KU LEUVEN

FACULTEIT INGENIEURSWETENSCHAPPEN

Avoiding local minima in Deep Learning: a nonlinear optimal control approach

Jan Scheers

Thesis voorgedragen tot het behalen van de graad van Master of Science in de ingenieurswetenschappen: wiskundige ingenieurstechnieken

Promotor:
Prof. dr. ir. Panos Patrinos

Academiejaar 2020 – 2021

Preface

I would like to thank everybody who kept me busy the last year, especially my promoter and my assistants. I would also like to thank the jury for reading the text. My sincere gratitude also goes to my friends and my family.

Jan Scheers

Contents

Abstract

Chapter 1

Introduction

1.1 Artificial Neural Networks

Artifical Neural Networks (ANNs) are a very popular machine learning model. They are known to be very expressive, leading to low statistical bias. With enough neurons, ANNs can approximate any function. They are especially useful for learning from very large data sets. But it is not entirely clear what the optimization of an ANN converges to, as the loss surface is highly non-convex. Nonetheless a number of results show that for wide enough networks, there are few "bad" local minima.

ANNs are composed of 'neurons', which are in some ways analogous to biological neurons.Each neuron is a nonlinear function transforming the weighted sum of its inputs:

$$y = \sigma(w_1 x_1 + w_2 x_2 + ... + w_n x_n)$$

With w_i the weights, x_i the inputs and σ the activation function. This is the McCulloch-Pitts neuron model.[REF] The most commonly used activation function σ is the Rectified Linear Unit (ReLU):

$$\sigma(x) = x^+ = \max(0, x)$$

A visual representation is shown in figure **??**b. A full network is built by connecting layers of neurons as shown in figure **??**a. An ANN can also be expressed as a combination of function composition and matrix multiplication.

$$f(W, x) = W_L \sigma(W_{L-1} \sigma(...W_1 \sigma(W_0 x)...))$$

where W_n are the matrixes of the connection weights and L is the depth of the network.

Optimal Control	Neural Network	Notation
decision variables	weight parameters	W
state variables	(neuron) activation	z

1.2 Backpropagation

Backpropagation is the usual algorithm for training an ANN. Training of a network is done by minimizing the loss function C. For regression problems this will be often be a squared error loss, while for classification tasks the cross entropy is used.

$$\underset{W}{\text{minimize}} \quad C(W) = \sum_{j=0}^{N} ||f(W, x^j) - y^j||^2$$

with x^j the input vectors, y^j the target output and N the number of data points

Backpropagation computes the gradient of the loss function C with respect to the weight matrices W. It has two steps: in the first step the output of the network is calculated using the current weights and input v. The activation values and derivatives of each Then the error is propagated backward and the gradient is calculated.

Then any gradient descent method can be used to find the step update.

1.3 Neural Networks in Optimal Control Theory

A neural network can also be interpreted as a dynamical system.

$$\begin{aligned} z_0 &= x \\ z_{k+1} &= \sigma(W_k z_k), \quad k = 0, ..., L-1 \\ y &= W_H z_L \end{aligned}$$

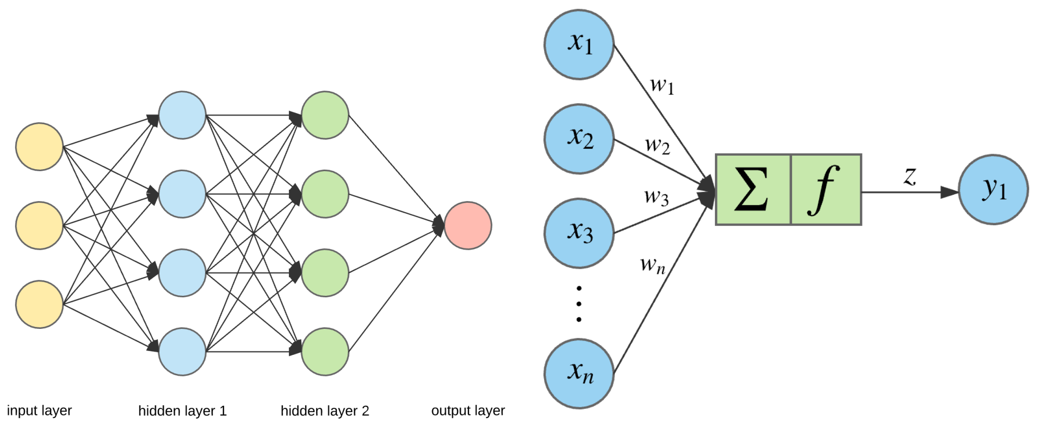


FIGURE 1.1: Feedforward Deep Neural Network and Single Neuron - McCulloch-Pitts model. (Retrieved from https://towardsdatascience.com)

In this way optimization methods from control theory can be applied. In particular, training a neural network can be formulated as the following Optimal Control Problem (OCP)

$$\begin{aligned} \underset{W}{\text{minimize}} \quad & \sum_{j=0}^{N} ||W_L z_L^j - y^j||^2 \\ \text{subject to} \quad & z_{k+1}^j = \max(W_k z_k^j, 0), \quad k = 0, \dots, L-1, j = 1, \dots, N \end{aligned} \tag{1.1}$$

There are two main direct approaches to solving an OCP. First is the sequential approach, where the states are eliminated using the dynamics. This is equivalent to the backpropagation algorithm which is the current standard method. [ref mizutani]

The other approach is the simultaneous approach, where the state variables and the dynamics are kept as constraints. In control theory this approach often works better for highly nonlinear problems, which is certainly the case for training neural networks. The simultaneous approach is novel to neural networks and will be the topic of this thesis.

The disadvantage of this method is the number of variables that need to be optimized is much larger. For a fully connected neural network of width W, each layer will contain W^2 weights. Combined with a depth D, that gives approximately W^2D weight variables to be optimized for both the backpropagation and simultaneous approach. Adding the states as variables however adds another WDN variables, where N is the number of samples in a training batch. The advantage of this method is that relaxing the states makes the problem more smooth, and will hopefully allow the optimization to converge more often to a good solution and not land in a bad local minimum.

1.4 Goal of the Thesis

Chapter 2

Initial exploration

In this chapter an initial exploration of the problem is done. The backpropagation algorithm is compared relative to the simultaneous approach for a couple small regression problems.

For the backpropagation algorithm the experiments were done using the Neural Network Toolbox in MATLAB version 2018a. The training was done using the `trainlm` procedure which implements a Levenberg-Marquardt backpropagation algorithm.

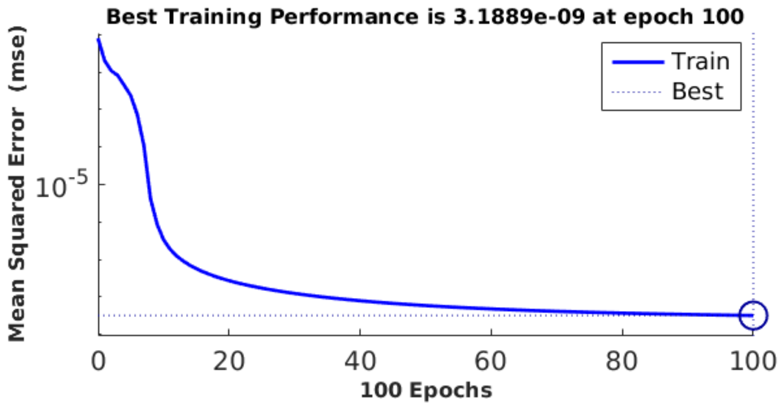
For the simultaneous approach the problems were set up using the YALMIP version R20190425 optimization library, implementing the OCP detailed in equation **??**. This problem was then solved using MATLAB's `fmincon` procedure.

2.1 First experiment

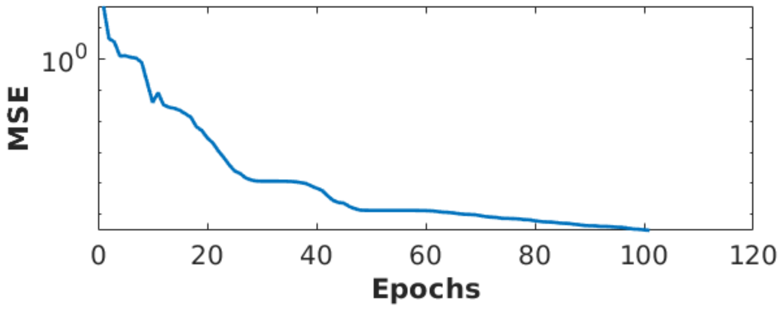
The first experiment conducted was to apply both algorithms to a test problem. A small neural network is constructed with 2 hidden layers with each layer containing 3 nodes with tansig activation function. The activation function was chosen because it works well for a small network. This network is then trained to approximate a piece of a sine function. Both algorithms are trained for 100 epochs. Figure **??** shows the training performance for a training run of each algorithm. Both perform well, but the simultaneous approach is much slower. This can be due to the fact that the new algorithm is not well optimized.

The backpropagation algorithm converges every time for this problem, taking anywhere between 10 and 1000 iterations. The stopping criteria is that the validation error increases for 6 consecutive iterations.

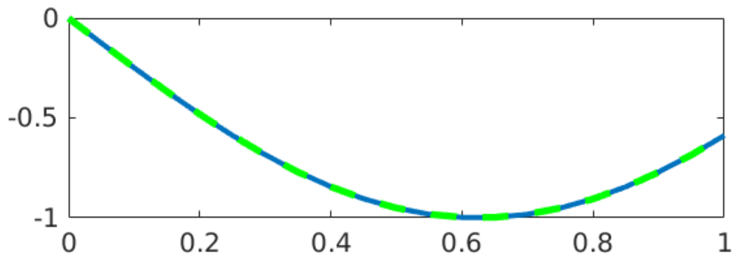
The simultaneous approach also converges if the intial conditions are set correctly. The weight variables are randomly initialized and the state variables are initialized by simulating the network once using the input vector, ensuring the initial point is feasible. The method converges every time, but it runs much slower. Its not known if this is due to the difference in optimization of the algorithms and the fact that the backpropagation algorithm is running on my GPU instead of the CPU.



(a) Training performance of backpropagation



(b) Training performance of simultaneous approach



(c) Sine function

Figure 2.1: Performance of algorithms for simple regression problem

2.2 Second experiment

For this experiment again the same regression problem of the previous section is considered but with a different network. Here a network of two layers is used, with 8 neurons in each layer, but using a ReLU activation function.

The backpropagation function will almost always converge for this problem.

For the simultaneous approach the RELU activation function will have to be reformulated, in order to have smooth constraints. The ReLU function can be transformed as follows:

$$\begin{gathered}
x^j_{k+1} = \max(W_k x^j_k, 0) \\
\Updownarrow \\
x^j_{k+1} = -\min(-W_k x^j_k, 0) \\
\Updownarrow \\
\min(x^j_{k+1} - W_k x^j_k) = 0 \\
\Updownarrow \\
(x^j_{k+1} - W_k x^j_k)^\top x^j_{k+1} = 0, \\
x^j_{k+1} \geq 0, x^j_{k+1} - W_k x^j_k \geq 0
\end{gathered}$$

But even using these smooth constraints, the algorithm will usually not converge. It might be that this is due to the use of the fmincon optimization method, which is very general. In the next chapter the simultaneous approach will be rewritten in python using a more specific algorithm.

2.3 Further exploration

There are many options that can be explored to further compare these algorithms.

- Activation function: ReLU is the most popular activation function in the field. Others are tansig, sigmoid, SoftPlus, leaky ReLU, etc.
- Network size: Networks can be up to thousands of neurons wide and hundreds of layers deep.
- Network architecture: There is a huge variety of possible network architectures. Convolutional neural networks for example are very popular for image recognition.
- Test problems: Neural networks have many applications. Some applications could benefit more from this training method than others.
- Optimization algorithm: fmincon is quite a general method, a more specific method might perform better

- Stopping criteria and initial conditions

  These will be explored in the next chapters

Chapter 3

Python implementation

In this chapter the simultaneous approach is examined more closely and implemented into python. Instead of using `fmincon` which is a very general black box method, a more specific algorithm should both run faster and converge more often. For this the Augmented Lagrangian Method was chosen.

3.1 Augmented Lagrangian Method

Instead of using fmincon, now an Augmented Lagrangian Method is used to solve the optimal control problem. The OCP equations

$$\begin{aligned} &\underset{W}{\text{minimize}} && \frac{1}{2}\sum_{j=0}^{N} ||W_H z_H^j - y^j||^2 \\ &\text{subject to} && 0 = z_{k+1}^j - \sigma(W_k x_k^j + b_k), \quad k = 0, \dots, H-1, j = 1, \dots, N \end{aligned}$$

are represented as a nonlinear least squares problem

$$\begin{aligned} &\min && \frac{1}{2}||F(x)||_2^2 \\ &\text{s. t.} && h(x) = 0 \end{aligned}$$

The ALM method solves this problem by adding both a penalty and a lagrangian term. After rewriting, the nonlinear least squares problem looks like this

$$\begin{aligned} \mathcal{L}_c(x, \lambda) &= \frac{1}{2}||F(x)||_2^2 + < \lambda, h(x) > + \frac{c}{2}||h(x)||_2^2 \\ &= \frac{1}{2}||F(x)||_2^2 + \frac{c}{2}||h(x) + \lambda/c||_2^2 - \frac{1}{2c}||\lambda||_2^2 \\ &= \frac{c}{2}\left|\left| \begin{bmatrix} F(x)/\sqrt{c} \\ h(x) + \lambda/c \end{bmatrix} \right|\right|^2 \end{aligned} \tag{3.1}$$

In the inner loop of the algorithm the least squares problem is solved for x^k up to a certain tolerance.

$$x^k \text{ s. t. } ||\nabla_k \mathcal{L}_{c_k}(x^k, \lambda^k)||_2 \leq \epsilon \tag{3.2}$$

The langrangian parameters *lambda* are then updated using the rule:

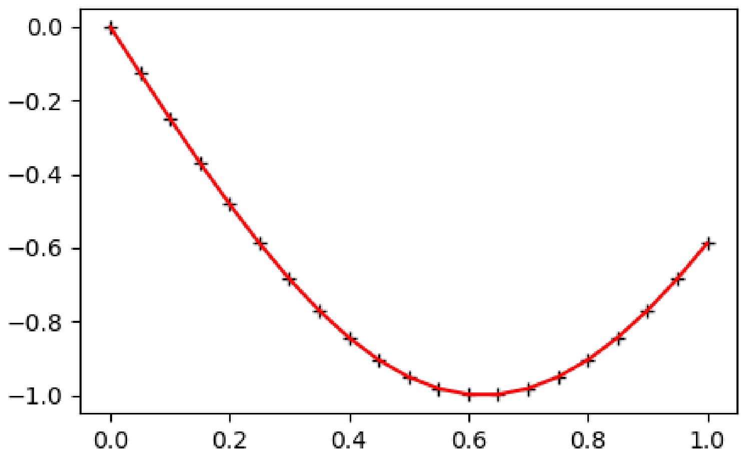
$$\lambda^{k+1} = \lambda^k + c_k h(x^k) \tag{3.3}$$

A new penalty parameter c^{k+1} is chosen and the algorithm continues. REFER nocedal wright,

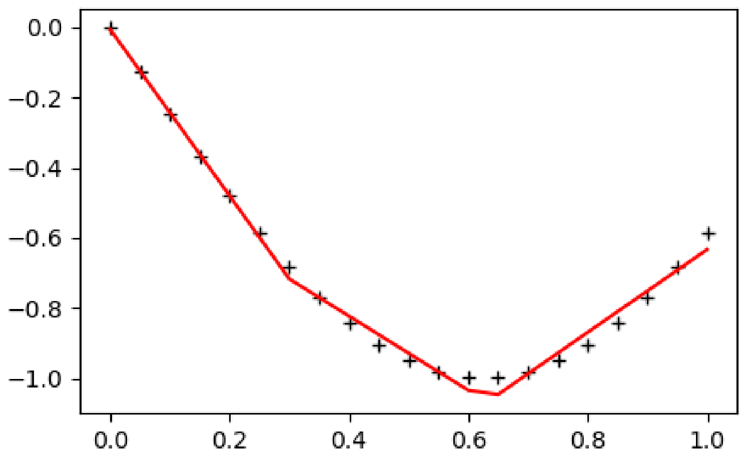
3.2 Jacobian

To solve the least squares problem, the Jacobian matrix must be calculated. It has a relatively sparse structure because there are no distant connections in the neural net, each layer is only connected to the next one and the previous one.

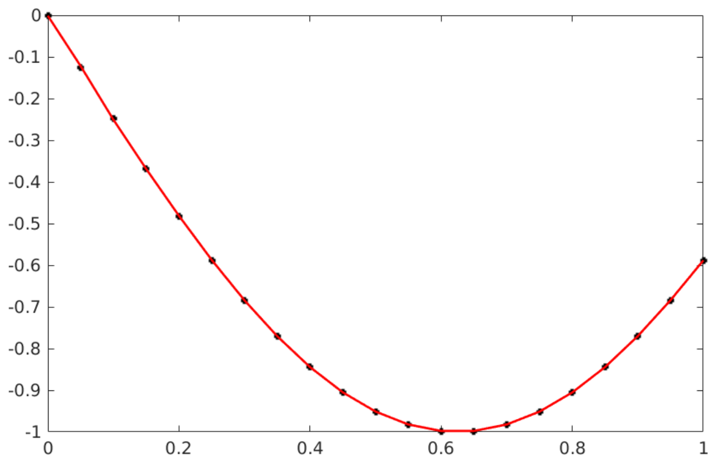
Neural networks obviously have many possible architectures, so a simple fully connected rectangular feedforward network is considered. It has an input dimension I, an output dimension O, and it has D hidden layers of width W. The weight matrixes have $I \times W + O \times W + (D-1) \times W \times W$ parameters, the bias vectors have $D \times W + O$ parameters and the state vectors have $D \times W \times N$ parameters. On the other hand $\mathcal{L}_c(x, \lambda)$ will have an output dimension of $D \times W \times N + O \times N$. The dimension of the Jacobian will be $(D \times W \times N + O \times N) \times (D \times W \times N + O + (D + I + O) \times W + (D-1) \times W^2)$. Therefore the Jacobian will be taller than it is wide when $N \geq 1 + (D+I+O) \times W/O + (D-1) \times W^2/O$. Written out completely the Jacobian will look like .... Figure



(A) Training performance of simultaneous approach, with tansig activation function



(B) Training performance of simultaneous approach, with ReLU activation function



(C) Training performance of backpropagation, with ReLU activation function

Figure 3.1: Performance of algorithms for simple regression problem

	$\nabla\mathcal{L}$	W_{0_1}	W_{0_2}	...	W_{0_W}	b_0
		I	I	...	I	W
F	O*N	0	0	...	0	0
h_1	N	$-x\sigma'(W_{0_1}x + b_{0_1})$	0	...	0	$-\sigma'(W_{0_1}x + b_{0_1})$
	N	0	$-x\sigma'(W_{0_2}x + b_{0_2})$	...	0	$-\sigma'(W_{0_2}x + b_{0_2})$
	...	...	...	...	...	...
	N	0	0	...	$-x\sigma'(W_{0_W}x + b_{0_W})$	$-\sigma'(W_{0_W}x + b_{0_W})$
h_2	W*N	0	0	...	0	0
...	...	...	...	...	...	...
h_D	W*N	0	0	...	0	0

	$\nabla\mathcal{L}$	W_{i_1}	W_{i_2}	...	W_{i_W}	b_1
		W	W	...	W	W
F	O*N	0	0	...	0	0
h_1	W*N	0	0	...	0	0
...	...	...	...	...	...	...
h_{i+1}	N	$-z_1\sigma'(W_{i_1}z + b_{i_1})$	0	...	0	$-\sigma'(W_{i_1}x + b_{i_1})$
	N	0	$-z_1\sigma'(W_{i_2}z + b_{i_2})$	...	0	$-\sigma'(W_{i_2}x + b_{i_2})$
	...	...	...	...	...	...
	N	0	0	...	$-z_1\sigma'(W_{i_W}z + b_{i_W})$	$-\sigma'(W_{i_W}x + b_{i_W})$
...	...	...	...	...	...	...
h_D	W*N	0	0	...	0	0

	$\nabla\mathcal{L}$	W_{D_1}	W_{D_2}	...	W_{D_O}	b_D
		W	W	...	W	O
F	N	$-\frac{z_D}{\sqrt{c}}\sigma'_O(W_{D_1}x + b_{D_1})$	0	...	0	$-\frac{1}{\sqrt{c}}\sigma'_O(W_{D_1}x + b_{D_1})$
	N	0	$-\frac{z_D}{\sqrt{c}}\sigma'_O(W_{D_2}x + b_{D_2})$	...	0	$-\frac{1}{\sqrt{c}}\sigma'_O(W_{D_2}x + b_{D_2})$
	...	...	...	...	...	...
	N	0	0	...	$-\frac{z_D}{\sqrt{c}}\sigma'_O(W_{D_O}x + b_{D_O})$	$-\frac{1}{\sqrt{c}}\sigma'_O(W_{D_O}x + b_{D_O})$
h_1	W*N	0	0	...	0	0
...	...	...	...	...	...	...
h_D	W*N	0	0	...	0	0

Square Diagonal Matrices

	$\nabla\mathcal{L}$	z_{i_1}	z_{i_2}	...	z_{i_W}
		N	N	...	N
F	O*N	0	0	...	0
h_1	W*N	0	0	...	0
...	...	...	...	...	...
h_i	N	1	0	...	0
	N	0	1	...	0
	...	...	...	...	...
	N	0	0	...	1
h_{i+1}	N	$-W_{i_{1,1}}\sigma'(W_{i_1}z_i + b_{i_1})$	$-W_{i_{1,2}}\sigma'(W_{i_1}z_i + b_{i_1})$	...	$-W_{i_{1,W}}\sigma'(W_{i_1}z_i + b_{i_1})$
	N	$-W_{i_{2,1}}\sigma'(W_{i_2}z_i + b_{i_2})$	$-W_{i_{2,2}}\sigma'(W_{i_2}z_i + b_{i_2})$	...	$-W_{i_{2,W}}\sigma'(W_{i_2}z_i + b_{i_2})$
	...	...	...	...	...
	N	$-W_{i_{W,1}}\sigma'(W_{i_W}z_i + b_{i_W})$	$-W_{i_{W,2}}\sigma'(W_{i_W}z_i + b_{i_W})$	...	$-W_{i_{W,W}}\sigma'(W_{i_W}z_i + b_{i_W})$
...	...	...	...	...	...
h_D	W*N	0	0	...	0

	$\nabla\mathcal{L}$	z_{D_1}	z_{D_2}	...	z_{D_W}
		N	N	...	N
F	N	$-W_{D_{1,1}}\sigma'_O(W_{D_1}z_D + b_{D_1})$	$-W_{D_{1,2}}\sigma'_O(W_{D_1}z_D + b_{D_1})$	...	$-W_{D_{1,W}}\sigma'_O(W_{D_1}z_D + b_{D_1})$
	N	$-W_{D_{2,1}}\sigma'_O(W_{D_2}z_D + b_{D_2})$	$-W_{D_{2,2}}\sigma'_O(W_{D_2}z_D + b_{D_2})$	...	$-W_{D_{2,W}}\sigma'_O(W_{D_2}z_D + b_{D_2})$
	...	...	...	...	...
	N	$-W_{D_{O,1}}\sigma'_O(W_{D_O}z_D + b_{D_O})$	$-W_{D_{O,2}}\sigma'_O(W_{D_O}z_D + b_{D_O})$	...	$-W_{D_{O,W}}\sigma'_O(W_{D_O}z_D + b_{D_O})$
h_1	W*N	0	0	...	0
...	...	...	...	...	...
h_D	N	1	0	...	0
	N	0	1	...	0
	...	...	...	...	...
	N	0	0	...	1

How to read figure

3.3 Algorithmic Verification of Jacobian

The Jacobian in the previous section was derived by hand. In this section will be explained how the Jacobian was verified algorithmically.

By Algorithmic Differentation the numerical value for the Jacobian can be deduced. For this the AlgoPy python module was used. By adding code from this packet to the calculation of the neural network, the Jacobian is calculated along with the network. This result was then compared to the analytical result for a number of different network configurations, confirming the correctness of the analytical derivation.

3.4 Alternative Representation

In this section we explain an alternative representation which is mathematically the same. Figure **??** shows the jacobian, but with the rows corresponding to the loss function put at the bottom. It shows a diagonal structure, because each layer in this feedforward net is only connected to the adjacent layers.

3.5 Testing

In this section the tests from the previous chapter are run again, this time using the ALM algorithm. The least squares problem in the inner loop is solved using the `least_squares` method in `numpy 1.20.1`, which is provided with the Jacobian calculated in the previous section. This time the stopping criterion is that the cost function described in equation **??** is less than a tolerance of $1e^{-6}$.

3.5.1 Test 1

Again a small regression problem is run, with 2 layers of 3 hidden nodes, using the tansig activation function. The result is plotted in Figure **??**.

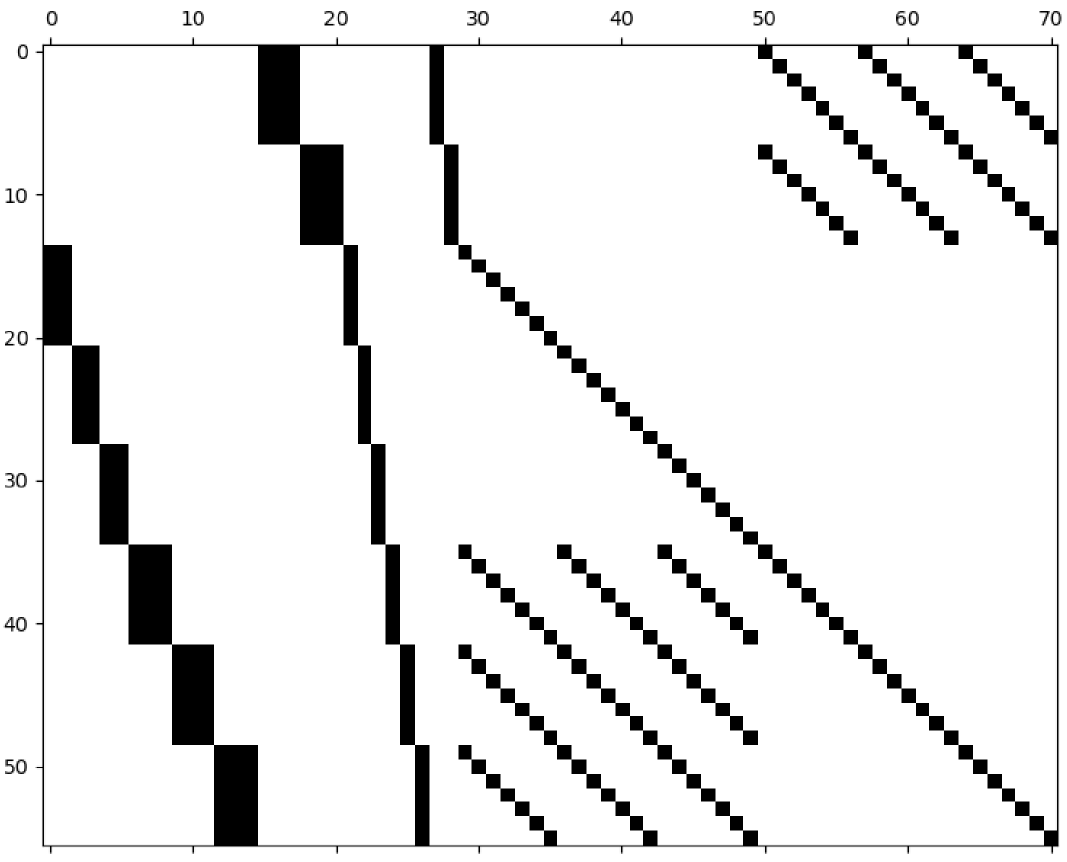


Figure 3.2: Nonzero elements of jacobian, for network with I=2,O=2,W=3,D=2,N=7

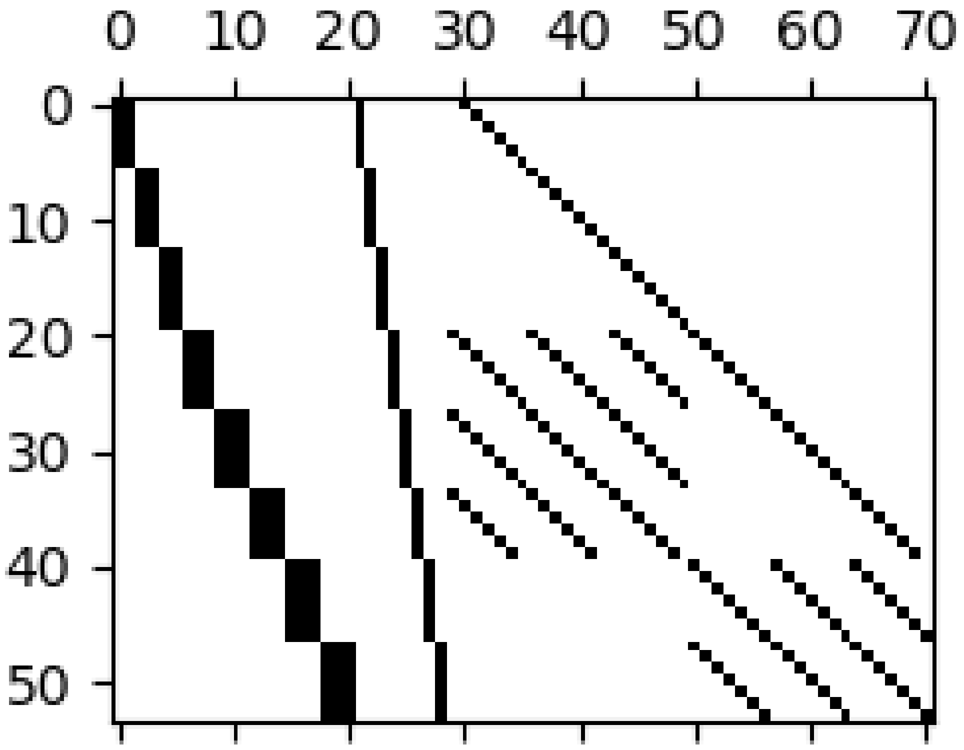


FIGURE 3.3: Nonzero elements of jacobian, for network with I=2,O=2,W=3,D=2,N=7, rearranged

Chapter 4

Tests

This chapter discusses several tests to compare the newly proposed method with backpropagation. Each test will be described in detail. The reference code to which we compare our experiments is the backpropagation method of Tenserflow.

The code was executed on ...

4.1 The First Topic of this Chapter

4.1.1 Item 1

Sub-item 1

Sub-item 2

4.1.2 Item 2

4.2 The Second Topic

4.3 Conclusion

Chapter 5

Conclusion

The final chapter contains the overall conclusion. It also contains suggestions for future work and industrial applications.

Appendices

Appendix A

Source code

This appendix contains the source code of the experiments.

A.1 First experiment source

```
N = 21;
xin = linspace(0,1,21);
y = -sin(.8*pi*x);

w1 = sdpvar(3,1);
b1 = sdpvar(3,1);
x1 = sdpvar(3,N);
w2 = sdpvar(3,3,'full');
b2 = sdpvar(3,1);
x2 = sdpvar(3,N);
w3 = sdpvar(3,1);
b3 = sdpvar(1,1);


assign(w1,2*rand(3,1)-1);
assign(b1,2*rand(3,1)-1);
assign(x1,tansig(value(w1*xin+repmat(b1,1,N))));
assign(w2,2*rand(3,3)-1);
assign(b2,2*rand(3,1)-1);
assign(x2,tansig(value(w2*x1 +repmat(b2,1,N))));
assign(w3,2*rand(3,1)-1);
assign(b3,2*rand(1,1)-1);

res = w3'*x2 + b3 - y;
obj = res*res';
%
f1 = (x1-(w1*xin+repmat(b1,1,N)));
```

```
f2 = (x2-(w2*x1 +repmat(b2,1,N)));
% con = [f1 >= 0; x1 >= 0; f1.*x1 <= 0;
%        f2 >= 0; x2 >= 0; f2.*x2 <= 0];
% con = [x1 == max(w1*xin+repmat(b1,1,N),0);
%        x2 == max(w2*x1 +repmat(b2,1,N),0)];
con = [x1 == tansig(w1*xin+repmat(b1,1,N));
       x2 == tansig(w2*x1 +repmat(b2,1,N))];
ops = sdpsettings('usex0',1);
ops.fmincon.MaxFunEvals = 20000;
ops.fmincon.MaxIter = 200;

optimize(con,obj,ops);

%%
x1s = tansig(value(w1)*xin+value(b1));
x2s = tansig(value(w2)*x1s+value(b2));
ys = value(w3)'*x2s+value(b3);

hold off
plot(xin,y,'Linewidth',3);
hold on
plot(xin,ys,'g--','Linewidth',4);
```

A.1.1 Second experiment source

```
clear
N = 21;W = 10;
xin = linspace(0,1,21);
y = -sin(.8*pi*xin);

w1 = sdpvar(W,1);
b1 = sdpvar(W,1);
x1 = sdpvar(W,N);
w3 = sdpvar(W,1);
b3 = sdpvar(1,1);


assign(w1,2*rand(W,1)-1);
assign(b1,2*rand(W,1)-1);
assign(x1,poslin(value(w1*xin+repmat(b1,1,N))));
assign(w3,2*rand(W,1)-1);
assign(b3,2*rand(1,1)-1);

res = w3'*x1 + b3 - y;
obj = res*res';
```

```
%
f1 = (x1-(w1*xin+repmat(b1,1,N)));
%f2 = (x2-(w2*x1 +repmat(b2,1,N)));
con = [f1 >= 0; x1 >= 0; f1.*x1 <= 0;];
%        f2 >= 0; x2 >= 0; f2.*x2 <= 0];
% con = [x1 == max(w1*xin+repmat(b1,1,N),0);
%        x2 == max(w2*x1 +repmat(b2,1,N),0)];
% con = [x1 == tansig(w1*xin+repmat(b1,1,N));
%        x2 == tansig(w2*x1 +repmat(b2,1,N))];
ops = sdpsettings('usex0',1);
ops.fmincon.MaxFunEvals = 20000;
ops.fmincon.MaxIter = 200;

optimize(con,obj,ops);

%%
x1s = poslin(value(w1)*xin+value(b1));
%x2s = tansig(value(w2)*x1s+value(b2));
ys = value(w3)'*x1s+value(b3);

hold off
plot(xin,y,'Linewidth',3);
hold on
plot(xin,ys,'g--','Linewidth',4);
```