Bio-inspired Computing in R

Deliverable 1: 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:

Date:

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.

Contents

1 Introduction

1.1 Purpose

The purpose of this document is to give an overview of the domain of the project; to identify and describe the motivations and objectives of the project; and to give initial plans of how to overcome foreseeable problems. Supporting technical literature relevant to the project domain is also discussed.

1.2 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.

2. **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.

3. **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.

4. **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.

5. **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.

6. **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.

2 Bio-inspired Computing

2.1 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).

2.2 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).

2.3 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.

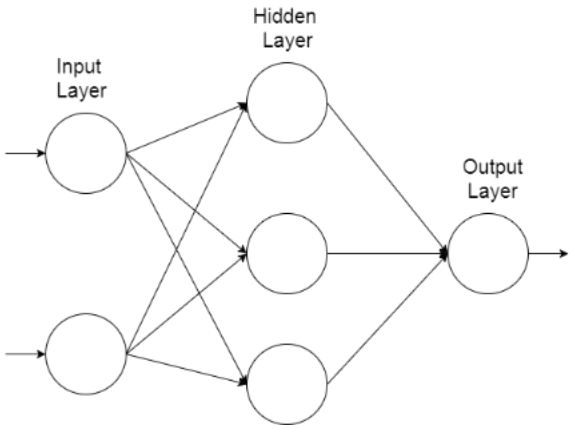

Figure 2-1: An example of a feed-forward neural network topology

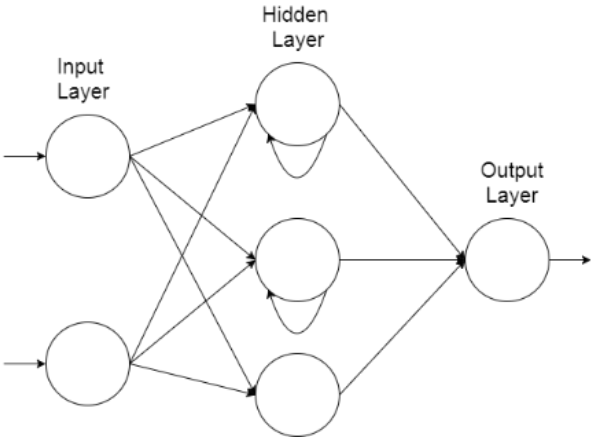

Figure 2-2: An example of a recurrent neural network topology

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).

2.4 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.

2.4.1 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).

2.4.2 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.

2.5 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.

2.5.1 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 $\{x, y, 2, 5, 1\}$ may look like the example shown in Figure 2-3 or Figure 2-4.

2.5.2 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.

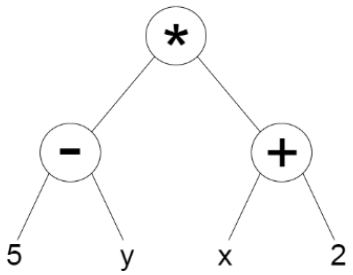

Figure 2-3: A tree built using the full method

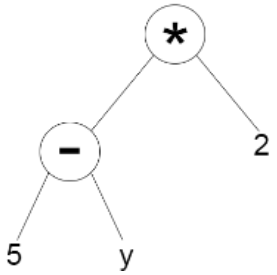

Figure 2-4: A tree built using the grow method

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.

2.5.3 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.

2.5.4 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 $5 - y$ so it must be evaluated twice.

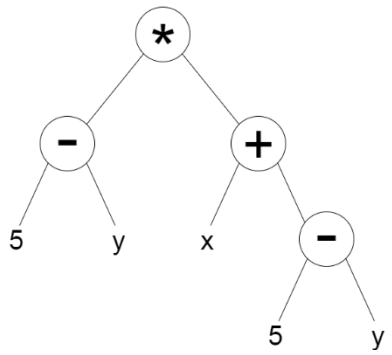

Figure 2-5: A tree with two subtrees containing $5 - y$

2.5.5 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.

3 Availability of Bio-inspired Algorithms in R

3.1 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

3.2 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

3.3 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

3.4 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

3.5 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 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

4 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. 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.

4.1 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.

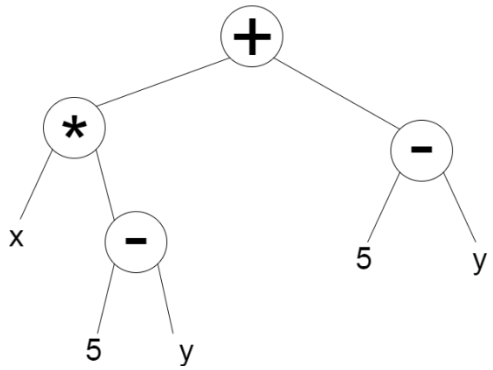

Figure 4-2: A tree with repeated subtrees of 5-y

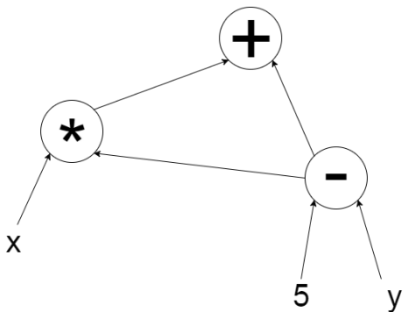

Figure 4-1: A graph reusing the 5-y subgraph

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).

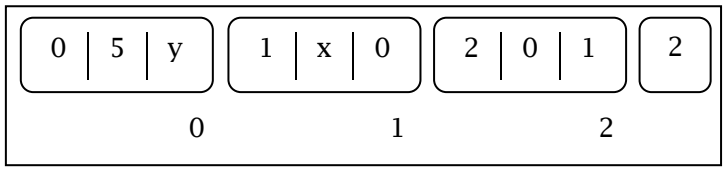

Figure 4-3: A genome representing the graph from Figure 4-2.

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).

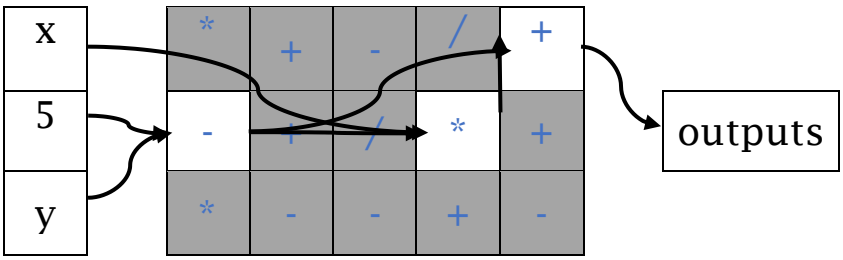

Figure 4-4: A two-dimensional grid representing the graph from Figure 4-2.

4.2 Operators in Cartesian Genetic Programming

5 Requirements Analysis

6 R Packages

6.1 Process of Package Creation

What a package contains - https://cran.r-project.org/doc/contrib/Leisch-CreatingPackages.pdf

http://r-pkgs.had.co.nz/package.html

6.2 Packages and Software Tools to Aid in the Process

Devtools

RStudio

Roxygen2

Testthat

Travis

7 Evaluation Strategy

8 Project Management

8.1 Project Schedule

8.1.1 Work Breakdown Structure

8.1.2 Project Timetable

8.2 Risk Analysis

8.2.1 Risk Identification

8.2.2 Risk Management

8.3 Professional, Legal, Ethical and Social Issues

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10 Appendices