

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

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

Promotor:

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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.

 $Jan\ Scheers$

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Abstract

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 and a bias:

$$y = \sigma(w_1 x_1 + w_2 x_2 + \dots + w_n x_n + b)$$
(1.1)

 w_i are the weights, x_i are the inputs to the neuron, which come either from a previous neuron, or are fed into the network, σ is the activation function, and finally a bias b is also added to the sum. This is the McCulloch-Pitts neuron model.[REF] The most commonly used activation function σ is the Rectified Linear Unit (ReLU):

$$\sigma(x) = x^{+} = \max(0, x) \tag{1.2}$$

Many other activation functions are possible, such as the sigmoid function $(\frac{1}{1+e-x})$ or the tansing function (tanh(x)).

A visual representation is shown in figure 1.1b. A full network is built by connecting layers of neurons as shown in figure 1.1a. An ANN can also be expressed as a combination of function composition and matrix multiplication, ignoring for a moment the bias vectors.

$$f(W,x) = W_L \sigma(W_{L-1}\sigma(...W_1\sigma(W_0x)...))$$
(1.3)

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

1.2 Neural Network Training

Training a neural network is an optimization problem as we will discuss in this section. Ruoyu Sun covers in [5] the current theory and algorithms for optimizing deep neural networks, upon which much of this section is based.

In a supervised learning problem a dataset of inputs and desired outputs is given: $x_i \in \mathbb{R}^{d_x}, y_i \in \mathbb{R}^{d_y}, i = 1, \dots, n$ with x_i the input vectors, y_i the desired output vectors and n the number of data points. We want the network to predict the output y_i based on the information in x_i , i.e. we want the network to learn the underlying mapping that connects the data. A standard fully connected network can be expressed as a combination of function composition and matrix multiplication as follows:

$$f_W(x) = W_L \sigma(W_{L-1} \sigma(...W_1 \sigma(W_0 x)...))$$
(1.4)

where L is the depth of the network, W_j are matrixes of dimension $d_j \times d_{j-1}$, $j = 1 \dots L$ containing the connection weights and σ is the activation function. The bias vectors b_i have been omitted from this equation for clarity.

We want to pick the parameters of the neural network so that the predicted output $\hat{y}_i = f_W(x_i)$ is as close as possible to the true output y_i for a certain distance metric $l(\cdot,\cdot)$. Thus the optimization problem can be written as follows:

minimize
$$F(W) = \sum_{j=0}^{N} l(y_j, f_W(x_j))$$
 (1.5)

In this thesis only regression problems will be considered, where l(x, y) is the quadratic loss function $l(x, y) = ||x^2 - y^2||$. For classification problems cross entropy loss is the most common cost function: $l(x, y) = x \log(y) + (1 - x) \log(y)$.

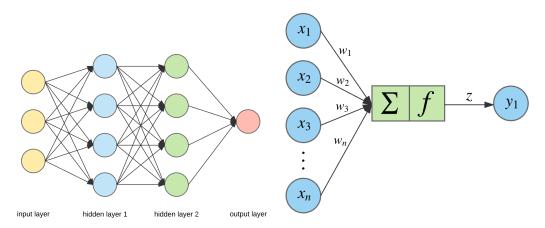


FIGURE 1.1: Feedforward Deep Neural Network and Single Neuron - McCulloch-Pitts model. (Retrieved from https://towardsdatascience.com)

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

Most methods for solving equation 1.5 are based on gradient descent (GD). This algorithm uses the gradient of the loss function to search for a local minimum:

$$W_{k+1} = W_k - \eta_k \nabla F(W_k) \tag{1.6}$$

where η_k is the step size (a.k.a. "learning rate") and $\nabla F(W_k)$ is the gradient of the loss function at the k-th iterate.

1.3 Backpropagation

Backpropagation is the current standard algorithm for calculating the gradient in equation 1.6. It was discovered and popularised in the context of neural networks by Rumelhart, Hinton & Williams (1986) ??, but in the context of optimal control the techniques for calculating this gradient were discovered in 1960 by Kelley 3.1c and Bryson 3.1c. It has been shown that reformulatin

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.

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

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 inputs. The activation values and derivatives of each neuron are stored. Then the error and gradient are calculated from the end of the network to the start, i.e. backwards.

Finally any gradient descent method can be used to find a step update. This is repeated until a stopping criterion is met.

1.4 Neural Networks in Optimal Control Theory

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

$$z_0 = x$$

$$z_{k+1} = \sigma(W_k z_k), \quad k = 0, ..., L - 1$$

$$y = W_H z_L$$

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)

minimize
$$\sum_{j=0}^{N} ||W_L z_L^j - y^j||^2$$

subject to $z_{k+1}^j = \max(W_k z_k^j + b^j, 0), \quad k = 0, \dots, L-1, j = 1, \dots, N$ (1.7)

1.5 Simultaneous Approach

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.

1.6 Goal of the Thesis

- implement simultaneous approach
- compare speed
- compare reliability/convergence

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 1.7. 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 3.1c 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.

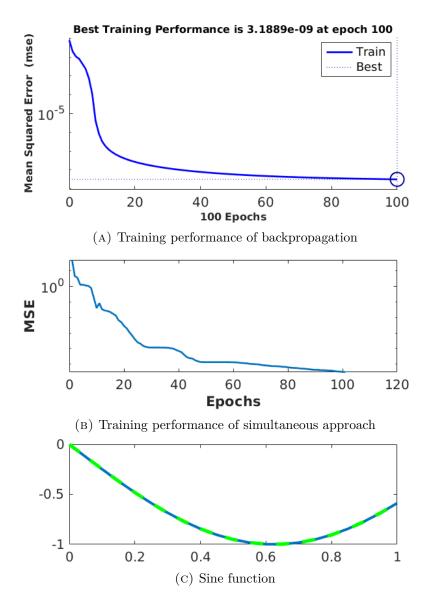


Figure 2.1: Performance of algorithms for simple regression problem

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:

$$x_{k+1}^{j} = \max(W_{k}x_{k}^{j}, 0)$$

$$\updownarrow$$

$$x_{k+1}^{j} = -\min(-W_{k}x_{k}^{j}, 0)$$

$$\updownarrow$$

$$\min(x_{k+1}^{j} - W_{k}x_{k}^{j}) = 0$$

$$\updownarrow$$

$$(x_{k+1}^{j} - W_{k}x_{k}^{j})^{\top}x_{k+1}^{j} = 0,$$

$$x_{k+1}^{j} \ge 0, x_{k+1}^{j} - W_{k}x_{k}^{j} \ge 0$$

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

2. Initial exploration

• Stopping criteria and initial conditions

These will be explored in the next chapters

The option that will be explored in the next chapter, will be changing the optimization algorithm. The fmincon method will be replaced by a specifically written algorithm, exploiting the structure of the problem.

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 (ALM) is used to solve the optimal control problem. The Optimal Control Problem described in equation 1.7, which is printed here again:

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

is represented as a nonlinear least squares problem

min
$$\frac{1}{2}||F(x)||_2^2$$

s. t. $h(x) = 0$

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

$$\mathcal{L}_{c}(x,\lambda) = \frac{1}{2} ||F(x)||_{2}^{2} + \langle \lambda, h(x) \rangle + \frac{c}{2} ||h(x)||_{2}^{2}$$

$$= \frac{1}{2} ||F(x)||_{2}^{2} + \frac{c}{2} ||h(x) + \lambda/c||_{2}^{2} - \frac{1}{2c} ||\lambda||_{2}^{2}$$

$$= \frac{c}{2} ||\int_{h(x) + \lambda/c}^{F(x)/\sqrt{c}} ||^{2}$$
(3.1)

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

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

The Langrangian parameters lambda are then updated using the rule:

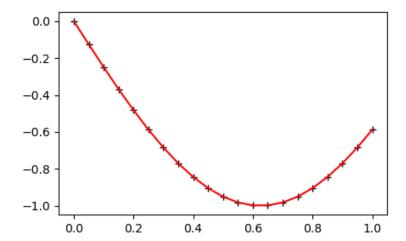
$$\lambda^{k+1} = \lambda^k + c_k h(x^k) \tag{3.3}$$

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

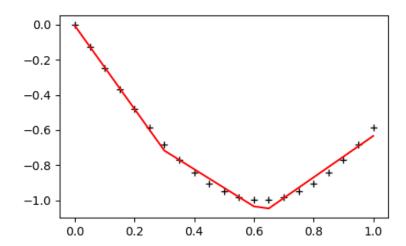
3.2 Jacobian

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.

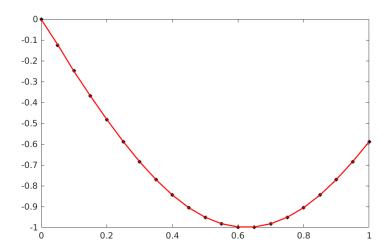
Neural networks obviously have many possible architectures, so a simple fully connected rectangular feedforward network is considered. It has an input dimension I, an output dimension O, and it has D hidden layers of width W. The weight matrixes have $I \times W + O \times W + (D-1) \times W \times W$ 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 Table 3.1



(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 $% \left(1\right) =\left(1\right) \left(1\right)$

Figure 3.1: Performance of algorithms for simple regression problem

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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 them to be equal within a small tolerance. The code is available at https://github.com/jan-scheers/thesis

3.4 Alternative Representation

In this section we explain an alternative representation which is mathematically the same. Figure 3.3 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 3.1 is less than a tolerance of $1e^{-6}$. Figure 3.1a and Figure 3.1b show the result of these two tests.

-	$\nabla \mathcal{L}$	W_{0_1}	$W_{0}{}_{2}$		W_{0W}	b_0	
	O*N	I 0	I			0	
$\frac{F}{h_1}$	N N	$\frac{0}{-x\sigma'(W_{0_{1}}x+b_{0_{1}})}$	0		0)
701	N	0	$-x\sigma'(W_{0_2}x+b_{0_2})$		0	$-\sigma'(W_{0_1}x + b_{0_1} - \sigma'(W_{0_2}x + b_{0_2})$)
			•••				
	N W*N	0	0	–	$\frac{x\sigma'(W_0{}_W x + }{0}$	b_{0_W}) $-\sigma'(W_{0_W}x + b_{0_W}$	_V)
h_2	W "IN		···		Ü	U	
h_D	W*N	0	0		0	0	
	$\nabla \mathcal{L}$	W_{i_1}	W_{i_2}		W _i	b_1	
		W	\overline{W}^2		$\overset{W_{i_{W}}}{\mathbb{W}}$	W	
F	O*N	0	0		0	0	
h_1	W*N	0	0		0	0	
h_{i+1}	N	$\frac{\cdots}{-z_1\sigma'(W_{i_1}z+b_{i_1})}$	0		0	$-\sigma'(W_i, x + b_i,$)
	N	0	$-z_1\sigma'(W_{i_2}z+b_{i_2})$		0	$-\sigma'(W_{i_1}x + b_{i_1} - \sigma'(W_{i_2}x + b_{i_2})$)
	 N			–	$z_1 \sigma'(W_{i_W} z +$	•••	
							<u> </u>
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	$-\frac{1}{\sqrt{c}}\sigma'_{O}(W_{D_{1}}x+b) \\ -\frac{1}{\sqrt{c}}\sigma'_{O}(W_{D_{2}}x+b)$	$p_{D_1})$
	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		z	$\frac{D}{\sigma}\sigma'$ (Wp. x -	$\frac{1}{2} h_{\rm D} = \frac{1}{2} \sigma' (W_{\rm D} + x + b)$,,)
$\overline{h_1}$	W*N	0	0		$\frac{\sqrt{c}}{0}$	$+b_{D_O}$) $-\frac{1}{\sqrt{c}}\sigma_O'(W_{D_O}x+b)$	D_O
h_D	W*N	0	0		0	0	
	$ abla \mathcal{L}$		uare Diagonal Matrices	3		~.	
	V L	$egin{array}{c} z_{i_1} \ \mathrm{N} \end{array}$	$egin{array}{c} z_{i_2} \ \mathrm{N} \end{array}$			$\overset{z_{i_W}}{\operatorname{N}}$	
\overline{F}	O*N	0	0			0	
h_1	W*N	0	0			0	
$\frac{\dots}{h_i}$	 N	1	0		•••	0	
	N	0	1			Ō	
	 NI						
h_{i+1}	N N	$\frac{0}{-W_{i_{1,1}}\sigma'(W_{i_{1}}z_{i}+b_{i_{1}})}$	$\frac{0}{-W_{i_{1,2}}\sigma'(W_{i_{1}})}$	$\gamma: + h:$		$\frac{1}{W_{i_{1},W}\sigma'(W_{i_{1}}z_{i}+b_{i_{1}})}$	
<i>re1</i> +1	N	$-W_{i_{2,1}}\sigma'(W_{i_{2}}z_{i}+b_{i_{2}})$	$-W_{i_{2,2}}\sigma'(W_{i_{2}})$	$z_i + b_{i_2}$		$W_{i_{1},W}\sigma'(W_{i_{1}}z_{i}+b_{i_{1}})$	
	N	$-W_{i_{W,1}}\sigma'(W_{i_{W}}z_{i}+b_{i_{W}})$	$-W_{i_{W,2}}\sigma'(W_{i_{W}}$	$z_i + b_{i_W}$	V	$V_{i_{W,W}}\sigma'(W_{i_{W}}z_{i}+b_{i_{W}})$	
h_D	w*N	0	0			0	
-	\(\nabla c\)						
	$\nabla \mathcal{L}$	$\overset{z_{D_1}}{\scriptscriptstyle{\rm N}}$	$^{z_{D_2}}_{ m N}$			$\overset{z_{D_W}}{\operatorname{N}}$	
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	$V_{D_{1,W}}\sigma'_{O}(W_{D_{1}}z_{D}+b_{D_{1}})$	
	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	$V_{D_2,W} \sigma_O'(W_{D_2} z_D + b_{D_2})$	
	 N	$-W_{D_{O,1}}\sigma_{O}'(W_{D_{O}}z_{D}+b_{D_{O}}z_{D})$	$-W_{D_{C,2}}\sigma'_{O}(W_{D_{C,2}})$	$z_D + b_D$	W	$\sum_{D_{O,W}} \sigma_O'(W_{D_O} z_D + b_{D_O})$	
$\overline{h_1}$	W*N	0,1 0, -0 - 20	0	-0		0	
h_D	N N	1 0	0 1		***	0 0	
					•••		
	N	0	0			1	

Table 3.1: Jacobian of feedforward neural network

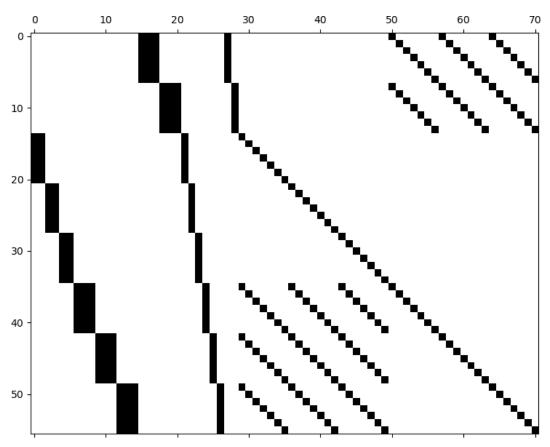


Figure 3.2: Nonzero elements of Jacobian, for network with $I{=}2{,}O{=}2{,}W{=}3{,}D{=}2{,}N{=}7$

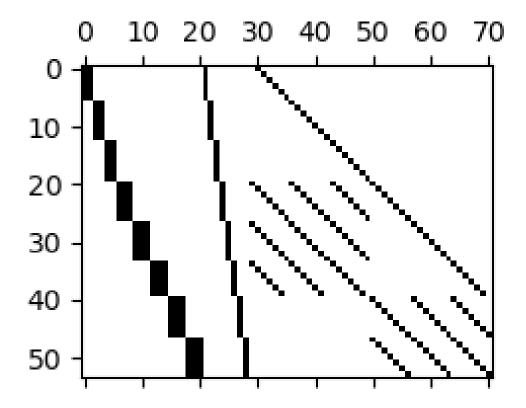


Figure 3.3: Nonzero elements of Jacobian, for network with I=2,O=2,W=3,D=2,N=7, rearranged

Tests

- [5]
 - Optimization for deep learning: theory and algorithms
 - Goals of optimization
 - Problem formulation
 - Gradient descent:
 - Tips tricks
 - State of the art algorithms
- [2]

"The Kelley-Bryson gradient formulas for such problems have been rediscovered by neural- network researchers and termed back propagation"

• [1]

Practical Augmented lagrangian method

- [3] "Indeed the loss surface of neural networks optimization problems is highly non-convex: it has a high number of saddle points which may slow down the convergence (4). A number of results (3; 13; 14) suggest that for wide enough networks, there are very few "bad" local minima, i.e. local minima with much higher cost than the global minimum"
- [4] Original Backpropagation paper

4.1 Needed

- Basic Neural network intro
- Optimal control reference
- Simultaneous approach

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 \ge 0; x2 \ge 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);
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 \ge 0; x1 \ge 0; f1.*x1 <= 0;];
         f2 \ge 0; x2 \ge 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);
```

Bibliography

- [1] E. G. Birgin and J. M. Martínez. Practical augmented Lagrangian methodsPractical Augmented Lagrangian Methods, pages 3013–3023. Springer US, Boston, MA, 2009.
- [2] S. E. Dreyfus. Artificial neural networks, back propagation, and the kelley-bryson gradient procedure. *Journal of Guidance, Control, and Dynamics*, 13(5):926–928, 1990.
- [3] A. Jacot, F. Gabriel, and C. Hongler. Neural tangent kernel: Convergence and generalization in neural networks, 2020.
- [4] D. E. Rumelhart, G. E. Hinton, and R. J. Williams. Learning representations by back-propagating errors. *Nature*, 323(6088):533–536, Oct 1986.
- [5] R. Sun. Optimization for deep learning: theory and algorithms, 2019.