

Bio-inspired Computing in R

Final Year Dissertation

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**Declaration of own work**

I, Ryan Porteous confirm that this work submitted for assessment is my own and is expressed in my own words. Any uses made within it of the works of other authors in any form (e.g., ideas, equations, figures, text, tables, programs) are properly acknowledged at any point of their use. A list of the references employed is included.

Signed:

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Date: 23/04/18

**Abstract**

R has become the first-choice language for data scientists. However, it is typically not the first choice for people developing and implementing bio-inspired algorithms. Consequently, it can be hard for data scientists to make use of bio-inspired methods. This project will look at the current availability of bio-inspired algorithms in R, identify holes in the provision, and develop a package to fill in one of these holes.

**Acknowledgements**

Firstly, I would like to thank my supervisor, Dr Michael Lones for providing his time, feedback and continuous guidance throughout the project. Also, for proposing the topic and supporting my design choices as the project progressed. Finally, for introducing me to the exciting area of Genetic Programming.

I would also like to thank my second reader, Dr Katrin Lohan, also for her feedback during the project.

Finally, I would like to thank my friends and family for providing support through my studies and always encouraging me to push myself further.

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# Introduction

## Aims and Motivations

Bio-inspired computing is a field which takes inspiration for its algorithms from a variety of nature’s systems such as evolution, and the way populations of animals interact with each other in an environment. This collection of algorithms can be applied to various areas and can also be used as a searching method to solve NP-hard problems due to the way the search space can be explored. R is a programming language which has become more popular in recent years as can be seen in the TIOBE Index (TIOBE, 2017). It is among the first-choice of languages for statisticians and data miners, with competition being mainly from Python, but is not the first-choice for those who are interested in implementing bio-inspired algorithms. Due to this, it can be hard for R users to apply bio-inspired methods to problem due to their limited availability.

The primary aims of this project can be defined as:

1. **Investigate the availability of bio-inspired algorithms in R**

I will begin by identifying the main areas of bio-inspired computing and searching for implementations of these algorithms available through the Comprehensive R Archive Network (CRAN). CRAN is a network which provides a central platform for R users to upload the software packages that they have developed and provide access to them for other users.

1. **Identify implementations to be improved or built upon, and areas where no solution exists**

From the implementations found in the previous step, I will assess how the solution has been implemented, what the solution provides and if it can be improved upon. Where no solution exists, this will be identified as an area that can be developed.

1. **To learn the fundamentals of R**

As mentioned previously R is among the first-choice of languages for data mining which is a field I am interested in. Thus, I aim to learn the fundamentals of the R language and gain practical experience of using them.

1. **Produce an R Package to improve the availability of bio-inspired tools for R**

A package will be developed to improve upon an existing solution or to provide a solution where no solution exists. I will aim to follow the best practices when creating this package to maintain a high standard of code quality and maintainability.

1. **Produce an implementation of Cartesian Genetic Programming**

This is the area I have identified as needing improvement and have chosen to produce a package to provide access to this area.

1. **Release the package on CRAN**

I aim to release the package on CRAN so that the package will be freely available for other R users to make use of.

1. **Evaluate the usability of the package**It is essential that the package is easy for users to use with no previous knowledge of Genetic Programming. To provide this, a guide will be distributed with the package and a Usability Study will be carried out on this guide.
2. **Evaluate the functionality of the package and identify areas for improvement**

Evaluation is an important stage of software development and I plan to incorporate it into this project. I will assess what the created package provides and what could be added to it. I will also assess the performance of the package and suggest possible improvements.

## Overview of Document

In the document that follows, I will cover the research carried out in order to identify the area of bio-inspired computing that could use improvement. I will then show how I was able to develop and release a package to provide provision to this area, making sure to emphasise what areas of the package work well, and what areas could use improvement. Then the usability study will be discussed which highlighted that there are issues with the software guide that I have produced but still allows users with no background in the area, or with R to use it which is an important factor when releasing software. Finally, a self-reflective section will be covered where I will compare what my initial goals were to what I have achieved, and how I think my skills have developed through the project.

# Bio-inspired Computing

## Genetic Algorithms

Genetic Algorithms (GAs) are an evolutionary search heuristic which takes inspiration from the process of natural selection (Darwin & Wallace, 1998). The algorithm uses a population of solutions to the given problem where each solution is given a fitness value which defines how suitable this solution is in this domain. The fitness value which can either be maximised or minimised is given from a fitness function which is defined depending on the scenario. This fitness value is used in the selection process which mimics natural selection (Darwin & Wallace, 1998). Each solution has a probability relative to their fitness value of being chosen as a parent. Parent is a term used to refer to a solution from the current generation which will be used in the crossover process to produce a child. A child is a solution that will carry over to the next generation. Crossover is a process, or operator, where two parents are used to generate a child solution. The goal is to combine both parents while removing the negative characteristics of the parents so that the child will have an improved fitness. Another operator which is used is mutation. This randomly alters the child solution and can help to explore the search space quickly (Sivanandam & Deepa, 2008). One implementation of this according to (Moon et al. 2002) is to choose two random values in the solution and to swap them. This process is repeated until a pre-defined number of generations have completed, or a set number of generations have passed with no improvement.

Genetic Algorithms are used for solving optimisation problems which are problems that involve finding the optimal solution in a search space of all possible solution. It can be difficult to find the globally optimal solution due to the search landscape itself having many local maxima, noise or from other constraints according to (Kramer, 2017). The performance of GA’s are reduced significantly in problems which have very high dimensions and where the evaluation of the fitness function becomes very computationally intensive (Kar, 2016).

## Cellular Automata

Although Cellular Automata (CA) were originally outlined by von Neumann and Stanislaw Ulam with the motivation of modelling biological self-reproduction (Wolfram, 1983) they did not gain widespread interest until John Conway’s “Game of Life” was revealed in 1970 (Adamatzky, 2010). CA are mathematical models consisting of simple components with local interactions (Navid & Bagheri, 2013) which are made up a lattice consisting of cells. The lattice can be defined as an n-dimensional list of cells where the cells have two states, black or white. To evolve or update the lattice of cells we use discrete time where time 0 is the initial state of the lattice. In each generation, a set of rules is applied to each cell. In a one-dimensional list, the colour of a given cell at each step is dictated by the rules which consider the colour of the cell and it’s left and right neighbouring cells on the previous step (Wolfram, 2002). Thus, a simple rule may be defined as if the given cell and all surrounding cells were black in the previous step, then turn the given cell white. In a one-dimensional lattice, the lines of cells can be layered to provide a visual representation of their behaviour over time which is an important characteristic of CA. Of course, there is no reason why this definition cannot be expanded into using more than 2 states for each cell, or defining a cells neighbourhood as all surrounding cells such as in the Moore neighbourhood which applies to two-dimensional automata and is defined as the 8 cells surround a given cell (Adamatzky, 2010). Another common neighbourhood is the von Neumann neighbourhood (Weisstein, 2003) which uses the cells directly above, below, to the left, and to the right of a given cell. The boundaries of the lattice need conditions to handle the problem where a cell's neighbourhood is out of bounds. A common way of handling this problem is to wrap the lattice at the edges.

Cellular automata can be used for the modelling of different processes. One such process is the spread of forest fires (Ghisu et al. 2015). Another is using them to generate random numbers that can be used in encryption (Sarkar, 2000).

## Artificial Neural Networks

Inspired by biological neural networks, Artificial Neural Networks (ANN) are one of the most widely used bio-inspired techniques. McCulloch and Pitts (1943) are credited with the writing of the article which marked the beginning of Neurocomputing (Yadav et al. 2015). In the article they created a computational model for neural networks and showed that any arithmetic or logical function could be computed by a simple neural network. According to (Yadav et al. 2015) an artificial neural network is an information processing system that has performance characteristics also present in biological neural networks. Russell and Norvig (2009) formally define them as collections of nodes, or neurons, connected by directed links. Each link has a continuous weight value which governs the strength and sign of the link. Each node computes the weighted sum of its inputs and then applies an activation function to produce an output value. The activation function works as a threshold which allows a network to represent nonlinear functions. Russell and Norvig (2009) also explain how this node definition can be connected to form a network. There are two main options which are feed-forward networks and recurrent networks. A feed-forward network’s connections form a directed acyclic graph as the nodes can only send information forward. Nodes in a recurrent network receive their output values as inputs which allows them to support short-term memory. Figures 2-1 and 2-2 show examples of a feed-forward and recurrent network respectively.



Figure 2‑2: An example of a recurrent neural network topology

Figure 2‑1: An example of a feed-forward neural network topology

Due the amount of research applied to ANNs, there are many different topologies or arrangements and can be applied to a variety of problems. They are useful for identifying relationships between variables or recognising patterns within data (Zhang, 2009) and due to this are a common tool used in data mining where they have been applied to both supervised and unsupervised learning problems (Craven & Shavlik, 1997).

## Swarm Intelligence

Swarm Intelligence is an area of algorithms which have gained a lot of popularity due to their versatility and their efficiency in solving nonlinear design problems (Yang & Karamanoglu, 2013). I will cover two of the main swarm intelligence algorithms, namely Ant Colony Optimisation (ACO) and Particle Swarm Optimisation.

### Ant Colony Optimisation

This algorithm takes inspiration from real ant colonies. Ants use pheromone to mark paths leading to food to communicate its location indirectly to other ants (Khushaba et al. 2008). Khushaba et al. (2008) continue to explain the behaviour of ants foraging for food. The amount of pheromone deposited depends on the distance to the food source, and the quality and quantity of the food source. The paths that are shorter are visited more on average due to more pheromone existing on the path. After a period, the difference in the amount of pheromone between the path options is large enough so that future ants to come across the paths are likely to follow the path previously marked and reinforce the option with their own pheromone (Dorigo & Gambardella, 1997). The quality of a solution to a problem can be modelled as the concentration of pheromone on a path according to (Yang & Karamanoglu, 2013). Due to the solution being modelled this way, the algorithm generally produces routes and paths evident from their higher concentrations, thus ant algorithms are well suited to discrete optimisation problems.

The ACO was originally used to solve the Travelling Salesman Problem and was effective at finding good solutions (Khushaba et al. 2008). ACO has been applied as a searching method within feature selection problems namely in areas of face and speech recognition problems (Khushaba et al. 2008). Feature selection is the process of reducing data with high dimensions into a lower dimension while keeping as close to the same amount of information as possible (Khan & Baig, 2015).

### Particle Swarm Optimisation

The collective behaviour of different animal species is the basis for Particle Swarm Optimisation (PSO). Behaviours such as fish schooling, insect swarming, and birds flocking are examples of such behaviour (Saka et al. 2013). Many newer algorithms that are based on swarm intelligence have taken inspiration from different areas, but still share connections to components used within PSO, thus it can be said that PSO established the foundational ideas of swarm intelligence-based computation as Yang (2014) describes.

Particle Swarm Optimisation was developed by Eberhart and Kennedy (1995) and they state in this article that it can be used to solve many of the same problems as the previously described area, Genetic Algorithms, but does not suffer from some of the same difficulties. Since it can be used to solve the same types of problems, it is useful to compare the algorithms stating the differences. As mentioned previously, GA use operators known as mutation and crossover, but this is not present in PSO. Instead it uses random real-numbers and allows the particles to communicate with each other (Yang, 2014). Yang (2014) also continues to explain that PSO is easier to implement due to no encoding or decoding of the solution being used. Eberhart and Kennedy (1995) describe the PSO concept as being like a GA in that a starting population of random candidate solutions is used but differ in that each solution is given a velocity value and is then “flown” through hyperspace. Solutions in PSO are referred to as particles. Each of these particles has memory, which is not a feature in a GA. This stores a value called the pbest which is the coordinates of the best solution found so far in the search space. The gbest is also stored by the particle swarm optimiser which is the best solution found by any of the population of particles. The search space is explored by the particles moving through the space, the moves are decided by referring to the particles own performance so far and the collective performance of the entire swarm (Saka et al. 2013).

Cho et al. (2011) discuss some of the challenges faced by the PSO topology defined by Eberhart and Kennedy (1995). Using gbest helps particles to converge to a solution quickly as they are attracted to move towards the global best solution found by the swarm. This is a problem as often the particles are trapped in a local maximum because not enough of the search space was explored before converging. Another topology which Cho et al. (2011) describe is lbest. In this, particles can only communicate with a select number of other particles allowing for a more thorough exploration to take place, but convergence occurs slower than gbest.

## Genetic Programming

Genetic Programming (GP) is the last area of bio-inspired computing that I will cover and is an area interested in using natural selection to automatically evolve computer programs (Miller, 2011). Koza (1992) describes the structure of a GP algorithm by stating that it starts with an initial population consisting of randomly generated computer programs. These programs consist of functions and terminals defined according to the domain of the problem. Functions can be anything from arithmetic or programming operations to mathematical or programming functions. The collection of allowed functions is called the function set. These functions can branch into other functions or terminals. Terminals are the variables and constants allowed in the program. The collection of terminals is called the terminal set. Koza (1992) continues by stating that each of these programs are measured according to their fitness value, that is, how well it performs in the given problem. The algorithm performs in generation just like a GA and with each generation with the goal of improving the fitness values of the population each time.

### Tree-based Genetic Programming

In tree-based GP, programs are expressed in the form of parse trees or abstract syntax trees. The internal nodes of the tree are elements taken from the defined function set and the leaf nodes are elements taken from the terminal set. For example, a tree built using a function set defined as and a terminal set consisting of may look like the example shown in Figure 2-3 or Figure 2-4.

### Initialisation of the Population

There are different styles of initialising the population of random programs and Poli et al. (2008) outline the full and grow methods, as well as a combination of both known as ramped half-and-half.

In the full and grow methods, a user set maximum depth parameter is chosen and the random individuals of the population are generated so that they do not exceed this depth. Poli et al. (2008) define this depth as the number of edges that need to be traversed to reach a specific node from the tree’s root node. The full method is appropriately named as it generates full trees, meaning nodes are generated from the function set until the maximum depth is reached, and all the leaves are at the same depth. Each of these leaves may only be a terminal as choosing a function would cause the tree to exceed the maximum depth. The grow method allows for trees with more variation in the shapes and sizes then the full method. It differs by allowing any function or terminal to be selected until the user defined depth is reached.



Figure 2‑3: A tree built using the full method

Figure 2‑4: A tree built using the grow method

As Poli et al. (2008) state, the full and grow methods do not provide a wide array of tree shapes and sizes. Koza (1992) defines a method to combat this problem called ramped half-and-half. The method incorporates both the full and grow methods and is useful because often in GP the size or shape of the ideal solution is not known in advance. A maximum depth is still used but this time a range of depths from two to the maximum is used so that an equal number of trees is produced for each depth. For each value of depth, half of the trees are created using the full method and the other half are created using the grow method. Due to all full trees for a given depth having the same shape and grow trees shapes varying widely from each other, this allows the ramped half-and-half method to create a variety of sizes and shapes.

### Operators in GP

I mentioned previously in Section 2.1 that genetic algorithms are based on natural selection and since this is also true for GP, it uses the same steps and operators although they are defined very differently in practice. Namely these operators are selection, crossover and mutation. Selection is defined the same way for GP and uses the same selection method. Poli et al. (2008) describe the other two operators at a high level as follows. In crossover for GP, a child program is created by combining parts of two selected parent programs. Mutation in GP is defined as the creation of a new child program by altering a randomly selected part of a selected parent program. These operators are used to progressively help to improve the fitness of the programs while still allowing the search space to be explored by not applying too much pressure.

### Problems with Tree-Based Representation

Tree-based GP is one of the older methods of GP and as such has various problems associated with it. As Poli et al. (2008) state that in a high-performance environment, a tree-based representation can be too inefficient as it requires the storage and handling of many pointers. Another issue with a tree-based representation is that expressions in separate subtrees need to be re-evaluated multiple times wasting time and memory as well as adding complexity to the tree. An example of this is shown in Figure 2-5. Both the left and right subtrees have the expression so it must be evaluated twice.

Figure 2‑5: A tree with two subtrees containing

### Other Types of Genetic Programming

There are other types of GP which aim to improve upon some of the problems faced in a tree-based representation. Some examples of these are Cartesian GP (Miller, 1999), Linear GP and Probabilistic GP along with a variety of others.

# Availability of Bio-inspired Algorithms in R

In the following section, I will cover the areas of bio-inspired computing which were highlighted in the preceding section and briefly outline a few packages which provide access to each area.

## Genetic Algorithms

Access to the algorithms in this area are covered through the two packages mentioned in Table 3-1.

|  |  |  |  |
| --- | --- | --- | --- |
| Package Name | Implemented In | Provides | Source |
| GA | Entirely in R | Set of tools for implementing GA,  Can define own operators  Can define own fitness function | (Scrucca, 2013) |
| genalg | Entirely in R | Implementation of GA for multi-dimensional function optimisation | (Willighagen & Ballings, 2015) |

Table 3‑1: Packages providing access to genetic algorithms

## Cellular Automata

The package identified in Table 3-2 provides an implementation of one-dimensional cellular automata but as mentioned in Section 2.2, multi-dimensional CA exist and there is no access to these currently within R. This is an area which can be developed.

|  |  |  |  |
| --- | --- | --- | --- |
| Package Name | Implemented In | Provides | Source |
| CellularAutomaton | Entirely in R | one-dimensional cellular automata | (Hughes, 2013) |

Table 3‑2: Packages providing access to cellular automata

## Artificial Neural Networks

Due to Artificial Neural Networks having a wide range of uses, there are many implementations to cover the different topologies of ANNs. Although there are many packages identified, most of them are built purely in R. These could be improved slightly by implementing the computationally heavy parts in a more efficient language such as C or Java and interfacing to them from R. This is an area which could be improved.

|  |  |  |  |
| --- | --- | --- | --- |
| Package Name | Implemented In | Provides | Source |
| rnn | Entirely in R | Multi-Layered RNN,  Gated Recurrent Unit,  LSTM NN | (Quast, 2016) |
| rsnns | Entirely in R | An R interface to the Stuttgart Neural Network Simulator | (Mergmeir & Benitez, 2012) |
| neural | Entirely in R | Radial Basis Function and  Multi-layer Perceptron with an attached graphical interface | (Fritsch et al., 2016) |
| nnet | The neural network is implemented in C and an interface to it is provided in R | Feed-forward Neural Networks with a single hidden layer | (Venables & Ripley, 2002) |

Table 3‑3: Packages providing access to artificial neural networks

## Swarm Intelligence

Table 3-4 shows three packages which implement Particle Swarm Optimisation with “ppso” providing an optionally parallel solution. All three packages are built entirely in R meaning these could be improved slightly by writing code to perform the demanding tasks. This is an area which could be improved.

|  |  |  |  |
| --- | --- | --- | --- |
| Package Name | Implemented In | Provides | Source |
| pso | Entirely in R | Implementation of Particle Swarm Optimisation | (Bendtsen, 2012) |
| psoptim | Entirely in R | Implementation of Particle Swarm Optimisation | (Ciupke, 2016) |
| ppso | Entirely in R | Optionally parallelised Particle Swarm Optimisation | (Francke, n.d) |

Table 3‑4: Packages providing access to areas of swarm intelligence

## Genetic Programming

The package “rgp” provides an implementation of tree-based GP but as previously mentioned in Section 2.5.5, other types of GP exist. This package has also recently been removed from CRAN as the author is no longer actively supporting it. The archived versions of the software are still available however. This is an area which can be developed.

|  |  |  |  |
| --- | --- | --- | --- |
| Package Name | Implemented In | Provides | Source |
| rgp | R with computationally heavy parts written in C | Implementation of tree-based GP | (Flasch et al., 2014) |

Table 3‑5: Packages providing access to genetic programming

# Genetic Programming

While I have identified Cellular Automata as an area that could be developed, ultimately, I have chosen to build upon Genetic Programming. The reasoning behind this choice is that access to the area is limited and I also find this area more interesting that CA. Also, GP has more practical uses than CA has within the field of data science. As mentioned in Section 2.5.5, other areas of GP exist and one of these is Cartesian Genetic Programming (CGP). This is the area I would like to develop a package to provide access to.

## Cartesian Genetic Programming

Cartesian Genetic Programming is a form of graph-based GP. Graph-based GP shares some similarities with tree-based GP in the way that programs are represented but also has some important distinctions. Graphs are like trees but represent the links between nodes using arrows showing directions and allow for cycles which allows for the reuse of previously calculated subgraphs. This solves one of the issues involved with tree-based GP (Miller, 2011). Figure 4-1 and Figure 4-2 show how a graph representation can reuse previously evaluated expressions.

Figure 4‑2: A graph reusing the 5-y subgraph

Figure 4‑1: A tree with repeated subtrees of 5-y

One way to represent a program in CGP is to use a list of integers referred to as a genome. A genome in CGP has a set size which stops this method of GP suffering from bloat which is a common problem in other methods (Turner & Miller, 2017). This set size is a maximum length of the genome and phenotypes of any size less than this can be produced allowing varied sizes of phenotypes. As Turner and Miller (2017) describe, a genome is composed of function genes, connection genes and output genes. Function genes contain integers which are corresponding entries in a function look-up-table. This look-up-table is similar to the function set described previously except that each function is mapped to an integer. Connection genes specify where the inputs for the function come from, and output genes specify where the output of the genome comes from. The structure of a genome for the graph in Figure 4-2 can be seen in Figure 4-3. The first value in each group is the function gene and the others are connection genes. The connection genes can either specify the inputs to the program or other groups. This can be seen in group 1 where “x” is an input to the program and “0” is group 0. The last group containing a single value is an output gene which specifies that the output of the genome comes from group 2. The function table for this genome can be specified as subtract (0), multiply (1), add (2).

|  |  |  |
| --- | --- | --- |
| 0 | 5 | y |
|  |  |  |

|  |  |  |
| --- | --- | --- |
| 1 | x | 0 |
|  |  |  |

|  |  |  |
| --- | --- | --- |
| 2 | 0 | 1 |
|  |  |  |

|  |
| --- |
| 2 |
|  |

0 1 2

*Figure 4-3: A genome representing the graph from Figure 4-2.*

Another way of representing programs in CGP which is more visual is shown in Figure 4-4. In this representation the grid imposes a restriction on the maximum size of the program, but this grid still needs to be large enough to still allow for expressiveness and evolvability. The squares in each column are not allowed to be connected to other nodes in the same column as Miller and Smith (2006) describe. Miller and Smith (2006) also describe an additional parameter on the representation that defines how many columns away a column can connect to, this is known as level-back. The squares on the right show the input values to the program. The squares in the two-dimensional grid show a random selection of functions from a function set. The square on the right marked as outputs has the same meaning as it does in the representation show in Figure 4-3, it marks which parts of the program the output result can be taken from. The arrows mark the direction and destination of the values being passed. The grid contains many functions which were unused in this execution which are represented by the greyed-out squares. During evolution subgraphs can also become greyed-out through mutation and become active at any point. Overestimating the size of the grid allows for more subgraphs to fade in and out of being used. This has been shown to be very

beneficial in the evolutionary search involved in CGP (Miller & Smith, 2006).

*Figure 4-4: A two-dimensional grid representing the graph from Figure 4-2.*

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| x |  | \* | + | - | / | + |  |  |
| 5 |  | - | + | / | \* | + |  | outputs |
| y |  | \* | - | - | + | - |  |  |

# Implementations of CGP in Other Languages

## JCGP

JCGP is an implementation of CGP in Java created by Eduardo Pedroni (2013). It implements the most commonly used evolutionary strategies as well as mutation methods while also allowing the user to define their own. It also allows the user to select whether the function nodes contain mathematical operators used for Symbolic Regression or whether they contain logic gates for a digital circuit representation. Again, the user can define their own set of function nodes by either selecting a subset of the functions provided by JCGP or to provide a completely different set. The key feature of JCGP is that it has an attached Graphical User Interface (GUI) to allow the user to view the chromosomes as they evolve. The ability to manually change the connections or function of each node in the chromosome is also supported. An interesting feature of JCGP is that it supports the ability to step through the generations of the evolutionary process which makes it clear to see how the chromosome changes over time. Another feature is that it allows the user to save the parameters they have set to a file which can then be loaded and used again later. Files containing the structure of the chromosomes can also be loaded but they architecture of the chromosome must be the same as the parameters in the program.

## CGP-Library

CGP-Library is a cross-platform implementation of CGP written in C (Turner, 2014). It implements classic CGP as well as Recurrent CGP and the ability to use them with Artificial Neural Networks. It provides a C source and header file to be compiled along with the user’s own source code allowing the user to use the library. This library also features the ability to view the structure of a chromosome by using the open source Graphvis (Graphviz.org, n.d) software which displays the structure of the chromosome in a graph format. User defined functions, selection operators and reproduction operators can also be added easily.

## CGP for ECJ

ECJ is an evolutionary computation system written in Java which supports a variety of evolutionary computation techniques. Although its origins are in Genetic Programming, it only provides Tree-Based GP. ECJ also supports plugins and there is a plugin developed to provide Cartesian Genetic Programming called CGP for ECJ (Oranchak, 2009). It supports real-valued and integer representations of the genomes. The plugin also includes a collection of sample problems and associated scripts and parameters files to run them. The plugin also includes three symbolic regression problems which can be run using either the integer representation or the real-valued representation. Classification problems are also included where each problem uses the real-valued representation. The classification problems are configured by default to split the dataset into a test set of 30% of instances and a training set of 70% of instance but this parameter can be altered.

# R Package Creation and Development Tools

The availability and broad range of packages in R has been one of the main reasons for the success of R as a language. R is distributed with many standard or base packages which make up the R source code. There are more benefits to an R package than being an easy way to structure and share functions and datasets, packages can also be dynamically loaded and unloaded at runtime meaning they only occupy memory while being used.

There are different versions of packages. The diagram shown in Figure 6-1 shows the differences between the types of packages.

*Figure 6-1: The differences between versions of R packages. Taken from R Packages (Wickham, 2015)*

To create a package in RStudio there is a convenient menu to allow you to do so. After doing this the created package will contain the three minimal components. The first is a /R directory to contain code written in R. The next is a DESCRIPTION file which describes the function of the package and contains the details of who created the package and what the dependencies are. This is the information shown on the CRAN page for a certain package. The last is the NAMESPACE file which is vital for releasing the package on CRAN as it helps to encapsulate the package and reduce the conflicts it will have with the naming conventions of other packages. It does this by specifying which functions are available from outside of the package which are indicated with the export tag.

## Packages and Software to aid Development

I have used various packages during development which reduced the learning curve of creating R packages, ultimately saving time throughout the project. These packages were also useful in helping to create a pipeline for writing R code, updating any associated documentation, and running tests to ensure the software still works as expected.

### roxygen2

The package “roxygen2” (Wickham et al., 2017) provides a way of automatically generating documentation for a package. When used it adds a basic skeleton of keywords to the comment section above a function. Figure 6-2 shows a simple example of what happens when pressing the command from within R studio “Insert Roxygen Skeleton. After filling in the skeleton, entering the command “roxygen2::roxygenise()” in the console will create documentation files for each function. Updating the documentation is as easy as running the command again as it recognises which parts have changed. This also updates the NAMESPACE file saving time and reducing the chance of errors from writing the NAMESPACE file manually.

*Figure 6-2: Example of code with a roxygen2 skeleton*

#' Title

#'

#' @param x

#' @param y

#'

#' @return

#' @export

#'

#' @examples

mult <- function(x, y) {

return(x \* y)

}

### testthat

The R package “testthat” (Wickham, 2016) aims to make testing of software as painless as possible. It provides functions that make it easy to describe what a function is expected to do and can run tests automatically as code or tests are changed. It also displays test progress visually and shows which expectations passed or failed. Using this package helped to quickly identify any areas where behaviour has changed from what was expected, and also helped to catch a lot of cases I did not originally consider when writing various functions.

### devtools

The aim of “devtools” (Wickham & Chang, 2017) is to make package development easier by providing functions to simplify many tasks. It provides convenient functions for installing and building packages, as well as incorporating documentation and testing into it by utilising the packages I have previously mentioned. Using this package, it is easy to create a simple workflow for when changes are made to code so that documentation is always updated, and unit tests are performed. “Devtools” also provides various functions for helping to release R packages onto CRAN as this process has significant overhead.

### lintr

I will be using the “lintr” (Hester, 2017) package which checks that code written is compliant with a specific style and highlights any differences. The style I set this package to follow was Google’s R style guide. This helped to increase the quality and readability of the code.

### RStudio

RStudio (RStudio, 2016) is a free open-source integrated development environment (IDE) for the R programming language. It includes an R console, a code editor, tools for debugging, and provides an interface displaying which functions and variables are stored within the current environment. It also provides the features that can be expected from an IDE such as code prediction and direct support to version control facilities.

### ggplot2

This R package “ggplot2” (Wickham & Chang, 2016) is a plotting framework for R which builds upon the base graphics that R provides but abstracts the more awkward parts. It is very simple to get started using this package as all that is required is specifying which data to use for each axis and the package will handle the rest. This is the package that I used to allow users to view the results as a graph.

### plotly and shiny

Creating an interactive visualisation of the results of my program was something I assumed would have to wait until a further revision until I found the packages “plotly” (Sievert et al., 2017) and “shiny” (Chang et al., 2017). “plotly” provides a way to easily turn plots created in “ggplot2” into interactive web visualisations. These visualisations then were displayed in a web browser using “shiny”.

## R Workflow

These packages helped to develop two workflows to follow when I was writing R code which helped to automate tasks and keep different areas of my package consistent with one another.

### Documentation Changes

The first workflow was used whenever a new function was defined, and I added documentation for it inside a “roxygen” skeleton, or changes were made to existing documentation. The workflow consisted of:

1. Editing an R source file
2. Using “devtools::load\_all()” which saves any changes made to source files and reloads the updated versions into the environment.
3. Using “devtools::document()” which uses “roxygen2” to generate any new documentation files and update any existing files with changes. This also keeps the NAMESPACE file up to date with the documentation.

This workflow ensured that any changes made were reflected in the packages various forms of documentation.

### Functionality or Test Changes

The second workflow was utilised when a new function was defined, or an existing function was changed; or whenever new tests were added, or existing tests were changed. This workflow consisted of:

1. Editing an R source file
2. Using “devtools::load\_all()” which saves any changes made to source files and reloads the updated versions into the environment.
3. Using “devtools::test()” which makes use of the “testthat” package to run all tests. Each test is run, and the outcome of each test is shown.
4. Repeat this process until all tests pass.

# Design

## Requirements Analysis

As I did not have previous experience of using Genetic Programming it was not initially clear what functionality the package I produced should have. To gain a better understanding of the important features of a GP package I investigated the implementations of CGP discussed in Section5, as well as an existing R package known as “rgp” which has been briefly mentioned in Section 3.5.

This project has now been released to the public but was originally planned to be a personal project so the requirements that follow have changed from when they were originally outlined. I originally aimed for the package to provide a broad range of customisation and functionality but when it came to development, it was decided that some of the requirements were either no longer practical or their priority was not as high as originally thought. Nevertheless, I will include the original requirements and discuss any changes made to these in Section 11.2.

The project is aimed towards users from a technical background, but it is still essential that the project is easy to use as they may not have knowledge in the field of Genetic Programming but still wish to use the software. Any prior knowledge should prove advantageous in their ability to pick up the package. The software will be provided with documentation describing the purpose and how to use each component as well as a guide for getting started in using the software.

The requirements of the package can be split into three main categories:

1. Allow users to perform Cartesian Genetic Programming on a set of data containing the desired results.
2. Allow users to change the parameters of the program and define their own where necessary.
3. Observe results from the program through textual outputs and graphs.

The following requirements will be assessed using the MoSCoW method which is used to assign priorities to requirements. The four categories are Must have, Should have, Could have, and Won’t have. Each requirement will be given a Requirement ID to allow them to be easily referred to through the remainder of this document. The first number refers to the main category identified above, and the second number is the unique number of the requirement within the category.

### Functional Requirements

|  |  |  |
| --- | --- | --- |
| Requirement ID | Description | Priority |
| FR1-1 | The package shall implement Cartesian Genetic Programming | Must |
| FR1-2 | The package shall allow users to run the evolutionary process on a population of chromosomes | Must |
| FR1-3 | The package shall allow users to step through each generation in the evolutionary process | Could |
| FR1-4 | The package shall allow users to pause and resume the evolutionary process | Could |
| FR1-5 | The package shall allow users to load a file containing the desired results | Must |
| FR1-6 | The package shall measure the fitness of a solution compared to the desired result | Must |
| FR1-7 | The package shall be able to construct classifier models for a given dataset | Could |
| FR1-8 | The package shall be able to build regression models through evolution. | Must |
| FR1-9 | The package shall allow existing R data structures to be passed into the program | Should |
| FR2-1 | The package shall provide a symbolic regression function set consisting of mathematical operations | Must |
| FR2-2 | The package shall provide a logical function set consisting of logic gates | Should |
| FR2-3 | The package shall provide the (μ *+ λ)* and Tournament Selection operators to be used | Must |
| FR2-4 | The package shall provide mutation methods to be used | Must |
| FR2-5 | The package shall allow users to choose a function set from the included choices | Should |
| FR2-6 | The package shall allow users to choose a selection operator from the included choices | Should |
| FR2-7 | The package shall allow users to choose a mutation method from the included choices | Should |
| FR2-8 | The package shall allow users to define their own function set | Should |
| FR2-9 | The package shall allow users to select a subset of the functions from a function set | Could |
| FR2-10 | The package shall allow users to define their own selection operators | Could |
| FR2-11 | The package shall allow users to define their own mutation methods | Could |
| FR2-12 | The package shall allow users to change the parameters of the program such as:   * Number of columns in chromosome * Number of rows in chromosome * Number of generations to run * The levels-back parameter * The population size | Must |
| FR2-13 | The package shall provide multiple functions to be used for calculating the fitness of a solution | Should |
| FR3-1 | The package shall display the results in a textual format in the R console | Must |
| FR3-2 | The package shall create an output file containing the results | Should |
| FR3-3 | The package shall display the results in a plotted graph | Could |
| FR3-4 | The package shall output an R data structure containing the results through its return value to be used elsewhere | Could |
| FR3-5 | The package shall allow users to load previous experiments to view the results as a graph | Could |

Table 7-1: Functional Requirements of the package

### Non-functional Requirements

The following non-functional requirements are arranged into categories of:

1. Performance

2. Visualisation

3. Usability

4. Robustness

The requirements are given a Requirement ID in the same manner as the Functional Requirements which is used to categorise them. The first number refers to the category of non-functional requirement identified above, and the second number is the unique number of the requirement within the category.

|  |  |  |
| --- | --- | --- |
| Requirement ID | Description | Priority |
| NFR1-1 | The packages computationally intensive parts shall will be written in C, C++ or Java to improve performance | Should |
| NFR1-2 | Only active nodes shall be processed when decoding the chromosome to improve performance | Should |
| NFR1-3 | The package shall stop execution when a solution has been found | Must |
| NFR2-1 | The created graphs shall be visually clear and understandable to the user | Must |
| NFR2-2 | The textual format shall be understandable and only contain necessary information | Must |
| NFR3-1 | The package shall provide convenient methods of abstracting away from the lower level functionality | Should |
| NFR4-1 | The package shall minimise errors that cause it to fail | Must |

Table 7-2: Non-functional requirements of the package

## Program Structure

In a previous project of mine, I created a Genetic Algorithm to solve the Travelling Salesman Problem and I feel the way I structured this project was effective. The structure is simple, but I feel it helps to understand which parts of the program are related. Although object-oriented programming is possible in R, the style I have used is a functional style and thus does not enforce the structure created. The package I have produced is a larger scale project than my previous project, so the structure was required to be extended slightly. Each file in the package contains related functions. As covered in Section 10.2 when I discuss the correctness of the package, the unit tests are grouped into tests that correspond to each file. The file “main.R” contains the function used to run the program so I chose to give it this name as it contains the main function of the program. Another example is “population.R” which contains the functions which are required to create the initial population. As previously mentioned, the style of programming I have used does not enforce this structure.

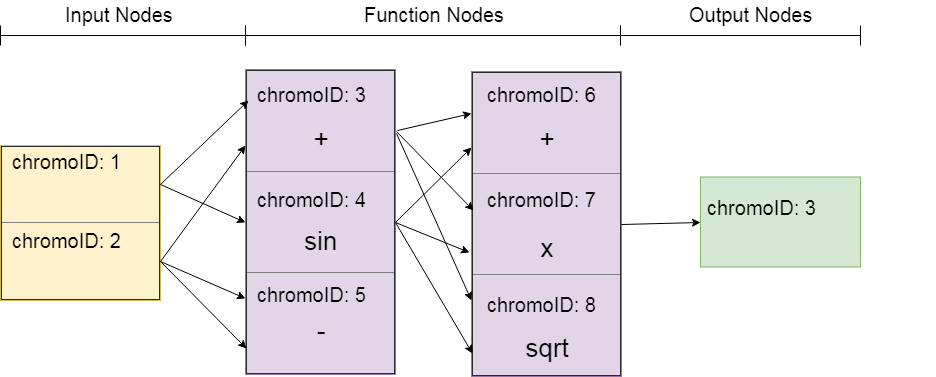
## Structure of a Solution

Instead of using the integer-based representation shown previously in Section 4-3, I chose to use the more intuitive grid-based representation shown previously in Section 4-4. This was so that it is simpler to visualise the resulting graph since a grid can be drawn and filled in with the actual values used in the program.

### The Grid Representation

The grid is composed of different types of nodes which are input nodes, function nodes, and output nodes. Input nodes are the nodes which are loaded with values to be propagated through the structure of function nodes. Function nodes are nodes which apply a selected function to its input values and store the result within them. Function nodes may have one or two inputs depending on the chosen function. Output nodes are nodes which simply select which node of the solution is used to give the overall result of the solution. Each of these nodes is given a unique identifier “chromoID” so that any node can be uniquely identified, and it is easy to tell which type of node it is from this ID. An example structure is shown below in Figure 7-3. In this example, there are two input nodes, a 2x3 grid of function nodes, and a single output node. Example functions are also shown in the function node structure to show that function nodes with different functions take a different number of inputs. The inputs for a node are shown using arrows. The structure created is a feed-forward graph.

Figure 7-3: The structure of a solution using the grid representation



### Structure of Types of Nodes

As each node has different components, each must be created differently from the others. The components of each is mentioned above in Section 7.3.1 but these components must be formalised into how they will be stored in R. The first and simplest component was the “chromoID”, this was simply stored as an integer. The next was the “value” that the node could take, this was stored as a numeric so that real numbers can be used. Both components so far are common to all types of nodes. The diagram in Figure 7-3 can be misleading as although the graph is a feed-forward graph, each node does not store where its value is sent to, it’s the reverse, each node stores where its value comes from. This is the next component known as “inputs” and is present in function nodes and output nodes. This was represented as a vector of integers where each integer is the “chromoID” of the node which is used as input. The final component which is only present in function nodes is the “funcID”. This is simply the unique identifier for the function from the function set. The function set as discussed in Section 3 and 4 is the list of functions that the program can use. The structure of each list can be seen in Figure 7-4. Of course, with each node having common components it makes sense in an object-oriented style to have a node superclass and have each of these inherit from it but as previously stated, I have not used an object-oriented style.

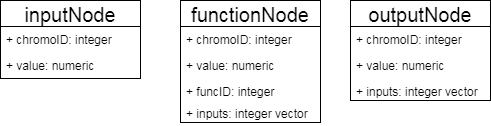


Figure 7-4: Structure of each type of node

### Choosing the Correct Data Structure

The next step was to choose a data structure to store each type of node. I wanted the representation used to store solutions to reflect the representation shown above so that it was easy to translate from a visual display to the actual representation used inside the program. I feel this ability would greatly benefit others and myself when trying to decipher what the solution is doing, and how it is structured. Choosing the correct data structures to use is an important part of any software project and it can have detrimental effects if an incorrect choice is made.

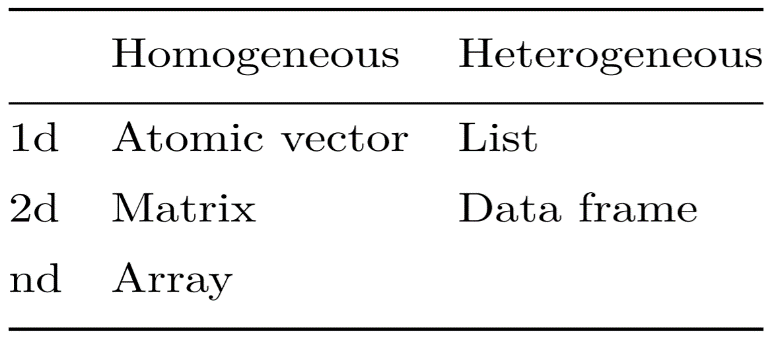


Figure 7-5: R Data Structures (taken from Hadley Wickham’s Advanced R)

R has a variety of data structures available to the developer. These are shown above in Figure 7-4 which is taken from the book, Advanced R (Wickham, 2014). The data structure I opted to use were data frames. This was for several reasons. The first being that as previously mentioned I wanted the data structure to be easily translatable to the visual representation and this required a two-dimensional data frame. This narrowed my choice down to matrices, arrays or data frames. The next reason was that the data to be stored into the structure was the data for each node. This means that the homogenous data structures could not be used since the data to be stored inside each node also was not homogenous. This left only one choice which was data frames. The way this approach was implemented is discussed in Section 8.1.

## Designing the Programs Flow

To design the flow of the program, I wrote down what processes are repeated in an Evolutionary Algorithm and then wrote these into basic pseudocode which is shown in Figure 7-5. The steps shown here are the absolute minimum structure of an Evolutionary Algorithm and help to understand where the evolutionary steps happen. While there are extra steps that will be included in the final version of the main algorithm, this is the structure I based the flow of the program from.

main function {

create initial population

calculate fitness of initial population

**while** maximum generations is not reached and a solution has not  
 been found

store the best solution found so far

perform selection and create the new population

calculate the fitness of the new population

check if a solution has been found

**end while**

store the best solution found

**return** the best solution found

}

Figure 7-5: Pseudocode showing structure of main function

## Designing a Decoding Algorithm

Decoding is the process of getting an output value from a solution with given inputs. One method to do this is to start at the output node of a solution and to recursively work down through the solution and calculate the value at each step back up the solution. This is the method I plan to use as this allows only the nodes which are connected to the output node to be used. An algorithm for this is shown in Figure 7-6. The algorithm repeatedly calls itself on each of the nodes it takes as input until it finds an “inputNode” which is a node that has the value to be propagated through the solution. This value is then passed through the solution as each function node applies its function to it before finally producing an output value.

decode(node) {

**if** this node is an inputNode

**return** this nodes value

**else**

Store the inputs to this node

firstValue = decode the value of the first input

**if** there are two inputs to the node

secondValue = decode the value of the second input

result = apply this nodes function to firstValue and  
 secondValue

**else**

result = apply this nodes function to firstValue

**end if**

**end if**

**return** result

}

Figure 7-6: Pseudocode for a decoding algorithm

## Designing how to Calculate Fitness

The fitness of a solution is the measure of how suitable the solution is to a given problem so calculating the fitness of a solution is an essential element of this package as highlighted by the functional requirement, FR1-6. I aim to distribute multiple fitness functions with the package to allow the user to choose the function which best applies to their scenario as mentioned in FR2-13. To allow for this, it is essential that the method I use to calculate fitness must be customisable. The pseudocode shown in Figure 7-7 is the structure for a function which calculates the fitness of a given solution. To calculate the fitness, it compares what result was given by decoding the solution and compares this to the expected value provided by the dataset passed as a parameter. This is repeated for every entry in the dataset which gives the total error for this given solution. The “fitnessFunction” parameter is the fitness function that the user has chosen to use to calculate fitness.

calculateFitness (solution, dataset, fitnessFunction) {

create a list to store results

**for each** entry in dataset

load the solution's inputs with the entry from dataset

decode this solution to get an output value

store this output value in the results list

**end for**

create a list so store the results and the expected

output from the dataset

get a fitness value by passing this list into

the fitnessFunction

**return** the fitness value

}

Figure 7-7: Pseudocode for an algorithm for calculating fitness of a solution

The fitness functions I plan to provide are functions which calculate the Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE). Both functions will accept a list which contains the predicted value and the actual value where the predicted value is the value given by decoding, and the actual value is the value from the dataset, and both functions will return the error calculated.

There will also be a convenience function provided for calculating the fitness of the entire population. This function will simply call the “calculateFitness” described above and store the result into the solution.

# Implementation

In this section I will cover the important parts of the package I have created known as caRtesian. Where there is a corresponding design section, I will link back to this and discuss how this design was converted into an implementation.

## Structure of a Solution

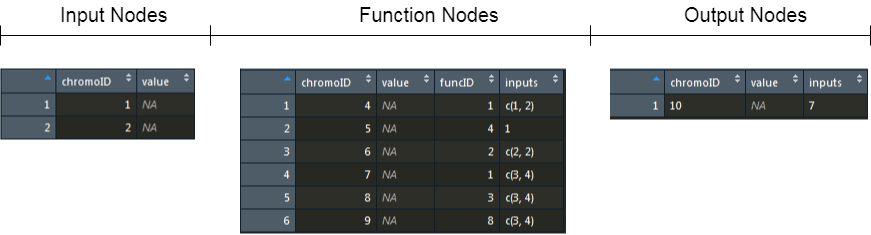
The design of a solution is covered in Section 7.3 as well as what information is required to be stored in the various types of nodes. This section will cover how this was implemented in R. The original idea was to use a data frame to represent the grid of nodes and store a node into each entry so that all nodes could be represented under one structure, but this solution proved to be more difficult to work with than it was worth. Instead, I still opted to use data frames but to use a different data frame for each node type, this meant there were three data frames in total. The different components were each given their own column in the respective data frame and each row in the data frame corresponded to a node. This meant that a solution was no longer represented in a two-dimensional manner as I had planned. The structure of each data frame is shown below in Figure 8-1. The data frames represent the solution shown in Figure 7-3.

Figure 8-1: Data frames containing the structure used in Figure 7-3

It is easy to see how the input nodes and the output nodes map to the diagram in Figure 7-3, but it is not so easy to understand the structure of the function nodes. This data frame could represent a 2x3 grid, or a 3x2 grid and although this results in the same number of nodes, the resulting shape is very different. This is exactly what I aimed to avoid but a sacrifice was required to be made in either the difficulty of working with the nodes stored directly into a data frame entry, or with the translation of the data structure used to a visual representation. Once each of these data frames have been created they are combined into a list where each element is a data frame and they are given appropriate names making them easy to refer to. The list is shown below in Figure 8-2. This list is named “solution” and is then stored into a larger list which contains the entire population of solutions.

## Function Sets

solution list[3] List of length 3

inputNodes list[3 x 2] A data.frame with 3 rows and 2 columns

functionNodes list[6 x 4] A data.frame with 6 rows and 4 columns

outputNodes list [1 x 3] A data.frame with 1 rows and 3 columns

Figure 8-2: Showing the structure of the “solution” list

The function set is the set of functions that a node can use to apply to its input values. There are various requirements that relate to the functionality surrounding function sets which are FR2-1, FR2-5, FR2-8 and FR2-9. These collectively describe the amount of customisation that should be allowed within the package concerning the function set. Since the users of the package are expected to have experience of using the R language, a solution to provide these requirements has been implemented. Different functions have been provided in the package which return different selections of mathematical functions to use. Each of these different selections can then be combined with another, or a subset can be taken easily by using simple vector manipulation. A helper function “constructFuncSet” has also been provided to help with the case where the user would like to construct their own function set entirely instead of using the provid0ed sets.

The definition of each function contained in a set are stored within a vector composed of the functions name and its arity. Each of these definitions is then combined into a singular vector which is finally stored into a data frame. To use one of these functions stored, a function built into R known as “do.call” is used where the first parameter is the name of the function and the second parameter is a list of the arguments to the function to be called. An example showing how R’s arithmetic functions are stored and can be called is shown below in Figure 8-3.

#Singular Vector of Function Definitions

functionDefs <- c(c("+", 2),

c("-", 2),

c("\*", 2),

c("/", 2))

#Data Frame of Function Definitions

funcName arity

1 + 2

2 - 2

3 \* 2

4 / 2

#Returns the result of 1 + 2

do.call("+", list(1, 2))

Figure 8-3: How function sets are represented and can be used

An admittedly better approach to storing the functions contained in a function set is to store the function directly and store the number of arguments to the function as the arity. I discuss this approach and the issues associated with it in Section 9.2.

## Creating the Initial Population

As discussed in Section 8.1 created solutions are stored into a larger list. This larger list is known as the population. I will discuss how valid solutions were created by initialising each solution with values.

### Creating the Input Nodes

As mentioned previously there are three types of nodes: input nodes, function nodes, and output nodes. The first type of nodes that I created were input nodes. These are created using the “generateInputs” function. The function takes “inputSize” as a parameter which is the number of input fields present in the dataset used with the program. The program also requires random constants to be available to use as input to function nodes so this “inputSize” variable is increased by one to allow for the constant to be stored here. This solution only allows for one constant to be used through the whole solution. Issues relating to this approach are discussed in Section 9.4. As discussed in Section 8.1 data frames are used to represent each type of node so the next step was to create a data frame to store the input nodes. The data frame created was the length of “inputSize” and each column was initialised with values. The “chromoID” of each row was initialised from one to “inputSize”. This resulted in each input node having a unique identifier as required. The next step was to initialise the “value” field where each value was set to “NA” since there were no values to store yet and then convert this to a numeric type so that the appropriate space is allocated in memory to hold the information that will be stored here eventually. Allocating the correct amount of space initially saves computation time later as dynamically growing structures in R are slow. Then the row to store the random constant was given the constant value that it will use for the remainder of this solutions life time. Lastly, the data frame containing the input nodes was returned.

### Creating the Function Nodes

Next the function nodes were created. These were created using the “generateFunctionNodes” function. This function takes several parameters which are: the starting “chromoID” to use, the number of rows and columns to be used in the function node structure, the levels back which is a new parameter and will be discussed in this section, and finally the function set containing the functions each node can use. In the same manner as with the input nodes, the appropriate data frame is created first with the correct types in each column before information was loaded into the data frame. This is achieved by the “createFunctionNodesStructure” found in Appendix A.

The next part of this function caused me some issues and I have since found a more elegant solution to this. Both the issues and the new solution are discussed in Section 9.3. The problem was how to restrict where a function node could take its input values from which is what the levels back parameter specifies. The levels back parameter specifies how many columns back a given function node can take values from. Every function node regardless of the levels back can take an input node as input. This was made more difficult due to the nodes being stored into a data structure which did not truly represent the two-dimensional structure I had hoped for. The way I implemented this was to create a matrix which initially contains the “chromoID” of each node in the input node structure created previously. The number of rows in the matrix is equal to the number of levels back add one. A row represents a column within the function node data frame that is valid to be used as input, and there is one extra row to store the input nodes since these can also be used as inputs. The number of columns was initially set to the number of input nodes, but this caused issues when the there were more rows required in the function node structure than there were in the input nodes. These issues are also discussed in Section 9.3. The solution currently used takes the maximum value of either the number of input nodes, or the number of rows required. However, this too brings its own associated problem. The first time the valid input matrix is created, the matrix is filled with the “chromoID” of each input node. A row of the matrix is then replaced after one column of function nodes has been created which the intended functionality. However, there are still multiple rows of input nodes which leads to a bias when using the sampling function to choose an input since there is at least double the chance to pick an input node compared to a function node. An example showing this bias is shown below in Figure 8-4. To combat this a wrapper for the “sample” function was implemented which removes any “NA” values which are caused when there are more input nodes than function nodes to enter, and then removes any duplicates. This allows for unbiased sampling.

There is then a nested loop where the outer loop iterates over the number of columns and the other moves down through the number of rows. The inner loop creates a function node with the values it will use and stores it in the correct position. The “chromoID” of the node created is added to a vector which is the vector that will be placed into the matrix containing the valid input locations after the inner loop completes.

Initial Matrix which Matrix after one column  
contains only input of function nodes has

node chromoIDs been added. Notice the

double entry in row 1 and 3

[,1] [,2] [,3] [,1] [,2] [,3]

[1,] 1 2 3 [1,] 1 2 3

[2,] 1 2 3 [2,] 4 5 6

[3,] 1 2 3 [3,] 1 2 3

Figure 8-4: Matrices showing the bias after function nodes have been added

Each node is given a unique identified again, it is also assigned a random function that it will use from the function set and the number of inputs this function expects are also generated.

### Creating the Output Nodes

The process of creating the output nodes is much simpler than the function nodes and is very similar to the input nodes. I designed this section of the program with the idea in mind that I would like the program to have multiple output values possible, but this idea was scrapped in later stages due to it being a lot more difficult to work with. The “chromoID” and “value” fields were created in the same way as with the input nodes. Output nodes also have input values but there are no restrictions as with the function nodes and can take their value from anywhere in the solution so calculating the input value for an output node is as simple as selecting a random “chromoID”.

### Wrapping Up

After creating the three different types of nodes, they are wrapped into a single list and given names making them easier to refer to. They are then stored in a larger list called “population” and returned to the main function of the program.

## Decoding

## Calculating the Fitness of a Solution

# Issues Faced During Implementation

The issues that I was confronted with during implementation are discussed in this section and where possible a solution to a given issue will also be discussed. There are issues discussed that do not relate to the areas covered in Section 8 but are still relevant and should be discussed.

## Choosing the correct Data Structures

Data frames in R are built up from lists of vectors, so it is possible using lists would have been a better approach but as I said, I wanted a two-dimensional structure. The issues relating to the choice of data frames are discussed in Section 9.1.

## Storing a Function directly in a List

As mentioned in Section 8.2, a better approach to representing function sets would have been to use lists and to store the function directly. This removes the need to use the “do.call” function since the function can simply be called with arguments passed to it. I attempted to use this approach but since this part of the package was still early in the development process, I had trouble with this. The trouble was how to calculate the arity of the functions to be used. I understood how to calculate the arity of a function that I created, and this could be done through calling the “formals” function and then counting the length of the returned values. However, this approach did not work for R’s mathematical operators since they part of R’s base package. When the “formals” function was used on these, “NULL” was returned. This is due to the functions of R’s base package being known as primitives. Some of R is implemented in C and primitive functions are exactly that, they store the C code that implements the function and are compiled at build time (Cran.r-project.org, 2018). These functions do not have formals and instead have “args” so to get the number of arguments to a primitive function, first “args” must be applied and then “formals”. This is the approach I would like to use upon refactoring of this project but will also require changes elsewhere in the program wherever the function sets are used.

One problem with this approach is that the basic arithmetic operators “+”, “-“, “\*”, and “/” cannot be stored this way as they raise syntax errors. To store these wrapper functions would have to be implemented that call these operators and the wrapper functions would be stored into the function set.

## Checking Valid Inputs to a Function Node

As mentioned in Section 8.3.2, issues were faced when computing the valid inputs to a given node. A working version was created quite quickly which I assumed to work but it assumed that the number of rows to use in the function node structure would be the same as the number of input nodes which is a terrible assumption to make. This was down to a mistake in the values I chose to test this functionality with. However, the issue did not arise until later in development and the problem was confusing to find since there was no error produced but instead, just unexpected behaviour.

When creating the function nodes, once the most recent column was created it was to replace the no longer valid inputs in the matrix but when there were more nodes created than there were columns in the matrix, it would cause values to be cut off. For example, if there were two input nodes and four function nodes were just generated, then when adding these function nodes to the matrix two values would be lost.

As my R skills have developed through this project and I am more aware of different functions available to an R developer I found a new more elegant way to implement this functionality. This method was to use the “getValidInputs” function I have created which can be found in Appendix B. This function takes as an argument the “chromoID” of the node to get the valid inputs of, the “functionNodeRange” which is simply the “chromoID” of each function node, and lastly a list containing the rows, columns and levels back used to create the function nodes. This function puts each of the identifier of each of the function nodes into a matrix similarly to before but this time it is structured in the same format as the function nodes meaning they have the same number of columns and rows. The function which simplifies the issues I was having before is “which”. This function returns the indices of an object where an expression is true. I had used this function previously in my program, but I did not know about the optional “arr.ind” which instead returns the row and column of where an expression true. This allowed me to find the index of the column containing the given node which then allowed me to find the valid columns through some operations applied on this column index. A subset was then taken from the matrix containing the identifiers of the function nodes by using the resulting valid columns. This produced all the valid input nodes for a given node. This was then converted to a vector and returned.

This implementation is much simpler and easier to debug so the old implementation will be replaced with this in the next version of the software.

## Allowing the use of Multiple Random Constants

A GP library should provide the ability to use random constant values in its solutions so that functions such as can be represented. My implementation does this through adding an extra input node and storing a random integer inside between -10 and 10. This allows the value chosen for this random constant to be retained through the life time of the solution and can be used multiple times.

Later in development I encountered the problem where a function which requires two distinct constants could not be represented. Due to how late this problem was discovered and the design of some earlier parts, the amount of work to rectify this problem was large and would require extensive testing to ensure the behaviour of the program did not change. Despite this, I will continue to discuss my attempts to solve this problem and explain a solution which will be attempted in a future version of the package.

The first solution I tried was to store the function which returns a random value into the input node data frame instead of the random value it returns. This would allow for multiple constants to be used through the program since each time it would be used, a random number would be returned. The issue with here is that this meant the behaviour of the solution would change each time it was used. For example, if a solution used a random constant then it would call the function which returns a random value. The next time this function is used it would return another random value which may well be the same value, but this is unlikely. More concretely, if the solution represented a function such as and random constant was set as 5 which produced no error meaning it was a perfect solution, the next time it was called this random constant could be a 6 which is no longer the correct solution.

This solution is partly correct, but I must implement some manner of retaining the random constant value returned. One way of doing this is to create a new type of node called a constant node which is structured similarly to an input node in that it only has a unique identifier and a value. Each time a random constant is to be used it will either sample a new value or use on of the already existing constants. Any constant values that are no longer used by any node in the solution should be removed to avoid excess memory being used. Another way to do this which may require less refactoring of code is to add a field to the function node structure which can store a random constant if it chooses to use one. However, I feel the first solution is more sensible.

## Decoding Process

## Allowing the Selection Method to be Changed

## Mutation producing Invalid Solutions

## Division by Zero

A problem was encountered when decoding the solution and propagating the input data through each of the function nodes to get an output value for the solution. To understand the problem an example must first be given. Given a dataset of random inputs called x which are in the from 0 to 10, and an output value y which is the result of the function . The solution could correctly identify to choose a random constant value of 10 and divide this by the input value. This could work perfectly for every input except when the input value was 0. Division by zero in most programming languages results in a crash but with R, the value is represented as “Inf” for Infinite. This would result in this solution not being selected during the next generation since its fitness is extremely high even though it is a perfect solution. I opted to remove the division function which is admittedly a poor decision on my behalf as this makes the example function given above very difficult to represent.

A solution to this issue is to use a protected division operator which returns a result of one when dividing by zero. This approach is discussed in Cartesian Genetic Programming (Miller, 2011).

## Plotting Average Fitness over Generations

## Releasing Software

# Evaluation

To evaluate this project, I have performed a usability study that has highlighted some usability issues with the guide that I have produced. This study will be covered in detail. I will also discuss the correctness of my software and cover the process of writing unit tests using the “testthat” package.

## Usability Study

### caRtesian – Getting Started (User Guide)

I created a user guide which is to be distributed along with package I have developed. This guide is important as it is the mechanism for teaching users how to use the basic functionality of the package. The guide aims to give a quick overview of Cartesian Genetic Programming and for users to be able to use the package without any previous knowledge of the area. Users who have experience with Evolutionary Algorithms will potentially pick up the commands quicker since they use terminology they will be familiar with. It is assumed that readers of this guide will have some previous experience using the R language, but it is not a requirement. The guide can be found in Appendix C.

The guide, “caRtesian – Getting Started” contains commands for users to run and an explanation as to what each command accomplishes. Through running each of these commands, the user will be able to set up the required variables, run the main function of the program, and to view the results that it produces. Installation instructions are also included.

As previously mentioned, the usability study I carried out has highlighted some issues with the user guide and these will be improved in a future version.

### Usability Study

## Correctness

I made extensive use of the “testthat” package throughout development as running tests was a core part of my workflow. Using this package, I added unit tests for the functions that I created. This was important as it helped to ensure that my program was working in the way I expected. Using unit tests are also a good way of detecting any behavioural changes that occur in my program caused by later changes. This was important when restructuring some existing functions as the tests acted as a safety net catching anything unintended. Unit tests also serve as a form of documentation in an R package and are distributed within the package.

### Approach to Unit Testing

Where possible I followed Test-First Programming (Madeyski, 2010) which involves defining tests first that the code about to be written should pass. Using this method, it encouraged me to think more about the structure of the function I was about to write, and I feel that the functions written using this method are more concise and well-structured.

However, as I this was my first project where I have used unit testing, and my first large project in R, I found it difficult at some points to know what a function was expected to do until I had written it. Where this was the case, I would aim to implement as little of the function as required and then write a unit test to capture this behaviour.

### Unit Testing using testthat

Unit testing in “testthat” aims to make testing as painless as possible (Wickham, 2011). It provides a visual display of which tests have passed or failed so it is straightforward to get an indication of where in your code something is not working as intended.

Test files are R scripts composed of a hierarchical structure. This structure is made up of expectations, tests and contexts. A “context” is used to group multiple tests into related functionality. In my package I have grouped tests into a file for each R source file and set the “context” as the file name. The next part is the “test\_that” statement which groups related expectations into one function and further helps with tracking down any failed tests. The last is the expectations or “expect\_that” statements. An example of this structure can be seen below in Figure 8-10.

context("funcSet")

test\_that("constructFuncSet returns a data frame of the correct structure", {

dummyFunctions <- c(c("add", 2),

c("subtract", 2),

c("sqrt", 1))

maxColumns <- 2

funcSet <- constructFuncSet(dummyFunctions)

expect\_equal(ncol(funcSet), maxColumns)

expect\_equal(nrow(funcSet), length(dummyFunctions) / maxColumns)

expect\_is(funcSet, "data.frame")

expect\_is(funcSet$funcName, "character")

expect\_is(funcSet$arity, "integer")

})

Figure 8-10: Example of testthat test structure

The “expect\_that” statements I mentioned previously are shown here as “expect\_equal” and “expect\_is” as this is less verbose than the “expect\_that” version. For example, the “expect\_is(x, y)” is actually “expect\_that(x, is.a(y))”. I used the less verbose option as I believe it does not reduce readability of each of the tests and saves time from remembering the syntax of many different expectation statements. These statements as well as the “test\_that” statement read as sentences. For example, the “test\_that” statement reads as “test that constructFuncSet returns a data frame of the correct structure”, and one of the above “expect\_is” statement reads as “expect funcSet is a data.frame”.

Using the testing workflow I mentioned in Section 6.2.2 the tests for my package produce the output shown in Figure 8-11. The contexts are shown on the right side with the time taken to run each of the tests inside, and the outcome of each test is displayed on the left. In this case all tests have passed so are marked as “OK”.

> devtools::test()

Loading caRtesian

Testing caRtesian

√ | OK F W S | Context

√ | 8 | dataHandler

√ | 22 | fitness [0.3 s]

√ | 6 | funcSet

√ | 6 | main [1.2 s]

√ | 54 | population [0.6 s]

√ | 6 | selection [0.2 s]

√ | 15 | utility [0.2 s]

== Results ============================================================

Duration: 2.7 s

OK: 117

Failed: 0

Warnings: 0

Skipped: 0

Figure 8-11: Output from using devtools::test() to run the tests in the caRtesian package shwoing

For completeness I will also show what is displayed when a test is failed. This is not a real case as I have edited the test in Figure 8-10 to purposely fail but it shows the informative output of “testthat”. This can be seen in Figure 8-12. The context that contains the failed test is marked with a red “x” and an entry is put into the “F” column. This shows that a test has failed. The line number of the failed test, and a description of the failing test and error received is then displayed below the context. This is what allowed me to quickly identify where problems were and quickly address them. The total number of passing tests, failed tests, tests that have raised warnings, and skipped tests is also summarised at the end.

> devtools::test()

Loading caRtesian

Testing caRtesian

√ | OK F W S | Context

√ | 8 | dataHandler [0.1 s]

√ | 22 | fitness [0.4 s]

x | 5 1 | funcSet

-----------------------------------------------------------------------

test-funcSet.R:18: failure: constructFuncSet returns a data frame of the correct structure

funcSet$arity inherits from `integer` not `numeric`.

-----------------------------------------------------------------------

√ | 6 | main [1.2 s]

√ | 54 | population [0.6 s]

√ | 6 | selection [0.2 s]

√ | 15 | utility [0.3 s]

== Results ============================================================

Duration: 3.0 s

OK: 116

Failed: 1

Warnings: 0

Skipped: 0

Figure 8-12: Output from using devtools::test() when a test fails in the caRtesian package

### Unit Tests highlighting need for Refactoring

When creating the functions of the package which create the initial population and populate it with the correct structure of nodes I found that I was using a lot of parameters to each of the functions. This felt like bad practice and felt like my code was tightly coupled as some of these parameters were unrelated to what the function was intended to do. My original solution to this issue was to use global variables. When R is evaluating a variable, if it is not defined in the current environment, it will then investigate the global environment. This also felt like bad practice as it was not clear by simply looking at a function what it was intended to do as there were variables being referenced from outside the scope of the function. However, I chose to continue with this approach.

When the time came to implement unit tests it was clear this approach was a bigger problem than having extra parameters to functions. Wherever a global variable was used, I needed to also define this global variable within each context that required it. An example is shown below in Figure 8-13.

cgp <- function(-PARAMETERS OMMITTED-) {

#Double arrow to assign the variable into the global environment

inputSize <<- 2

...

initPopulation(popsize = 5)

}

initPopulation <- function(popsize) {

...

#Using a variable defined outside of this functions scope

generateInputs(inputSize)

...

}

library(caRtesian)

context("population")

#Must also define this global variable again here

inputSize <<- 2

test\_that("initPopulation returns the correct number of solutions", {

...

})

Figure 8-13: Structure of code and associated test when using global variables

This example looks different from the code distributed in the final version as this was early in the development process. The parameters to the “cgp” function have been omitted as they are not important for this example. Also, where appropriate code has been missed out or marked with “…” to shows steps take place before the line shown. The example shows a variable defined globally in the “cgp” function called “inputSize”. It then shows a call to the “initPopulation” function but does not pass the “inputSize” as a parameter. The “inputSize” is used within this function when calling “generateInputs” even though it is defined out of this function’s scope. So far, this global variable has been assigned once. The global variable must also be initialised before any tests that use this variable can be run since tests are run under a different environment to the package. This means this same variable has been assigned twice and must be assigned in every test file that requires it. In this case it is not clear why “inputSize” is being defined in the first place since “initPopulation” does not use it as a parameter as previously mentioned.

Without adding unit tests to my software, I may not have removed the use of global variables and thus the quality of my code would have suffered in that readability would be reduced for outside users.

## Performance of Package

Write here about how profvis

Write here about how I should minimise the number of times the fitnessFunction is called by not re-evaluating any solutions which currently have a fitness since these have not been changed. If a solution is new, it’s fitness value will be Inf.

Can also write about how it is possible to speed this up by instead of decoding, extract the function that the solution represents and apply this instead. I currently decode every time I loop.

Maybe I can profvis the fitness function to see where problems actually are.

# Reflection

## What I achieved vs initial aims

## What I achieved vs Requirements

## How R skills have developed

## R as a language

Throughout the implementation of this package I have aimed to increase the efficiency of my scripts wherever I knew how. The main area where I have increased efficiency is that I make sure to allocate the correct length to vectors and lists when creating them instead of building these dynamically and allowing R to handle this.

# Further Work

# Conclusions

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# Appendices

## Appendix A – createFunctionNodesStructure

#' createFunctionNodesStructure

#'

#' Creates a data frame containing the structure of a function node. The data

#' frame is the length set in the generateFunctionNodes parameters.

#'

#' @param rowsRequired the number of rows to create

#'

#' @return the data frame created

#'

createFunctionNodesStructure <- function(rowsRequired) {

#Create integer vectors containing rowsRequired NA values

naColumn <- rep(as.integer(NA), rowsRequired)

#Create a data frame with the length required to store the function nodes

functionNodes <- data.frame(chromoID = naColumn,

value = as.numeric(naColumn),

funcID = naColumn)

#Add a column to store a vector specifiying the input nodes

functionNodes$inputs <- vector(mode = "list", length = nrow(functionNodes))

return(functionNodes)

}

## Appendix B – getValidInputs

#' getValidInputs

#'

#' Determines the valid range of input chromoIDs for a given chromoID

#'

#' @param chromoID the chromoID to calculate the range of

#' @param functionNodeRange all the chromoIDs contained in functionNodes

#' @param functionNodeStructure the parameters used to create functionNodes

#'

#' @return the valid chromoIDs

#'

getValidInputs <- function(chromoID, functionNodeRange, functionNodeStructure) {

#Put the functionNode chromoIDs into a matrix

functionNodeMatrix <- matrix(functionNodeRange,

nrow = functionNodeStructure$rows,

ncol = functionNodeStructure$cols)

#Find the column index containing chromoID

column <- which(functionNodeMatrix == chromoID, arr.ind = TRUE)[[1, 2]]

#Get the columns that are in the levelsBack range

validColumns <- (column - functionNodeStructure$levelsBack):(column - 1)

validColumns <- validColumns[validColumns >= 1]

#Extract the chromoIDs from the validColumns

validChromoIDs <- functionNodeMatrix[, validColumns]

return(as.vector(validChromoIDs))

}

## Appendix C – caRtesian – Getting Started (User Guide)