Keen: Kotlin Genetic Algorithms Framework

Thesis for the degrees of
Civil Engineer in Computer Science
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Ignacio Slater Muñoz
Departamento de Ciencias de la Computación
Facultad de Ciencias Físicas y Matemáticas
Universidad de Chile.
Thesis Author

Nancy Hitschfeld. PhD.
Departamento de Ciencias de la Computación
Facultad de Ciencias Físicas y Matemáticas
Universidad de Chile
Thesis Supervisor

Alexandre Bergel. PhD.
Relational AI
Switzerland
Second Supervisor

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Abstract

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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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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Contents

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) [12] 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 highest[4] 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.

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[1]See definition A.6 on page 75

[2]See definition A.11 on page 76

[3]Not 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.17 on page 76) simultaneously.

[4]In 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] [4, 5, 12, 13] 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: *population* ← initializePopulation()   ▷ Creates a random population of individuals
2: evaluate(*population*)   ▷ Calculates the fitness of each individual
3: **repeat**
4:     *parents* ← selectParents(*population*)   ▷ Selects a subset of individuals as parents
5:     alter(*offspring*)   ▷ Applies genetic operators to offspring, creating variations
6:     *population* ← selectSurvivors(*population, offspring*)   ▷ 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(*population*)   ▷ 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 genes[8] 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 $(\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_n)$*, and a representation* **G** *with n chromosomes of length* $(m_1, m_2, \ldots, m_n)$ *where each chromosome is encoded using the alphabet* $\mathcal{A}_i$*, the cardinality of the search space S is defined as:*

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[5]Also known as Simple Genetic Algorithms (SGA) [12], or Traditional Genetic Algorithms (TGA) [13].
[6]See definition A.10 on page 76.
[7]See definition A.9 on page 76
[8]See definition A.7 on page 75.
[9]See [37].
[10]See definition A.4 on page 75.

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

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 [4], 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 $\phi : S \to \mathbb{R}^n$, 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 $\Phi : \mathbb{P} \to \mathbb{R}^{m \times n}$ 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:

$$\phi_{\mathbf{G}} = \sum_{i=1}^{n} g_i \tag{1.2}$$

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.

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[11]This is known as the *One Max* problem [33] or *Ones Counting* problem [37].

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 $i \in \{1, \ldots, N\}$. Let σ be the survival rate, a parameter controlling the degree of elitism. This is the proportion of individuals that

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[12]Since 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

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

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 operator[14] 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:

$$p_i = \frac{f_i}{\sum_{j=1}^{N} f_j} \tag{1.3}$$

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

Individual	Fitness	Selection Probability
I_1	2	50%
I_2	1	25%
I_3	0	0%
I_4	1	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 40. 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.

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[13]The 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.

[14]See section 4.3.1 on page 41 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*

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

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 40.

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

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

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:

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[15]This is referred to as *crossing-over* in [4].

[16]See section 4.3.3 on page 48.

$$I_1 \quad \boxed{1 \; 1 \; 0 \; 0} \quad \phi_1 = 2$$

$$I_2 \quad \boxed{0 \; 0 \; 0 \; 1} \quad \phi_2 = 1$$

$$O_1 \quad \boxed{0 \; 0 \; 0 \; 0} \quad \phi_1' = 0$$

$$O_2 \quad \boxed{1 \; 1 \; 0 \; 1} \quad \phi_2' = 3$$
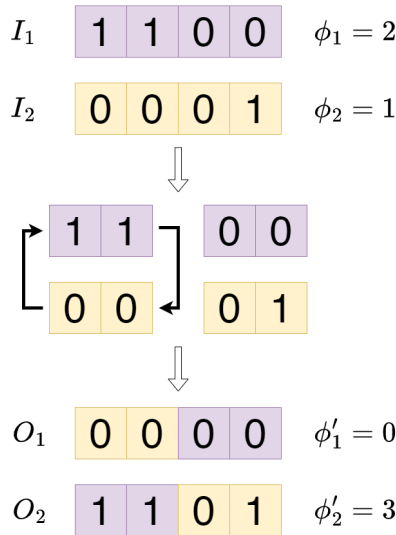
Figure 1.1: Single-point crossover

Generation 0 → Generation 1

$\mathbf{I}$	$\mathbf{\Phi_I}$	$\mathbf{O}$	$\mathbf{\Phi_O}$
$\begin{bmatrix}1100\\0001\end{bmatrix}$	$\begin{bmatrix}2\\1\end{bmatrix}$	$\begin{bmatrix}0000\\1101\end{bmatrix}$	$\begin{bmatrix}0\\3\end{bmatrix}$
$\begin{bmatrix}0001\\0100\end{bmatrix}$	$\begin{bmatrix}1\\1\end{bmatrix}$	$\begin{bmatrix}0101\\ \cdot \end{bmatrix}$	$\begin{bmatrix}2\\ \cdot \end{bmatrix}$

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, · 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

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

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 $\to$ Generation 1

I	$\mathbf{\Phi_I}$	**O**	$\mathbf{\Phi_O}$
$\begin{bmatrix} 0000 \\ 1101 \\ 0101 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 3 \\ 2 \end{bmatrix}$	$\begin{bmatrix} 1111 \\ 0010 \\ 1010 \end{bmatrix}$	$\begin{bmatrix} 4 \\ 1 \\ 2 \end{bmatrix}$

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.

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[17]See appendix B.12 on page 84.
[18]See section 4.3.2 on page 42.

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 1[19] 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 $\phi_{\mathbf{G}} = 4$.

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.

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[19] $P = \{11\textcolor{red}{00}, 00\textcolor{red}{0}1, 00\textcolor{red}{00}, 01\textcolor{red}{00}\}$

[20] $P' = \{0001, 11\textcolor{red}{1}1, 00\textcolor{red}{1}0, 10\textcolor{red}{1}0\}$

	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) [5, 7, 11, 12] 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.

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[21]For a formal definition of program induction, refer to definition A.16 on page 76.

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:     $parents \leftarrow$ selectParents($population$)   ▷ Parent selection for reproduction
5:     alter($offspring$)   ▷ Apply genetic operators to offspring
6:     $population \leftarrow$ 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** fittest($population$)   ▷ Return the best solution found

---

1.3.1 Representation and Evaluation

Representation

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,[22] 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 illustrate this with an example 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 [5]. In this example, our goal is to use symbolic regression to approximate the function

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

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

The next step in preparing our GP setup is to define the primitive set, which includes the functions and terminals that the algorithm can use to construct candidate solutions. In this case, we will use the following set of functions and terminals:

- Functions: 1. + (Addition) 2. − (Subtraction) 3. × (Multiplication) 4. / (Division) 5. sin (Sine) 6. cos (Cosine) 7. pow (Power)

- Terminals: 1. x (The variable x) 2. $\{c \mid c \in [1, 7] \land c \in \mathbb{Z}\}$ (An ephemeral constant)[23]

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.

---

[22]For example, by applying genetic operators.
[23]See definition A.5 on page 75.
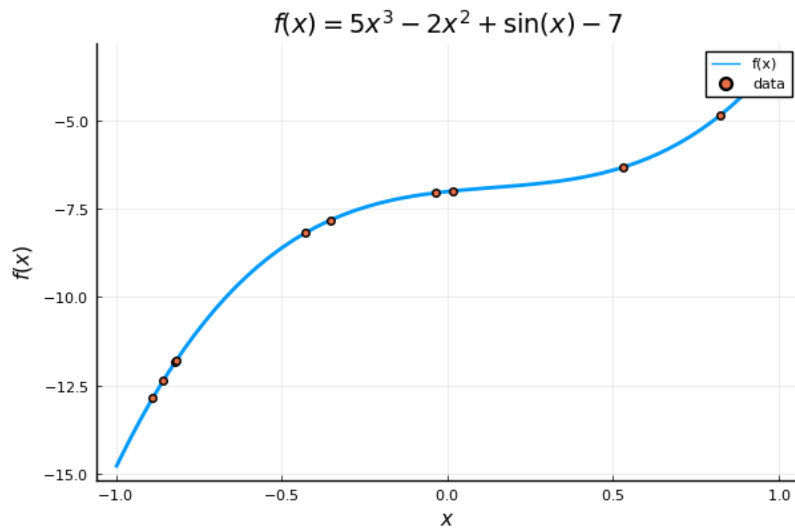
Figure 1.3: A set of points generated from the function $5x^3 - 2x^2 + \sin(x) - 7$

x	y
0.889 160	-12.872 629
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 $5x^3 - 2x^2 + \sin(x) - 7$
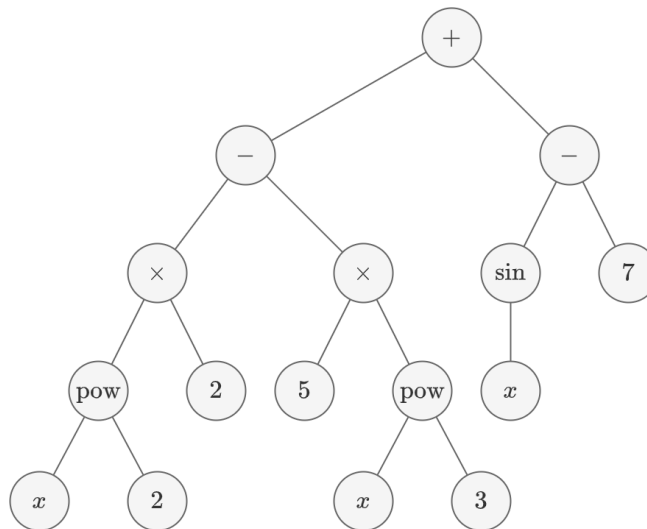
Figure 1.4: A possible tree representation of the program $5x^3 - 2x^2 + \sin(x) - 7$

Note that this definition arises the possibility of having a program that has an infinite number of nodes, as the tree can grow indefinitely. This leads the search to be unsuccessful since the probability of finding a solution is close to zero, for example, the probability of finding a solution on the initial population would be: $\lim_{x \to \infty} \frac{1}{x} = 0$. To avoid this issue of potentially infinite trees, we typically impose certain *constraints* on the generation of the trees. The most common constraints are the *maximum height* of the tree and the *maximum number of nodes* in the tree.

Search space

Using this representation, we can define the *genotype* of the individuals to contain only one *chromosome* which is composed of a single *gene*[24] that is the tree representation of the program. Recalling the definition of cardinality presented in definition 1.1 on page 6, we can see that the cardinality of the search space will be the number of possible trees that can be generated using the primitive set and the maximum height of the tree.

Lemma 1.1. *Let $\mathbb{T}_H$ be the set of all possible **labeled trees** of height H, with $H \in \mathbb{N}$. Given the sets $\mathcal{T}$ and $\mathcal{F}$ corresponding to the possible labels of terminal nodes (nodes that do not have children) and the possible labels of internal nodes (nodes that have children) respectively, the number of trees in $\mathbb{T}_H$ is given by the following recurrence relation:*

$$|\mathbb{T}_H(\mathcal{T}, \mathcal{F})| = \begin{cases} |\mathcal{T}| & \text{if } H = 0 \\ \sum_{f \in \mathcal{F}} |\mathbb{T}_{H-1}(\mathcal{T}, \mathcal{F})|^{A(f)} & \text{if } H > 0 \end{cases} \tag{1.5}$$

where $A(f)$ is the arity of the node f.

Proof. For the proof, we will use induction on the height of the tree. For the sake of brevity, we will use the notation $|\mathbb{T}_H(\mathcal{T}, \mathcal{F})| = |\mathbb{T}_H|$.

Base case: $H = 0$ If the height of the tree is 0, then the tree is composed of a single node, which is a terminal node. Thus, the number of possible trees is equal to the number of possible terminal nodes, which arises:

$$|\mathbb{T}_0| = |\mathcal{T}|$$

Base case: $H = 1$ If the height of the tree is 1, then the tree is composed of a root node, which is an internal node, and a set of children, which are terminal nodes. Suppose that the root node has the label $f \in \mathcal{F}$ and arity $A(f)$.

Since the children are terminal nodes, each children can have any of the labels in $\mathcal{T}$. Thus, the number of trees rooted at f is equal to the number of possible combinations of $A(f)$ elements (with repetition and order) from the set $\mathcal{T}$, this is:

$$\prod_{i=1}^{A(f)} |\mathcal{T}| = |\mathcal{T}|^{A(f)}$$

Since the root node can have any of the labels in $\mathcal{F}$, the number of possible trees of height 1 is equal to:

$$|\mathbb{T}_1| = \sum_{f \in \mathcal{F}} |\mathcal{T}|^{A(f)}$$

---

[24]Although the most common representation is to have a single gene referencing the root of the tree, several variations that use multi-gene chromosomes have been proposed, such as Koza's *Automatically Defined Functions* [7], Angeline and Pollack's *Genetic Library Builder* [6, 8], or Rosca and Ballard's *Adaptive Representation* [9].

Inductive step: $H > 1$ Suppose the statement holds true for $H = h$. We aim to prove that the statement also holds true for $H = h + 1$.

Since a terminal node cannot have children,[25] each tree of height $h + 1$ has a root with one of the labels from the set $\mathcal{F}$, and the remaining h layers are fully formed subtrees of height h.

For a given node label $f \in \mathcal{F}$ with arity $A(f)$, each child is the root of a subtree of height h. Given our inductive assumption, there are $|\mathbb{T}_h|$ possible such subtrees.

Since all subtrees are independent, the number of possible trees with the root f is $|\mathbb{T}_h|^{A(f)}$, which is the product of $|\mathbb{T}_h|$ over the arity of f.

We can sum this quantity over all $f \in \mathcal{F}$ to get the total number of possible trees of height $h + 1$:

$$|\mathbb{T}_{h+1}| = \sum_{f \in \mathcal{F}} |\mathbb{T}_h|^{A(f)}$$

$\square$

Lemma 1.2. *Let $\mathbb{T}_{\leq H}$ be the set of all possible **labeled trees** of height $h \leq H$, with $H \in \mathbb{N}$ and $h \in \mathbb{N}$. Given the sets $\mathcal{T}$ and $\mathcal{F}$ corresponding to the possible labels of terminal nodes and the possible labels of internal nodes respectively, the number of trees in $\mathbb{T}_{\leq H}$ is given by the following recurrence relation:*

$$|\mathbb{T}_{\leq H}(\mathcal{T}, \mathcal{F})| = \begin{cases} |\mathcal{T}| & \text{if } H = 0 \\ |\mathbb{T}_H(\mathcal{T}, \mathcal{F})| + |\mathbb{T}_{\leq H-1}(\mathcal{T}, \mathcal{F})| & \text{if } H > 0 \end{cases} \tag{1.6}$$

Where $\mathbb{T}_H$ is the set of all possible trees of height H.

Proof. For the sake of simplicity, we will use the notation $|\mathbb{T}_{\leq H}| = |\mathbb{T}_{\leq H}(\mathcal{T}, \mathcal{F})|$ and $|\mathbb{T}_H| = |\mathbb{T}_H(\mathcal{T}, \mathcal{F})|$.

The set $\mathbb{T}_{\leq H}$ can be partitioned into two disjoint sets: the set of all possible trees of height H and the set of all possible trees of height $h < H$. Thus we have:

$$|\mathbb{T}_{\leq H}| = |\mathbb{T}_H| + |\mathbb{T}_{\leq H-1}|$$

$\square$

Theorem 1.1. *Let $\mathbb{T}_{\leq H}$ be the set of all possible **labeled trees** of height $h \leq H$, with $H \in \mathbb{N}$ and $h \in \mathbb{N}$. Given the sets $\mathcal{T}$ and $\mathcal{F}$ corresponding to the possible labels of terminal nodes and the possible labels of internal nodes respectively, the number of trees in $\mathbb{T}_{\leq H}$ is given by the following recurrence relation:*

$$|\mathbb{T}_{\leq H}(\mathcal{T}, \mathcal{F})| = \begin{cases} |\mathcal{T}| & \text{if } H = 0 \\ \left(\sum_{h=0}^{H-1} \sum_{f \in \mathcal{F}} |\mathbb{T}_h(\mathcal{T}, \mathcal{F})|^{A(f)} \right) + |\mathcal{T}| & \text{if } H > 0 \end{cases} \tag{1.7}$$

Where $\mathbb{T}_H$ is the set of all possible trees of height H and $A(f)$ is the arity of the node f.

Proof. From lemma 1.2 we know the number of trees of height H or less is given by:

$$|\mathbb{T}_{\leq H}| = |\mathbb{T}_H| + |\mathbb{T}_{\leq H-1}|$$

Then, by applying lemma 1.1 on the preceding page, we get:

---

[25]This could also be interpreted as a terminal node having an arity of 0, or that all terminal nodes are leaves.

$$|\mathbb{T}_{\leq H}| = \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{H-1}|^{A(f)}\right) + |\mathbb{T}_{\leq H-1}|$$

By unrolling the recurrence relation, we get:

$$
\begin{aligned}
|\mathbb{T}_{\leq H}| &= \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{H-1}|^{A(f)}\right) + |\mathbb{T}_{\leq H-1}| \\
&= \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{H-1}|^{A(f)}\right) + \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{H-2}|^{A(f)}\right) + \cdots + \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{1}|^{A(f)}\right) + \left(\sum_{f \in \mathcal{F}} |\mathbb{T}_{0}|^{A(f)}\right) + |\mathbb{T}_0| \\
&= \left(\sum_{h=0}^{H-1} \sum_{f \in \mathcal{F}} \mathbb{T}_h(\mathcal{T}, \mathcal{F})|^{A(f)}\right) + |\mathcal{T}|
\end{aligned}
$$

$\square$

With this result, we can now calculate the cardinality of the search space of the genetic programming algorithm for a given maximum height H, since a program can be seen as a *labeled tree*. Then, given the set $\mathcal{T} = \{x, c\}$ and the set $\mathcal{F} = \{+, -, \times, /, \sin, \cos, \exp, \log\}$, where

$$A(f) = \begin{cases} 2 & \text{if } f \in \{+, -, \times, /, \text{pow}\} \\ 1 & \text{if } f \in \{\sin, \cos\} \end{cases}$$

Given that the height of the AST of the target program is 4, we can use 5 as the maximum height of the programs in the search space (to allow a little of "breathing room" to the generated programs). Noting that, since c can be one of 7 possible values, $|\mathcal{T}| = 8$, we can calculate the cardinality of the search space as follows:

$$
\begin{aligned}
|\mathcal{S}| = |\mathbb{T}_{\leq 5}(\mathcal{T}, \mathcal{F})| &= \left(\sum_{h=0}^{4} \sum_{f \in \mathcal{F}} |\mathbb{T}_h(\mathcal{T}, \mathcal{F})|^{A(f)}\right) + 8 \\
&\approx 9.531\,142 \times 10^{37} \\
&\approx 10^{38}
\end{aligned}
$$

Thus, the search space of the genetic programming algorithm is of the order of 10^{38} programs.[26] It should be easy to see that the size of the search space make it unfeasible to perform an exhaustive search. This is why we need to use a heuristic search algorithm, such as genetic programming. In fig. 1.5 on the following page we can see how the number of trees of height less or equal to h rapidly increases as h increases.

Evaluation

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* $\text{MSE} : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ *defined as:*

---

[26]This value was computed using the script shown in listing C.1 on page 89.
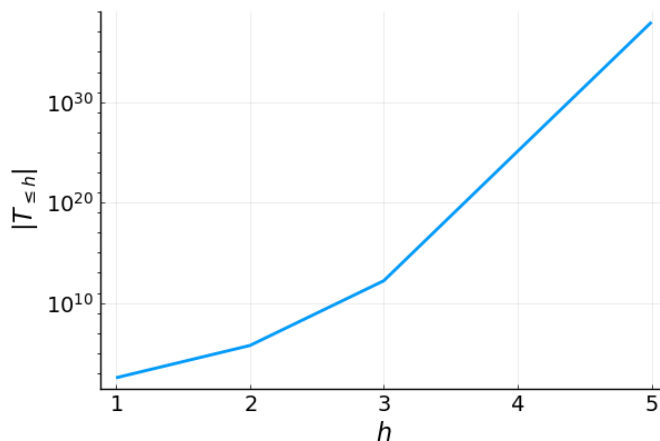
Figure 1.5: Total number of trees of height less or equal to h for $h \in \{0, \ldots, 5\}$ and $\mathcal{T} = \{x, c\}$ and $\mathcal{F} = \{+, -, \times, /, \sin, \cos, \text{pow}\}$. Note that the Y axis is in logarithmic scale.

$$\text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2 \tag{1.8}$$

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 page 16. Suppose also that $\mathsf{P}[\mathbf{x}]$ is the set of points generated by evaluating P on the points of $\mathbf{x}$, and that $\mathsf{P}(x)$ is the result of evaluating P on the point x. Then, we can define the fitness of P as:

$$\phi_{\mathsf{P}} = \text{MSE}(\mathbf{y}, \mathsf{P}[\mathbf{x}]) = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{y}_i - \mathsf{P}(\mathbf{x}_i))^2 \tag{1.9}$$

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* [5]. In this method, a maximum height is defined, and the algorithm then creates a random tree with a given minimum height and a maximum height.

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

The grow method then proceeds to recursively generate the trees with random nodes until a terminal node is selected or the maximum height 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 height between l and h

1: **function** grow($\mathbf{t}$, $\mathbf{f}$, d)
2:    $c \leftarrow \emptyset$
3:    **if** $d = n \ \vee \ \left(d \geq l \ \wedge \ \text{random}() < \dfrac{|\mathbf{t}|}{|\mathbf{t}| + |\mathbf{f}|} \right)$ **then**
4:       **return** a random node from $\mathbf{t}$
5:    **else**
6:       $f \leftarrow$ a random node from $\mathbf{f}$
7:       **for** i **in** $1 \ldots \text{arity}(f)$ **do**
8:          $c_i \leftarrow$ 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 size of the longest path from the root to a leaf is a number $n \in [l, h]$.

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 height of $h = 3$, a minimum height of $l = 1$, and the primitives set defined in the previous section, the algorithm could generate the population: $\mathbf{P} = \{\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3, \mathbf{I}_4\} = \left\{ \frac{3}{\sin(2)} \times 5^3,\ 7 - (5 + \sin(x)),\ 7 + 2,\ 5x^2 \right\}$, as shown in fig. 1.6 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.

$$\text{MSE}(\mathbf{y}, \mathbf{I}_1[\mathbf{x}]) = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - \mathbf{I}_1(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} \left(\mathbf{y}_i - \frac{3}{\sin(2)} \cdot 5^3 \right)^2$$
$$\approx 177\,596.851\,131$$

$$\text{MSE}(\mathbf{y}, \mathbf{I}_2[\mathbf{x}]) = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - \mathbf{I}_2(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - 7 - (5 + \sin(x_i)))^2$$
$$\approx 137.398\,836$$

$$\text{MSE}(\mathbf{y}, \mathbf{I}_3[\mathbf{x}]) = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - \mathbf{I}_3(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - (7 + 2))^2$$
$$\approx 331.924\,267$$

$$\text{MSE}(\mathbf{y}, \mathbf{I}_4[\mathbf{x}]) = \frac{1}{10} \sum_{i=1}^{10} (\mathbf{y}_i - \mathbf{I}_4(\mathbf{x}_i))^2 = \frac{1}{10} \sum_{i=1}^{10} \left(\mathbf{y}_i - 5x^2 \right)^2$$
$$\approx 138.079\,865$$

With this, we can assign a fitness to each individual in the population as shown in table 1.12 on the following page.

(a) $\mathbf{I}_1 = \dfrac{3}{\sin(2)} \times 5^3$

(b) $\mathbf{I}_2 = 7 - (5 + \sin(x))$

(c) $\mathbf{I}_3 = 7 + 2$
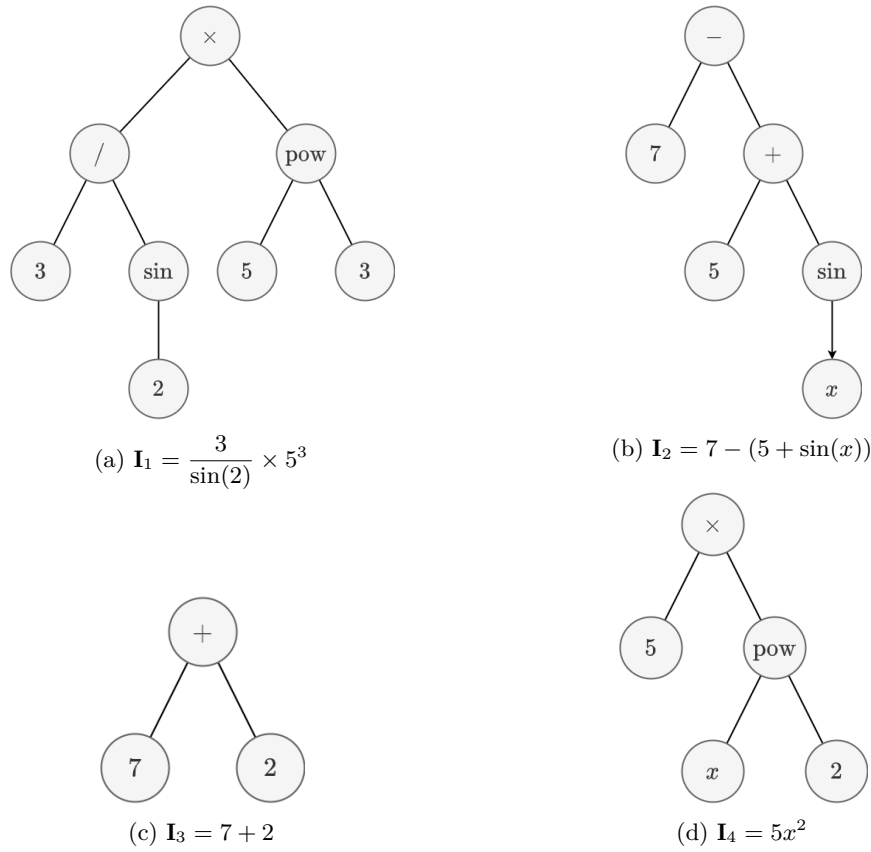
(d) $\mathbf{I}_4 = 5x^2$

Figure 1.6: A population of random trees.

A summary of the population's fitness is shown in table 1.13.

Generation 0

Individual	Program	Depth	Fitness
$\mathbf{I}_1$	$\frac{3}{\sin(2)} \times 5^3$	3	177 596.851 131
$\mathbf{I}_2$	$7 - (5 + \sin(x))$	3	137.398 836
$\mathbf{I}_3$	$7 + 2$	1	331.924 267
$\mathbf{I}_4$	$5x^2$	2	138.079 865

Table 1.12: Population of individuals in generation 0

	Fitness	Individual
Best	137.398 836	$\mathbf{I}_2$
Worst	177 596.851 131	$\mathbf{I}_1$
Average		44 551.063 525
Standard Deviation		88 697.238 974

Table 1.13: Fitness of the 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.

A graphical representation of the population is shown in fig. 1.7 on the facing page. It is clear from the figure that

the worst individual is $\mathbf{I}_1$.

Figure 1.7: 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 height of these trees, signifying th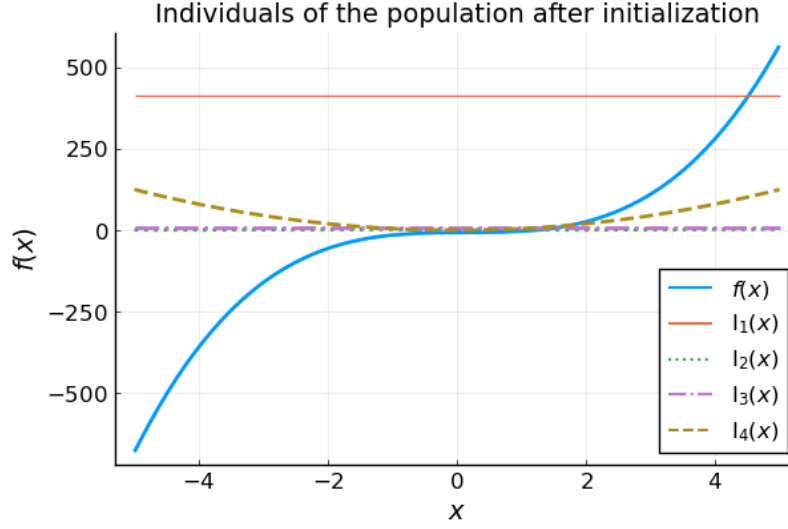e length of the longest path from the root to a leaf, is determined randomly within a specified range. Each tree is recursively populated with random nodes until a terminal node is chosen or the maximum height is reached. Once a random population of trees is created, the fitness of each individual, based 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 height 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 [14]. 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:

$$\phi'(I) = \left(\sum \Phi_{\mathbf{P}}\right) - \phi_I \tag{1.10}$$

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:

$$p_i = \frac{\phi'(\mathbf{P}_i)}{\sum_{j=1}^{N} \phi'(\mathbf{P}_j)} \tag{1.11}$$

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
$I_1(x)$	607.402 968	0.113 615%
$I_2(x)$	178 066.855 263	33.307 633%
$I_3(x)$	177 872.329 832	33.271 246%
$I_4(x)$	178 066.174 234	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. 1.8.
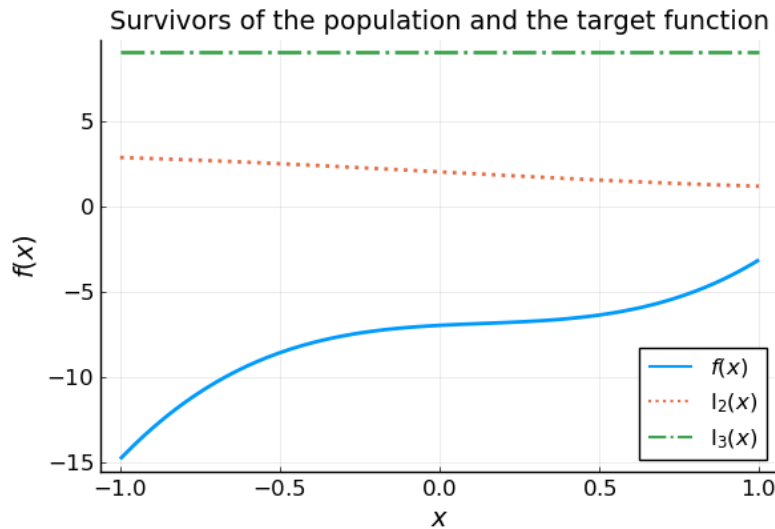
Figure 1.8: Comparison between the survivors and the target function.

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.

1.3.4 Variation

Analogous to GA, the individuals in a GP population undergo a variation process. For the symbolic regression problem under consideration, we introduce variation using two specific operators: *crossover* and *mutation*.

Crossover

Variation operators in Genetic Programming (GP) must maintain the syntactic correctness of the programs or individuals. For crossover, this implies that the resultant offspring must be syntactically correct programs.

The crossover operator used in Genetic Algorithms (GAs), described in section 1.2.4 on page 10, is not typically suitable for GP, as it does not guarantee the syntactic correctness of the resulting individuals. Though there could be instances where the crossover operator used in GAs is applicable to GP, as depicted in chapter 7 on page 63, these are not common scenarios.

The choice of operator in GP depends on the representation of the individuals.

For tree-based GP, the fundamental crossover operator is the *subtree crossover*, referenced in section 4.3.3 on page 49.

This operator selects a random node from each parent and exchanges the subtrees rooted at these nodes. Usually, a constraint similar to the one used for generating the initial population is applied to this operator to prevent the creation of overly large trees.

Assuming we select two individuals, $\mathbf{I}_1$ and $\mathbf{I}_2$, from the population, the subtree crossover operator chooses a random node from each individual, say $\clubsuit = 7$ from $\mathbf{I}_1$ and $\diamondsuit = x^2$ from $\mathbf{I}_2$. The subtrees rooted at these nodes are then interchanged, as shown below:

$$
\begin{aligned}
\chi(\mathbf{I}_2, \mathbf{I}_4) \quad &= \chi(\clubsuit - (5 + \sin(x)), 5\diamondsuit) \\
&= (\diamondsuit - (5 + \sin(x)), 5\clubsuit) \\
\Leftrightarrow \quad (\mathbf{O}_1, \mathbf{O}_2) \quad &= (x^2 - (5 + \sin(x)), 5 \cdot 7)
\end{aligned}
$$

where χ signifies the subtree crossover operator between two individuals. The crossover of $\mathbf{I}_1$ and $\mathbf{I}_2$ is depicted in fig. 1.9.
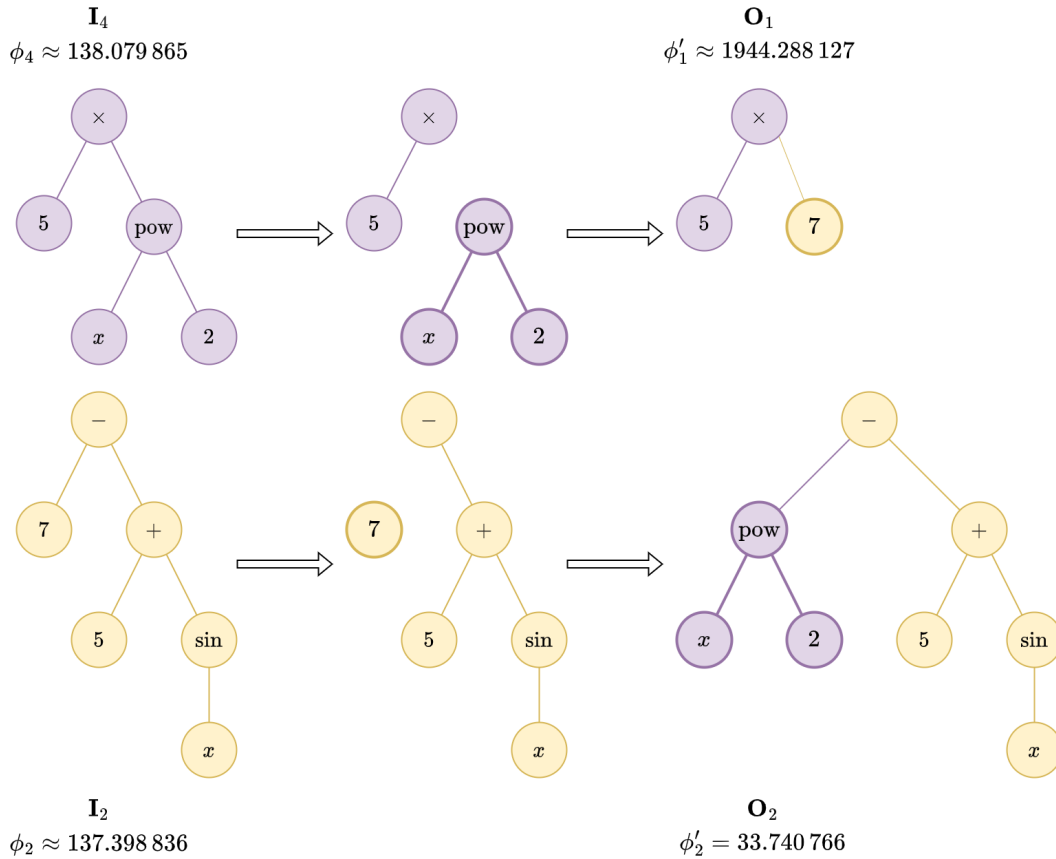

Figure 1.9: Crossing over of $\mathbf{I}_2 = 7 - (5 + \sin(x))$ and $\mathbf{I}_4 = 5x^2$, producing $\mathbf{O}_1 = x^2 - (5 + \sin(x))$ and $\mathbf{O}_2 = 5 \cdot 7$.

Following the application of the subtree crossover operator, the fitness of the individuals in the population is

evaluated as shown in table 1.17 on the next page. A summary of the population's fitness is given in table 1.18 on the facing page.

Generation 1

Individual	Program	Fitness
$\mathbf{I}_2$	$7 - (5 + \sin(x))$	137.398 836
$\mathbf{I}_3$	$7 + 2$	331.924 267
$\mathbf{O}_1$	$5 \cdot 7$	1944.288 127
$\mathbf{O}_2$	$x^2 - (5 + \sin(x))$	33.740 766

Table 1.15: Population after applying the subtree crossover operator.

	Fitness	Individual
Best	33.740 766	O_2
Worst	1944.288 127	O_1
Average	611.837 999	
Standard deviation	896.858 214	

Table 1.16: Fitness summary of the population after applying the subtree crossover operator.

A notable improvement in the population's fitness is observed after the application of the subtree crossover operator. Comparing the results from table 1.13 on page 22, we find that the average fitness (or error) has dropped from 44 551.063 525 to 611.837 999, equating to an improvement of approximately 98.627%.

$$\frac{\bar{\Phi}_i - \bar{\Phi}_X}{\bar{\Phi}_i} = \frac{44\,551.063\,525 - 611.837\,999}{44\,551.063\,525} \approx 98.627\%$$

where $\bar{\Phi}_i$ is the average fitness of the population after initialization and $\bar{\Phi}_X$ is the average fitness of the population after applying the subtree crossover operator.

A reduction in the population's fitness standard deviation, from 88 697.238 974 to 896.858 214, is also seen. This decrease of around 98.989% indicates that the population's diversity has reduced.

$$\frac{\sigma_i - \sigma_X}{\sigma_i} = \frac{88\,697.238\,974 - 896.858\,214}{88\,697.238\,974} \approx 98.989\%$$

where σ_i is the standard deviation of the fitness of the population after initialization and σ_X is the standard deviation of the fitness of the population after applying the subtree crossover operator.

Diversity here is a measure of population's dispersion, and a decline in diversity may signal that the population is not converging towards a solution (too much diversity) or is converging prematurely (too little diversity).

In the following section, we discuss the mutation operator, which can be used to introduce diversity into the population, thereby preventing premature convergence.

Mutation

Mutation, another crucial genetic operator, introduces new genetic material into the population, thus maintaining genetic diversity and preventing premature convergence to suboptimal solutions. In the context of GP, the mutation operator modifies a program in the population, while ensuring the resultant individual's syntactic correctness.

In tree-based GP, a common form of mutation is the *point mutation* [11, 37], which selects a random node from an individual and replaces it with a random primitive with the same arity. This operator is similar to the bit-flip mutation operator used on section 1.2.4 on page 12. As with bit-flip mutation, point mutation can also be applied

with a certain probability to each node in an individual, meaning that more than one node can be mutated in a single individual.

Suppose we mutate all the individuals in the population resulting from the crossover operation in section 1.3.4 on page 24, and that exactly one node is mutated in each individual. Let the selected nodes be $\clubsuit = \sin$ in $\mathbf{I}_2$, $\spadesuit = 7$ in $\mathbf{I}_3$, $\heartsuit = 5$ in $\mathbf{O}_1$, and $\diamondsuit = 2$ in $\mathbf{O}_2$. Then, a possible result of applying the point mutation operator can be:

$$M\left(\begin{bmatrix} I_2 \\ I_3 \\ O_1 \\ O_2 \end{bmatrix}\right) = M\left(\begin{bmatrix} 7 - (5 + \clubsuit(x)) \\ \spadesuit + 2 \\ \heartsuit \cdot 7 \\ x^{\diamondsuit} - (5 + \sin(x)) \end{bmatrix}\right) = \left(\begin{bmatrix} 7 - (5 + \clubsuit'(x)) \\ \spadesuit' + 2 \\ \heartsuit' \cdot 7 \\ x^{\diamondsuit'} - (5 + \sin(x)) \end{bmatrix}\right) = \left(\begin{bmatrix} 7 - (5 + \cos(x)) \\ 6 + 2 \\ 6 \cdot 7 \\ x^3 - (5 + \sin(x)) \end{bmatrix}\right)$$

Here, $\clubsuit'$, $\spadesuit'$, $\heartsuit'$, and $\diamondsuit'$ are random primitives with the same arity as $\clubsuit$, $\spadesuit$, $\heartsuit$, and $\diamondsuit$, respectively. That being, $\clubsuit' = \cos$, $\spadesuit' = 6$, $\heartsuit' = 6$, and $\diamondsuit' = 3$.

The fitness of the individuals in the population after applying the subtree mutation operator is then evaluated. The results of this fitness evaluation are shown in **??** on page ??. A summary of the fitness of the population is presented in **??** on page ??.

Generation 1

Individual	Program	Fitness
$\mathbf{I}_2$	$7 - (5 + \sin(x))$	137.398 836
$\mathbf{I}_3$	$7 + 2$	331.924 267
$\mathbf{O}_1$	$5 \cdot 7$	1944.288 127
$\mathbf{O}_2$	$x^2 - (5 + \sin(x))$	33.740 766

Table 1.17: Population after applying the subtree crossover operator.

	Fitness	Individual
Best	33.740 766	O_2
Worst	1944.288 127	O_1
Average	611.837 999	
Standard deviation	896.858 214	

Table 1.18: Fitness summary of the population after applying the subtree crossover operator.

Just like the crossover operator, mutation can also significantly influence the fitness and diversity of the population. By generating new structures in the population, mutation can help prevent stagnation and maintain diversity, thus avoiding premature convergence to suboptimal solutions.

In the next section, we discuss the combination of crossover and mutation operators and their role in navigating the search space effectively.

Chapter 2

Relevant Work (State of the Art)

In this chapter, we will explore the current state of the art in the field of genetic algorithm frameworks. While the theory of genetic algorithms is not a recent development, the application of these algorithms continues to evolve[1] with the advancement of various programming languages and tools. Therefore, our focus in this chapter will be on current and actively developed frameworks widely used for studying and implementing genetic algorithms.

Specifically, we will look into Agile Artificial Intelligence in Pharo, DEAP, Jenetics, ECJ, and GeneticSharp. Each section will provide a brief overview of the framework along with basic code samples to highlight their syntax and outline their unique features and differences. We believe this approach will provide a comprehensive perspective on the versatility and diversity of tools available in this field.

This state-of-the-art review does not only offer insights into the current trends and tools in genetic algorithms but also sets the stage for our contribution - a genetic algorithm framework in Kotlin.

2.1 Agile Artificial Intelligence in Pharo

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[1]No pun intended.

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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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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2.6 Other Libraries

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Chapter 3

Introduction

3.1 Motivation

The birth of artificial intelligence (AI) as we understand it today can be traced back to the mid-20th century, when Alan Turing posed the provocative question: "Can machines think?" [1]. From that moment on, the field has grown dramatically, developing an extensive range of applications that continue to expand and evolve.

One of the early attempts to simulate evolution artificially dates back to 1954 when Nills Aall Barricelli [3] defined evolution as a purely statistical process. This pioneering work laid the foundations for the field of *evolutionary computation* (EC), setting the criteria for a system to be deemed evolutionary. Barricelli posited that such a system's components must be capable of reproduction and mutation, enabling evolution via natural selection or survival of the fittest.

Furthering these principles, John Holland's seminal work, *Adaptation in Natural and Artificial Systems* [4], introduced *genetic algorithms* (GA), a revolutionary approach to solving optimization problems inspired by the mechanisms of natural selection and genetics. This established the foundation for the field of *evolutionary algorithms* (EA), spurring the development of numerous techniques and algorithms, including genetic algorithms, genetic programming, and evolutionary strategies.

Despite the demonstrated success of evolutionary algorithms in solving complex optimization problems, from scheduling and data mining to machine learning and beyond, their implementation can be cumbersome, often requiring a significant amount of repetitive coding. As AI adoption continues to grow, so does the need for streamlined, user-friendly libraries and frameworks that enable efficient experimentation and implementation of these powerful algorithms.

One promising platform for the development of such a framework is the *Kotlin programming language* [31]. *Kotlin* boasts an intuitive syntax, static typing, and seamless interoperability with *Java* [22, 23, 32], making it a compelling choice for AI and EC practitioners. The language's stature has been recognized officially in Android app development [21], and it enjoys growing popularity among developers, with over 60% of Android developers now using it [20]. Additionally, Kotlin is ranked as the ninth fastest-growing language globally from 2021 to 2023, according to a study by GitHub [36], surpassing Python by 0.4%.

The Kotlin Multiplatform feature further enhances the language's appeal by enabling code sharing across a multitude of platforms, including JVM, JavaScript, Android, iOS, and native desktop applications. This capability fosters increased productivity and consistency in development work.

Given these strengths, the main goal of this thesis is to leverage *Kotlin* to design and implement a novel genetic algorithms framework, contributing to the ever-expanding usage of *Kotlin* in the AI community. We anticipate that this framework will expedite research and applications in the field, accelerating the pace of innovation in evolutionary computation.

3.2   Hyphotesis and Research Questions

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3.3   Objectives

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3.4 Methodology

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3.5 Structure

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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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6.3   Solution

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6.4 Results

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6.5   Conclusion

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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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7.3   Solution

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7.4 Results

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7.5 Conclusion

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Chapter 8

Conclusions

8.1 Summary

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8.2 Contributions

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8.3 Future Work

8.3.1 Genetic Algorithms

Genetic Operators

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8.3.2   Genetic Programming

Primitive Set

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Genetic Operators

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8.3.3   Multi-Objective Evolution

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8.3.4   Neuroevolution

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8.3.5 Coevolution

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8.3.6 Evolution Strategy

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8.3.7 Other evolutionary algorithms

Ant Colony Optimization

Artificial Immune Systems

Differential Evolution

Estimation of Distribution Algorithms

Evolutionary Programming

Grammatical Evolution

Particle Swarm Optimization

8.3.8 Crash Reproduction

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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Appendix A

Glossary

In this appendix we present a glossary of terms used throughout this document that may be unfamiliar to the reader and are not defined in the main text.

A

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

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

Definition A.3 (Arity). *The number of arguments a function takes, or the number of children a node has in a tree.*

C

Definition A.4 (Chromosome). *Representation of a single column of genetic information of a candidate solution to a given optimization problem.*

Formally, a chromosome is a vector $\mathbf{c} = (g_1, g_2, \ldots, g_n)$, where g_i is a gene (see definition A.7).

E

Definition A.5 (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.6 (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.7 (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.8 (Generation)**.** *Number of iterations performed by an evolutionary algorithm.*

Definition A.9 (Genotype)**.** *Representation of the full genetic information of a candidate solution to a given optimization problem.*

Formally, a genotype is a matrix $\mathbf{G} = (\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_n)$, where $\boldsymbol{c}_i$ is a chromosome (see definition A.4 on the previous page).

I

Definition A.10 (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.9) and $\mathbf{f}$ is the fitness value of the individual.

M

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

P

Definition A.13 (Parameter optimization)**.** *Optimization problem where the solution is a set of parameters that optimize a given function.*

Definition A.14 (Phenotype)**.** *Same as definition A.10.*

Definition A.15 (Population)**.** *Set of candidate solutions to a given optimization problem.*

Definition A.16 (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.17 (Search space)**.** *Set of all candidate solutions to a given optimization problem.*

Definition A.18 (Selector)**.** *See definition 1.4 on page 9.*

V

Definition A.19 (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 55.

B.1 Ackley Function

In the field of optimization, especially within evolutionary algorithms and swarm intelligence, the *Ackley function* serves as a prevalent benchmark function. Named after *David H. Ackley*, who introduced it during his research,[1] this function is particularly challenging for optimization algorithms due to its property of possessing a large number of local minima, despite having a single global minimum. This trait can often cause such algorithms to become entrapped in local minima.

Definition B.1 (Ackley Function). *The* Ackley Function, *denoted as $f : \mathbb{R}^2 \to \mathbb{R}$, is mathematically expressed as:*

$$f(x, y) = -20\,e^{-0.2\sqrt{0.5(x^2+y^2)}} - e^{0.5\,[\cos(2\pi x)+\cos(2\pi y)]} + e + 20 \tag{B.1}$$

This function is evaluated within the range x, $y \in [-5, 5]$.

The global minimum of the Ackley function is located at $f(0, 0) = 0$. Visualizations of the Ackley function are depicted as a contour plot and a surface plot in fig. B.1.
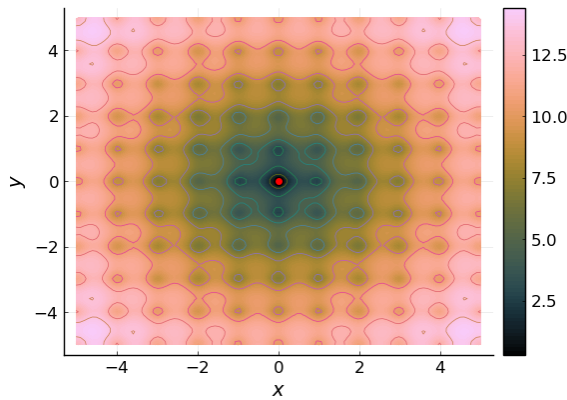
(a) Contour plot of the Ackley Function
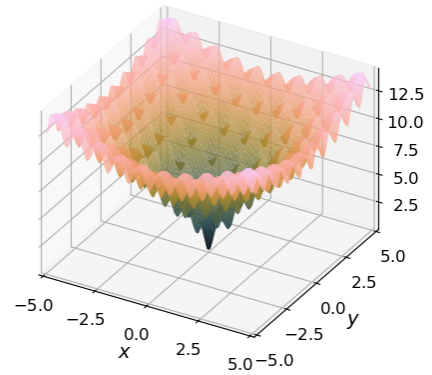
(b) Surface plot of the Ackley Function

Figure B.1: Illustrations of the Ackley Function with the global minimum indicated by a red dot.

---

[1]Ackley, D. H. (1987) "A connectionist machine for genetic hillclimbing", Kluwer Academic Publishers, Boston MA.

B.2 Beale Function

Unveiled by Beale in 1958[2], the Beale function is recognized for its multimodal characteristics and sharp peaks that define the domain's corners.

Definition B.2 (Beale Function). *The* Beale Function, *symbolized as $f : \mathbb{R}^2 \to \mathbb{R}$, is expressed by the equation:*

$$f(x, y) = (1.5 - x + xy)^2 + (2.25 - x + xy^2)^2 + (2.625 - x + xy^3)^2 \tag{B.2}$$

It's evaluated within the domain $x,\, y \in [-4.5,\, 4.5]$.

The global minimum of the Beale function is found at $f(3,\, 0.5) = 0$. Both contour and surface plots of the Beale function are depicted in fig. B.2.
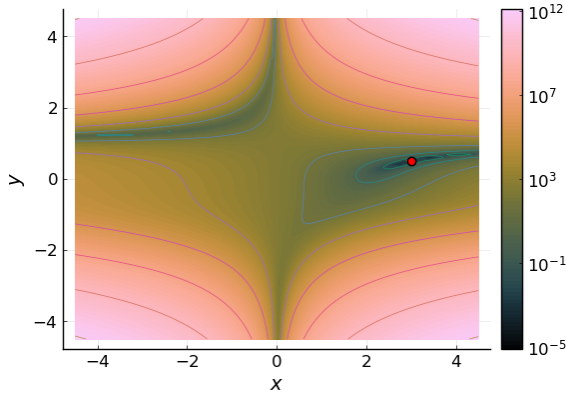
(a) Contour plot of the Beale Function   (b) Surface plot of the Beale Function
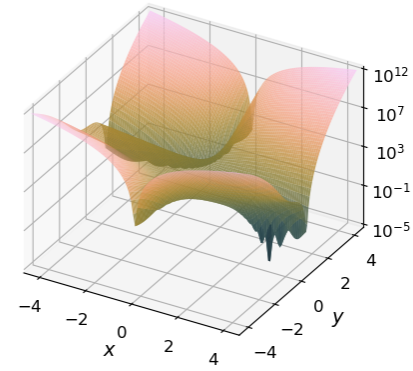
Figure B.2: Visual representation of the Beale Function

B.3 Booth Function

The Booth function is a quadratic test problem used in the optimization field, specifically tailored for algorithms that handle two-dimensional search spaces.

Definition B.3 (Booth Function). *The* Booth function, $f : \mathbb{R}^2 \to \mathbb{R}$, *is defined as:*

$$f(x, y) = (x + 2y - 7)^2 + (2x + y - 5)^2 \tag{B.3}$$

where:

- *$x,\, y \in \mathbb{R}$ represent the decision variables.*

The global minimum of the Booth function is $f(1, 3) = 0$. The function is usually constrained to the square $[-10, 10]^2$. A contour plot and a surface plot of the Booth function are illustrated in fig. B.3 on the next page.

B.4 Bukin Function N.6

The *Bukin function N.6*, a two-dimensional benchmark problem, is renowned for its inherent complexity and frequent utilization in assessing optimization algorithms. Notable for a sharply defined, deep valley, the Bukin function N.6 presents distinct hurdles for optimization techniques owing to its abrupt discontinuity and non-differentiability at $x = 0$.

---

[2]Beale, E. M. (1958). "On an Iterative Method for Finding a Local Minimum of a Function of More than One Variable".
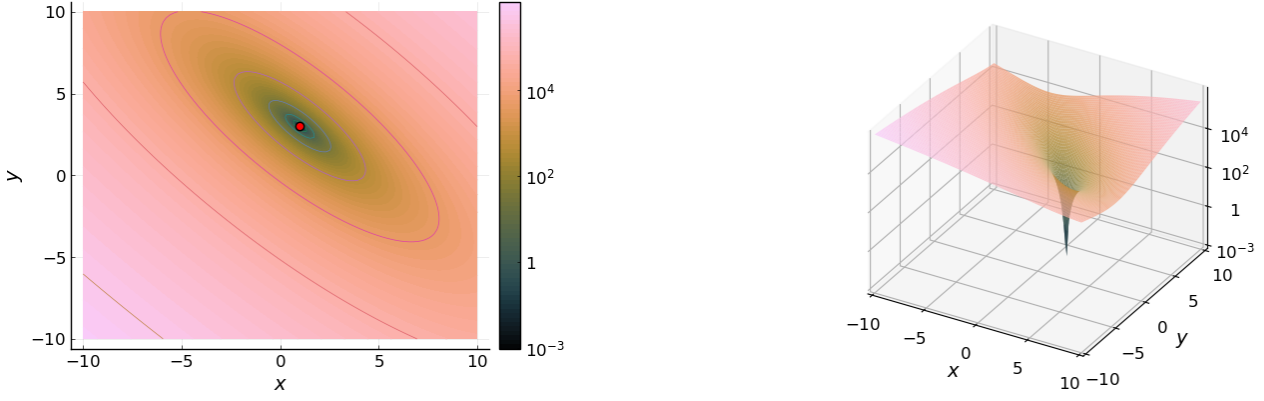
Figure B.3: Booth Function

Definition B.4 (Bukin Function N.6)**.** *The* Bukin function N.6, *given by* $f : \mathbb{R}^2 \to \mathbb{R}$*, is mathematically represented as:*

$$f(x, y) = 100\sqrt{|y - 0.01x^2|} + 0.01|x + 10| \tag{B.4}$$

The decision variables, $x, y \in \mathbb{R}$*, typically have the prescribed domains:* $-15 \leq x \leq -5$ *and* $-3 \leq y \leq 3$ *respectively.*

The function attains its global minimum at $(x, y) = (-10, 1)$, yielding a value of zero. The Bukin function N.6, due to its unique characteristics, offers a striking visualization. A profound ridge, extending diagonally across the domain, forms a distinguishing feature. The contour and surface plots illustrating the Bukin function N.6 are presented in fig. B.4.

(a) Contour plot of Bukin function N.6

(b) Surface plot of Bukin function N.6
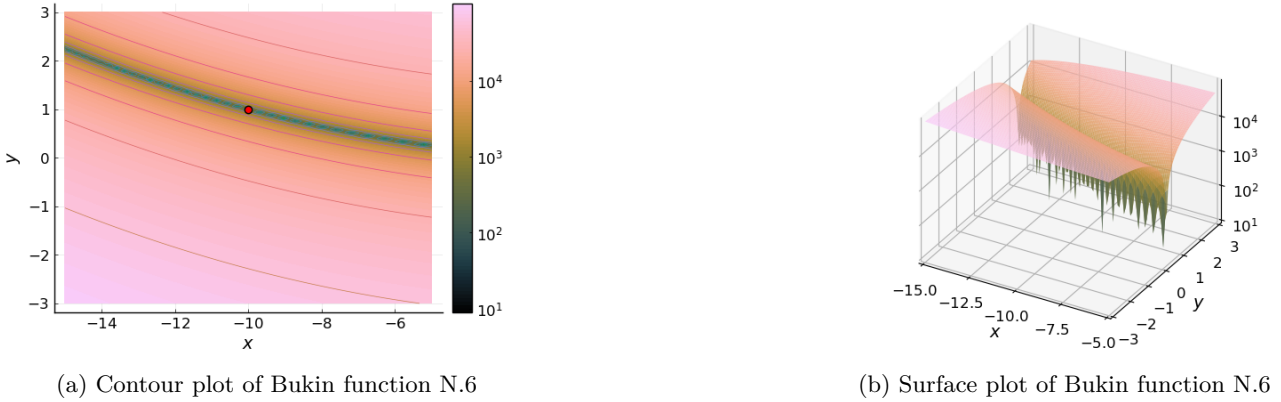
Figure B.4: Contour and Surface Plots of Bukin Function N.6

B.5 The Cross-in-Tray Function

The Cross-in-Tray function, known for its utility in testing optimization algorithms, poses a challenge due to its numerous local minima and four identical global minima, thereby making it an effective benchmark for evaluating an algorithm's capability to escape local optima and locate global optima.

Definition B.5 (Cross-in-Tray Function)**.** *The* Cross-in-Tray Function*, denoted as a mapping from* $\mathbb{R}^2 \to \mathbb{R}$*, is formally defined as:*

$$f(x,\, y) = -0.0001 \left[\left| \sin(x) \sin(y) \exp\left(\left| 100 - \frac{\sqrt{x^2 + y^2}}{\pi} \right| \right) \right| + 1 \right]^{0.1} \tag{B.5}$$

This function is usually evaluated over the domain $-10 \le x, y \le 10$.

This function exhibits four identical global minima located at $(\pm 1.349\,41, \pm 1.349\,41)$, with each of these points having the function value of $f(x,\, y) = -2.062\,61$.

In fig. B.5, contour and surface plots are presented to provide a visual understanding of the function's intricate topology.
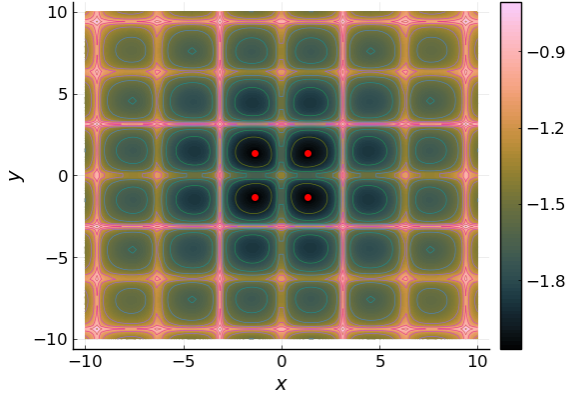
(a) Contour plot showcasing the complex landscape of the Cross-in-Tray function. The red dot denotes the location of the global minimum.
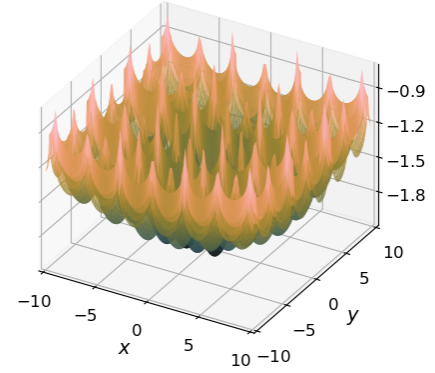
(b) Surface plot providing a 3D representation of the Cross-in-Tray function, enhancing the visualization of its global and local minima.

Figure B.5: Contour and surface plots illustrating the topological complexity of the Cross-in-Tray function

B.6   Easom Function

The *Easom function* is a well-known unimodal benchmark function employed in the evaluation of optimization algorithms. It gains its name from Charles Easom and is distinctively recognized by its 'needle'-like global minimum. This feature presents a demanding task for optimization algorithms due to its confined optimal search space.

Definition B.6 (Easom Function)**.** *The* Easom function*, defined for $f : \mathbb{R}^2 \to \mathbb{R}$, is formally expressed as:*

$$f(x,\, y) = -\cos(x)\cos(y)\exp\left(-((x-\pi)^2 + (y-\pi)^2)\right) \tag{B.6}$$

Here, $x,\, y \in \mathbb{R}$ constitute the decision variables.

The global minimum of the Easom function is situated at the coordinates $f(\pi,\, \pi) = -1$.

The intricate structure and narrow optimal space of the Easom function are clearly revealed in its contour and surface plots.

B.7   Eggholder Function

The *Eggholder function* is a widely-used non-convex function in the field of optimization, particularly for benchmarking optimization algorithms. The function is notorious for its multitude of local minima, presenting a complex search space that challenges the robustness and capability of an optimization algorithm to locate the global minimum.
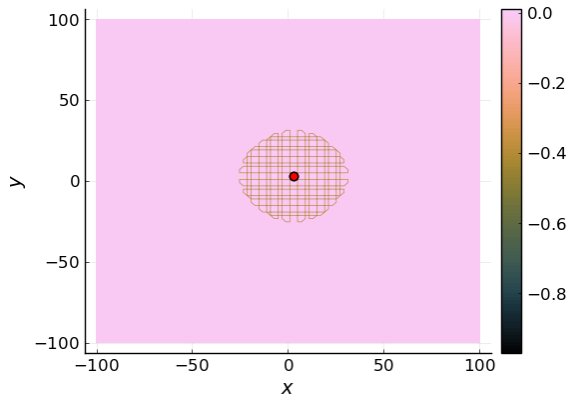
(a) Contour plot of the Easom function with the global minimum represented by the red dot
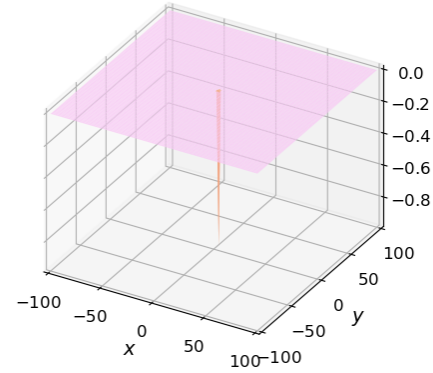
(b) Surface plot of the Easom function
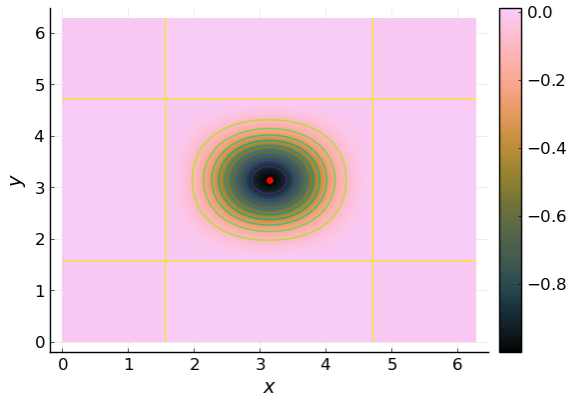
(c) Contour plot of the Easom function in the vicinity of the global minimum, $[0, 2\pi]$.
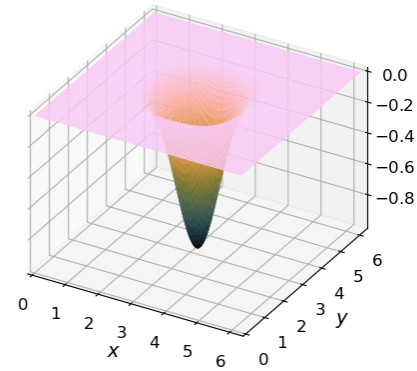
(d) Surface plot of the Easom function in the vicinity of the global minimum, $[0, 2\pi]$.

Figure B.6: Contour and surface visualizations of the Easom function

Definition B.7 (Eggholder Function). *Formally, the Eggholder Function is represented as a mapping $\mathbb{R}^2 \to \mathbb{R}$, and is mathematically defined as:*

$$f(x, y) = -(y + 47) \sin\left(\sqrt{\left|\frac{x}{2} + (y + 47)\right|}\right) - x \sin\left(\sqrt{|x - (y + 47)|}\right) \tag{B.7}$$

where the typical domain for evaluation spans $-512 \leq x, y \leq 512$.

The Eggholder function's global minimum resides at $(512, 404.2319)$, delivering a function value of $f(x, y) = -959.6407$.

Visual representations of the function can enhance understanding of its complexity. Figure fig. B.7 on the following page offers both contour and surface plots of the Eggholder function.

B.8 Goldstein-Price Function

The *Goldstein-Price function*, believed to be proposed by individuals named Goldstein and Price, is a challenging multimodal function recognized for its landscape densely populated with local minima. This function serves as a standard benchmark in the field of optimization, testing the efficacy of various algorithms. The precise origins of this function, however, remain elusive in academic literature.
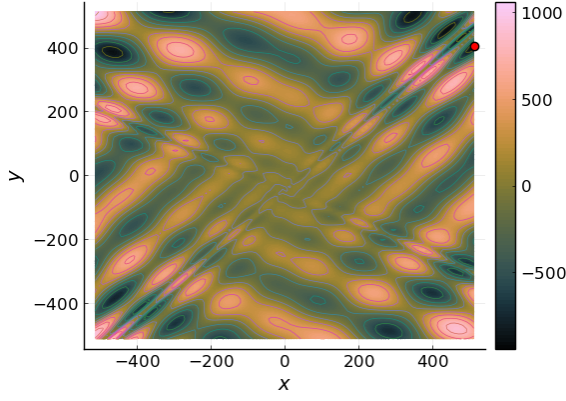
(a) A contour plot of the Eggholder function, displaying its intricate landscape. The red dot signifies the location of the global minimum.
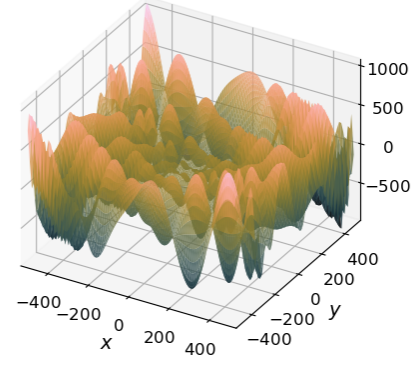
(b) A 3D surface plot of the Eggholder function, allowing a more comprehensive visualization of its local and global minima.

Figure B.7: Contour and surface visualizations of the Eggholder function, showcasing its intricate topology

Definition B.8 (Goldstein-Price Function). *The Goldstein-Price function, denoted as $f : \mathbb{R}^2 \to \mathbb{R}$, is formally articulated as follows:*

$$f(x, y) = \left[1 + (x + y + 1)^2 \cdot (19 - 14x + 3x^2 - 14y + 6xy + 3y^2)\right] \\ \cdot \left[30 + (2x - 3y)^2 \cdot (18 - 32x + 12x^2 + 48y - 36xy + 27y^2)\right] \tag{B.8}$$

The function's global minimum is located at $f(x^*, y^*) = 3$ with $(x^*, y^*) = (0, -1)$. Evaluations of the Goldstein-Price function are typically performed within the range $x, y \in [-2, 2]$.
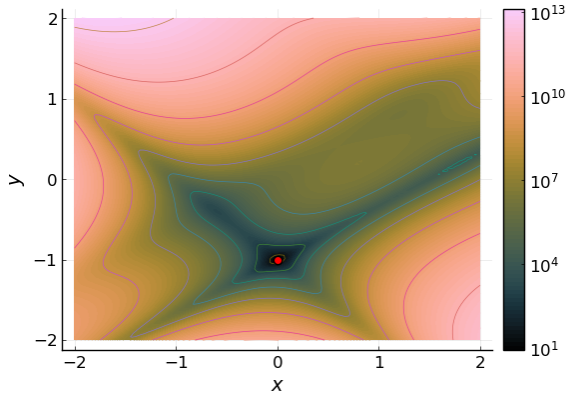
(a) Contour plot.
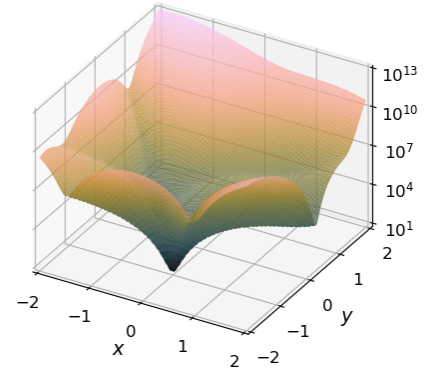
(b) Surface plot.

Figure B.8: Visual representations of the Goldstein-Price function

B.9 Himmelblau's Function

The *Himmelblau's function*, attributed to David Mautner Himmelblau,[3] is a significant benchmark function in the realm of optimization, renowned for its complex multi-modal nature. Himmelblau, an American engineer, made substantial contributions to systems engineering and optimization theory.

---

[3]Himmelblau, D. (1972). "Applied Nonlinear Programming". McGraw-Hill. ISBN 0-07-028921-2.

Definition B.9 (Himmelblau's Function)**.** *The* Himmelblau's function*, symbolized as* $f : \mathbb{R}^2 \to \mathbb{R}$*, is formally described as:*

$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2 \tag{B.9}$$

Here, $x, y \in \mathbb{R}$ *are the decision variables, with the domains* $\{x \mid -10 \le x \le 10\}$ *and* $\{y \mid -10 \le y \le 10\}$.

Distinguished by its four minima, located at $(3, 2)$, $(-2.805118, 3.131312)$, $(-3.779310, -3.283186)$, and $(3.584428, -1.848126)$, all roughly equating to zero, this function showcases its complexity.

Figure B.9 portrays the multi-modal landscape of Himmelblau's function through contour and surface plots, underlining its inherent intricacy, and as such, its utility in the evaluation of optimization techniques.
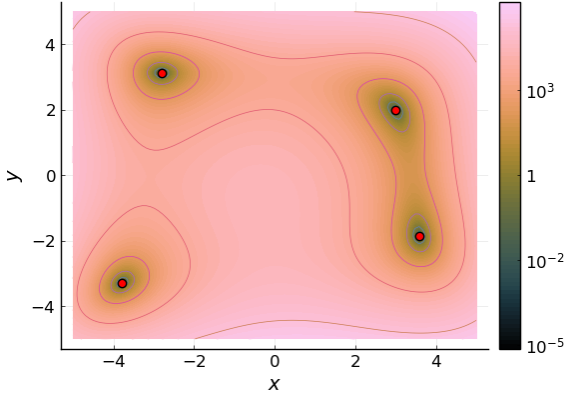
(a) Contour plot of Himmelblau's function, the minima are signified by the red dots
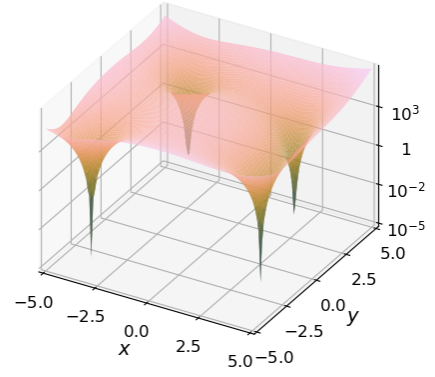
(b) Surface plot of Himmelblau's function

Figure B.9: The detailed multi-modal structure of Himmelblau's function illustrated through contour and surface plots

B.10   Lévi Function N.13

The *Lévi function N.13* is a noteworthy two-dimensional function frequently employed in the field of optimization algorithms for performance testing. Its complex, sinuous landscape, teeming with numerous local minima, presents a significant challenge to optimization procedures.

Definition B.10 (Lévi Function N.13)**.** *The* Lévi function N.13*, denoted as* $f : \mathbb{R}^2 \to \mathbb{R}$*, is formally defined as follows:*

$$f(x, y) = \sin^2(3\pi x) + (x - 1)^2 \cdot (1 + \sin^2(3\pi y)) + (y - 1)^2 \cdot (1 + \sin^2(2\pi y)) \tag{B.10}$$

where $x, y \in \mathbb{R}$ *are the decision variables.*

The Lévi function N.13 finds its global minimum at $f(1, 1) = 0$. The complex topology of this function is visually captured in the contour and surface plots shown in Figure B.10.

B.11   Matyas Function

The *Matyas function*, known for its simplicity and convex nature, is a standard test problem in the field of optimization algorithms. Despite its apparent simplicity, it provides invaluable insights into an algorithm's performance and behavior.
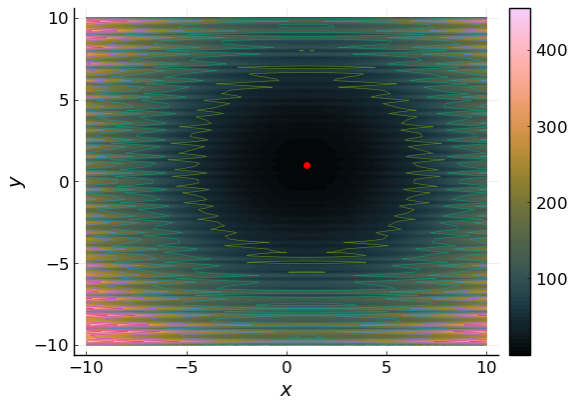
(a) Contour plot of the Lévi function N.13
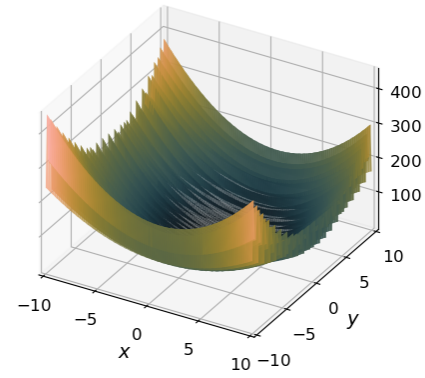
(b) Surface plot of the Lévi function N.13

Figure B.10: Contour and Surface Representations of the Lévi Function N.13

Definition B.11 (Matyas Function). *The* Matyas function*, denoted as* $f : \mathbb{R}^2 \to \mathbb{R}$*, is formulated as:*
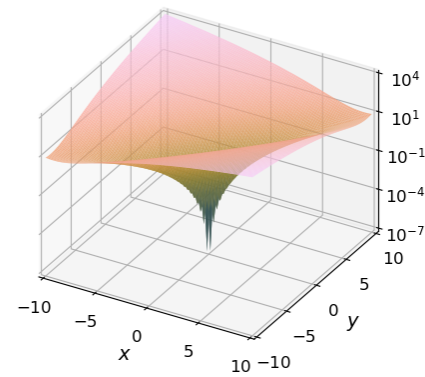
$$f(x,\, y) = 0.26(x^2 + y^2) - 0.48xy \tag{B.11}$$

where:

- $x,\, y \in \mathbb{R}$ *denote the decision variables.*

The Matyas function reaches its global minimum at the origin, with $f(0,0) = 0$. The contour and surface visualizations of the Matyas function, offering perspectives on its topographical attributes, are presented in fig. B.11.
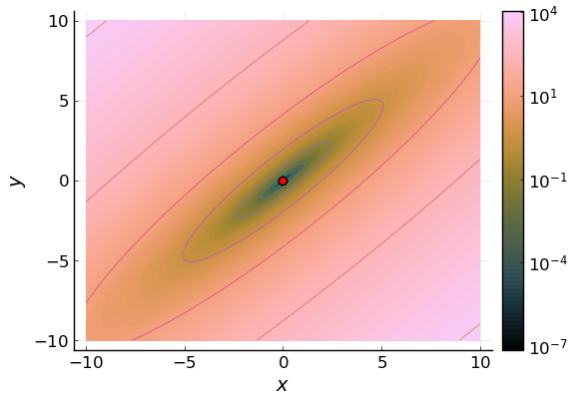
(a) Contour plot of the Matyas function with a red dot indicating the global minimum

(b) Surface plot of the Matyas function

Figure B.11: Contour and Surface Visualizations of the Matyas Function

B.12   Rastrigin Function

The Rastrigin function, first proposed by Rastrigin in 1974[4], is a prominent non-convex function utilized as a benchmark for optimization algorithms. This function is a classic example of non-linear multimodal optimization problems, known for their complexity due to the abundance of local minima.

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[4]Rastrigin, L. A. (1974). "Systems of extremal control." Mir, Moscow.

Definition B.12 (Rastrigin Function)**.** *The* Rastrigin function*, denoted as* $f : \mathbb{R}^n \to \mathbb{R}$*, is formulated as:*

$$f(\mathbf{x}) = An + \sum_{i=1}^{n} \left[\mathbf{x}_i^2 - A\cos(2\pi\mathbf{x}_i) \right] \tag{B.12}$$

Here,

- *n is the number of dimensions.*

- *$\mathbf{x}$ is a vector composed of n real numbers.*

- *A is a constant, typically set to 10.*

The global minimum of the Rastrigin function is situated at $\mathbf{x}^* = (0, \ldots, 0)$, with $f(\mathbf{x}^*) = 0$. It's particularly challenging due to its numerous local minima, distributed regularly throughout the search space. The function is predominantly evaluated within the hypercube $\mathbf{x} \in [-5.12, 5.12]^n$.

Visualizations of the Rastrigin function for $n = 2$ are presented in fig. B.12, showcasing both the contour plot and the 3D surface plot.
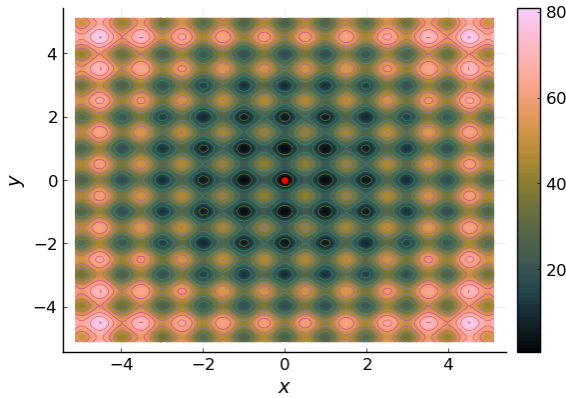
(a) Contour plot of the Rastrigin Function.
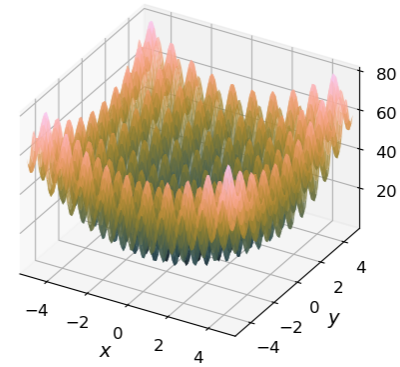
(b) 3D surface plot of the Rastrigin Function.

Figure B.12: Visualizations of the Rastrigin Function for $n = 2$, with the global minimum marked by a red dot.

B.13 The Rosenbrock Function

Introduced by Howard H. Rosenbrock in 1960[5], the Rosenbrock function is a non-convex function that serves as a benchmark for optimization algorithms. Despite its simplicity, it poses a challenge due to its characteristic landscape, a long, narrow, parabolic-shaped flat valley. While finding the valley is relatively simple, converging to the global minimum within it is notably difficult.

Definition B.13 (Rosenbrock function)**.** *The* Rosenbrock function*, denoted as* $f : \mathbb{R}^n \to \mathbb{R}$*, is defined by the following equation:*

$$f(\mathbf{x}) = \sum_{i=1}^{n-1} \left[100(\mathbf{x}_{i+1} - \mathbf{x}_i^2)^2 + (1 - \mathbf{x}_i)^2 \right] \tag{B.13}$$

In this equation:

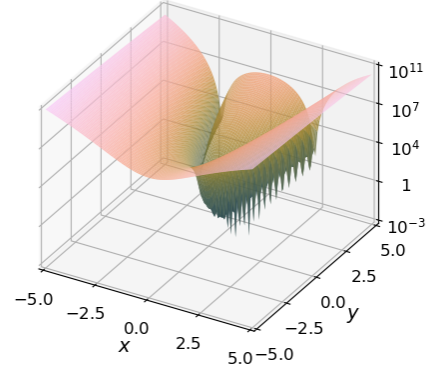- *n is the number of dimensions.*

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[5]Rosenbrock, H.H. (1960). "An automatic method for finding the greatest or least value of a function". The Computer Journal. 3 (3): 175-184. doi:10.1093/comjnl/3.3.175. ISSN 0010-4620.

- **x** *is a vector composed of n real numbers.*

The Rosenbrock function's global minimum is at $f(\mathbf{x}^*) = 0$, corresponding to the point $\mathbf{x}^* = (1, \ldots, 1)$. To illustrate the function's behavior for $n = 2$, fig. B.13 presents a contour plot and a surface plot.
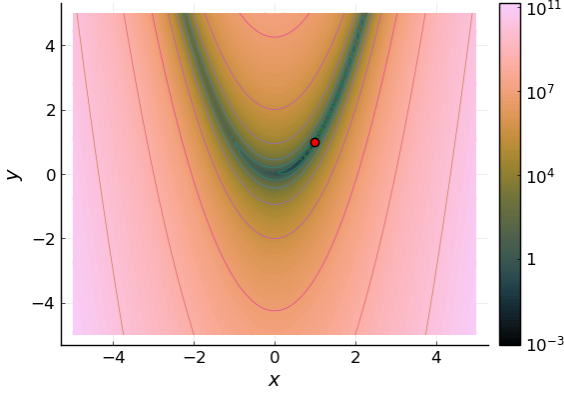
(a) Contour plot of the Rosenbrock function.   (b) Surface plot of the Rosenbrock function.

Figure B.13: Rosenbrock Function for $n = 2$, the red dot indicates the global minimum.

B.14   The Sphere Function

The sphere function serves as a prominent benchmark problem in the realm of optimization algorithms. This convex function's simplicity and well-defined nature make it ideal for gauging the performance of such algorithms.

Definition B.14 (Sphere Function). *The* sphere function, *denoted as $f : \mathbb{R}^n \to \mathbb{R}$, is formally described as:*

$$f(\mathbf{x}) = \sum_{i=1}^{n} \mathbf{x}_i^2 \tag{B.14}$$

Herein:

- $n \in \mathbb{N}$ *signifies the number of dimensions.*

- $\mathbf{x}_i \in \mathbb{R}$ *represents the i-th element of the vector* **x**.

The global minimum of the sphere function occurs at $f(\mathbf{x}^*) = 0$ with the input vector $\mathbf{x}^* = (0, \ldots, 0)$. The contour and surface plots showcasing the behavior of the sphere function for a two-dimensional input ($n = 2$) are illustrated in fig. B.14 on the facing page.
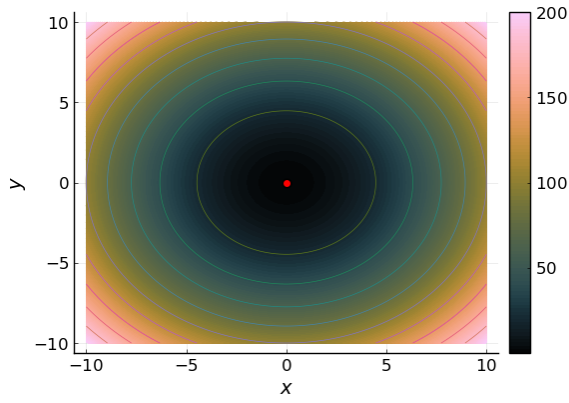
B.15   Three-Hump Camel Function

The *Three-Hump Camel function*, colloquially termed as the camel-back function, serves as a standard benchmark in the optimization algorithms testing landscape. This two-dimensional function earns its name from the characteristic tri-modal hump visual pattern it presents in a three-dimensional space, bearing resemblance to a camel's back.

Definition B.15 (Three-Hump Camel Function). *The* Three-Hump Camel function, *depicted as $f : \mathbb{R}^2 \to \mathbb{R}$, is formally expressed as:*
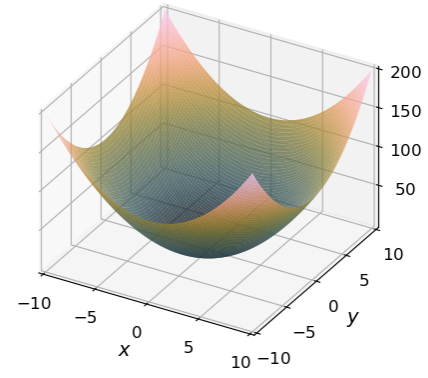
$$f(x, y) = 2x^2 - 1.05x^4 + \frac{x^6}{6} + xy + y^2 \tag{B.15}$$

*where $-5 \leq x \leq 5$ and $-5 \leq y \leq 5$.*

(a) Contour plot of the Sphere Function.

(b) Surface plot of the Sphere Function.

Figure B.14: Visual Representation of the Sphere Function with $n = 2$

The Three-Hump Camel function exhibits its global minimum at the origin, $f(0, 0) = 0$. Although its form appears straightforward, the function's multiple local optima pose considerable challenges for optimization algorithms, making it an excellent test case.
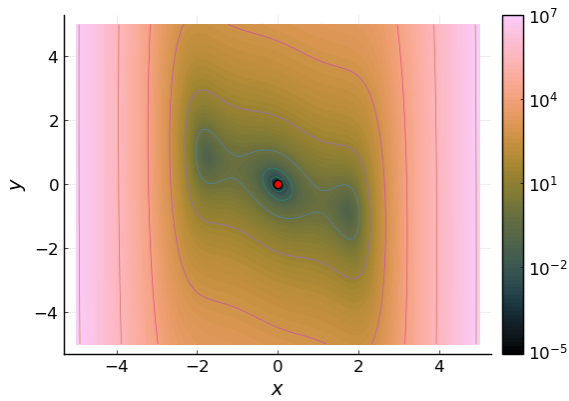
(a) Contour plot of the Three-Hump Camel function. The red dot signifies the global minimum.
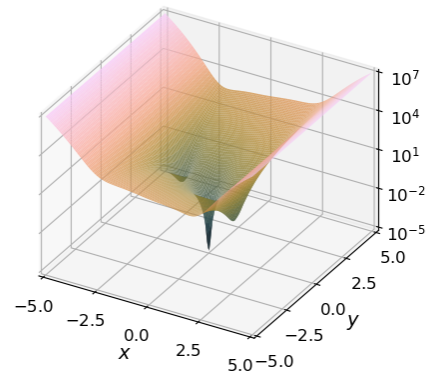
(b) Surface plot showcasing the characteristic tri-modal humps of the Three-Hump Camel function.

Figure B.15: Contour and surface visualizations of the Three-Hump Camel function
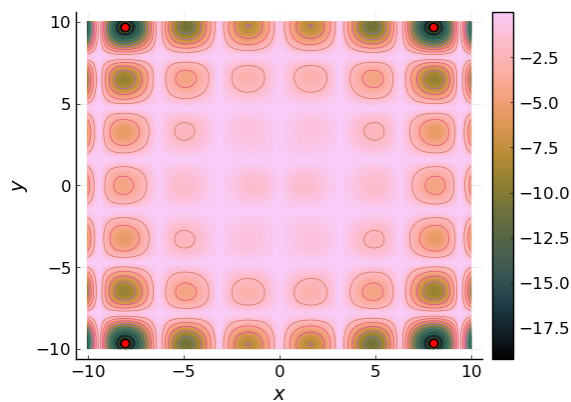
B.16   Hölder Table Function

The *Hölder Table function* is a two-dimensional real-valued function employed in various branches of mathematical analysis. Due to its intriguing properties and complex topography, it serves as a valuable tool for function approximation and numerical analysis studies.

Definition B.16 (Hölder Table function)**.** *The* Hölder Table function, *designated as* $f : \mathbb{R}^2 \to \mathbb{R}$, *is described by the equation*
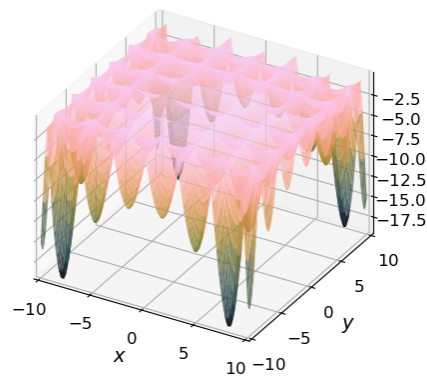
$$f(x, y) = - \left| \sin(x) \cos(y) \exp\left(\left| 1 - \frac{\sqrt{x^2 + y^2}}{\pi} \right| \right) \right| \tag{B.16}$$

This function is defined for $-10 \leq x, y \leq 10$.

The Hölder Table function peaks globally at $f(x^*, y^*) = 19.208\,5$ for $x^* = \pm 8.05502$ and $y^* = \pm 9.66459$. Its intricately structured landscape can be vividly illustrated through contour and surface plots, as depicted in fig. B.16.

(a) Contour visualization of the Hölder Table function. The global minimum points are denoted by red dots.

(b) Three-dimensional surface representation of the Hölder Table function.

Figure B.16: The Complex Topography of the Hölder Table Function: Contour and Surface Representations

Appendix C

Additional Listings

This appendix contains additional listings of the source code used in this thesis that are not essential to the understanding of the thesis. The listings are included here for completeness.

Listing C.1: Calculation of $|\mathbb{T}_{\leq 5}(\mathcal{T}, \mathcal{F})|$ for $\mathcal{T} = \{x, c\}$ and the set $\mathcal{F} = \{+, -, \times, /, \sin, \cos, \text{pow}\}$ using the *Julia* programming language.

```julia
arities = [2, 2, 2, 2, 1, 1, 2] # A ({+, −, ×, /, sin, cos, pow}) = {2, 2, 2, 2, 1, 1, 2}
terminals_size = 8   # |T| = |{x, 1, 2, 3, 4, 5, 6, 7}| = 8
# |T≤h|
t_leq(h :: Int) :: Int128 = if h == 0 # |T| if h = 0
  terminals_size
else   # (∑_{h=0}^{h−1} ∑_{f∈F} |T_h|^{A(f)}) + |T| if h > 0
  c_sum = terminals_size
  for i = 0:h - 1
    c_sum = c_sum + sum(t(i) .^ arities)
  end
  c_sum
end
# |T_h|
t(h :: Int) :: Int128 = if h == 0 # |T| if h = 0
  terminals_size
else   # ∑_{f∈F} |T_{h−1}|^{A(f)} if h > 0
  sum(t(h - 1) .^ arities)
end
res = t_leq(5)   # |T≤5(T, F)|
```

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