNDS_LOW,
                 up=BOUNDS_HIGH,
                 eta=CROWDING_FACTOR)

toolbox.register("mutate",
                 tools.mutPolynomialBounded,
                 low=BOUNDS_LOW,
                 up=BOUNDS_HIGH,
                 eta=CROWDING_FACTOR,
                 indpb=1.0/NUM_OF_PARAMS)

```

```

/usr/local/lib/python3.7/dist-packages/deap/creator.py:141: RuntimeWarning: /
RuntimeWarning)
/usr/local/lib/python3.7/dist-packages/deap/creator.py:141: RuntimeWarning: /
RuntimeWarning)

```

▼ Elitism Tools

```

def eaSimpleWithElitism(population, toolbox, cxpb, mutpb, ngen, stats=None,
                        halloffame=None, verbose=__debug__):
    """This algorithm is similar to DEAP eaSimple() algorithm, with the modificati
    halloffame is used to implement an elitism mechanism. The individuals containe
    halloffame are directly injected into the next generation and are not subject
    genetic operators of selection, crossover and mutation.
    """
    logbook = tools.Logbook()
    logbook.header = ['gen', 'nevals'] + (stats.fields if stats else [])

    # Evaluate the individuals with an invalid fitness
    invalid_ind = [ind for ind in population if not ind.fitness.valid]
    fitnesses = toolbox.map(toolbox.evaluate, invalid_ind)
    for ind, fit in zip(invalid_ind, fitnesses):
        ind.fitness.values = fit

    if halloffame is None:
        raise ValueError("halloffame parameter must not be empty!")

    halloffame.update(population)
    hof_size = len(halloffame.items) if halloffame.items else 0

    record = stats.compile(population) if stats else {}
    logbook.record(gen=0, nevals=len(invalid_ind), **record)

```

```

if verbose:
    print(logbook.stream)

# Begin the generational process
for gen in range(1, ngen + 1):

    # Select the next generation individuals
    offspring = toolbox.select(population, len(population) - hof_size)

    # Vary the pool of individuals
    offspring = algorithms.varAnd(offspring, toolbox, cxpb, mutpb)

    # Evaluate the individuals with an invalid fitness
    invalid_ind = [ind for ind in offspring if not ind.fitness.valid]
    fitnesses = toolbox.map(toolbox.evaluate, invalid_ind)
    for ind, fit in zip(invalid_ind, fitnesses):
        ind.fitness.values = fit

    # add the best back to population:
    offspring.extend(halloffame.items)

    # Update the hall of fame with the generated individuals
    halloffame.update(offspring)

    # Replace the current population by the offspring
    population[:] = offspring

    # Append the current generation statistics to the logbook
    record = stats.compile(population) if stats else {}
    logbook.record(gen=gen, nevals=len(invalid_ind), **record)
    if verbose:
        print(logbook.stream)

return population, logbook

```

▼ GA Workflow

```

# create initial population (generation 0):
population = toolbox.populationCreator(n=POPULATION_SIZE)

# prepare the statistics object:
stats = tools.Statistics(lambda ind: ind.fitness.values)
stats.register("max", numpy.max)
stats.register("avg", numpy.mean)

# define the hall-of-fame object:
hof = tools.HallOfFame(HALL_OF_FAME_SIZE)

print('*****')
start = time.time()
# perform the Genetic Algorithm flow with hof feature added:
population, logbook = eaSimpleWithElitism(population,

```

```
toolbox,  
cxpb=P_CROSSOVER,  
mutpb=P_MUTATION,  
ngen=MAX_GENERATIONS,  
stats=stats,  
halloffame=hof,  
verbose=True)
```

```
end = time.time()  
time_NNA = end - start  
print("Time Elapsed = ", time_NNA)
```

```
*****
```

gen	nevals	max	avg
0	100	500	18.35
1	94	500	20.6
2	93	500	23.76
3	94	500	38.88
4	93	500	48.58
5	93	500	50.68
6	92	500	62.93
7	93	500	47.7
8	92	500	59.98
9	94	500	75.68
10	95	500	55.81
11	85	500	76.89
12	93	500	79.83
13	92	500	73.48
14	85	500	66.83
15	96	500	69.02
16	94	500	98.28
17	95	500	91.89
18	93	500	92.16
19	93	500	100.52
20	90	500	112.75
21	89	500	112.59
22	92	500	149.5
23	95	500	177.98
24	96	500	228.95
25	89	500	239.97
26	91	500	298.21
27	91	500	277.71
28	95	500	356.53
29	93	500	426.83
30	94	500	426.92
31	93	500	371.19
32	92	500	415.99
33	91	500	447.65
34	90	500	431.27
35	94	500	445.97
36	91	500	448.41
37	91	500	449.5
38	88	500	470.01
39	93	500	473.17
40	90	500	460.75

Time Elapsed = 102.10462594032288

```
# print best solution found:  
best = hof.items[0]
```



```
6 : -----  
action = 0  
observation = [0.02157332 0.03104637 0.00890634 0.07124991]  
reward = 1.0  
totalReward = 6.0  
done = False  
  
7 : -----  
action = 1  
observation = [ 0.02219425  0.22603951  0.01033134 -0.21860977]  
reward = 1.0  
totalReward = 7.0  
done = False  
  
8 : -----  
action = 0  
observation = [0.02671504 0.03077141 0.00595914 0.07731411]  
reward = 1.0  
totalReward = 8.0  
done = False  
  
9 : -----  
.
```

```
cartPole.replayVideo()
```

0:00 / 0:00



```
# Replay the best solution - VIDEO version  
#env.close()  
show_video()
```

0:00 / 0:00

```
# find average score of 100 episodes using the best solution found:
print("Running 100 episodes using the best solution...")
scores = []
for test in range(100):
    scores.append(cartPole.getScore(best))
    print("scores = ", scores)
    print("Avg. score = ", sum(scores) / len(scores))
```

Part 4. What about the solution dependence on GA

- ▼ conditions?
- ▼ ... with various **RANDOM_SEED** ...

Results for various RANDOM_SEEDs

- ▼ RANDOM_SEED = 42

```
# Set the random seed
# for reproducibility of results:
RANDOM_SEED = 42
random.seed(RANDOM_SEED)

# Create the instance of the MountainCartPole class:
```



```

print('*****')
start = time.time()
# perform the Genetic Algorithm flow with hof feature added:
population, logbook = eaSimpleWithElitism(population,
                                          toolbox,
                                          cxpb=P_CROSSOVER,
                                          mutpb=P_MUTATION,
                                          ngen=MAX_GENERATIONS,
                                          stats=stats,
                                          halloffame=hof,
                                          verbose=True)

end = time.time()
time_666 = end - start
print("Time Elapsed = ", time_666)

```

gen	nevals	max	avg
0	100	107	13.16
1	94	107	15.3
2	90	195	21.15
3	92	195	22.12
4	90	309	28.75
5	93	500	40.27
6	93	500	51.37
7	92	500	55.92
8	89	500	60.71
9	91	500	52.74
10	90	500	46.15
11	89	500	48.56
12	94	500	48.64
13	96	500	50.98
14	92	500	72.16
15	91	500	63.82
16	92	500	77.75
17	90	500	82.13
18	96	500	101.53
19	93	500	109.37
20	88	500	127.58
21	93	500	177.51
22	94	500	218.88
23	94	500	238.59
24	95	500	248.42
25	95	500	243.61
26	93	500	254.23
27	90	500	286.46
28	94	500	338.73
29	94	500	376.32
30	94	500	411.44
31	89	500	434.94
32	92	500	437.33
33	91	500	434.47
34	92	500	440.55
35	92	500	461.34
36	88	500	460.73
37	91	500	445.49
38	87	500	451.93
39	95	500	433.93


```
time_1042 = end - start
print("Time Elapsed = ", time_1042)
```

```
*****
```

gen	nevals	max	avg
0	100	98	14.05
1	93	369	20.27
2	90	369	24.69
3	95	500	37.39
4	90	500	34
5	94	500	36.67
6	90	500	47.13
7	91	500	58.5
8	95	500	85.11
9	92	500	81.75
10	94	500	83.59
11	92	500	98.02
12	94	500	120.35
13	89	500	136.98
14	87	500	136.72
15	91	500	134.35
16	93	500	128.28
17	95	500	140.19
18	93	500	149.64
19	90	500	161.43
20	95	500	204.21
21	93	500	208.19
22	91	500	234.49
23	90	500	283.42
24	93	500	336.07
25	92	500	339.78
26	89	500	353.78
27	85	500	360.43
28	88	500	376.7
29	95	500	374.63
30	88	500	394.9
31	94	500	357.41
32	90	500	370.26
33	92	500	378.91
34	89	500	362.35
35	83	500	402.14
36	89	500	372.56
37	93	500	393.47
38	96	500	431.22
39	93	500	402.09
40	85	500	411.7

Time Elapsed = 108.02887892723083

```
# print best solution found:
best = hof.items[0]
print("Best solution: ", best)
print("Best FitnessMin = %1.5f" % best.fitness.values[0])
#print("Best Fitness = ", best.fitness.values[0])

# extract statistics:
maxFitnessValues_GA_1042, meanFitnessValues_GA_1042 = logbook.select("max", "avg")
```



```
# perform the Genetic Algorithm flow with hof feature added:
population, logbook = eaSimpleWithElitism(population,
                                          toolbox,
                                          cxpb=P_CROSSOVER,
                                          mutpb=P_MUTATION,
                                          ngen=MAX_GENERATIONS,
                                          stats=stats,
                                          halloffame=hof,
                                          verbose=True)

end = time.time()
time_1042_CR0p1 = end - start
print("Time Elapsed = ", time_1042_CR0p1)
```

```
*****
```

gen	nevals	max	avg
0	100	98	14.05
1	93	369	20.27
2	90	369	24.69
3	95	500	37.39
4	90	500	34
5	94	500	36.67
6	90	500	47.13
7	91	500	58.5
8	95	500	85.11
9	92	500	81.75
10	94	500	83.59
11	92	500	98.02
12	94	500	120.35
13	89	500	136.98
14	87	500	136.72
15	91	500	134.35
16	93	500	128.28
17	95	500	140.19
18	93	500	149.64
19	90	500	161.43
20	95	500	204.21
21	93	500	208.19
22	91	500	234.49
23	90	500	283.42
24	93	500	336.07
25	92	500	339.78
26	89	500	353.78
27	85	500	360.43
28	88	500	376.7
29	95	500	374.63
30	88	500	394.9
31	94	500	357.41
32	90	500	370.26
33	92	500	378.91
34	89	500	362.35
35	83	500	402.14
36	89	500	372.56
37	93	500	393.47
38	96	500	431.22
39	93	500	402.09
40	85	500	411.7

```
Time Elapsed = 106.09052872657776
```

```
# print best solution found:
```



```
halloffame=hof,  
verbose=True)
```

```
end = time.time()  
time_1042_CR0p2 = end - start  
print("Time Elapsed = ", time_1042_CR0p2)
```

```
*****
```

gen	nevals	max	avg
0	100	61	12.76
1	84	139	18.63
2	87	139	20.28
3	86	139	20.38
4	88	262	27.71
5	87	500	36.11
6	89	500	46.12
7	76	500	50.12
8	83	500	69.22
9	83	500	102.08
10	90	500	112.98
11	90	500	135.09
12	92	500	151.42
13	79	500	196.46
14	89	500	206.88
15	85	500	254.88
16	87	500	307.1
17	92	500	343.59
18	87	500	368.36
19	89	500	361.83
20	90	500	386.21
21	84	500	401.56
22	87	500	450.47
23	88	500	428.24
24	89	500	446.1
25	86	500	427.84
26	90	500	465.95
27	87	500	464.36
28	89	500	468.08
29	83	500	461.77
30	88	500	457.34
31	83	500	487.66
32	83	500	485.6
33	83	500	457.34
34	80	500	478.28
35	88	500	470.93
36	87	500	464.49
37	89	500	479.88
38	87	500	462.48
39	90	500	492.46
40	85	500	472.49

```
Time Elapsed = 137.8567316532135
```

```
# print best solution found:  
best = hof.items[0]  
print("Best solution: ", best)  
print("Best FitnessMin = %1.5f" % best.fitness.values[0])  
#print("Best Fitness = ", best.fitness.values[0])
```

```
# extract statistics:
```

gen	nevals	max	avg
0	100	98	14.05
1	57	98	15.38
2	76	413	23.66
3	66	413	32.9
4	65	413	40.32
5	71	413	54.39
6	65	413	76.21
7	57	500	101.52
8	65	500	127.46
9	62	500	165.06
10	74	500	164.39
11	66	500	185.03
12	74	500	168.55
13	59	500	244.16
14	63	500	310.33
15	70	500	359.5
16	61	500	422.41
17	73	500	444.25
18	63	500	481.18
19	66	500	467.12
20	60	500	470.3
21	74	500	484.17
22	69	500	481.37
23	64	500	479.4
24	71	500	484.64
25	65	500	470.95
26	64	500	468.52
27	74	500	472.32
28	67	500	476.02
29	66	500	477.52
30	61	500	492.61
31	72	500	469.78
32	59	500	469.91
33	68	500	464.12
34	68	500	478.64
35	64	500	464.44
36	72	500	481.83
37	65	500	474.61
38	67	500	470.35
39	69	500	453.34
40	64	500	455.02

Time Elapsed = 116.45055270195007

```
# print best solution found:
best = hof.items[0]
print("Best solution: ", best)
print("Best FitnessMin = %1.5f" % best.fitness.values[0])
#print("Best Fitness = ", best.fitness.values[0])

# extract statistics:
maxFitnessValues_GA_1042_CR0p4, meanFitnessValues_GA_1042_CR0p4 = logbook.select("
print('History of maxFitnessValues_GA =',maxFitnessValues_GA_1042_CR0p4)
print('History of meanFitnessValues_GA =',meanFitnessValues_GA_1042_CR0p4)
```

Best solution: [0.6272811775924462, 0.4841432610995863, 0.6791695047075679,
Best FitnessMin = 500.00000


```
P_CROSSOVER = 0.9 # probability for crossover
```

```
# Set the random seed
# for reproducibility of results:
RANDOM_SEED = 1042
random.seed(RANDOM_SEED)

# Create the instance of the MountainCartPole class:
#car = MountainCar(RANDOM_SEED)
cartPole = CartPole(RANDOM_SEED)
```

```
# create initial population (generation 0):
population = toolbox.populationCreator(n=POPULATION_SIZE)
```

```
# prepare the statistics object:
stats = tools.Statistics(lambda ind: ind.fitness.values)
stats.register("max", numpy.max)
stats.register("avg", numpy.mean)
```

```
# define the hall-of-fame object:
hof = tools.HallOfFame(HALL_OF_FAME_SIZE)
```

```
print('*****')
```

```
start = time.time()
```

```
# perform the Genetic Algorithm flow with hof feature added:
```

```
population, logbook = eaSimpleWithElitism(population,
                                           toolbox,
                                           cxpb=P_CROSSOVER,
                                           mutpb=P_MUTATION,
                                           ngen=MAX_GENERATIONS,
                                           stats=stats,
                                           halloffame=hof,
                                           verbose=True)
```

```
end = time.time()
```

```
time_1042_CR0p9 = end - start
```

```
print("Time Elapsed = ", time_1042_CR0p9)
```

```
*****
```

gen	nevals	max	avg
0	100	98	14.05
1	93	369	20.27
2	90	369	24.69
3	95	500	37.39
4	90	500	34
5	94	500	36.67
6	90	500	47.13
7	91	500	58.5
8	95	500	85.11
9	92	500	81.75
10	94	500	83.59
11	92	500	98.02
12	94	500	120.35
13	89	500	136.98
14	87	500	136.72

- BUT ... more important ... different levels of gene exchange.

▼ ... with various GA parameters ... like Mutation Probability

(let's try it as a self-guided learning!)

It takes a small change in $P_MUTATION$ variable.

▼ Comparison Plots

▼ Random Seed Dependence

▼ Fitness Function

```
sns.set_style("whitegrid")

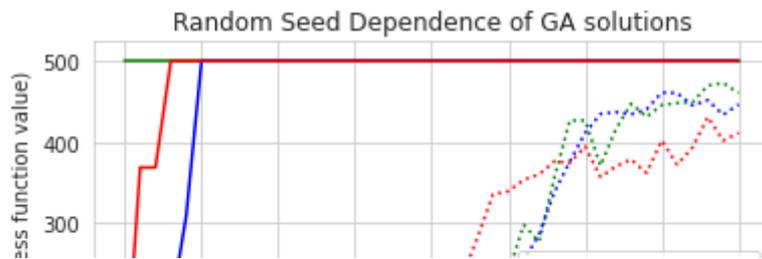
# Classic grid search solution
#plt.hlines(accuracy_classic_solution, 0, 5, linestyle = 'solid', label='Classic g

# NN architecture
plt.plot(maxFitnessValues_GA_42, color='green', label='42 (max)')
plt.plot(meanFitnessValues_GA_42, color='green', linestyle = 'dotted', label='42 (

# NN hyperparameter
plt.plot(maxFitnessValues_GA_666, color='blue', label='666 (max)')
plt.plot(meanFitnessValues_GA_666, color='blue', linestyle = 'dotted', label='666

# NN architecture + hyperparameter
plt.plot(maxFitnessValues_GA_1042, color='red', label='1042 (max)')
plt.plot(meanFitnessValues_GA_1042, color='red', linestyle = 'dotted', label='1042

plt.xlabel('Generation')
plt.ylabel('Max / Average (fitness function value)')
plt.title('Random Seed Dependence of GA solutions')
plt.legend(title='Random Number Seed')
plt.show()
```



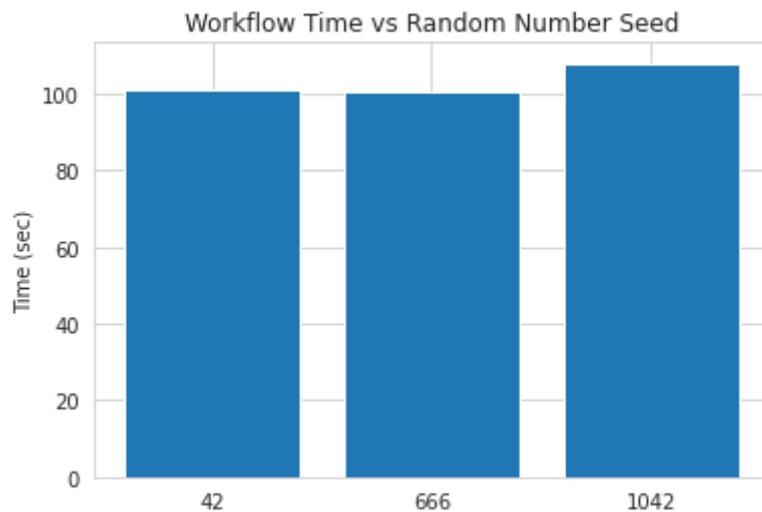
▼ Time

```

import matplotlib.pyplot as plt

x = ['42', '666', '1042']
y = [time_42, time_666, time_1042]
plt.bar(x, y)
plt.ylabel('Time (sec)')
plt.title('Workflow Time vs Random Number Seed')
plt.show()

```



▼ Crossover Probability Dependence

▼ Fitness Function

```

sns.set_style("whitegrid")

# Classic grid search solution
plt.hlines(accuracy_classic_solution, 0, 5, linestyle = 'solid', label='Classic g

# NN architecture
plt.plot(maxFitnessValues_GA_1042_CR0p1, color='green', label='0.1 (max)')
plt.plot(meanFitnessValues_GA_1042_CR0p1, color='green', linestyle = 'dotted', lab

```

```

# NN hyperparameter
plt.plot(maxFitnessValues_GA_1042_CR0p2, color='blue', label='0.2 (max)')
plt.plot(meanFitnessValues_GA_1042_CR0p2, color='blue', linestyle = 'dotted', label='0.2 (mean)')

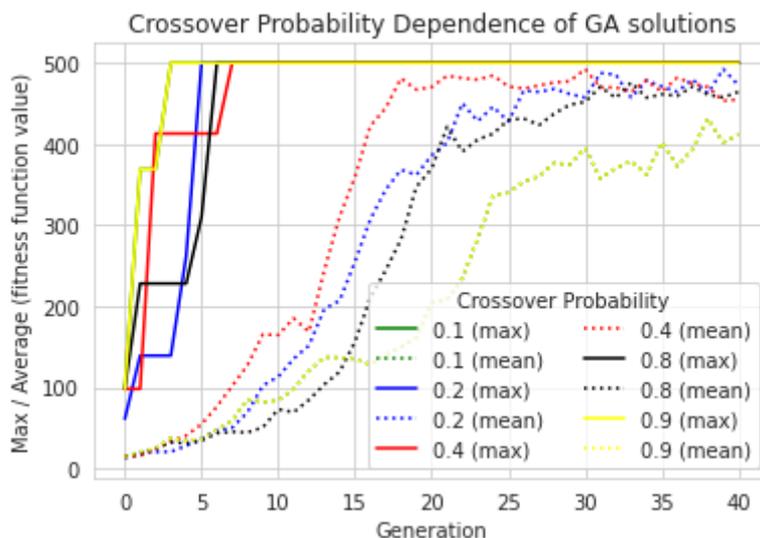
# NN architecture + hyperparameter
plt.plot(maxFitnessValues_GA_1042_CR0p4, color='red', label='0.4 (max)')
plt.plot(meanFitnessValues_GA_1042_CR0p4, color='red', linestyle = 'dotted', label='0.4 (mean)')

# NN architecture + hyperparameter
plt.plot(maxFitnessValues_GA_1042_CR0p8, color='black', label='0.8 (max)')
plt.plot(meanFitnessValues_GA_1042_CR0p8, color='black', linestyle = 'dotted', label='0.8 (mean)')

# NN architecture + hyperparameter
plt.plot(maxFitnessValues_GA_1042_CR0p9, color='yellow', label='0.9 (max)')
plt.plot(meanFitnessValues_GA_1042_CR0p9, color='yellow', linestyle = 'dotted', label='0.9 (mean)')

plt.xlabel('Generation')
plt.ylabel('Max / Average (fitness function value)')
plt.title('Crossover Probability Dependence of GA solutions')
plt.legend(title='Crossover Probability', ncol=2)
plt.show()

```



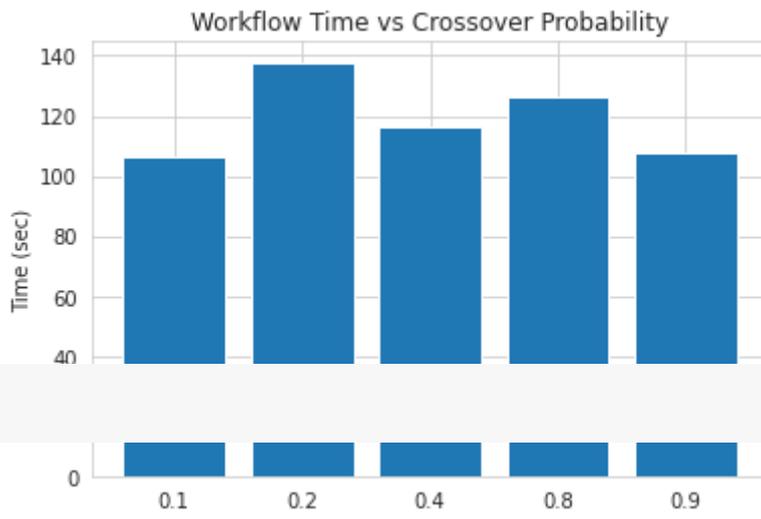
▼ Time

```

import matplotlib.pyplot as plt

x = ['0.1', '0.2', '0.4', '0.8', '0.9']
y = [time_1042_CR0p1, time_1042_CR0p2, time_1042_CR0p4, time_1042_CR0p8, time_1042_CR0p9]
plt.bar(x,y)
plt.ylabel('Time (sec)')
plt.title('Workflow Time vs Crossover Probability')
plt.show()

```



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▼ Lecture 08 - Neuroevolution - EvoJAX

based on (C) Google Brain, Yujin Tang, Yingtao Tian, David Ha works

Brief Content:

- EvoJAX installation (**every time after start of Colab VM!**),
- components needed for the EA workflow,
- *Reinforcement Learning (RL) problem*:
 - CartPole-v1
- policy gradients with parameter-based exploration,
- and others.

By the end of this lecture you will know:

- again, how to use the DEAP framework's built-in algorithms to produce concise code
- how to solve the *Reinforcement Learning* problem using a EA-based solutions for search of solutions,
- how to use policy gradients with parameter-based exploration,
- how to experiment with various settings of the GA and interpret the differences in the results.

▼ Pre-requisite

Before we start, we need to install EvoJAX from [EvoJAX-github](#) and import some libraries.

Note In our [paper](#), we ran the experiments on NVIDIA V100 GPU(s). Your results can be different from ours.

```
from IPython.display import clear_output, Image

!pip install evojax

clear_output()
```

```
import os
import numpy as np
import jax
import jax.numpy as jnp

from evojax.task.cartpole import CartPoleSwingUp
```

Saved successfully!



MLPolicy

```
from evojax.algo import MLP
from evojax import Trainer
from evojax.util import create_logger

# Let's create a directory to save logs and models.
log_dir = './log'
logger = create_logger(name='EvoJAX', log_dir=log_dir)
logger.info('Welcome to the tutorial on Neuroevolution algorithm creation!')

logger.info('Jax backend: {}'.format(jax.local_devices()))
!nvidia-smi --query-gpu=name --format=csv,noheader
```

```
EvoJAX: 2022-02-11 02:06:40,128 [INFO] Welcome to the tutorial on Neuroevolut
absl: 2022-02-11 02:06:40,137 [INFO] Unable to initialize backend 'tpu_driver
absl: 2022-02-11 02:06:40,322 [INFO] Unable to initialize backend 'tpu': INVA
EvoJAX: 2022-02-11 02:06:40,324 [INFO] Jax backend: [GpuDevice(id=0, process_
Tesla K80
```

▼ Introduction

EvoJAX has three major components: the *task*, the *policy network* and the *neuroevolution algorithm*. Once these components are implemented and instantiated, we can use a trainer to start the training process. The following code snippet provides an example of how we use EvoJAX.

```
seed = 42 # Wish me luck!

# We use the classic cart-pole swing up as our tasks, see
# https://github.com/google/evojax/tree/main/evojax/task for more example tasks.
# The test flag provides the opportunity for a user to
# 1. Return different signals as rewards. For example, in our MNIST example,
# we use negative cross-entropy loss as the reward in training tasks, and the
# classification accuracy as the reward in test tasks.
# 2. Perform reward shaping. It is common for RL practitioners to modify the
# rewards during training so that the agent learns more efficiently. But this
# modification should not be allowed in tests for fair evaluations.
hard = False
train_task = CartPoleSwingUp(harder=hard, test=False)
test_task = CartPoleSwingUp(harder=hard, test=True)

# We use a feedforward network as our policy.
# By default, MLPPolicy uses "tanh" as its activation function for the output.
policy = MLPPolicy(
    input_dim=train_task.obs_shape[0],
    hidden_dims=[64, 64],
    output_dim=train_task.act_shape[0],
    logger=logger,
)
```

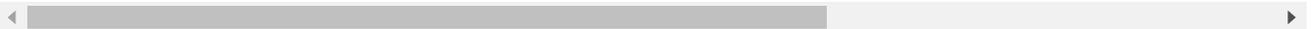
Saved successfully!



Algorithm.

```
# If you want to know more about the algorithm, please take a look at the paper:  
# https://people.idsia.ch/~juergen/nn2010.pdf  
solver = PGPE(  
    pop_size=64,  
    param_size=policy.num_params,  
    optimizer='adam',  
    center_learning_rate=0.05,  
    seed=seed,  
)  
  
# Now that we have all the three components instantiated, we can create a  
# trainer and start the training process.  
trainer = Trainer(  
    policy=policy,  
    solver=solver,  
    train_task=train_task,  
    test_task=test_task,  
    max_iter=600,  
    log_interval=100,  
    test_interval=200,  
    n_repeats=5,  
    n_evaluations=128,  
    seed=seed,  
    log_dir=log_dir,  
    logger=logger,  
)  
_ = trainer.run()
```

```
EvoJAX: 2022-02-11 02:06:43,518 [INFO] MLPPolicy.num_params = 4609  
EvoJAX: 2022-02-11 02:06:43,687 [INFO] Start to train for 600 iterations.  
EvoJAX: 2022-02-11 02:07:10,038 [INFO] Iter=100, size=64, max=712.8441, avg=6  
EvoJAX: 2022-02-11 02:07:29,392 [INFO] Iter=200, size=64, max=782.5107, avg=7  
EvoJAX: 2022-02-11 02:07:31,972 [INFO] [TEST] Iter=200, #tests=128, max=816.3  
EvoJAX: 2022-02-11 02:07:51,419 [INFO] Iter=300, size=64, max=920.6417, avg=8  
EvoJAX: 2022-02-11 02:08:10,756 [INFO] Iter=400, size=64, max=921.8397, avg=8  
EvoJAX: 2022-02-11 02:08:10,907 [INFO] [TEST] Iter=400, #tests=128, max=934.5  
EvoJAX: 2022-02-11 02:08:30,258 [INFO] Iter=500, size=64, max=932.7117, avg=8  
EvoJAX: 2022-02-11 02:08:49,644 [INFO] [TEST] Iter=600, #tests=128, max=955.2  
EvoJAX: 2022-02-11 02:08:49,652 [INFO] Training done, best_score=935.1467
```



```
# Let's visualize the learned policy.
```

```
def render(task, algo, policy):  
    """Render the learned policy."""  
  
    task_reset_fn = jax.jit(test_task.reset)  
    policy_reset_fn = jax.jit(policy.reset)  
    step_fn = jax.jit(test_task.step)  
    act_fn = jax.jit(policy.get_actions)  
  
    params = algo.best_params[None, :]  
    task_s = task_reset_fn(jax.random.PRNGKey(seed=seed)[None, :])  
    policy_s = policy_reset_fn(task_s)
```

Saved successfully! X

```
images = [CartPoleSwingUp.render(task_s, 0)]
done = False
step = 0
reward = 0
while not done:
    act, policy_s = act_fn(task_s, params, policy_s)
    task_s, r, d = step_fn(task_s, act)
    step += 1
    reward = reward + r
    done = bool(d[0])
    if step % 3 == 0:
        images.append(CartPoleSwingUp.render(task_s, 0))
print('reward={}'.format(reward))
return images
```

```
imgs = render(test_task, solver, policy)
gif_file = os.path.join(log_dir, 'cartpole.gif')
imgs[0].save(
    gif_file, save_all=True, append_images=imgs[1:], duration=40, loop=0)
Image(open(os.path.join(log_dir, 'cartpole.gif'), 'rb').read())
```

This tutorial walks you through the process of creating a new neuroevolution algorithm.

To contribute an algorithm implementation to EvoJAX, all you need to do is to implement the `NEAlgorithm` interface.

The interface is defined as the following and you can see the related Python file [here](#):

```
class NEAlgorithm(ABC):
    """Interface of all Neuro-evolution algorithms in EvoJAX."""

    pop_size: int

    @abstractmethod
    def ask(self) -> jnp.ndarray:
        """Ask the algorithm for a population of parameters.
        Returns
            A Jax array of shape (population_size, param_size).
        """
        raise NotImplementedError()

    @abstractmethod
    def tell(self, fitness: Union[np.ndarray, jnp.ndarray]) -> None:
        """Report the fitness of the population to the algorithm.
        Args:
            fitness - The fitness scores array.
        """
        raise NotImplementedError()

    @property
    def best_params(self) -> jnp.ndarray:
        raise NotImplementedError()

    @best_params.setter
    def best_params(self, params: Union[np.ndarray, jnp.ndarray]) -> None:
        raise NotImplementedError()
```

▼ Wrap an existing implementation

`NEAlgorithm` adopts the well-known “ask” and “tell” interfaces, where the former requests the algorithm to generate a population of parameters and the latter reports the parameters' fitness scores so that the algorithm can update its internal states. We think the conventional interface for the neuroevolution algorithms brings familiarity to the developers and thus reduces the

Saved successfully!



interface is also used by many existing algorithms, it is therefore possible for the practitioners to quickly plug in existing algorithms for sanity checks. In the first part of this tutorial, we will create an implementation that wraps [CMA-ES](#). Please take a look at this wonderful [tutorial](#) for more information about CMA-ES.

```
import cma
from evjax.algo.base import NEAlgorithm

class CMAWrapper(NEAlgorithm):
    """This is a wrapper of CMA-ES."""

    def __init__(self, param_size, pop_size, init_stdev=0.1, seed=0):

        self.pop_size = pop_size
        self.params = None
        self._best_params = None

        # We create CMA-ES in a simplest form.
        self.cma = cma.CMAEvolutionStrategy(
            x0=np.zeros(param_size),
            sigma0=init_stdev,
            inopts={
                'popsize': pop_size,
                'seed': seed if seed > 0 else 42,
                'randn': np.random.randn,
            },
        )

        # We jit-compile some utility functions.
        self.jnp_array = jax.jit(jnp.array)
        self.jnp_stack = jax.jit(jnp.stack)

    def ask(self):
        self.params = self.cma.ask()
        return self.jnp_stack(self.params)

    def tell(self, fitness):
        # CMA-ES minimizes, so we negate the fitness.
        self.cma.tell(self.params, -np.array(fitness))
        self._best_params = np.array(self.cma.result.xfavorite)

    @property
    def best_params(self):
        return self.jnp_array(self._best_params)

    @best_params.setter
    def best_params(self, params):
        self._best_params = np.array(params)
```

Saved successfully!



is extremely simple, we haven't used many options or functions provided by CMA-ES.

But let's plug in this implementation to our cart-pole earlier example and see how it works.

Alert Depending on your CPUs, running the following cell may take some time.

```
# Instead of PGPE, we use our CMAWrapper now.
solver = CMAWrapper(
    pop_size=64,
    param_size=policy.num_params,
    seed=seed,
)
trainer = Trainer(
    policy=policy,
    solver=solver,
    train_task=train_task,
    test_task=test_task,
    max_iter=600,
    log_interval=100,
    test_interval=200,
    n_repeats=5,
    n_evaluations=128,
    seed=seed,
    log_dir=log_dir,
    logger=logger,
)
_ = trainer.run()
```

```
EvoJAX: 2022-02-11 02:08:59,845 [INFO] Start to train for 600 iterations.
(32_w,64)-aCMA-ES (mu_w=17.6,w_l=11%) in dimension 4609 (seed=42, Fri Feb 11
EvoJAX: 2022-02-11 02:14:31,792 [INFO] Iter=100, size=64, max=643.9105, avg=4
EvoJAX: 2022-02-11 02:20:00,840 [INFO] Iter=200, size=64, max=692.3575, avg=5
EvoJAX: 2022-02-11 02:20:01,894 [INFO] [TEST] Iter=200, #tests=128, max=751.8
EvoJAX: 2022-02-11 02:25:27,575 [INFO] Iter=300, size=64, max=718.8022, avg=5
EvoJAX: 2022-02-11 02:31:06,983 [INFO] Iter=400, size=64, max=747.0325, avg=5
EvoJAX: 2022-02-11 02:31:07,139 [INFO] [TEST] Iter=400, #tests=128, max=706.6
EvoJAX: 2022-02-11 02:36:32,660 [INFO] Iter=500, size=64, max=725.8452, avg=6
EvoJAX: 2022-02-11 02:41:55,297 [INFO] [TEST] Iter=600, #tests=128, max=764.3
EvoJAX: 2022-02-11 02:41:55,305 [INFO] Training done, best_score=743.6188
```

The simple CMA-ES wrapper worked! However, we also notice that the training time increased significantly.

Although the task and the policy networks are accelerated by GPUs, the

`cma.CMAEvolutionStrategy` implementation we used in the code above relies on CPUs, and that is why we see the drop in training speed.

Nevertheless, being able to wrapper an existing algorithm and plug that in EvoJAX's training pipeline serves as sanity checks and helps debugging when you migrate algorithms to EvoJAX. Next, we will show you how to implement an algorithm in JAX from scratch.

We are going to implement a very simple version of PGPE, users interested in the algorithm can take a look at the [paper](#) and also check out some popular implementations ([example1](#), [example2](#)).

In a nutshell, PGPE samples the policy network parameters θ from Gaussian distributions. It maintains the means μ and the standard deviations σ of the Gaussian distributions, and then estimates the gradients of these parameters using the following formulae:

$$\Delta\mu_i = \alpha(r - b)(\theta_i - \mu_i), \Delta\sigma_i = \alpha(r - b) \frac{(\theta_i - \mu_i)^2 - \sigma_i^2}{\sigma_i}$$

where α is the learning rate and b is a baseline from the reward r .

The following code snippet provides a sample implementation of PGPE.

Note This simplified version ignores popular tricks such as converting the rewards to ranks, using modern optimizers for parameter update, etc.

```
from evojax.algo.base import NEAlgorithm

class SimplePGPE(NEAlgorithm):
    """A simplified version of PGPE."""

    def __init__(self, param_size, pop_size,
                 lr_mu=0.05, lr_sigma=0.1, init_stdev=0.1, seed=0):

        self.pop_size = pop_size
        assert pop_size % 2 == 0, "pop_size must be a multiple of 2."
        n_directs = pop_size // 2
        self.noises = jnp.zeros(param_size)
        self.params = jnp.zeros(param_size)
        self.mu = jnp.zeros(param_size)
        self.sigma = jnp.ones(param_size) * init_stdev
        self.rand_key = jax.random.PRNGKey(seed=seed)

    def ask_fn(key, mu, sigma):
        next_key, sample_key = jax.random.split(key=key, num=2)
        perturbations = jax.random.normal(
            key=sample_key, shape=(n_directs, param_size)) * sigma[None, :]
        params = jnp.vstack([perturbations, -perturbations]) + mu[None, :]
        return params, perturbations, next_key

    self.ask_fn = jax.jit(ask_fn)

    def tell_fn(rewards, mu, sigma, perturbations):
        fitness = jnp.array(rewards).reshape([2, n_directs])

        # To map to the formulae above:
        fitness - b) and (theta - mu) = perturbations
```

Saved successfully!

```
        s.mean(axis=0)
        b = jnp.mean(fitness)

        # Update the means.
        grad_mu = (
            (avg_fitness - b)[: , None] * perturbations
        ).mean(axis=0)
        new_mu = mu + lr_mu * grad_mu

        # Update the sigmas.
        # We constrain the change of sigma to prevent numerical errors.
        grad_sigma = (
            (avg_fitness - b)[: , None] *
            (perturbations ** 2 - (sigma ** 2)[None, :]) / sigma[None, :]
        ).mean(axis=0)
        new_sigma = jnp.clip(
            sigma + lr_sigma * grad_sigma, 0.8 * sigma, 1.2 * sigma)

        return new_mu, new_sigma

    self.tell_fn = jax.jit(tell_fn)

def ask(self):
    self.params, self.noises, self.rand_key = self.ask_fn(
        self.rand_key, self.mu, self.sigma)
    return self.params

def tell(self, fitness):
    self.mu, self.sigma = self.tell_fn(
        fitness, self.mu, self.sigma, self.noises)

@property
def best_params(self):
    return self.mu

@best_params.setter
def best_params(self, params):
    self.mu = jnp.array(params)
```

```
# Let's test our simple PGPE.
solver = SimplePGPE(
    pop_size=64,
    param_size=policy.num_params,
    seed=seed,
)
trainer = Trainer(
    policy=policy,
    solver=solver,
    train_task=train_task,
    test_task=test_task,
    max_iter=1000,
    log_interval=100,
    test_interval=200,
```

Saved successfully! ✕

```
    log_dir=log_dir,  
    logger=logger,  
)  
_ = trainer.run()
```

```
EvoJAX: 2022-02-11 02:41:55,585 [INFO] Start to train for 1000 iterations.  
EvoJAX: 2022-02-11 02:42:16,350 [INFO] Iter=100, size=64, max=413.9725, avg=1  
EvoJAX: 2022-02-11 02:42:35,561 [INFO] Iter=200, size=64, max=512.9973, avg=3  
EvoJAX: 2022-02-11 02:42:36,577 [INFO] [TEST] Iter=200, #tests=128, max=556.6  
EvoJAX: 2022-02-11 02:42:55,783 [INFO] Iter=300, size=64, max=523.7679, avg=4  
EvoJAX: 2022-02-11 02:43:14,984 [INFO] Iter=400, size=64, max=567.3138, avg=5  
EvoJAX: 2022-02-11 02:43:15,137 [INFO] [TEST] Iter=400, #tests=128, max=585.5  
EvoJAX: 2022-02-11 02:43:34,341 [INFO] Iter=500, size=64, max=586.1516, avg=5  
EvoJAX: 2022-02-11 02:43:53,552 [INFO] Iter=600, size=64, max=567.7144, avg=5  
EvoJAX: 2022-02-11 02:43:53,705 [INFO] [TEST] Iter=600, #tests=128, max=636.5  
EvoJAX: 2022-02-11 02:44:13,604 [INFO] Iter=700, size=64, max=592.1466, avg=4  
EvoJAX: 2022-02-11 02:44:32,814 [INFO] Iter=800, size=64, max=603.3476, avg=5  
EvoJAX: 2022-02-11 02:44:32,966 [INFO] [TEST] Iter=800, #tests=128, max=665.1  
EvoJAX: 2022-02-11 02:44:52,172 [INFO] Iter=900, size=64, max=632.6639, avg=5  
EvoJAX: 2022-02-11 02:45:11,339 [INFO] [TEST] Iter=1000, #tests=128, max=643.  
EvoJAX: 2022-02-11 02:45:11,346 [INFO] Training done, best_score=592.5771
```

Despite its simplicity, the training and test scores rise steadily. You can see our complete implementation of PGPE [here](#).

We hope this tutorial helps. Please let us (evojax-dev@google.com) know if you have any problems or suggestions, thanks!

Saved successfully! ✕

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Lecture 08 - Neuroevolution – EvoJAX – Additional Materials

Neuroevolution

<https://en.wikipedia.org/wiki/Neuroevolution>

EvoJAX

Paper:

<https://arxiv.org/abs/2202.05008>

<https://arxiv.org/pdf/2202.05008.pdf>

Codes + notebooks:

EvoJAX: Hardware-Accelerated Neuroevolution

<https://github.com/google/evojax>

Blogs:

EvoJAX: A Great Framework For Most Deep Tasks

<https://rezayazdanfar.medium.com/evojax-a-great-framework-for-most-deep-tasks-10adf685c152>

6 min read

Google Brain's EvoJAX Hardware-Accelerated Toolkit Significantly Improves Neuroevolutionary Computation

<https://medium.com/syncedreview/google-brains-evojax-hardware-accelerated-toolkit-significantly-improves-neuroevolutionary-7943f92adb>

4 min read

Presentation from co-author with reviewers:

EvoJAX: Hardware-Accelerated Neuroevolution

https://www.youtube.com/watch?v=vfz0XfZ_AbM

1:22:08

EvoJAX: Hardware-Accelerated Neuroevolution

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ABSTRACT

Evolutionary computation has been shown to be a highly effective method for training neural networks, particularly when employed at scale on CPU clusters. Recent work have also showcased their effectiveness on hardware accelerators, such as GPUs, but so far such demonstrations are tailored for very specific tasks, limiting applicability to other domains. We present EvoJAX, a scalable, general purpose, hardware-accelerated neuroevolution toolkit. Building on top of the JAX library, our toolkit enables neuroevolution algorithms to work with neural networks running in parallel across multiple TPU/GPUs. EvoJAX achieves very high performance by implementing the evolution algorithm, neural network and task all in NumPy, which is compiled just-in-time to run on accelerators. We provide extensible examples of EvoJAX for a wide range of tasks, including supervised learning, reinforcement learning and generative art. Since EvoJAX can find solutions to most of these tasks within minutes on a single accelerator, compared to hours or days when using CPUs, our toolkit can significantly shorten the iteration cycle of evolutionary computation experiments.

EvoJAX is available at <https://github.com/google/evojax>

ACM Reference Format:

Yujin Tang, Yingtao Tian, and David Ha. 2022. EvoJAX: Hardware-Accelerated Neuroevolution. In *2022 Genetic and Evolutionary Computation Conference (GECCO '22)*, July 9–13, 2022, Boston, USA. ACM, New York, NY, USA, 4 pages. <https://doi.org/10.1145/3520304.3528770>

1 INTRODUCTION

Hardware accelerators have played an important role in advancing the state-of-the-art for deep learning (DL), enabling rapid training of neural networks and shorter research iteration cycles for their development [12]. But much of this progress is restricted to systems that rely on gradient descent, a highly effective optimization method when we provide it with a well-defined objective function. But in areas such as artificial life, complex systems, computational biology, and even classical physics [18], much of the interesting behaviors we observe take place near the chaotic states, where a system is constantly transitioning between order and disorder. It can be argued that intelligent life and even civilization are all complex systems operating at the *edge of chaos* [3, 16]. If we wish to study these systems, we need efficient methods to simulate and find solutions in complex systems.

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<https://doi.org/10.1145/3520304.3528770>

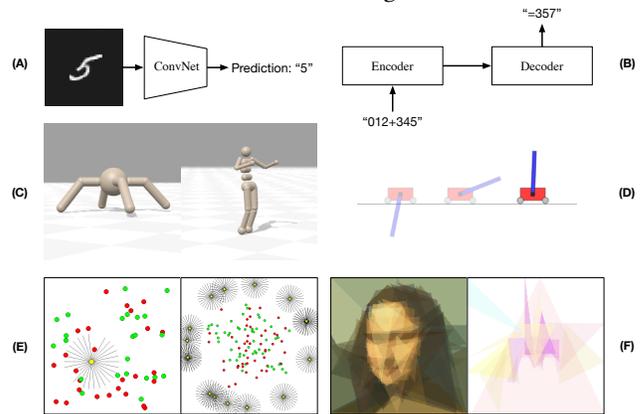


Figure 1: EvoJAX Examples. (A) MNIST classification. (B) Seq2Seq learning. (C) Robotic control. (D) Cart-pole swing up. (E) Left: WaterWorld wherein the agent (yellow) tries to get food (green) while avoiding poison (red). Right: A version of WaterWorld with multiple agents. (F) Abstract painting with only triangles. Left: Painting a concrete image. Right: Painting the concept “Walt Disney World”.

Neural networks are a promising approach for modeling complex systems [9, 19], and neuroevolution has made great progress in developing methods for evolving neural networks to solve a wide range of problems. Evolution-based methods have been shown to find state-of-the-art solutions for reinforcement learning (RL) [8, 13, 22, 25, 29]. A policy with non-differentiable operations can solve many more tasks than one that is fully differentiable [20, 27, 28, 33]. More importantly, the removal of the requirement of a differentiable policy also liberates the researchers’ mind, enabling higher levels of creativity for looking at problems and directions differently from the mainstream. In a sense, enabling researchers to use neural networks beyond gradient-based methods also enables the broader machine learning (ML) research community to explore in a way that is also less “grad student descent” [7]-based.

However, the progress of hardware-accelerated computational methods for evolution has not kept pace with ML, or even RL. Much of computational evolution is still conducted using CPU clusters, largely ignoring the recent breakthroughs in hardware accelerators such as GPUs/TPUs. Recent work started to demonstrate effectiveness of GPUs for neuroevolution [25], but so far such demonstrations are tailored for specific tasks [24], limiting their applicability to other domains. To enable greater access to hardware accelerators for neuroevolution researchers, we developed EvoJAX, a scalable, general purpose, neuroevolution toolkit. Building on the JAX library [1], our toolkit enables neuroevolution algorithms to work with neural networks running in parallel across multiple TPU/GPUs. EvoJAX achieves very high performance by implementing the evolution algorithm, neural network and task all in NumPy, which is compiled just-in-time to run on accelerators.

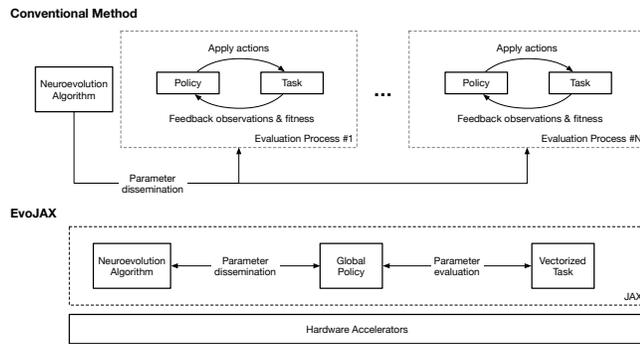


Figure 2: Architectural Overview of EvoJAX.

In this paper, we describe the design of EvoJAX and show how one can use and extend EvoJAX for neuroevolution research. We showcase several extensible examples of EvoJAX for a wide range of tasks, including supervised learning (image classification, seq-to-seq), RL (cart-pole swing-up [6], Brax locomotion [5], multi-agent water world), and generative art (image approximation with shapes, CLIP-guided abstract art [30]). We show that EvoJAX can find solutions to most of these tasks within minutes on GPU/TPUs, compared to hours or days when using CPUs. We believe our toolkit can significantly shorten the experimental iteration cycle for researchers working with evolutionary computation. We have also created several tutorials and notebooks as part of this open-source project to make adapting EvoJAX for novel use cases straightforward.

2 SYSTEM DESIGN

EvoJAX aims to improve the neuroevolution training efficiency by implementing the entire pipeline in modern ML frameworks that support hardware acceleration. We choose JAX[1] in our current implementation due to its wide variety of hardware support and its matured features of auto-vectorization, device-parallelism, just-in-time compilation, etc. As we will see in Section 4, as long as the component interfaces are properly implemented, EvoJAX also allows user extensions with other frameworks.

Figure 2 gives an overview of how EvoJAX works. There are three major components – the neuroevolution algorithm, the policy and the task. Although these components are common in conventional neuroevolution implementations, we highlight the key differences that make EvoJAX much more efficient:

Modern ML Optimizers Researchers and practitioners in the field of DL have been focusing on inventing optimization algorithms [21] and techniques [15, 32, 34] that are both fast and effective. Although these techniques were tailored for gradient-based optimizations, they can be directly applied to gradient estimation-based evolutionary algorithms [17, 23] too. By leveraging JAX-based libraries [1, 10, 11], EvoJAX not only achieves significant speed-up but also provides the users with the tools and the interfaces to develop their own implementations in a mature framework.

Global Policy In conventional neuroevolution implementations, it is a common practice to spawn multiple processes for parameters evaluation. To achieve hardware acceleration, the implementation adopts one of the DL frameworks and then each of the evaluation processes maintains a separate computational graph for the same policy. Unfortunately, most DL frameworks

are not designed for multi-process training scenarios and often cause difficulties. Moreover, when these processes are run on the same accelerator, maintaining identical copies of the computational graph is a waste of resource. Conforming to the “Single-Program, Multiple-Data” (SPMD) model [4], EvoJAX solves this by building a global policy and treat both the task observations and the policy parameters as data for the computational graph. This global policy design is easy to implement as it is consistent with DL frameworks, and in the experiments we observe high data-throughput.

Vectorized Tasks Same as the policies, conventional methods also create copies of the tasks in the spawned processes for independent parameters evaluations. To be compliant with EvoJAX’s global policy design, we propose to group these tasks in a vectorized form. In terms of implementation, this can be achieved by either creating the task in auto-vectorization supported frameworks or by creating a task observations collector on top of all the evaluation processes. EvoJAX adopts the first method.

Device Parallelism Thanks to the device-parallelism support in JAX, EvoJAX is capable of scaling its training procedure almost linearly to the available hardware accelerators. Utilizing EvoJAX’s training pipeline, this device parallelism is automatically managed and is transparent to the users. As we will see in Section 3, together with the previously mentioned features, EvoJAX significantly shortens the training time for novel and non-trivial tasks.

EvoJAX defines simple yet functionally complete interfaces for the three components, any implementations that are compliant with the interfaces can be seamlessly integrated (see Section 4).

Finally, in addition to the mentioned major components, EvoJAX also comes with a trainer and a simulation manager that help orchestrate and manage the training process. They contain detailed implementations of task roll-out seeds generation, efficient training loops, time profiling and logistics operations such as logging, testing and periodic model saving. Convenient as they are, we point out that EvoJAX is a flexible toolkit, where it is possible to use any component independently (e.g., using a custom training loop).

3 EVOJAX EXAMPLES

We provide a total of six examples (see Figure 1) to showcase the capacity, efficiency and the usage of EvoJAX online in the format of Python scripts and notebooks. The examples are designed to feature different aspects of EvoJAX and are in three categories: Supervised Learning Tasks, Control Tasks and Novel Tasks. As the experimental setups, “Robotic Control” was trained with TPUs, “Concrete and Abstract Painting” was trained with 8 NVIDIA V100 GPUs, and the rest were trained with 1 NVIDIA V100 GPU.

Supervised Learning Tasks They provide both the data and the ground-truth labels to train the policy. In EvoJAX, supervised learning tasks are modelled as single-step tasks, the examples in this category are thus isolated from other factors to prove the correctness and efficiency of our algorithms’ implementation.

- **MNIST Classification.** Here, we train a convolutional neural network (ConvNet) with 10K parameters with EvoJAX. Although MNIST is a solved problem in DL, it is non-trivial for neuroevolution in terms of achieving high test accuracy within a short time (e.g., in minutes). We show that EvoJAX can train the ConvNet to reach > 98% test accuracy within 5 minutes.

- **Seq2Seq Learning.** It has recently been shown that genetic algorithms (GA) can train large models [20]. Here, we show that EvoJAX is also capable of training a large network with hundreds of thousands of parameters. We adopt a seq-to-seq task where the policy is required to output a sequence after observing a query sequence. Concretely, the query is a sequence that represents the addition of two randomly generated integers (e.g., “012+345=”, we pad the numbers with leading 0’s so that they have equal lengths) and the result is a sequence representing the answer. Using an LSTM-based seq2seq [26] model, EvoJAX achieves > 99% test accuracy within tens of minutes.

While one would obviously use gradient-descent for such tasks in practice, the point is to show that neuroevolution can also solve them to some degree of accuracy within a short amount of time, which will be useful when these models are adapted within a more complicated task where gradient-based approaches may not work.

Control Tasks The purpose of including control tasks are twofold: 1) Unlike supervised learning tasks, control tasks in EvoJAX have undetermined number of steps, we thus use these examples to demonstrate the efficiency of our task roll-out loops. 2) We wish to show the speed-up benefit of implementing tasks in JAX and illustrate how to implement one from scratch.

- **Robotic Control.** Brax [5] is a differentiable physics engine implemented in JAX that simulates environments made up of rigid bodies, joints, and actuators. We show that it is easy to wrap Brax tasks in EvoJAX, and it takes EvoJAX tens of minutes to solve a robotic locomotion task on Colab TPUs.
- **Cart-Pole Swing Up.** Through this classic control task, we illustrate how a task is implemented from scratch in JAX and integrated into EvoJAX’s training pipeline. In our implementation, a user can command the initial states to be randomly sampled from a narrow (easy version) or a wide (hard version) range of possible settings, with the latter being much harder to solve. EvoJAX solves both versions within minutes.

Novel Tasks In this last category, we go beyond simple illustrations and show examples of novel tasks that are more practical and attractive to researchers in the genetic and evolutionary computation area, with the goal of helping them try out ideas in EvoJAX.

- **WaterWorld.** In this task [14], an agent tries to get as much food as possible while avoiding poisons. EvoJAX is able to train the agent in tens of minutes. Furthermore, we demonstrate that **multi-agents training** in EvoJAX is possible. Here, we spawn the entire population in the same task roll-out and directly measure each agent’s performance in a multi-agent world. This training scheme automatically generates task complexity beyond human design, and is beneficial for learning policies that can deal with interactions between agents and environmental uncertainties.
- **Concrete and Abstract Painting.** We reproduce the results from a computational creativity work [30]. The original work, whose implementation requires multiple CPUs and GPUs, could be accelerated on a single GPU efficiently using EvoJAX, which was not possible before. Moreover, with multiple GPUs/TPUs, EvoJAX can further speed up the mentioned work almost linearly. We also show that the modular design of EvoJAX allows its components be used independently – in this case it is possible to use only the

Table 1: Time Comparisons. We report the training time for both methods to achieve widely accepted test scores.

	Baseline	EvoJAX
MNIST	36 min	3 min
Cart-Pole Swing Up (Hard Version)	37 min	2 min
Locomotion (Ant) ¹	201 min	9 min

neuroevolution algorithms from EvoJAX while leveraging one’s own training loops and environment implantation.

We summarize EvoJAX’s benefit via these examples. First of all, EvoJAX brings significant training speed up. In Table 1 we show the time costs of training some popular tasks with both a conventional setup and EvoJAX.¹ On modest hardware accelerators, EvoJAX trains 10 ~ 20 times faster which leads to quicker idea iterations. Secondly, the capability of training multi-agents in a complex setting that is beyond human design supplies training environmental richness. And finally, EvoJAX puts the entire pipeline on unified hardware setups and that allows the practitioners to simplify complex hardware arrangements. As an example, for the substantial load of computation in our Abstract Painting example, the baseline needs to use both GPUs and CPUs, while EvoJAX only uses GPUs.

4 EXTENDING EVOJAX

A goal of EvoJAX is to provide researchers with an infrastructure that allows fast idea iterations. With EvoJAX it is possible to devise more effective neuroevolution algorithms, to explore novel policy architectures, and to experiment with new tasks. EvoJAX has carefully defined interfaces, as long as these interfaces are properly implemented, a user extended module can be integrated into the pipeline seamlessly.

```
import jax.numpy as jnp

class TaskState: obs: jnp.ndarray
class PolicyState: keys: jnp.ndarray
class NEAlgorithm:
    def ask(self) -> jnp.ndarray: pass
    def tell(self, fitness: jnp.ndarray) -> None: pass
class PolicyNetwork:
    def reset(self, states: TaskState) -> PolicyState: pass
    def get_actions(self, t_states: TaskState, params: jnp.ndarray,
                    p_states: PolicyState) \
        -> Tuple[jnp.ndarray, PolicyState]: pass
class VectorizedTask:
    def reset(self, key: jnp.ndarray) -> TaskState: pass
    def step(self, state: TaskState, action: jnp.ndarray) \
        -> Tuple[TaskState, jnp.ndarray, jnp.ndarray]: pass
```

Figure 3: Major Component Interfaces in EvoJAX.

Devising New Algorithms Users interested in inventing new neuroevolution algorithms should implement *NEAlgorithm* in Figure 3, which serves as the base class for all neuroevolution algorithms in EvoJAX. Being consistent with most conventional implementations, *NEAlgorithm* adopts the “ask” and “tell” interfaces, where the former requests the algorithm to generate a population of parameters and the latter reports the parameters evaluation results back to the algorithm for internal states update. Taking on the conventional interfaces for the neuroevolution algorithms not only brings familiarity to the developers and thus reducing the required

¹We use the code from [27] as the baseline. For the Locomotion task, we use PyBullet Ant in the baseline and Brax Ant in EvoJAX. The baseline is trained with 96 CPUs.

learning effort, but also allows the practitioners to quickly plug in existing algorithms for sanity checks by writing a simple wrapper.

Exploring Novel Policy Architectures *PolicyNetwork* in Figure 3 defines the policy interface, all policies in EvoJAX implement the *get_actions* method. The method puts no restrictions on what the policy network should be or how it should behave, giving full freedom for neural architecture search (NAS). Because EvoJAX conforms to the SPMD model, *get_actions* accepts three parameters: the vectorized task states, the population parameters and the policy’s internal states. At the beginning of a roll-out, each individual in the population sees identical observations, they will then diverge due to the population’s different behaviors. Because JAX requires pure functions, the policy’s states (e.g., random seeds, LSTM cell states, etc) are passed to *get_actions* via a Flax [10] dataclass *p_states*, which is initialized by *PolicyNetwork.reset*. The method returns the actions and the updated policy states. At runtime, calling *get_actions* is equivalent to passing a batch of data through the model.

Experimenting with More Tasks In Figure 3, *VectorizedTask* forms the base for all EvoJAX tasks. Similar to OpenAI’s Gym environments [2], the interface defines the *reset* and the *step* methods. Following the pure-function principle of JAX, one major difference between EvoJAX tasks and Gym environments is that EvoJAX’s tasks do not keep internal states. Instead, these states are encapsulated in a *TaskState* instance and carried over the roll-out steps. Similar to *PolicyState*, users can inherit *TaskState* and create one’s own task specific state to encapsulate arbitrary information besides the environment observations. In most tasks, the initial states are generated via a procedure of randomness. The *reset* method thus accepts *key*’s that act as seeds for the random process.

5 LIMITATIONS AND FUTURE WORKS

EvoJAX is based on the JAX framework, which is based on the familiar NumPy and is thus friendly to researchers accustomed to such tools. However, practitioners may have to take effort to understand the subtleties of JAX in order to maximize its performance. The time spent on learning the JAX framework may translate to a delayed adoption of EvoJAX, hence much of our focus so far has been on creating examples and tutorials that others can use as templates to build upon. Another limitation of EvoJAX is the compatibility with existing non-parallelizable tasks. Although it is possible to create an observation collector on top of the evaluation processes to mimic the behavior of *VectorizedTask*, the operation involves inter-process communications that becomes a bottleneck, preventing such tasks from the benefit of hardware-acceleration.

In the future, we plan to release more neuroevolution algorithm implementations to EvoJAX in addition to PGPE [23, 31] in the current release. We will add more policies and tasks to both demonstrate a wider variety of examples in order to encourage greater adoption of EvoJAX, with the goal of further enhancing the computation tools available in evolutionary computation research.

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