

Keen: Kotlin Genetic Algorithms Framework

*Thesis for the degrees of
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Abstract

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And after the second paragraph follows the third paragraph. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

After this fourth paragraph, we start a new paragraph sequence. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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Chapter 1

Theoretical Framework

The objective of this chapter is to provide the reader with the theoretical background necessary to understand the rest of the document.

1.1 Evolutionary Algorithms

In the field of computational intelligence, evolutionary algorithms (EA) [7] are a family of algorithms inspired by the process of natural selection. They are part of the larger field of evolutionary computation,¹ which is a subfield of metaheuristics.²

EAs are algorithms that perform optimization or learning tasks by evolving solutions to a given problem. These tasks may range from function optimization to machine learning or game AI development. EAs have three main characteristics:

- **Population-based:** These algorithms work with a population of solutions, allowing them to explore the search space in parallel.³
- **Fitness-oriented:** The solutions in the population are evaluated using a fitness function, which is a problem-dependent function that assigns a value to each solution based on its quality. The goal of the algorithm is to find the solution with the highest⁴ fitness.
- **Variation-driven:** The candidate solutions are modified using genetic operators, such as mutation, crossover, and selection, to create new solutions. These operators are usually based on the biological processes of mutation and recombination.

While these principles serve as the foundation for most EAs, it's important to note that some variants may prioritize some principles over others, or introduce new principles. This diversity allows EAs to be adapted to a wide range of problems and scenarios.

¹See definition A.5 on page 63

²See definition A.10 on page 64

³Not to be confused with parallelization, which is a technique used to speed up the execution of an algorithm by running it in parallel on multiple processors. “Parallel” in this context means that the algorithm is exploring multiple points in the search space (definition A.16 on page 64) simultaneously.

⁴In some cases, the goal is to minimize the fitness function, in which case the algorithm will aim to find the solution with the lowest fitness.

1.2 Genetic Algorithms

Genetic Algorithms (GA)⁵ [3, 4, 7, 8] are a type of EA where a *population* of *individuals*⁶ representing candidate solutions to an optimization problem evolves towards better solutions. Each individual is defined by its location in the search space, known as its *genotype*⁷, and its fitness value, computed by a *fitness function*. At a high level, GA is an automatic method for problem-solving, starting from a *high-level statement* of the desired outcome, without needing the user to predefine the solution's form or structure.

The classical GA operates as follows:

Algorithm 1 Genetic Algorithm

1:	<i>population</i> \leftarrow initializePopulation()	▷ Creates a random population of individuals
2:	evaluate(<i>population</i>)	▷ Calculates the fitness of each individual
3:	repeat	
4:	<i>parents</i> \leftarrow selectParents(<i>population</i>)	▷ Selects a subset of individuals as parents
5:	alter(<i>offspring</i>)	▷ Applies genetic operators to offspring, creating variations
6:	<i>population</i> \leftarrow selectSurvivors(<i>population</i> , <i>offspring</i>)	▷ Selects individuals for the next generation
7:	until termination condition is met	▷ Could be a pre-defined number of generations, a desired fitness level, etc.
8:	return fittest(<i>population</i>)	▷ Returns the most fit individual

Here, initializePopulation() generates a random population of individuals, while evaluate(*population*) assesses the fitness of each individual in the population.

The algorithm then continually performs the following steps until a termination condition is met:

1. selectParents(*population*) chooses a subset of individuals from the population to parent the next generation.
2. alter(*offspring*) modifies the offspring to introduce variability ("new genetic material") into the population.
3. evaluate(*offspring*) computes the fitness of each new individual.
4. selectSurvivors(*population*, *offspring*) selects the individuals that will survive to the next generation.

Finally, the algorithm returns the most fit individual in the population.

The exact implementation of each of these steps depends on the specific problem at hand. Factors such as the problem's complexity, the representation of individuals, or even the computational resources available, can greatly influence the choice of methods used for initialization, selection, alteration, and survivor selection.

1.2.1 Representation and Evaluation

One of the most important aspects of a GA is the representation of the individuals. The representation is the encoding of potential solutions to the problem into a form that can be manipulated by the algorithm. This defines the search space of the algorithm, and it is one of the main factors that determines the performance of the algorithm.

The most general representation of an individual is a matrix of genes⁸ called the *genotype*⁹ of the individual, where each column of the matrix is called a *chromosome*¹⁰.

Definition 1.1 (Cardinality of the search space). *The cardinality of the search space is the number of different individuals that can be represented by the encoding.*

Formally, given a vector of alphabets $(\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_n)$, and a representation \mathbf{G} with n chromosomes of length (m_1, m_2, \dots, m_n) where each chromosome is encoded using the alphabet \mathcal{A}_i , the cardinality of the search space S is defined as:

⁵Also known as Simple Genetic Algorithms (SGA) [7], or Traditional Genetic Algorithms (TGA) [8].

⁶See definition A.9 on page 64.

⁷See definition A.8 on page 64.

⁸See definition A.6 on page 63.

⁹See [25].

¹⁰See definition A.3 on page 63.

$$|S| = \prod_{i=1}^n |\mathcal{A}_i|^{m_i} \quad (1.1)$$

Note that this definition assumes that the chromosomes are independent, which may not be the same for all evolutionary algorithms.

Remark. In the original publication of the GA [3], the genotype was known as the environment (E) and the search space was defined as a class \mathcal{E} of all possible environments.

To illustrate this concept, consider the following problem: given a binary string of length n , find the string that has the most ones.¹¹ In this case, we can use a single column matrix \mathbf{G} to represent the individual, where each gene $g_i \in \mathcal{A}$ represents the i -th bit of the string, where $\mathcal{A} = \{0, 1\}$ is the alphabet containing the two possible values of a bit.

Then,

$$|S| = \prod_{i=1}^1 |\mathcal{A}|^n = 2^n$$

Knowing this, we can conclude that an exhaustive search of the search space would require evaluating 2^n individuals, and thus the algorithm would have a time complexity of $\mathcal{O}(2^n)$.

This is a very simple example, but we can see how a naive search algorithm would have a very high time complexity. This would be of the utmost importance in a real world problem, where the search space would be much larger.

With a representation defined, we can now define an evaluation method for the individuals, which is done using a *fitness function*.

Definition 1.2 (Fitness function). A fitness function is a function $\phi : S \rightarrow \mathbb{R}^n$, where S is the search space and n is the number of objectives of the optimization problem, that takes a genotype as input and returns a vector of real numbers representing how close the individual is to the global optimum of each objective.

The fitness function is usually defined by the user of the algorithm, and it is problem dependent.

Definition 1.3 (Batch fitness function). A batch fitness function $\Phi : \mathbb{P} \rightarrow \mathbb{R}^{m \times n}$ is a function that maps a population to a matrix of real numbers, where m is the number of individuals in the population and n is the number of objectives of the optimization problem.

The one max problem is a maximization problem with a single objective, so the fitness function would be defined as follows:

$$\phi_{\mathbf{G}} = \sum_{i=1}^n g_i \quad (1.2)$$

In the *Representation and Evaluation* section, we examined the key aspect of a genetic algorithm (GA) — the representation of individuals, their encoding and search space. The performance of a GA significantly depends on how solutions are encoded to form individuals. We use the concepts of genotype, chromosome, and gene to describe the individual's representation. The cardinality of the search space, defined as the total number of different individuals that can be represented, is crucial as it impacts the algorithm's complexity. We introduced the “One Max” problem as an example, using a binary string representation. The fitness function, which evaluates individuals' fitness, plays a critical role in navigating the search for optimal solutions. In the “One Max” problem, the fitness function sums the binary string elements, representing the number of ones in the string.

¹¹This is known as the *One Max* problem [22] or *Ones Counting* problem [25].

1.2.2 Initialization

GA operates on a group of individuals called a *population*. The algorithm designer must define the size of the population, and how to initialize it. The initialization process is usually random, but it can also be guided by some prior knowledge about the problem being solved. For example, if the problem is to find a solution to a maze, the population could be initialized with individuals that represent paths from the start to the end of the maze. This would speed up the search process, since the algorithm would not have to start from scratch.

Once the population is initialized, the algorithm performs an evaluation of each individual in the population, and assigns a *fitness value* to each individual. This is done in an effort to learn something about the problem, and to guide the search process towards better solutions.

In the case of the *One Max* problem, there is no prior knowledge about the problem, so the population via a blind search of the search space (in other words, the initialization is random). This is done by generating a random binary string of length n for each individual in the population.

Let's assume that we have a population of size 4, and that the length of the binary strings is $n = 4$.

The initialization process could generate the following individuals:¹²

Generation 0		
Individual	Binary string	Fitness
I_1	1100	2
I_2	0001	1
I_3	0000	0
I_4	0100	1

Table 1.1: Population of individuals in generation 0

	Fitness	Individual
Best	2	I_1
Worst	0	I_3
Average	1	
Standard deviation	0.817	

Table 1.2: Fitness of the individuals in generation 0

In the initialization phase of a genetic algorithm, we define and setup the population of individuals to be used in the search process. This population can be randomly generated or informed by some prior knowledge about the problem at hand. Each individual is evaluated to determine its fitness, guiding the algorithm's search for optimal solutions. In our "One Max" problem example, we initialized a population of four individuals with binary strings of length $n = 4$ and evaluated their fitness. This setup marks the beginning of the evolutionary process, setting the stage for the subsequent stages of selection (section 1.2.3), crossover (section 1.2.4 on page 10), and mutation (section 1.2.4 on page 12).

1.2.3 Selection

Once initialization is complete, the Genetic Algorithm (GA) enters its main loop, where the core evolutionary processes take place. In the GA, a mechanism that simulates natural selection operates, providing fitter individuals with higher chances of survival and breeding opportunities.

Suppose that we have a population P of N individuals, each with a fitness value f_i , where $i \in \{1, \dots, N\}$. Let σ be the survival rate, a parameter controlling the degree of elitism. This is the proportion of individuals that

¹²Since the nature of genetic algorithms is stochastic, the initialization process could generate different individuals each time the algorithm is run. For this example, we selected a specific set of individuals in a way that makes it easier to get a grasp of the algorithm.

will survive (unmodified) to the next generation. The GA will then select $\lfloor \sigma N \rfloor$ individuals to survive to the next generation, and $\lceil (1 - \sigma)N \rceil$ individuals to be replaced by the offspring.¹³

Definition 1.4 (Selection operator). *An operator used to select individuals from a population.*

Formally, a selection operator is a function

$$\Sigma : \mathbb{P} \times \mathbb{N} \times \cdots \rightarrow \mathbb{P}; (P, n, \dots) \mapsto \Sigma(P, n, \dots)$$

where:

- \mathbb{P} is the set of populations;
- \mathbb{N} is the set of positive natural numbers;
- P is a population;
- n is the number of individuals to select from P ;
- $\Sigma(P, n)$ is the population of n individuals selected from P .

The selection operator is typically implemented as a *stochastic* operator, introducing some randomness into the selection process.

As an illustration, consider a *roulette wheel* selection operator¹⁴ applied to a population of four individuals with a survival rate of 0.25. In this selection scheme, each individual is assigned a selection probability proportional to its fitness value (assuming higher fitness is better). The selection probability of an individual i is calculated as follows:

$$p_i = \frac{f_i}{\sum_{j=1}^N f_j} \quad (1.3)$$

In our example, the selection probabilities are detailed in table 1.3.

Individual	Fitness	Selection Probability
I_1	2	0.5
I_2	1	0.25
I_3	0	0.0
I_4	1	0.25

Table 1.3: Selection probabilities for the individuals in the example population.

The selection operator then selects individuals at random, each with a probability equal to their selection probability. Suppose I_2 is selected to survive to the next generation, then I_1 , I_3 , and I_4 will be replaced by the offspring.

This section has introduced the concept of selection in GAs, which will be explored further in section 4.3.1 on page 32. Next, we will delve into variation operators responsible for generating the offspring that will replace the individuals not selected to survive to the next generation.

1.2.4 Variation

Variation is the process of creating new individuals from existing ones in the pursuit of exploring the solution space. This is crucial in a Genetic Algorithm (GA) to avoid premature convergence to sub-optimal solutions. In a GA, variation is achieved by applying *variation operators* to the individuals in the population. The most common variation operators are *crossover* and *mutation*, which will be explored in this section.

¹³The sole purpose of employing both *floor* and *ceiling* functions is to guarantee that the total number of individuals chosen for survival and replacement equals N , which makes these functions interchangeable in this context.

¹⁴See section 4.3.1 on page 33 for a detailed description of the roulette wheel selection operator.

Definition 1.5 (Variation operator). *A variation operator is used to create new individuals from existing ones. Formally, it is a variadic function represented as*

$$\varphi : \mathbb{P} \times \mathbb{R} \times \cdots \rightarrow \mathbb{P}; (P, \rho, \dots) \mapsto \varphi(P, \rho, \dots)$$

where:

- \mathbb{P} is the set of all possible populations,
- \mathbb{R} is the set of real numbers,
- P is the population to be varied,
- ρ is the probability of applying the operator to an individual in the population.

The additional arguments depend on the specific implementation of the variation operator. The role of these arguments will be clarified in section 4.3 on page 32.

Crossover

The variation operator in genetic algorithms often involves a procedure known as *crossover*, which emulates the process of genetic recombination observed in nature.¹⁵ This process involves the exchange of genetic material between two individuals to create a new generation.

Definition 1.6 (Crossover operator). *A crossover operator is a variation operator that is used to create new individuals from existing ones by performing a recombination of their genetic material.*

Formally, it is a variadic function represented as

$$\Xi : \mathbb{P} \times \mathbb{R} \times \cdots \rightarrow \mathbb{P}; (P, \rho, \dots) \mapsto \Xi(P, \rho, \dots)$$

where:

- \mathbb{P} is the set of all possible populations,
- \mathbb{R} is the set of real numbers,
- P is the population to be varied,
- $\rho \in [0, 1]$ is the probability of applying the operator to an individual in the population.

For the problem under consideration, we utilize a simplified form of the *single-point crossover*¹⁶ operator. This operator selects the first half of the genes from two parent individuals and generates two new offspring by interchanging these selected genes.

For instance, consider two parent individuals selected via the *roulette wheel* selector described earlier: $I_1 = 1100$ and $I_2 = 0001$. The single-point crossover operator selects the first half of the genes from each parent, i.e., 11 from I_1 and 00 from I_2 , and produces a pair of new chromosomes with the first half, and produces two new offspring by exchanging these selected parts: $O_1 = 1101$ and $O_2 = 0000$ (as illustrated in fig. 1.1 on the next page).

Following another iteration of the single-point crossover operator, we can generate a result as shown in table 1.4 on the facing page, leading to a new population $\mathbf{O} = \{(0000, 0), (1101, 3), (0101, 2)\}$.

If we now use these offspring as-is to create the next generation, we would obtain the population shown in table 1.5 on the next page:

¹⁵This is referred to as *crossing-over* in [3].

¹⁶See section 4.3.3 on page 40.

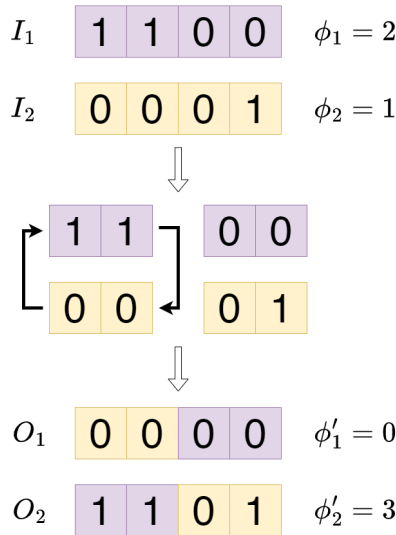


Figure 1.1: Single-point crossover

Generation 0 \rightarrow Generation 1			
I	Φ_I	O	Φ_O
$\begin{bmatrix} 1100 \\ 0001 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0000 \\ 1101 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 3 \end{bmatrix}$
$\begin{bmatrix} 0001 \\ 0100 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0101 \\ \cdot \end{bmatrix}$	$\begin{bmatrix} 2 \\ \cdot \end{bmatrix}$

Table 1.4: Illustration of the single-point crossover operation. In this procedure, two parent individuals are selected and a cut point is chosen. Each offspring is then formed by combining the genes from the parents: one gets the genes from the first part of the first parent and the second part of the second parent, while the other gets the genes from the first part of the second parent and the second part of the first parent. Here, \cdot represents a “discarded” value (since according to the survival rate, only three offspring need to be produced).

Generation 1		
Individual	Binary String	Fitness
I_2	0001	1
O_1	0000	0
O_2	1101	3
O_3	0101	2

Table 1.5: Population after applying the single-point crossover operator. Note that I_2 is the survivor of the previous generation picked in section 1.2.3 on page 8.

	Fitness	Individual
Best	3	O_2
Worst	0	O_1
Average	1.25	
Standard deviation	1.291	

Table 1.6: Fitness of the population after applying the single-point crossover operator. “Best” refers to the individual with the highest fitness, and “Worst” refers to the individual with the lowest fitness

As observed from table 1.6 on the preceding page, the average fitness of the population has increased from 1 to 1.25, and the fitness of the best individual has improved from 2 to 3. This improvement showcases how the crossover operator helps guide the search towards superior solutions.

While the crossover operation has indeed enhanced the average fitness of the population, to further augment genetic diversity within the population and prevent premature convergence to suboptimal solutions (local optima), the introduction of a *mutation* operator is often beneficial. This operation will be discussed in the next section.

Mutation

One limitation of the crossover operator is its reliance on existing genetic material in the population.

This constraint can lead to premature convergence, particularly for problems with numerous local optima such as the *Rastrigin function* optimization.¹⁷

To counteract this and introduce *diversity* in the population, we use the *mutation* operator.

This operator alters the genetic material of an individual within the population according to a specific probability.

Definition 1.7 (Mutation operator). *A mutation operator is a function that alters the genetic material of individuals within a population based on a certain probability, thereby producing a new population.*

Formally, a mutation operator is a variadic function

$$M : \mathbb{P} \times \mathbb{R} \times \cdots \rightarrow \mathbb{P}; (P, \mu, \dots) \mapsto M(P, \mu, \dots)$$

where:

- \mathbb{P} represents the set of all possible populations;
- \mathbb{R} represents the set of real numbers;
- P is the current population;
- μ represents the mutation rate—the probability that an individual in the population will undergo mutation.

The other arguments are specific to the mutation operator being used.

For instance, in the “One Max” problem, we can use a *bit-flip* mutation.¹⁸ This operator scans each gene in an individual and substitutes it with its complement according to a predetermined probability.

Suppose we set the *mutation rate* $\mu = 1$, and apply the mutation operator to the population resulting from the crossover operation described in section 1.2.4 on page 10. As shown in ?? on page ??, the resulting population would be $\mathbf{O} = \{(1111, 4), (0010, 1), (1010, 3)\}$.

Generation 0 → Generation 1			
I	$\Phi_{\mathbf{I}}$	O	$\Phi_{\mathbf{O}}$
$\begin{bmatrix} 0000 \\ 1101 \\ 0101 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 3 \\ 2 \end{bmatrix}$	$\begin{bmatrix} 1111 \\ 0010 \\ 1010 \end{bmatrix}$	$\begin{bmatrix} 4 \\ 1 \\ 2 \end{bmatrix}$

Table 1.7: Illustration of the *bit-flip* mutation operator applied to the population resulting from the crossover operation in section 1.2.4 on page 10.

If the mutated offspring were used to generate the next population, as shown in table 1.8 on the next page, you can observe the increased diversity.

¹⁷See appendix B.1 on page 65.

¹⁸See section 4.3.2 on page 34.

Generation 1		
Individual	Binary String	Fitness
I_2	0001	1
O'_1	1111	4
O'_2	0010	1
O'_3	1010	2

Table 1.8: Population after applying the *bit-flip* mutation operator to the population resulting from the crossover operation in section 1.2.4 on page 10.

	Fitness	Individual
Best	4	O'_1
Worst	0	(I_2, O'_2)
Average	2	
Standard deviation	1.414	

Table 1.9: Fitness of the population after applying the *bit-flip* mutation operator to the population resulting from the crossover operation in section 1.2.4 on page 10.

Clearly, the mutation operator has introduced diversity into the population. In the original population, no individual had a 1¹⁹ in the third position. Therefore, the crossover operator could never produce an individual with a 1 in that position. But the mutation operator has introduced three individuals with a 1 in the third position.²⁰

In conclusion, the mutation operator plays a crucial role in genetic algorithms by introducing diversity into the population and preventing premature convergence to local optima. It facilitates a more thorough exploration of the search space, allowing new and potentially beneficial traits to emerge. However, it's essential to note that a high mutation rate might disrupt advantageous traits, while a low rate might not sufficiently prevent premature convergence. The specific mutation operator and the mutation rate used are crucial factors in shaping the genetic algorithm's search process.

With this, the variation process is complete, and we can proceed to the next step of the genetic algorithm.

1.2.5 Termination

After each generation – when a new population is fully created – the genetic algorithm verifies if the termination criteria have been met. If so, the algorithm terminates and returns the best individual identified. Otherwise, the process continues to the next generation.

Consider a scenario where the termination criterion is defined as the discovery of an individual possessing the maximum number of ones, represented as 1111. This would correspond to a condition where $\phi_G = 4$.

Recall that we found the individual 1111 after applying the variation operators to the population. As a result, the termination criterion is met and the genetic algorithm concludes its process.

It's worth noting that not all search space has been explored, as demonstrated in table 1.10 on the following page. The algorithm's fitness-oriented search strategy means it performs a guided, rather than exhaustive, search. However, the increasing fitness of the population's individuals across generations indicates convergence towards an optimal solution.

For small search spaces like in our example, the distinction between this algorithm and a purely random search may seem minimal. But for larger search spaces, as explored later in this thesis, the difference becomes highly significant.

¹⁹ $P = \{1100, 0001, 0000, 0100\}$

²⁰ $P' = \{0001, 1111, 0010, 1010\}$

	00	01	10	11
00				
01				
10				
11				

Table 1.10: Candidates from the search space that were explored by the genetic algorithm. Cells that are coloured in dark gray represent candidates that were explored by the genetic algorithm. Each individual is defined by the row and column that it occupies in the search space, where the row represents the first 2 bits of the individual and the column represents the last 2 bits of the individual; e.g. the individual 0001 is located in the first row and second column of the table.

It's important to underline that genetic algorithms, being stochastic in nature, do not guarantee discovery of the optimal solution. Their effectiveness depends on various factors such as the fitness function, the representation scheme, the variation operators, and the selection strategy. These components and their impact on performance across different problems will be thoroughly examined in this thesis.

In summary, the termination phase of the genetic algorithm represents a crucial step in determining the overall process outcome. By utilizing a targeted termination criterion – such as the discovery of an individual with the highest possible fitness score – the algorithm effectively navigates the search space. While not exhaustive in its exploration, the algorithm uses a fitness-oriented strategy to guide its trajectory towards an optimal solution. It's essential to recognize the inherent limitations of genetic algorithms due to their stochastic nature. Despite these, their potential to outperform random searches, especially in large search spaces, is considerable. However, success relies heavily on choosing appropriate parameters and procedures, a topic to be explored in-depth in subsequent sections of this thesis.

1.3 Genetic Programming

Genetic Programming (GP) [4, 5, 6, 7] is a specialized branch of Evolutionary Algorithms (EA) which focuses on evolving a population of computer programs to solve a given problem. One can perceive GP as an extension of Genetic Algorithms (GA), the key distinction being the problem each approach solves: GA optimizes parameters to enhance a given function, whilst GP induces programs.²¹

Despite these differences, GP and GA share various characteristics such as the utilization of a population of individuals, the employment of a fitness function to evaluate the individuals, and the application of genetic operators to generate new individuals. Notwithstanding, GP adopts a unique representation for the individuals and unique genetic operators.

Remark. *Although GP operates a fitness-guided search in the space of computer programs, it can be deemed as an optimization problem, akin to GA.*

Each individual in a GP population embodies a computer program composed of a set of primitives, referred to as *functions* and *terminals*. An intuitive way to comprehend primitives is by visualizing a composite pattern where the functions equate to composite objects and the terminals to leaf objects (refer to fig. 1.2 on the facing page). An *abstract syntax tree* (AST) is an example of a program representation where the functions correspond to the internal nodes, and the terminals to the leaf nodes.

The general GP algorithm is represented in algorithm 2 on the next page, which closely resembles the GA algorithm with the main disparity being the nature of the *genetic operators* in GP.

In the ensuing sections, we will delve into the fundamental components of a GP algorithm and elucidate them through an example.

²¹For a formal definition of program induction, refer to definition A.15 on page 64.



Figure 1.2: The composite structure of a GP individual, illustrating the relationship between functions and terminals

Algorithm 2 Outline of the Genetic Programming algorithm, showcasing its structural similarities with the Genetic Algorithm

- 1: Generate an initial population by recursively building random programs.
 - 2: Execute each program and assign a fitness value to it.
 - 3: **repeat**
 - 4: $parents \leftarrow \text{selectParents}(population)$ ▷ Parent selection for reproduction
 - 5: $alter(offspring)$ ▷ Apply genetic operators to offspring
 - 6: $population \leftarrow \text{selectSurvivors}(population, offspring)$ ▷ Survivor selection to form next generation
 - 7: **until** termination condition is met ▷ Termination can be a fixed number of generations, or a satisfactory fitness level, etc.
 - 8: **return** $\text{fittest}(population)$ ▷ Return the best solution found
-

1.3.1 Representation and Evaluation

As with GAs, the representation of the individuals is one of the most important aspects of a GP. The representation is the encoding of potential solutions to the problem into a form that can be manipulated, executed and evaluated by the algorithm.

Various methods exist for program representation, such as utilizing an abstract syntax tree, a linear sequence of instructions, a stack of instructions, or a combination of these approaches. However, the most common representation is the *tree representation*, where the program is represented as a composite data structure like the one shown in the introduction to this section.

Let's consider the following problem: given a set of n points in the plane, find the curve that best fits the points. This is a very common problem in statistics, and it is known as the *symbolic regression* problem [4]. In this instance, we aim to conduct a symbolic regression of the function

$$f(x) = 5x^3 - 2x^2 + \sin(x) - 7; x \in [-1, 1] \quad (1.4)$$

using this function, we can generate a set of random points in the curve as shown in fig. 1.3 on the following page and table 1.11 on the next page.

The next step would be to define the primitive set, that is the set of functions and terminals that will be used to build the programs. In this case, we will use the following set of functions and terminals:

- Functions:
 - +: Addition
 - -: Subtraction
 - ×: Multiplication
 - /: Division
 - sin: Sine
 - cos: Cosine

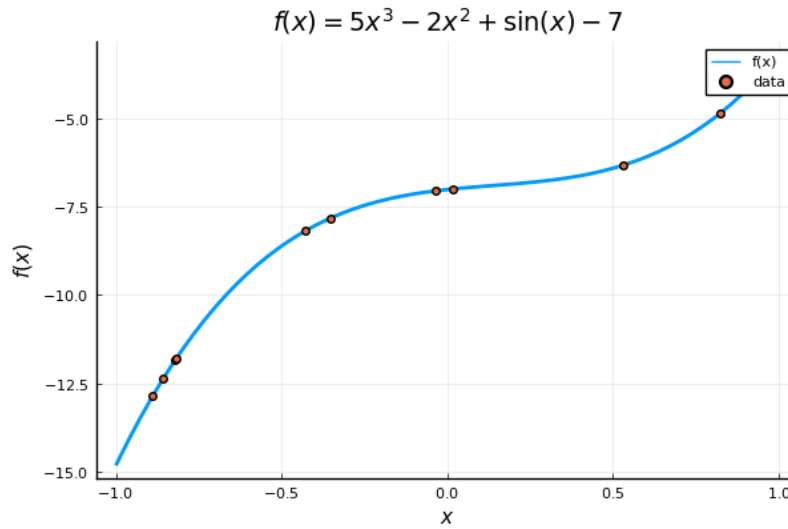


Figure 1.3: A set of points generated from the function $5x^3 - 2x^2 + \sin(x) - 7$

x	y
-0.889 160	-12.872 628
-0.856 103	-12.358 361
-0.821 295	-11.851 004
-0.818 193	-11.807 452
-0.429 859	-8.183 442
-0.352 328	-7.812 033
-0.035 776	-7.038 557
0.017 450	-6.983 134
0.529 010	-6.314 804
0.821 101	-4.848 557

Table 1.11: A set of points generated from the function $5x^3 - 2x^2 + \sin(x) - 7$

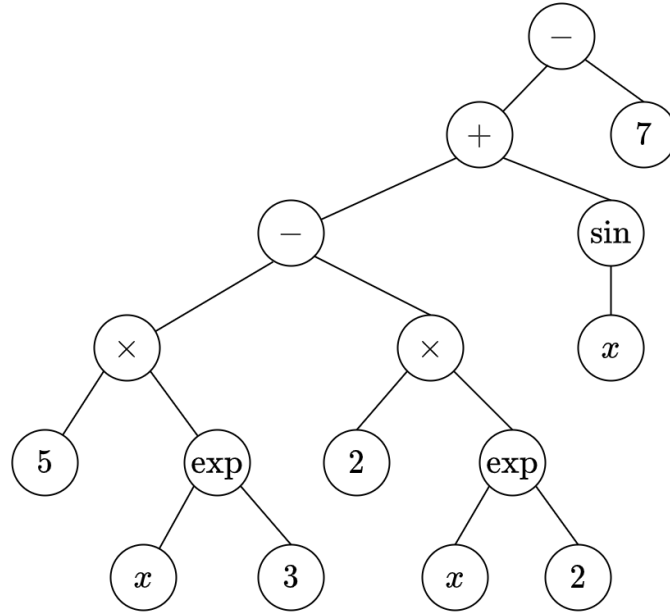
- exp: Exponential
- log: Logarithm
- Terminals:
 - x : The variable x
 - $c \in 1 \dots 7$: An ephemeral constant²²

Using this set of functions and terminals, we can represent the program as a tree, as shown in fig. 1.4 on the next page.

Now, we need to define how to evaluate the fitness of a program. Again, there are many ways to do this, but a common way is to use the *mean squared error* (MSE) between the points and the program.

Definition 1.8 (Mean Squared Error). *If a vector of n predictions is generated from a sample of n data points on all variables, and \mathbf{y}_i is the i -th observed value and $\hat{\mathbf{y}}_i$ is the i -th prediction, then the MSE of the predictor is a function $\text{MSE} : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ defined as:*

²²See definition A.4 on page 63.

Figure 1.4: A tree representation of the program $5x^3 - 2x^2 + \sin(x) - 7$

$$\text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{n} \sum_{i=1}^n (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2 \quad (1.5)$$

The MSE is a common measure of the quality of an estimator, used in many *machine learning* problems.

In our case, we will use the MSE to evaluate the fitness of a program. Consider a program P and two sets of points, \mathbf{x} and \mathbf{y} , as outlined in table 1.11 on the facing page. Suppose also that $P[\mathbf{x}]$ is the set of points generated by evaluating P on the points of \mathbf{x} , and that $P(x)$ is the result of evaluating P on the point x . Then, we can define the fitness of P as:

$$\phi_P = \text{MSE}(\mathbf{y}, P[\mathbf{x}]) = \frac{1}{n} \sum_{i=1}^n (\mathbf{y}_i - P(\mathbf{x}_i))^2 \quad (1.6)$$

This section elucidated the pivotal aspects of Genetic Programming (GP), focusing on representation of individuals and their evaluation. Individuals, potential solutions to a problem, can be encoded in several ways including tree representation. A common statistical problem, symbolic regression, was illustrated using a set of points on a curve from a function involving both polynomial and trigonometric elements. By defining a set of functions and terminals, these points were represented as a tree. The fitness of an individual program was assessed using the Mean Squared Error (MSE) between the points on the curve generated by the function and the points produced by the program. Thus, in the context of this problem, the fittest individual is the one that minimizes this error, i.e., best fits the curve. The methods described here underscore the versatility and applicability of GP to various types of problems. This method of representation and evaluation provides a robust basis for generating evolving populations of programs. In the next sections we will discuss the mechanisms for generating these populations and the evolutionary operators that act on them.

1.3.2 Initialization

As with other evolutionary algorithms, the algorithm starts by generating a population of random individuals.

There are many ways to generate random individuals, but a very common (and simple) method is the *grow method* [4]. In this method, a maximum depth is defined, and the algorithm then creates a random tree with a depth between 0 and the maximum depth.

Definition 1.9 (Depth of a tree). *The depth of a tree is defined as the length of the longest (non backtracking) path from the root to a leaf.*

Remark. *A tree with a depth of 0 is a tree with only one node, the root.*

Remark. *The tree in fig. 1.4 on the previous page has a depth of 5, as the longest path from the root to a leaf is*

$$- \rightarrow + \rightarrow - \rightarrow \times \rightarrow \exp \rightarrow x$$

The grow method then proceeds to recursively generate the trees with random nodes until a terminal node is selected or the maximum depth is reached. This method is shown in algorithm 3.

Algorithm 3 The grow method for generating random trees

Require: $l \in \mathbb{N}, h \in \mathbb{N}$

Require: $l \leq h$

Require: a random integer n such that $l \leq n \leq h$

Require: \mathbf{t} and \mathbf{f} are the sets of terminal and function nodes respectively, where $\mathbf{t} \neq \emptyset$ and $\mathbf{f} \neq \emptyset$

Ensure: a random tree with a depth between l and h

```

1: function grow( $\mathbf{t}, \mathbf{f}, d$ )
2:    $c \leftarrow \emptyset$ 
3:   if  $d = n \vee \left( d \geq l \wedge \text{random}() < \frac{|\mathbf{t}|}{|\mathbf{t}| + |\mathbf{f}|} \right)$  then
4:     return a random node from  $\mathbf{t}$ 
5:   else
6:      $f \leftarrow$  a random node from  $\mathbf{f}$ 
7:     for  $i$  in  $1 \dots \text{arity}(f)$  do
8:        $c_i \leftarrow \text{grow}(\mathbf{t}, \mathbf{f}, d + 1)$ 
9:        $c \leftarrow c \cup \{c_i\}$ 
10:    end for
11:    return a tree with root  $f$  and children  $c$ 
12:  end if
13: end function

```

With this method, the algorithm can generate trees where the depth of the shortest path from the root to a leaf is l and the depth of the longest path is h .

Now that the algorithm can generate random trees, it can generate a random population of trees by generating a random tree for each individual in the population. Assuming a population size of $p = 4$, a maximum depth of $h = 3$, a minimum depth of $l = 1$, and the primitives set defined in the previous section, the algorithm could generate the population shown in fig. 1.5 on the next page.

The next step is to calculate the fitness of each individual in the population. If we recall, the fitness function is the MSE between the expected output and the actual output of the individual.

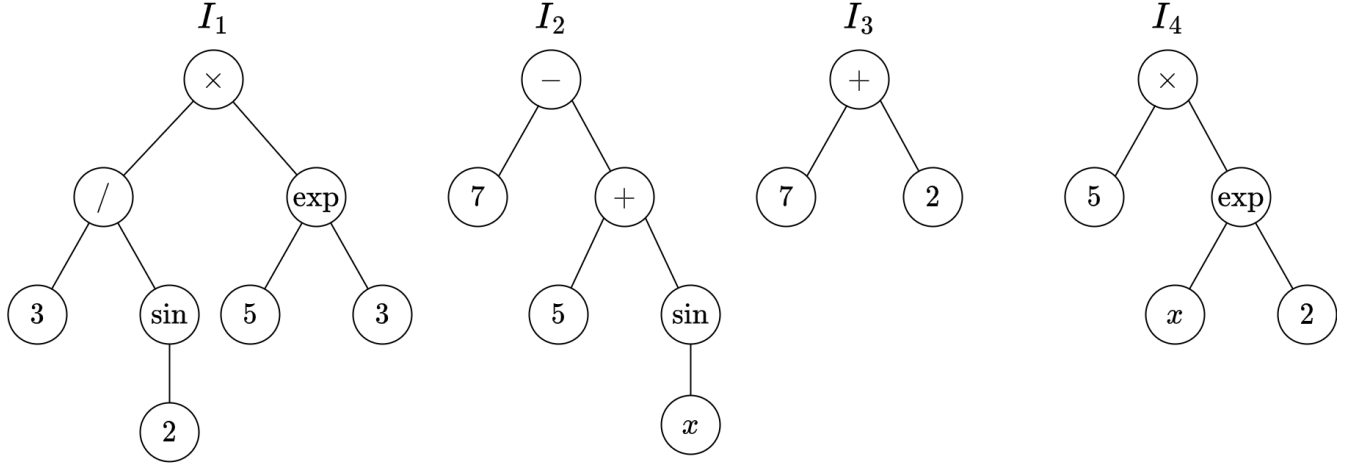


Figure 1.5: A population of random trees.

$$\begin{aligned}
 \text{MSE}(\mathbf{y}, I_1[\mathbf{x}]) &= \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - I_1(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} \left(\mathbf{y}_i - \frac{3}{\sin(2)} \cdot 5^3 \right)^2 \\
 &= 177596.85113055952 \\
 \text{MSE}(\mathbf{y}, I_2[\mathbf{x}]) &= \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - I_2(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - 7 - (5 + \sin(x_i)))^2 \\
 &= 137.39883553479902 \\
 \text{MSE}(\mathbf{y}, I_3[\mathbf{x}]) &= \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - I_3(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - (7 + 2))^2 \\
 &= 331.9242673984617 \\
 \text{MSE}(\mathbf{y}, I_4[\mathbf{x}]) &= \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - I_4(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - 5x^2)^2 \\
 &= 138.07986538961543
 \end{aligned}$$

With this, we can assign a fitness to each individual in the population as shown in table 1.12. A summary of the population's fitness is shown in table 1.13 on the next page.

Generation 0			
Individual	Program	Depth	Fitness
I_1	$\frac{3}{\sin(2)} \times 5^3$	3	177 596.851 131
I_2	$7 - (5 + \sin(x))$	3	137.398 836
I_3	$7 + 2$	1	331.924 267
I_4	$5x^2$	2	138.079 865

Table 1.12: Population of individuals in generation 0

We can observe that the worst individual has an error significantly larger than the best individual. This is to be expected, as the MSE is a measure of the error that escalates exponentially with the difference between the expected and actual output.

	Fitness	Individual
Best	137.398 836	I_2
Worst	177 596.851 131	I_1
Average	44 551.063 525	
Standard Deviation	88 697.238 974	

Table 1.13: Fitness of the individuals in generation 0

A graphical representation of the population is shown in fig. 1.6. It is clear from the figure that the worst individual is I_1 .

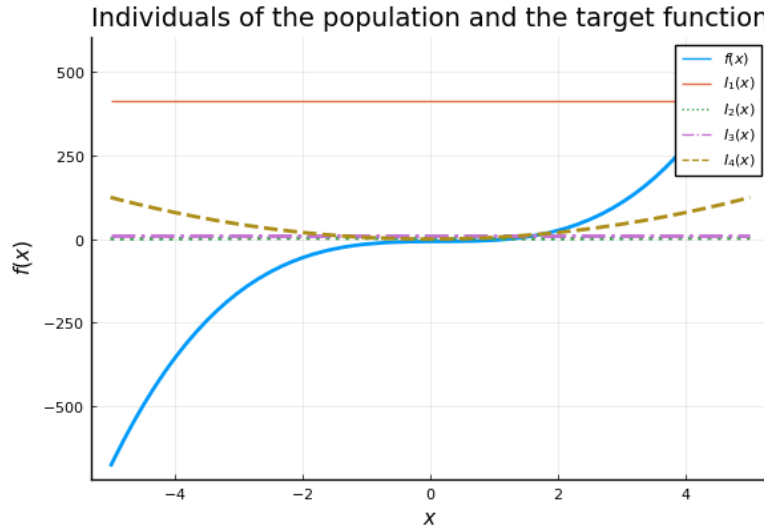


Figure 1.6: Graphical representation of the population in generation 0 compared to the expected output.

In summary, the initialization stage of the genetic programming algorithm, a population of random individuals, represented as trees, was generated using the “grow method”. The depth of these trees, signifying the length of the longest path from the root to a leaf, is determined randomly within a specified range. Each tree is recursively populated with random nodes until a terminal node is chosen or the maximum depth is reached. Once a random population of trees is created, the fitness of each individual, based on the Mean Squared Error (MSE) between the expected and actual output, is calculated. This results in the assignment of fitness scores to all individuals, facilitating the evaluation and selection process in the succeeding stages of the algorithm. The output of this process is a random population of trees with fitness scores and depth measurements, ready for the next steps of selection, crossover, and mutation.

1.3.3 Selection

The selection process in Genetic Programming (GP) is similar to that of Genetic Algorithms (GA). However, unique modifications have been proposed for the standard process in GP, which consider the semantics, or the functional behavior, of the programs being evolved [9]. This work will not delve into this topic, as it is beyond the scope of this document.

For the problem under study, we use a selection process similar to the one used in the *One Max* problem (a simple optimization problem where the objective is to maximize the number of ones in a binary string). The equation for calculating the selection probability will diverge from eq. (1.3) on page 9, as it presumes the fittest individual is the one with the highest fitness value. In contrast, the symbolic regression problem, which is our focus, considers the individual with the lowest fitness value as the fittest.

For this particular case of the symbolic regression problem, we adjust our approach to selection. We introduce a

corrected fitness function, ϕ' , defined as:

$$\phi'(I) = \left(\sum \Phi_{\mathbf{P}} \right) - \phi_I \quad (1.7)$$

Here, ϕ_I signifies the fitness of individual I , and $\Phi_{\mathbf{P}}$ represents the *batch fitness function* defined in definition 1.3 on page 7 applied to the population \mathbf{P} . We then define the selection probability for an individual \mathbf{P}_i as:

$$p_i = \frac{\phi'(\mathbf{P}_i)}{\sum_{j=1}^N \phi'(\mathbf{P}_j)} \quad (1.8)$$

In this equation, N stands for the size of the population.

With this methodology, we calculate the selection probabilities for the population as illustrated in table 1.14. The outcome shows that the individual with the highest error has a considerably low probability of being selected, while the other individuals have roughly equal chances.

Individual	Fitness	Selection Probability
I_1	177 596.851 131	0.113 616%
I_2	137.398 836	33.307 633%
I_3	331.924 267	33.271 246%
I_4	138.079 865	33.307 505%

Table 1.14: Selection probabilities for the symbolic regression problem.

Assuming a *survival rate* of 50%, let's consider that the selection process favors I_2 and I_3 as survivors due to their higher selection probabilities (as shown in the previous table). In this scenario, I_1 and I_4 are identified as the ones to be replaced by the offspring in the next generation. A comparison between the survivors and the target function is shown in fig. 1.7.

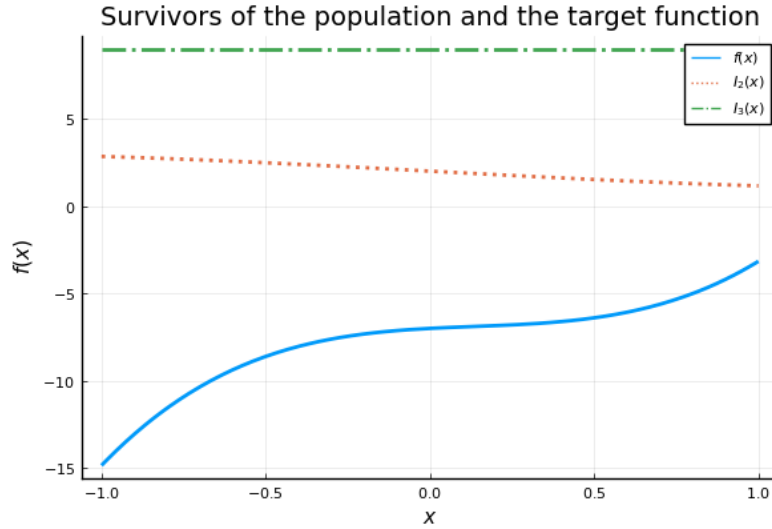


Figure 1.7: Comparison between the survivors and the target function.

To conclude, this section discussed the selection process in Genetic Programming (GP), noting that it largely mirrors that of Genetic Algorithms (GA) with some differences. These differences primarily focus on the semantics of the programs being evolved. The symbolic regression problem, necessitates a corrected fitness function and an adjusted selection probability equation. We outlined how these modifications are implemented and computed selection probabilities for a hypothetical population. A survival rate of 50% resulted in two individuals being

selected as survivors and two being marked for replacement in the next generation. This lays the groundwork for the next phase of the process, which is variation.

Chapter 2

Relevant Work (State of the Art)

2.1 Agile Artificial Intelligence in Pharo

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2.2 DEAP

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2.3 Jenetics

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2.4 *ECJ*

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2.5 *GeneticSharp*

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Chapter 3

Introduction

3.1 Motivation

The notion of learning machines has been around since the 1950s, when Alan Turing [1] asked a simple question: “Can machines think?”. Since then, the field of artificial intelligence has grown exponentially, with new applications being developed every day.

The first ideas on artificially simulating evolution date back to 1954, when Nils Aall Barricelli [2] proposed a definition of evolution as a pure statistical process, establishing the basis for the field of *evolutionary computation* (EC). In this work, Baricelly states that in order for a system to be considered an evolutionary system, its components must satisfy the following conditions:

1. Be able to reproduce.
2. Be able to undergo hereditary changes (mutations) in order to permit evolution by a process of survival of the fittest.

John Holland [3] will later formalize these ideas in his book *Adaptation in Natural and Artificial Systems*, where he introduces the concept of *genetic algorithms* (GA), a method for solving optimization problems based on the principles of natural selection and genetics. Holland’s work will be the basis for the field of *evolutionary algorithms* (EA).

3.2 Hypothesis and Research Questions

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3.4 Methodology

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Chapter 4

Keen: Kotlin Evolutionary Algorithms Framework

4.1 Introduction

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4.2 Architecture

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4.3 Genetic Operators

4.3.1 Selection

Random Selector

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Roulette Wheel Selector

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Tournament Selector

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4.3.2 Mutation

Bit Flip Mutator

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Random Mutator

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Swap Mutator

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Inversion Mutator

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4.3.3 Crossover

Combine Crossover

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Mean Crossover

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Ordered Crossover (OX)

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Partially Mapped Crossover (PMX)

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Position Based Crossover (PBX)

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Single-Point Crossover

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Single-Node Crossover

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4.4 Genetic Algorithms

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4.5 Genetic Programming

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4.6 Parallelism

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4.7 Extensibility

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4.8 Conclusion

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Chapter 5

Case Study: Real Function Optimization

5.1 Introduction

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5.2 Problem Description

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5.3 Solution

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5.4 Results

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5.5 Conclusion

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Chapter 6

Case Study: Knapsack Problem

6.1 Introduction

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6.2 Problem Description

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Chapter 7

Case Study: Crash Reproduction

7.1 Introduction

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7.2 Problem Description

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Chapter 8

Conclusions

8.1 Summary

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8.3 Future Work

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and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

After this fourth paragraph, we start a new paragraph sequence. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Appendix A

Glossary

In this appendix we present a glossary of terms used throughout this document as a reference for the reader.

A

Definition A.1 (Alteration). *See section 1.2.4 on page 9*

Definition A.2 (Alterer). *See definition 1.5 on page 10.*

C

Definition A.3 (Chromosome). *Representation of a single column of genetic information of a candidate solution to a given optimization problem.*

Formally, a chromosome is a vector $\mathbf{c} = (g_1, g_2, \dots, g_n)$, where g_i is a gene (see definition A.6).

E

Definition A.4 (Ephemeral Constant). *A constant that is randomly generated at the start of the program and remains constant throughout the execution of the program.*

This is used to represent constant values in the program.

Definition A.5 (Evolutionary computation). *Family of algorithms for global optimization inspired by the process of natural selection.*

This typically involves processes mimicking natural selection, mutation, recombination, and survival of the fittest. The solutions to a problem are encoded as a set of “individuals” in a “population”. Over multiple generations, these individuals are selected and modified (via genetic operators like crossover and mutation) in order to find better solutions.

G

Definition A.6 (Gene). *Representation of a single component of a candidate solution to a given optimization problem.*

Formally, for a multi-dimensional function f , a gene is an element g in the domain of f .

Definition A.7 (Generation). *Number of iterations performed by an evolutionary algorithm.*

Definition A.8 (Genotype). *Representation of the full genetic information of a candidate solution to a given optimization problem.*

Formally, a genotype is a matrix $\mathbf{G} = (\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n)$, where \mathbf{c}_i is a chromosome (see definition A.3 on the preceding page).

I

Definition A.9 (Individual). *A candidate solution to a given optimization problem.*

Formally, an individual is a pair (\mathbf{G}, \mathbf{f}) , where \mathbf{G} is the genotype (see definition A.8) and \mathbf{f} is the fitness value of the individual.

M

Definition A.10 (Metaheuristics). *Problem-independent algorithmic method that yields a sufficiently good solution within reasonable time for an optimization problem, especially for complex problems where an exact solution is not crucial.*

Definition A.11 (Mutator). *See definition 1.7 on page 12.*

P

Definition A.12 (Parameter optimization). *Optimization problem where the solution is a set of parameters that optimize a given function.*

Definition A.13 (Phenotype). *Same as definition A.9.*

Definition A.14 (Population). *Set of candidate solutions to a given optimization problem.*

Definition A.15 (Program induction). *Inference of an algorithm or program featuring recursive calls or repetition control structures, starting from information that is known to be incomplete, called the evidence, such as positive and negative I/O examples or clausal constraints.*

S

Definition A.16 (Search space). *Set of all candidate solutions to a given optimization problem.*

Definition A.17 (Selector). *See definition 1.4 on page 9.*

V

Definition A.18 (Variadic function). *Function that accepts a variable number of arguments.*

Appendix B

Test Functions for Optimization

This appendix contains the test functions used in the numerical experiments in chapter 5 on page 47.

B.1 Rastrigin Function

The Rastrigin function is a non-convex function used as a performance test problem for optimization algorithms. It is a typical example of non-linear multimodal function. It was first proposed by Rastrigin in 1974.¹

Definition B.1 (Rastrigin Function). *The Rastrigin function, $f : \mathbb{R}^n \rightarrow \mathbb{R}$, is defined as:*

$$f(\mathbf{x}) = An + \sum_{i=1}^n [\mathbf{x}_i^2 - A \cos(2\pi\mathbf{x}_i)] \quad (\text{B.1})$$

where:

- n is the number of dimensions.
- \mathbf{x} is a vector of n real values.

The global minimum of the Rastrigin function is $f(\mathbf{x}^*) = 0$ at $\mathbf{x}^* = (0, \dots, 0)$. The function has many local minima, which are regularly distributed. The A parameter controls the depth of the local minima. The function is usually evaluated on the hypercube $\mathbf{x} \in [-5.12, 5.12]^n$. A contour plot and a surface plot of the Rastrigin function for $n = 2$ are shown in fig. B.1.

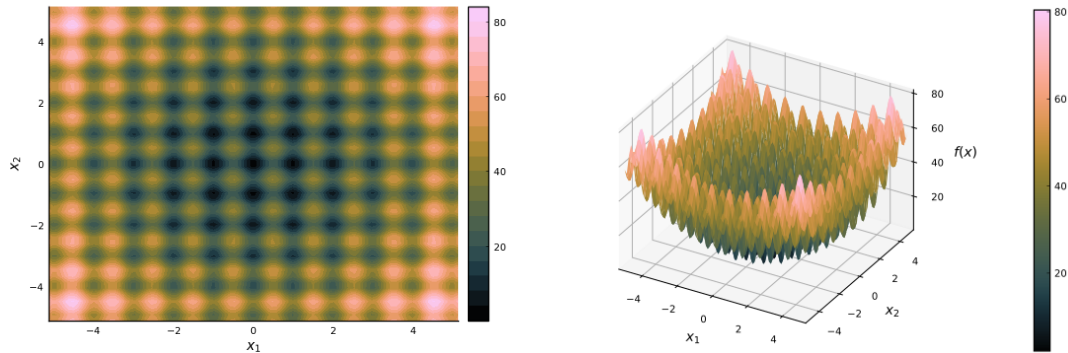


Figure B.1: Rastrigin Function for $n = 2$

¹Rastrigin, L. A. “Systems of extremal control.” Mir, Moscow (1974).

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