
SYMBOLIC REGRESSION

PROJECT FOR
ARTIFICIAL NEURAL NETWORKS

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Chapter 1

Introduction

This project was made as an year-end project for the theoretical part of the class Artificial Neural Networks on Department of Applied Informatics and Multimedia at Technical Eductional Institute of Crete. The task was to find an application of neural networks on the internet, and process it from a theoretical point of view. To introduce basic procedures which are done in order to get the result of neural network.

The chosen application of neural networks is a diploma thesis from The Faculty of Applied Informatics on The University of Tomas Bata in Czech republic in Zlin. This thesis is dealing with analytical programming (special type of evolutionary algorithms) in order to make the optimization of neural networks. It is comparing the algorithm SOMA (evolutionary type of algorithm) to the learning process with backpropagation algorithm and nonlinear interlacing. I decided, that I will focus this project on the algorithm of backpropagation.

Problem which is solved in this project is a symbolic regression, which is very popular in the world of artificial intelligence these days. As it is said on the website www.symbolicregression.com: "Symbolic regression is a function discovery approach for analysis and modeling of numeric multivariate data sets for a purpose of getting insights about data-generating systems."

There is a lot of researches focused on symbolic regression, one of them is taking place on my home university (Brno University of Technology), which is dealing with this problem by cartesian genetic programming, combined with coevolution. In the end of this project I am also comparing the results of neural networks to the results of cartesian genetic programming. After a comparison of the performance on the basic symbolic regression problems, which were solved by neural networks in the mentioned thesis, I am trying to predict the success of neural networks on much more difficult functions

which I decided to use as testbenches in this theoretical project.

I have chosen this topic mainly because of the topic my bachelor's thesis which is dealing with competitive coevolution in cartesian genetic programming applied to symbolic regression and its comparssion to coevolution of fitness predictors. Now, thanks to this project, I can also compare success of my algorithms t the success of neural networks in solving symbolic regression.

Chapter 2

Application description

The neural network which I am trying to describe in this project should be a neural network solving symbolic regression. Symbolic regression is a topic, which is now very popular in the field of artifical intelligence. We try to solve it not only with artifical neural networks, but also with genetic programming and genetic algorithms.

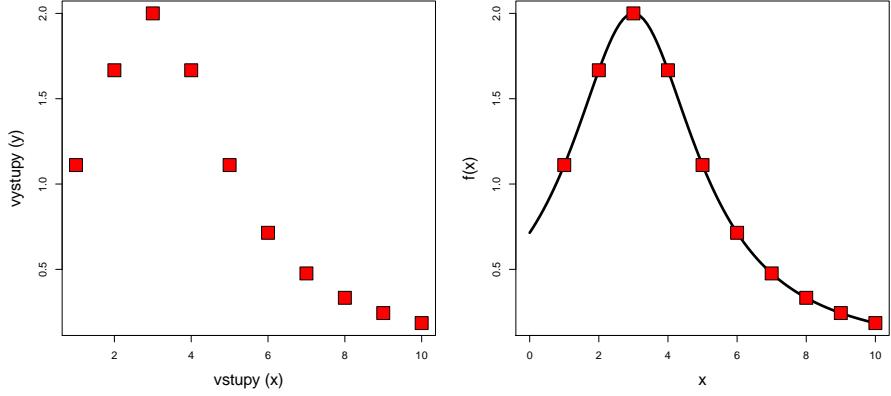
In this chapter I am going to bring near the problematics of symbolic regression, approximate what do we expect from the general symbolic regression to do and how we will change it for the symbolic regression used in this project. Then, after the description of symbolic regression, I will introduce you the two functions which I chose for this project as a test benchmarks.

2.1 Symbolic regression

Symbolic regression is an approach to the function discovery. It is used for modeling and analyzing numerical data in order to get a purpose about data-generating systems. As the name suggest, the method by which the insights are to be generated, is regression.

The term symbolic regression is representing the process of interleaving some curve through the known data. This curve is usually expressed as a mathematical function. For a long time it used to be a qualification of humans only, but how time passes, it starts to be possible also with an artifical intelligence.

Symbolic regression works as it is shown on the picture 2.1. As you can see on the left side, there is an input of symbolic regression, on the right side is the desired output. If we have a function, which takes one number (let's say x) as an input and gives us one output (let's say y), we can logically organize this pairs into vectors (x, y) . If you have vectors in the shape



(a) input of symbolic regression

(b) output of symbolic regression

Figure 2.1: Symbolic regression

of (x, y) , it is natural to draw it in a 2D plot like we can see on the picture 2.1.

On the right side of the picture, we can see our desired output. We want the symbolic regression (or symbolic function identification) to find the some of the relations between the inputs and outputs. In more details, we need to identify which of the inputs is more important than other and how is it related to the changes in the output. In order to predict, what would be the function value of some input which we didn't train the network on. In this example the value is always according to the function f as follows.

$$f(x) = \frac{10}{5 + (x - 3)^2} \quad (2.1)$$

The goal of symbolic regression is in getting the relation between x and y onto whole field of real numbers from our input, which are only vectors (x_1, x_2, \dots) identificating points in the plane, space or multidimensional space, which the searched function goes through.

As a demonstration of more difficult problem which can be solved by symbolic regression, I am adding another possible input displayed as a 3-dimensional plot (figure 2.2. This plot is corresponding to the following function.

$$f(x_1, x_2) = \frac{(x_1 - 3)^4 + (x_2 - 3)^3 - (x_2 - 3)}{(x_2 - 2)^4 + 10} \quad (2.2)$$

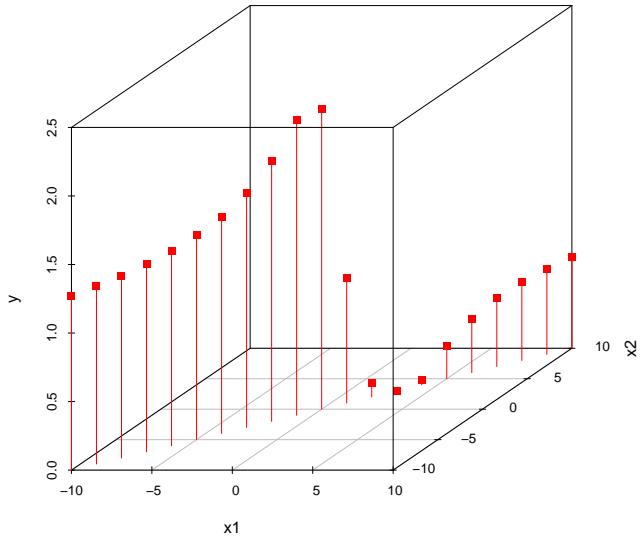


Figure 2.2: Symbolic regression

This function is also called rational polynomial function in 2 dimensions and is used in the community working on symbolic regression as a prove, that their algorithm can solve even the most challenging functions.

2.1.1 Our way of interpreting symbolic regression

For this project, we will want something little bit different from symbolic regression. Usually we want it to tell us straightly the function in the shape of $y = f(x)$, but here, in this project, we will not really want it to show us the function. We will want the neural network to train to count all possible inputs of the function (in our case all the real numbers) and after, if we give it some input vector, which is not in the training patterns, we expect it to count the correct output. If we go deeper, we can imagine it as a formula inside the neural network, but we will not interpret it like this, we will only wait for the outputs.

2.2 Test benchmarks

For symbolic regression we start from the basic tests with elementary functions (e.g. $y = x^2$) in the beginning to prove that the method is suitable to

solve symbolic regression. As we already know, that symbolic regression is solvable with neural networks (proven also in [5]), we can continue in function discovery on more difficult functions. I decided to prepare two testing sets for two different functions to try the symbolic regression on them.

I decided to use toy benchmarks from the website symbolicregression.com¹, which is officially the place where all the people from the community share their results, compare them to other results and check if their symbolic regression is properly working. The testbenches I have concretely chosen from the symbolic regression website are testbench number 3: Salustowitz function in 2 dimensions and testbench number 5: unwrapped ball function in 2 dimensions.

2.2.1 Salustowitz function 3D

$$f(x_1, x_2) = e^{-x_1} x_1^3 \cos(x_1) \sin(x_1) (\cos(x_1) \sin^2(x_1) - 1)(x_2 - 5) \quad (2.3)$$

We can see the plot of the Salustowitz function on the figure 2.3, which is plotted in the ranges as follow:

$$\begin{aligned} x_1 &\in \langle 0, 10 \rangle \\ x_2 &\in \langle 0, 10 \rangle \end{aligned} \quad (2.4)$$

2.2.2 Unwrapped Ball 3D

$$f(x_1, x_2) = \frac{10}{5 + (x_1 - 3)^2 + (x_2 - 3)^2} \quad (2.5)$$

We can see the plot of the Unwrapped Ball function on the figure 2.4, which is plotted in the ranges as follow:

$$\begin{aligned} x_1 &\in \langle 0, 10 \rangle \\ x_2 &\in \langle 0, 10 \rangle \end{aligned} \quad (2.6)$$

¹<http://symbolicregression.com/?q=node/5>

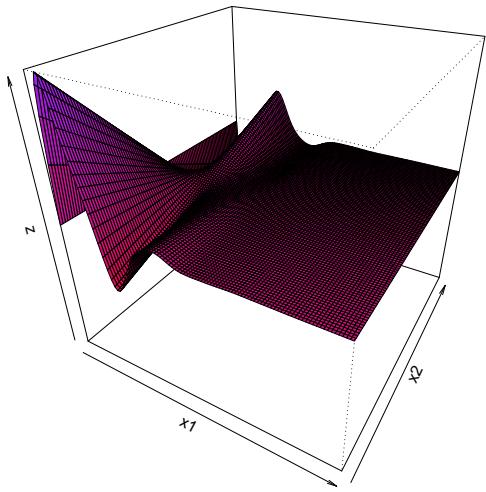


Figure 2.3: Salustowicz function

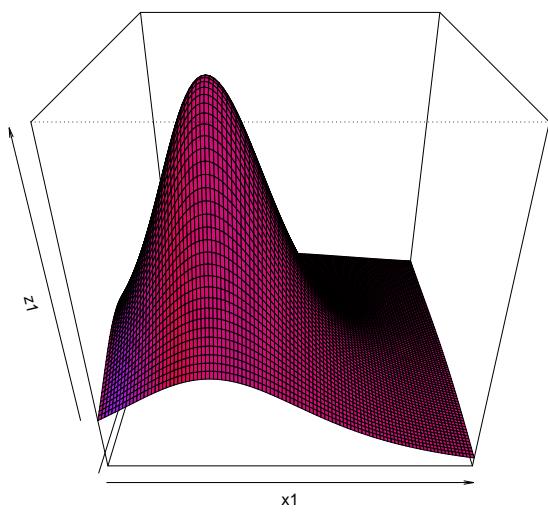


Figure 2.4: Unwrapped Ball function

Chapter 3

Neural network architecture

I am going to dedicate this chapter to the architecture of the used neural network. In the beginning I am going to talk about the number of neurons and their organization in the network. Then I will speak about the training patterns, how to create and preprocess them, how to make sure that the values will be small enough to be usable for neural network. Then I will speak about the way how I create the data for this specific type of neural network and in the end of the chapter the discussion about activation function, BIAS and other fixed parametres as learning rate will take place.

3.1 Perceptron

Each neuron in designed neural network works as a simple perceptron. Let's describe a work of a perceptron. Schematic picture of perceptron is on the picture 3.1. In a general case, neuron receives vector x as an input. Each component of the vector (so called characteristic value of the vector) is multiplied by factor w (weight) and is added together with remaining characteristic values of the vector and with coefficient called bias as well. Bias can also be often seen realized as an unit input multiplied by coefficient b .

Output of each perceptron is set by following equation:

$$out = act.function \left(\sum w_i x_i + bias \right) \quad (3.1)$$

In this equation activation function is one of the used functions, as defined below, in the chapter 3.6. Sum goes through all the inputs of the neuron, each weighted.

A neural network consists of a set of neurons that are connected to each other and the identity of the connection is determined by the weight w . In

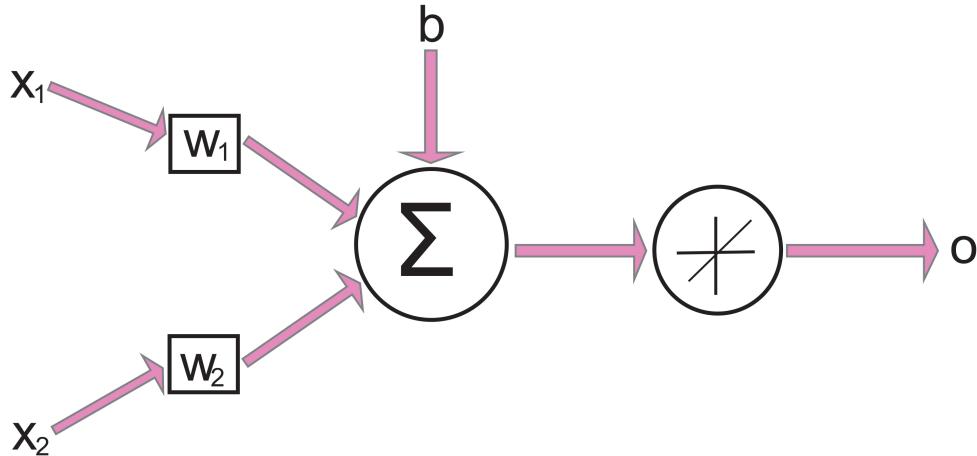


Figure 3.1: Neural network architecture

multilayer neural networks, there are different layers, where each consists of a set of neurons. It must be mentioned that in a neural network is not necessary the number of neurons of each level to be the same. Also it is not necessary all neurons to implement the same transfer function.

The training of a neural network is to regulate the network connections in order to implement a particular function, and the network to give or to reach/approach a desired output. The arrangement of the connections is done by adjusting the weights. Goal of the network's training is also the setting of biases. [1]

3.2 Architecture

As it is already proven in the publication [5], if you are working on symbolic regression through neural networks, you can use several different neural networks. As a best suitable network for 3D functions was found a network with two inputs, one output (as the function requires) and two layers (which mean one hidden layer). We can see this neural network on the picture 3.2.

On this picture (3.2) we can see a neural network, where individual layers are distinguished by shades of grey. The darker shade is for the first layer, the input layer, which doesn't count any functions. It just takes the input and passes it to the next layer. With the lighter shade of grey I drew the hidden and the output layer.

As we can see on the picture, there are 4 active neurons, each of them has a BIAS and inputs. Neurons in the hidden layer have two inputs, neurons

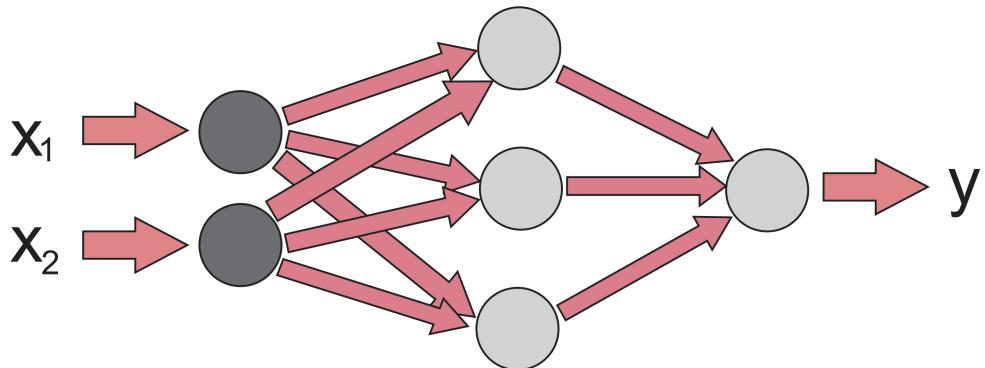


Figure 3.2: Neural network architecture

in the output layer have three inputs. If we count one weight for each input and BIAS for each neuron, we can say, that the state of learning of our neural network can be expressed as 13 values. If we give numbers from up to down and from left to right and use the numbers of both connected nodes as an index for each weight, we can describe whole neural network by vector of 13 dimensions as follow:

$$net = [w_{13}, w_{23}, w_{14}, w_{24}, w_{15}, w_{25}, w_{36}, w_{46}, w_{56}, B_3, B_4, B_5, B_6] \quad (3.2)$$

3.3 Inputs

About inputs of the neural network is known, that it should be small numbers. In the neural networks classes we were working with numbers belonging to the interval $\langle 0, 1 \rangle$. In order to be in consent with our classes I will continue in keeping the inputs in small numbers.

As I defined before, in the chapter 2.2, I am testing the neural network on two functions, both of them defined on the same interval. Some of my inputs can look like this:

$$[3, 5.7] \quad (3.3)$$

If it not in the shape how it is suitable for neural network, so I will do a mathematical transformation for my input vector in order to keep the values small. As my inputs are always in the interval $\langle 0, 10 \rangle$, to get it into the interval $\langle 0, 1 \rangle$, I will do the simple operation: divide all the inputs by 10. The input vector defined in the equation 3.3 will now look like this:

$$[0.3, 0.57] \quad (3.4)$$

3.4 Outputs

In the previous chapter we have been speaking about the transformation of data on the input of the neural network. We decided to divide all the data we put into the network by 10. Of course we are still looking for the same function, but on 10 times smaller domain, so we have to recount desired outputs for all input patterns.

This means, that we are creating completely new set of patterns, which fits better the neural network learning process. After we finish learning, we can take input from any part of whole domain and make it a new pattern in order to test if the neural network found solution which is suitable for whole domain.

3.5 Generating data

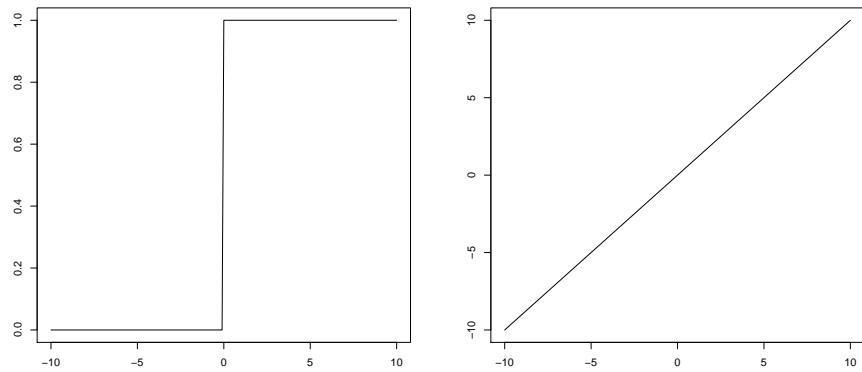
The best way of generating training and testing patterns for our networks is doing it automatically in some supporting software. The way of creating it depends on the way how we want to run our neural network application. In case we have got the neural network learning function as a binary file and run it from operating system on our computer, the best way to keep our data is in a data file. We can load the data from a data file in every run. Other way is designing the application of neural networks directly for the problem which we are trying to solve. In that case we can write the training patterns directly into the code of our application.

For our application we are using MATLAB script file, which is designed for our specific task, so we can write the data statically into the data vector in the beginning of the code.

For both cases, it is useful to generate the data automatically, code used for generation of data for our second testbench could look like it is shown in the algorithm 1.

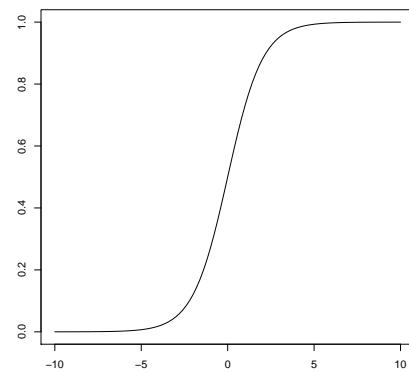
3.6 Activation functions

In neural networks we use activation functions to correct the output of each neuron to keep it in the interval, where we want to have it. The most known functions and functions which we are using in our lessons are hard limit function (so called step function), pure linear function and sigmoid function. Their graphs are displayed on the figure 3.3.



(a) Hard limit function

(b) Linear function



(c) Sigmoid function

Figure 3.3: Used activation functions.

```

data generation()
begin
    |   y = 0;
    |   for x = 0; x != 10 ; x += 0.1 do
    |       |   y += 0.1;
    |       |   write(x);
    |       |   write(y);
    |       |   write(10 / (5 + (x - 3)3 + (y - 3)2))
    |       |   write(newline);
    |   end
end

```

Algorithm 1: Data generation algorithm

In the neural networks application which is described in this project, it was decided to use two types of activation functions. For all neurons in the hidden layer we are using sigmoid activation function in order to keep the values small. For the neuron in the output layer we are using linear activation function. The harm limit activation function doesn't have its place in this application. It is caused by the type of the problem. Hard limit function is usually used in the problems of a classificatory character in order to separate patterns belonging to one group (e.g. 0) from patterns belonging to the other group (e.g. 1). [3]

3.7 Other parameters

Parameters, which I am going to discuss in this section are mainly the starting values of all trained magnitudes. Due to the fact, that the application uses also evolutionary algorithms in order to train the network, the initial weights and biases are set randomly, as it is usual in evolutionary algorithms for initial population.

3.8 Learning algorithms

In the application there were used three types of learning process:

1. Backpropagation algorithm
2. Nonlinear interlacing
3. SOMA algorithm

Knowledge from our course covers only one of them in detail, so I decided to devote this project mainly to backpropagation algorithm and a way of

learning through it. Weights updating in backpropagation algorithm can work in two different ways:

Sequential update - sequential (so called online) update means, that every time we let one pattern go through a network, we count error, which gives us necessary values for counting the δ (deltas) of the output layer, and then we continue backwards until we get to the first layer. Then, after updating all weights, we load the next pattern to repeat whole procedure.

Batch update - this type of update means, that as a first task, we count errors and deltas for all patterns. After that, we count an average delta and count the weight changes only once, after counting all patterns with initial weights.

In application which I have chosen for this project, the online update version of this algorithm is used. For completeness, let's now define equations used in the backpropagation algorithm [2].

$$\delta_k = o_k(1 - o_k)(t_k - o_k) \quad (3.5)$$

$$\delta_h = o_h(1 - o_h) \sum_{k \in outputs} w_{h,k} \delta_k \quad (3.6)$$

$$\begin{aligned} w_{i,j} &= w_{i,j} + \delta w_{i,j} \\ \Delta w_{i,j} &= \eta \delta_j x_{i,j} \end{aligned} \quad (3.7)$$

The equation 3.5 is counted for each output unit k , the equation 3.6 is valid for all hidden units with number h . The set of equations 3.7 is used for updating weights after all.

Chapter 4

Results

Result of this application is to prove that neural networks are able to solve this kind of problem successfully. In the application which I am starting from, the author was using two basic 3D functions, which are shown on plots 4.1. Equations according to this functions are following.

$$f(x_1, x_2) = 0.5x_1 + 2x_2 \quad (4.1)$$

$$f(x_1, x_2) = 0.5x_1^6 + 2x_2^3 \quad (4.2)$$

The results of used functions are shown in the table ???. Tests were done on the same set as was training. Success was measured in standard deviation from the desired value.

As an experiment, I am now trying to estimate error, which can be reached on my tesbenches. My estimations come out from comparsion of the linear and polynomic functions next to Salustowitz and Unwrapped Ball functions in cartesian genetic programming with coevolution. As I said before, the success rate is much worse in these much more dificult functions. As an experimental result, I framed the table ?? to predict awaited results. To prove if the errors which this neural network really reaches are corresponding to my predictions, we will need to do more research and testing.

As it was proven in [4], the success rate (number of succesful solutions from 100)in basic linear or polynomial functions is 1.25 times worse in the

f_{linear}	10^{-3}
$f_{polynom}$	10^{-6}

Table 4.1: Application results

$f_{Salustowitz}$	$10^{-5} - 10^{-2}$
$f_{UnwrappedBall}$	$10^{-2} - 10^{-1}$

Table 4.2: Predicted results for my testbenches

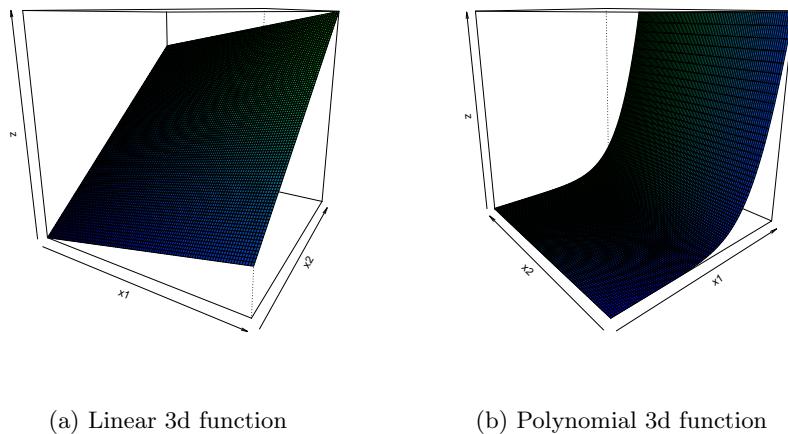


Figure 4.1: Testbenches used in original application

Salustowitz function (our testbench no. 1) and 4 times worse in the Unwrapped Ball function.

Chapter 5

Conclusions

In this project I described the symbolic regression problem in general, I found an application on the internet which deals with symbolic regression realized by neural networks. It is an application of the character of proving that it is possible to solve symbolic regression with neural networks.

I also introduced the application which deals with symbolic regression by cartesian genetic programming (CGP) using coevolution. As these two ways of programming are very close, due to both of them are parts of main streams in artificial intelligence, I decided to presume, that the ratio of success will be analogic in both of them. So I started from ratio between problems solved by application which I was talking about and problems which I set to solve by neural networks and were already solved by CGP. I used the ratio which was reached by CGP to predict how good will be the application of neural networks for the same problem.

In this project, I was trying to describe the problem completely from basic theories well-founded by equations, pictures and 3D plots. I continued with my estimations of the following results of research. During working on this project, I made a complete overview of using basic neural networks for solving problems and how it is executed.

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