

SENIOR HONOURS PROJECT



University of
St Andrews

Freeing Neural Training Through Surfing

Georg Wölflein
170011885

Supervisor: Dr. Mike Weir

April 13, 2020

Word count: 3412 words

Abstract

TODO

Declaration

“I declare that the material submitted for assessment is my own work except where credit is explicitly given to others by citation or acknowledgement. This work was performed during the current academic year except where otherwise stated. The main text of this project report is 3412 words long, including project specification and plan. In submitting this project report to the University of St Andrews, I give permission for it to be made available for use in accordance with the regulations of the University Library. I also give permission for the title and abstract to be published and for copies of the report to be made and supplied at cost to any bona fide library or research worker, and to be made available on the World Wide Web. I retain the copyright in this work.”

Georg Wölflein

Contents

1	Introduction	5
2	Context survey	6
2.1	Neural networks	6
2.2	Implementation tools	6
3	Requirements specification	7
3.1	Ethics	7
I	Theory	8
4	Neural network theory	9
4.1	Supervised learning	9
4.2	Artificial neural networks	10
4.2.1	Single-layer network	12
4.2.2	Multi-layer perceptron	13
5	Neural network learning	15
5.1	Gradient descent with mean squared error	15
5.2	Local minimum problem	15
5.3	Simulated annealing	15
6	Neural surfing theory	16
6.1	Weight and output spaces	16
6.1.1	Relationship between weight and output space	17
6.1.2	Gradient descent from the perspective of weight and out- put space	20
6.2	Unrealizable regions	21
6.3	Goal-connecting paths	23
7	Problems	24
7.1	Stripe problem	24
8	Generalising neural surfing	25

II Framework	26
9 Design	27
10 Implementation	28
Bibliography	28

Chapter 1

Introduction

*Describe the problem you set out to solve and the extent of your success in solving it. You should include the aims and objectives of the project in order of importance and try to outline key aspects of your project for the reader to look for in the rest of your report. **TODO***

Chapter 2

Context survey

2.1 Neural networks

TODO

2.2 Implementation tools

- TensorFlow
- keras

TODO

Chapter 3

Requirements specification

Primary objectives:

1. Design a generic framework that can be used for various neural training algorithms with a clear set of inputs and outputs at each step. This framework should include benchmarking capabilities.
2. For a simple case of this framework (when the dimensionality of the control space and output space are suitably low), implement a visualisation tool that shows the algorithm's steps.
3. Implement a particular training algorithm for the framework that uses potential field techniques.
4. Evaluate the performance of this and other algorithms on tasks of differing complexity, especially with regard to the local minimum problem and similar issues.

Secondary objectives:

1. Investigate how this approach can be generalized to other numerical optimisation problems.

3.1 Ethics

There are no ethical considerations. All questions on the preliminary self-assessment form were answered with “NO” and hence no ethics form had to be completed.

Part I

Theory

Chapter 4

Neural network theory

4.1 Supervised learning

Definition 1 (Regression model). In machine learning, a regression model f is defined as a mathematical function of the form

$$f(\mathbf{x}) = \hat{y} = y + \epsilon \quad (4.1)$$

that models the relationship between a D -dimensional feature vector $\mathbf{x} \in \mathbb{R}^D$ of independent (*input*) variables and the dependent (*output*) variable $y \in \mathbb{R}$. Given a particular \mathbf{x} , the model will produce a *prediction* for y which we denote \hat{y} . Here, the additive error term ϵ represents the discrepancy between y and \hat{y} .

Definition 2 (Labelled dataset). A labelled dataset consists of N tuples of the form $\langle \mathbf{x}_i, y_i \rangle$ for $i = 1, \dots, N$. For each feature vector \mathbf{x}_i (a row vector), the corresponding y_i represents the observed output, or *label* [Burkov, 2019]. We use the vector

$$\mathbf{y} = [y_1 \quad y_2 \quad \cdots \quad y_N]^\top \quad (4.2)$$

to denote all the labelled outputs in the dataset, and the $N \times D$ matrix

$$\mathbf{X} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \cdots \quad \mathbf{x}_N]^\top \quad (4.3)$$

for representing the corresponding feature vectors.

Supervised learning A supervised learning algorithm for a regression task infers the function f given in (4.1) from a set of *labelled training data* of the form explained previously. We use the vector

$$\hat{\mathbf{y}} = [\hat{y}_1 \quad \hat{y}_2 \quad \cdots \quad \hat{y}_N]^\top \quad (4.4)$$

to denote the prediction that f produces for each training sample.

4.2 Artificial neural networks

Artificial neural networks (ANNs) take inspiration from the human brain and can be regarded as a set of interconnected neurons. More formally, an ANN is a directed graph of n neurons (referred to as *nodes* or *units*) with weighted edges (*links*). Each link connecting two units i and j is directed and associated with a real-valued weight $w_{i,j}$.

A particular unit i 's *excitation*, denoted z_i , is calculated as the weighted sum

$$z_i = \sum_{j=1}^n w_{j,i} a_j + b_i \quad (4.5)$$

where $a_j \in \mathbb{R}$ is another unit j 's *activation* and $b_i \in \mathbb{R}$ is the i th unit's *bias*. Notice that in this model, if there exists no link between unit i and a particular j then simply $w_{i,j} = 0$ and therefore j will not contribute to i 's excitation.

The unit i 's activation is its excitation applied to a non-linear *activation function*, $g : \mathbb{R} \rightarrow \mathbb{R}$. We have

$$a_i = g(z_i) = g\left(\sum_{j=1}^n w_{j,i} a_j + b_i\right). \quad (4.6)$$

Activation functions In its original form, McCulloch and Pitts defined the neuron as having only binary activation [McCulloch and Pitts, 1943]. This means that in our model from (4.6), we would require $a_i \in \{0, 1\}$ and hence an activation function of the form $g_{\text{thres}} : \mathbb{R} \rightarrow \{0, 1\}$ which would be defined¹ as

$$g_{\text{thres}}(x) = \begin{cases} 0 & x < 0 \\ 1 & x \geq 0 \end{cases}. \quad (4.7)$$

Commonly used activation functions in modern neural networks include the sigmoid

$$g_{\text{sig}}(x) = \frac{1}{1 + e^{-x}} \quad (4.8)$$

and the rectified linear unit (ReLU)

$$g_{\text{ReLU}} = \begin{cases} 0 & x < 0 \\ x & x \geq 0 \end{cases} \quad (4.9)$$

which are depicted in Figure 4.1. Unlike g_{step} , these activation functions are differentiable which is an advantage for being able to use gradient descent [Russell and Norvig, 2010, p. 729].

Rectified units do not suffer from the *vanishing gradient effect* [Glorot et al., 2011]. This phenomenon occurs with sigmoid activation functions when they

¹In fact, McCulloch and Pitts defined the activation to be zero when $x < \theta$ for a threshold parameter $\theta \in \mathbb{R}$ and one otherwise, but in our model the bias term b_i acts as the threshold.

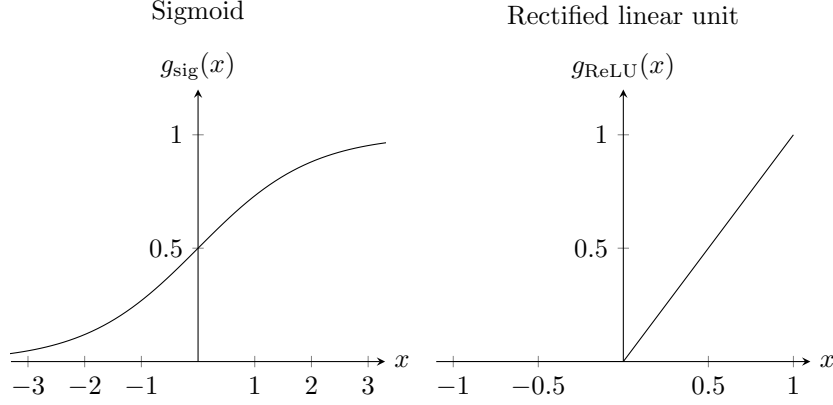


Figure 4.1: Plots of the the two most common activation functions.

reach high saturation, i.e. when the input is significantly far from zero such that the gradient is almost horizontal. However, the vanishing gradient problem is usually not prevalent in shallow² networks so the sigmoid function still remains popular [Neal, 1992].

Particularly in deep neural networks, different neurons (grouped in *layers*, see Section 4.2.2) often have different activation functions [Burkov, 2019], but for the purposes of this report it is more convenient (in terms of notation) to have the activation function be the same for all neurons, so it does not need to be supplied as a parameter to the function describing the particular neural network. Much of the work in this report can easily be generalized to designs with multiple activation functions. This is because the algorithms explained in this report do not concern themselves with the specifics of the activation functions, as long as they are non-linear.

ANNs as regression models We can employ an ANN to model a regression problem of the form given in (4.1). To do so, we need at least $D + 1$ neurons in the network. We consider the first D units to be the *input* neurons, and the last neuron, n , is the output unit. Furthermore, we require $w_{j,k} = 0$ for $j, k \in \mathbb{Z}^+$ where $j \leq n$ and $k \leq D$ to ensure that there are no links feeding into the input neurons.

To obtain the prediction \hat{y} given the D -dimensional feature vector \mathbf{x} , we set the activation of the i th unit to the value the i th element in \mathbf{x} for $i = 1, \dots, D$. Then, we propagate the activations using (4.6) until finally the prediction is the activation of the last neuron, $\hat{y} = a_n$. This process is often called *forward propagation* or *forward pass* [Burkov, 2019].

²Shallow networks refer to ANNs with few layers.

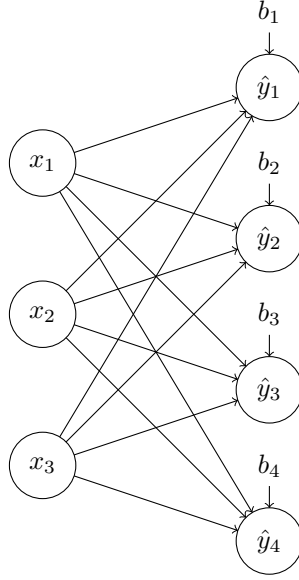


Figure 4.2: A single-layer perceptron with three input and four output neurons.

4.2.1 Single-layer network

We introduce a single-layer network (SLN) as a type of ANN which consists of two conceptual layers, an input and an output layer. Every input node is connected to every output node, but there are no intra-layer links (i.e. there are no links between any two input nodes or any two output nodes), as shown in Figure 4.2. This is what we call a *fully-connected feedforward* architecture. SLN architectures will always form a *directed acyclic graph* (DAG) because there are no intra-layer or backwards connections.

We purposefully use the term SLN instead of single-layer perceptron (SLP) to avoid confusion. A SLP has only one output unit and uses the threshold activation function given in (4.7) [Rosenblatt, 1958]. In our definition of a SLN we allow more than one output and impose no restrictions on g , except that the same activation function is used for every output neuron. We still use the term ‘single layer’ because the input layer, lacking any incoming weight or bias connections, is not considered to be a ‘proper’ layer.

Let us consider a SLN with m inputs and n outputs. Since every output unit i only has connections from every input unit j , we can adapt (4.6) to give the activation of a particular output neuron i as

$$a_i = y_i = g(z_i) = g\left(\sum_{j=1}^m w_{j,i}x_j + b_i\right) = g(\mathbf{w}_i^T \mathbf{x} + b_i) \quad (4.10)$$

where $\mathbf{w}_i = [w_{1,i} \ w_{2,i} \ \cdots \ w_{m,i}]^\top$ represents the weights of all the edges that connect to output unit i . This is all we need to formally define a SLN.

Definition 3 (Single-layer network). A SLN with m inputs and m outputs is the vector-valued function $\mathbf{S} : \mathbb{R}^m \rightarrow \mathbb{R}^n$ defined as

$$\mathbf{S}(\mathbf{x}; \mathbf{W}, \mathbf{b}) = \mathbf{g}(\mathbf{W}^\top \mathbf{x} + \mathbf{b}) \quad (4.11)$$

where the $m \times n$ matrix

$$\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \cdots \ \mathbf{w}_n] = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,1} & w_{m,2} & \cdots & w_{m,n} \end{bmatrix} \quad (4.12)$$

captures all weights and the vector

$$\mathbf{b} = [b_1 \ b_2 \ \cdots \ b_n]^\top \quad (4.13)$$

represents the biases. The vector-valued activation function $\mathbf{g} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is simply the activation function $g : \mathbb{R} \rightarrow \mathbb{R}$ applied pointwise to a vector, i.e.

$$\mathbf{g}(\mathbf{z}) = [g(z_1) \ g(z_2) \ \cdots \ g(z_n)]^\top$$

for the vector of excitations $\mathbf{z} = [z_1 \ z_2 \ \cdots \ z_n]^\top$.

Unlike the formula for a regression model, a SLN is a vector-valued function, due to the fact that there are multiple outputs. Note that when $n = 1$, we reach the same form as in (4.1). Moreover, if we additionally use the threshold activation function from (4.7), we arrive at the SLP model given by Rosenblatt [1958].

4.2.2 Multi-layer perceptron

A multi-layer perceptron³ (MLP) is a fully-connected feedforward ANN architecture with multiple layers which we will define in terms of multiple nested functions as in Burkov [2019].

Definition 4 (Multi-layer perceptron). A MLP M with m inputs and L layers is the mathematical function $M : \mathbb{R}^m \rightarrow \mathbb{R}$ defined as the nested function

$$M(\mathbf{x}; \mathcal{W}, \mathcal{B}) = \hat{y} = f_L(\mathbf{f}_{L-1}(\dots(\mathbf{f}_1(\mathbf{x})))) \quad (4.14)$$

where $\mathcal{W} = \mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_L$ are the weight matrices and $\mathcal{B} = \mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_L$ the bias vectors such that the nested functions are given by $\mathbf{f}_l(\mathbf{x}) = \mathbf{S}(\mathbf{x}; \mathbf{W}_l, \mathbf{b}_l)$ for $l = 1, \dots, L-1$. The outermost function f_L represents a SLN with only one output unit and is hence the scalar-valued function $f_L(\mathbf{x}) = S(\mathbf{x}; \mathbf{W}_L, \mathbf{b}_L)$.

³Unlike SLPs, the activation function in a MLP as defined in literature does not necessarily need to be the binary threshold function g_{thres} ; in fact, it is often one of the more modern activation functions explained in Section 4.2 [Hastie et al., 2017; Burkov, 2019]. Hence we can use the term ‘multi-layer perceptron’.

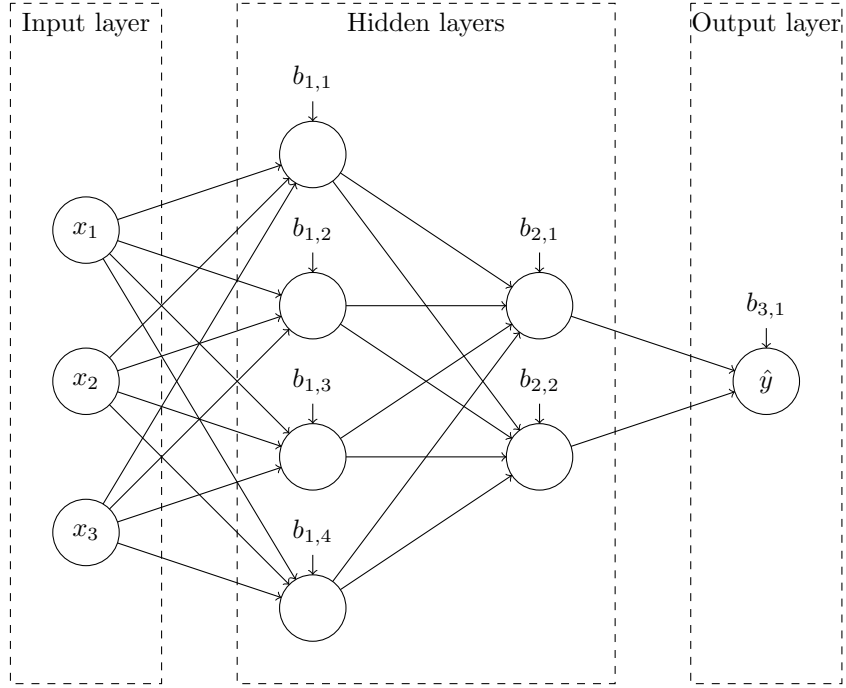


Figure 4.3: A multi-layer perceptron with three inputs and two hidden layers.

Notice that for every $l < L$, \mathbf{W}_l is a $n_l \times m_l$ matrix such that $n_l = m_{l+1}$ to ensure that the number of outputs of layer l is the number of inputs to layer $l + 1$. This means that the MLP has m_1 input neurons. Since the final layer has only one output unit, \mathbf{W}_L has only one row, and finally $n_L = 1$.

The graph representing this type of network consists of connecting the outputs of the SLN representing layer l with the inputs of the SLN representing layer $l + 1$, as shown in Figure 4.3. The layers between the input and output layers are referred to as *hidden* layers.

Since MLPs are simply nested SLNs, it follows that MLPs retain the DAG property and are therefore *feedforward* networks as well. In the forward pass, the activations are propagated from layer to layer (i.e. nested function to nested function) as in (4.11).

Chapter 5

Neural network learning

5.1 Gradient descent with mean squared error

5.2 Local minimum problem

5.3 Simulated annealing

Chapter 6

Neural surfing theory

6.1 Weight and output spaces

In Definition 4 we established that the tuple $\langle \mathcal{W}, \mathcal{B} \rangle$ along with the activation function is sufficient to fully define a MLP. Most importantly, we have $\mathcal{W} = \mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_L$ and $\mathcal{B} = \mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_L$ representing each layer's weight matrices and bias vectors, respectively.

Definition 5 (Weight space). The weight space \mathcal{W}_A of an artificial neural network A is the set of all possible assignments to its *trainable parameters*. The trainable parameters are its weights \mathcal{W} and biases \mathcal{B} . If A has P trainable parameters then its weight space is defined as

$$\mathcal{W}_A = \mathbb{R}^P. \quad (6.1)$$

Definition 6 (Output space). The output space \mathcal{O}_A of an artificial neural network A with one output neuron spans the space of all possible output predictions on the training set. From (4.4), the vector $\hat{\mathbf{y}}$ represents the prediction \hat{y} for all N training samples. The output space spans all possible assignments of $\hat{\mathbf{y}}$, so

$$\mathcal{O}_A = \mathbb{R}^N. \quad (6.2)$$

Lemma 1. *The weight space for a SLN S with m inputs and n outputs is $\mathcal{W}_S = \mathbb{R}^{n(m+1)}$.*

Proof. S 's trainable parameters are the weight matrix $\mathbf{W} \in \mathbb{R}^{m \times n}$ from (4.12) and bias vector $\mathbf{b} \in \mathbb{R}^n$ from (4.13). By Definition 5, the weight space encompasses all values of \mathbf{W} and \mathbf{b} , so

$$\mathcal{W}_S = \mathbb{R}^{m \times n} \times \mathbb{R}^n = \mathbb{R}^{mn+n} = \mathbb{R}^{(m+1)n}.$$

□

Lemma 2. *A MLP M with L layers where the number of inputs to layer l is given as m_l will have the weight space $\mathcal{W}_M = \mathbb{R}^P$ where $P = \sum_{l=1}^{L-1} (m_{l+1}(m_l + 1)) + m_L + 1$.*

Proof. By Definition 4, M is comprised of L SLNs which we will denote $\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_L$. This allows us to express the weight space of M as the product of the weight spaces of each of the SLNs,

$$\mathcal{W}_M = \prod_{l=1}^L \mathcal{W}_{S_l}.$$

For every layer l , the number of inputs to S_l will be the number of inputs to the l th layer, m_l . Let n_l denote the number outputs for each layer l . Then, by Lemma 1,

$$\mathcal{W}_{S_l} = \mathbb{R}^{n_l(m_l+1)}.$$

By splitting of the last factor in the product of weight spaces, we obtain

$$\mathcal{W}_M = \prod_{l=1}^{L-1} \mathcal{W}_{S_l} \times \mathcal{W}_{S_L} = \prod_{l=1}^{L-1} \mathbb{R}^{n_l(m_l+1)} \times \mathbb{R}^{n_L(m_L+1)}.$$

Notice that for any layer l , the number of outputs is equal to the number of inputs to the next layer, so $n_l = m_{l+1}$ except for the last layer where there is only one output unit leaving $n_L = 1$. This leaves

$$\begin{aligned} \mathcal{W}_M &= \prod_{l=1}^{L-1} \mathbb{R}^{m_{l+1}(m_l+1)} \times \mathbb{R}^{m_L+1} \\ &= \mathbb{R}^{\sum_{l=1}^{L-1} m_{l+1}(m_l+1)} \times \mathbb{R}^{m_L+1} \\ &= \mathbb{R}^{\sum_{l=1}^{L-1} m_{l+1}(m_l+1) + m_L + 1}, \end{aligned}$$

so $\mathcal{W}_M = \mathbb{R}^P$ with

$$P = \sum_{l=1}^{L-1} m_{l+1}(m_l + 1) + m_L + 1.$$

□

Remarks The significance of Lemma 2 is that we obtain a formula for the number of trainable parameters P in a MLP. By Definition 5, P determines the dimensionality of the weight space. On other other hand, Definition 6 states that the number of samples in the training set N determines the dimensionality of the output space. There is no relationship between P and N since the number of samples in the training set can be arbitrarily chosen. It follows that there is no relationship between the dimensionalities of \mathcal{W} and \mathcal{O} .

6.1.1 Relationship between weight and output space

We will now examine the nature of the mapping between the two spaces, and whether there exists a linear mapping. Note that linear mappings can exist between spaces of different dimensionalities [Rudin, 2006].

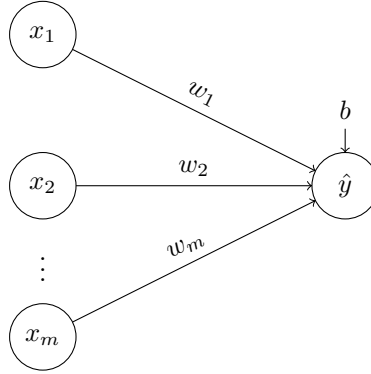


Figure 6.1: The DAG representing a SLN with m inputs and one output unit.

Definition 7 (Weight-output mapping). Given an artificial neural network $A : \mathbb{R}^m \rightarrow \mathbb{R}^n$ with m inputs and n outputs parameterized by a set of trainable parameters $\mathbf{w} \in \mathcal{W}_A$, the weight-to-output-space mapping $h_A : \mathcal{W}_A \rightarrow \mathcal{O}_A$ for a dataset with N m -dimensional feature vectors given by the matrix $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_N]^\top \in \mathbb{R}^{N \times m}$ is

$$h_A(\mathbf{w}) = \begin{bmatrix} A(\mathbf{x}_1; \mathbf{w}) \\ A(\mathbf{x}_2; \mathbf{w}) \\ \vdots \\ A(\mathbf{x}_N; \mathbf{w}) \end{bmatrix}.$$

TODO : explain confusion of the term weight-output mapping

Theorem 3. For a SLN S with one output unit, the function $h_S : \mathcal{W}_S \rightarrow \mathcal{O}_S$ is not a linear mapping.

Proof. Let S have m inputs, as depicted in Figure 6.1. Modifying the formula for a SLN given in Definition 3 (4.11) for the case where there is only one output unit, we obtain $\hat{y} = f_{\text{SLP}}(\mathbf{x}; \mathbf{w}^\top, b) = g(\mathbf{w}\mathbf{x} + b)$ where $\mathbf{x} = [x_1 \ x_2 \ \cdots \ x_m]^\top$ is the input feature vector.

We will consider a dataset with N samples where the input is given by the $N \times m$ matrix $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_N]^\top$ as in (4.3). By Definition 7, the mapping from weight to output space $h_S : \mathcal{W}_S \rightarrow \mathcal{O}_S$ is

$$h_S(\mathbf{w}) = \begin{bmatrix} g(\mathbf{w}^\top \mathbf{x}_1 + b) \\ g(\mathbf{w}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{w}^\top \mathbf{x}_N + b) \end{bmatrix}.$$

We will assume, by way of contradiction, that h is a linear mapping. From the definition of linear mappings, it must be true that $h(\mathbf{u} + \mathbf{v}) = h(\mathbf{u}) + h(\mathbf{v})$

for $\mathbf{u}, \mathbf{v} \in \mathcal{W}_S$ [Rudin, 2006]. On the LHS we have

$$h(\mathbf{u} + \mathbf{v}) = \begin{bmatrix} g((\mathbf{u} + \mathbf{v})^\top \mathbf{x}_1 + b) \\ g((\mathbf{u} + \mathbf{v})^\top \mathbf{x}_2 + b) \\ \vdots \\ g((\mathbf{u} + \mathbf{v})^\top \mathbf{x}_N + b) \end{bmatrix} = \begin{bmatrix} g(\mathbf{u}^\top \mathbf{x}_1 + \mathbf{v}^\top \mathbf{x}_1 + b) \\ g(\mathbf{u}^\top \mathbf{x}_2 + \mathbf{v}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{u}^\top \mathbf{x}_N + \mathbf{v}^\top \mathbf{x}_N + b) \end{bmatrix}$$

and on the RHS we get

$$h(\mathbf{u}) + h(\mathbf{v}) = \begin{bmatrix} g(\mathbf{u}^\top \mathbf{x}_1 + b) \\ g(\mathbf{u}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{u}^\top \mathbf{x}_N + b) \end{bmatrix} + \begin{bmatrix} g(\mathbf{v}^\top \mathbf{x}_1 + b) \\ g(\mathbf{v}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{v}^\top \mathbf{x}_N + b) \end{bmatrix} = \begin{bmatrix} g(\mathbf{u}^\top \mathbf{x}_1 + b) + g(\mathbf{v}^\top \mathbf{x}_1 + b) \\ g(\mathbf{u}^\top \mathbf{x}_2 + b) + g(\mathbf{v}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{u}^\top \mathbf{x}_N + b) + g(\mathbf{v}^\top \mathbf{x}_N + b) \end{bmatrix}.$$

We obtain

$$\begin{bmatrix} g(\mathbf{u}^\top \mathbf{x}_1 + \mathbf{v}^\top \mathbf{x}_1 + b) \\ g(\mathbf{u}^\top \mathbf{x}_2 + \mathbf{v}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{u}^\top \mathbf{x}_N + \mathbf{v}^\top \mathbf{x}_N + b) \end{bmatrix} = \begin{bmatrix} g(\mathbf{u}^\top \mathbf{x}_1 + b) + g(\mathbf{v}^\top \mathbf{x}_1 + b) \\ g(\mathbf{u}^\top \mathbf{x}_2 + b) + g(\mathbf{v}^\top \mathbf{x}_2 + b) \\ \vdots \\ g(\mathbf{u}^\top \mathbf{x}_N + b) + g(\mathbf{v}^\top \mathbf{x}_N + b) \end{bmatrix}.$$

Let $\alpha_i = \mathbf{u}^\top \mathbf{x}_i$ and $\beta_i = \mathbf{v}^\top \mathbf{x}_i$ for all i . Since $\mathbf{u}, \mathbf{v} \in \mathbb{R}^m$ and all $\mathbf{x}_i \in \mathbb{R}^m$, it follows that $\alpha_i, \beta_i \in \mathbb{R}$ for all i . Hence $g(\alpha + \beta + b) = g(\alpha + b) + g(\beta + b)$.

The only functions that satisfy g are functions that satisfy Cauchy's functional equation¹, but these solutions only apply when $b = 0$ and furthermore are linear, whereas the activation function g is non-linear. We arrived at a contradiction, thus disproving our initial assumption that h is a linear mapping, so it must be a non-linear mapping. \square

Corollary 3.1. *For any SLN S , the function $h_S : \mathcal{W}_S \rightarrow \mathcal{O}_S$ is not a linear mapping.*

Proof. We will generalize the results from Theorem 3 to SLNs with multiple outputs. Let S have m inputs and n outputs. We construct n smaller SLNs, S_1, S_2, \dots, S_n where each S_i has all m input units, but only the i th output unit. The DAG representing S_i will only contain links from the input nodes to output node \hat{y}_i (and, of course, the associated bias term b_i) as depicted in Figure 6.2.

Now, we can simulate the function of S by the construction

$$S(\mathbf{x}) = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} S_1(\mathbf{x}) \\ S_2(\mathbf{x}) \\ \vdots \\ S_n(\mathbf{x}) \end{bmatrix}.$$

By Theorem 3, each S_i does not have a linear mapping from weight space to output space, so S cannot have a linear mapping either. \square

¹Cauchy's functional equation is $f(a + b) = f(a) + f(b)$. For $a, b \in \mathbb{Q}$, the only solutions are linear functions of the form $f(x) = cx$ for some $c \in \mathbb{Q}$ [Reem, 2017].

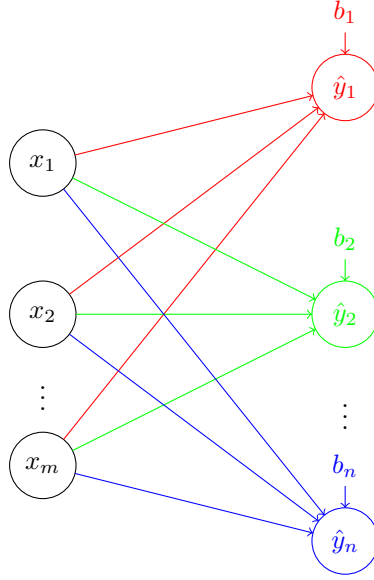


Figure 6.2: The DAGs representing the constructions of n SLNs with one output from a SLN with m inputs and n outputs. Each color represents one of the constructed smaller SLNs.

Corollary 3.2 (Weight-output mapping in general). *For any MLP M , $h_M : \mathcal{W}_M \rightarrow \mathcal{O}_M$ is not a linear mapping.*

Proof. Let M have L layers. By Definition 4, M is a nested function of L SLNs. Corollary 3.1 states that each of these SLNs does not have a linear mapping from weight to output space. Hence the composition of L SLNs that forms M does not have a linear mapping from weight to output space. \square

Remarks The findings from Corollary 3.2 are very significant. They show that there is no apparent relationship between weight and output space that we can easily determine analytically. If there were a straightforward mapping between weight and output space, we would be able to simply be able to determine the ideal weight configuration that would achieve our target \mathbf{y} in output space.

However, since this is not possible, the findings above set the scene for the neural surfing technique. One of the core assumptions is that at a small enough scale, the mapping between weight and output space is *locally linear*, or at least close enough.

6.1.2 Gradient descent from the perspective of weight and output space

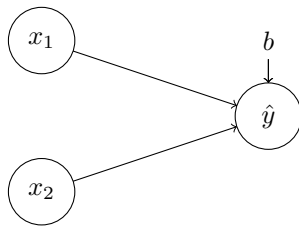


Figure 6.3: A simple MLP with one layer and two inputs (equivalently, a SLN with two inputs and one output).

TODO : Write about how SGD with MSE usually gets viewed from the perspective of error-weight space. However, it is interesting to look at the perspective of weight and output space. It becomes apparent that MSE can be thought of as greedily trying to reduce the Euclidean distance from $\hat{\mathbf{y}}$ to \mathbf{y} in output space.

6.2 Unrealizable regions

Definition 8 (Strongly unrealizable point). Given an artificial neural network A , a point $\mathbf{p} \in \mathcal{O}_A$ in output space is *strongly unrealizable* if and only if there exists no weight configuration $\mathbf{w} \in \mathcal{W}_A$ such that $h_A(\mathbf{w}) = \mathbf{p}$. In other words, it is impossible to attain \mathbf{p} .

Definition 9 (Strongly unrealizable region). Given an artificial neural network A , a *strongly* unrealizable region $\mathcal{U} \subset \mathcal{O}_A$ is a subspace of the output space where every point $\mathbf{p} \in \mathcal{U}$ is strongly unrealizable.

It is apparent that there exists no neural learning algorithm that can elicit a change in weight space that will attain a point in a strongly unrealizable region in output space. Hence we define a *weakly* unrealizable region for a particular neural learning algorithm as a region in output space that cannot be attained by a particular algorithm.

Lemma 4. *A strongly unrealizable region cannot encompass the whole output space.*

Proof. Let us consider an artificial neural network A . We will show that for every unrealizable region, $\mathcal{U} \subsetneq \mathcal{O}_A$. By Definition 9, $\mathcal{U} \subset \mathcal{O}_A$, so it remains to prove that every unrealizable region $\mathcal{U} \neq \mathcal{O}_A$.

Choose any weight configuration $\mathbf{w} \in \mathcal{W}_A$. Let the point $\mathbf{p} = h_A(\mathbf{w})$. We know that \mathbf{p} is *not* strongly unrealizable because \mathbf{w} achieves \mathbf{p} . Hence no unrealizable region can contain \mathbf{p} , so $\mathbf{p} \notin \mathcal{U}$ but $\mathbf{p} \in \mathcal{O}_A$. It follows that $\mathcal{U} \neq \mathcal{O}_A$. \square

Let us look at a couple of examples of unrealizable regions.

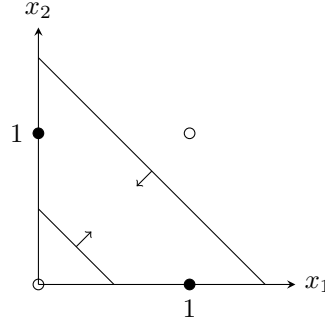


Figure 6.4: The locations of the two hyperplanes in input space acting as decision boundaries required to learn an XOR mapping. The filled-in dot represents an activation of 1 (true) and the circle represents 0 activation (false).

Example 1. A trivial example of an unrealizable region is predicting two different outputs for the same training sample. Consider a MLP M with one layer and two inputs, as shown in Figure 6.3. Let $\mathbf{x} \in \mathbb{R}^2$ be any point in input space. For this example, let the training data be the matrix $\mathbf{X} = [\mathbf{x} \quad \mathbf{x}]^T$. Now we can define an unrealizable region

$$\mathcal{U} = \left\{ \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} : p_1, p_2 \in \mathbb{R}, p_1 \neq p_2 \right\}$$

because $h_M(\mathbf{x})$ cannot produce two different outputs for the same value of \mathbf{x} .

Example 2 (XOR mapping). Let us look at a less contrived example. While it “is well known that any Boolean function [...] can be approximated by a suitable two-layer feed-forward network” [Blum, 1989], single-layer networks with non-decreasing activation functions can only learn a Boolean mapping that is *linearly separable* [Russell and Norvig, 2010, p. 723]. A linearly separable mapping has a linear decision boundary which means that there is only one linear hyperplane separating the two classes (true and false).

The XOR function is not linearly separable because it requires at least two linear decision boundaries, as shown in Figure 6.4. We will consider the same single-layer architecture from Figure 6.3 again, using the sigmoid activation function. The sigmoid is a non-decreasing function. Since we only have one unit (the output neuron) with this non-decreasing non-linear activation function, it follows that we can only have one decision boundary. We just showed that the XOR mapping requires two decision boundaries. Therefore, given the input matrix

$$\mathbf{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix},$$

the point $\mathbf{p} = [0 \ 1 \ 1 \ 0]^\top$ in output space is strongly unrealizable. So $\mathcal{U} = \{\mathbf{p}\}$ is an example of an unrealizable region.

TODO : What if \mathbf{y} is unrealizable? (XOR example demonstrates that)

6.3 Goal-connecting paths

Chapter 7

Problems

7.1 Stripe problem

Chapter 8

Generalising neural surfing

Generalize to classification as regression with multiple output variables

Part II

Framework

Chapter 9

Design

TODO

Chapter 10

Implementation

TODO

Bibliography

- Blum, E. K. (1989). Approximation of boolean functions by sigmoidal networks: Part i: Xor and other two-variable functions. *Neural Computation*, 1(4):532–540.
- Burkov, A. (2019). *The Hundred-Page Machine Learning Book*. Andriy Burkov.
- Glorot, X., Bordes, A., and Bengio, Y. (2011). Deep sparse rectifier neural networks. In Gordon, G., Dunson, D., and Dudík, M., editors, *Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics*, volume 15 of *Proceedings of Machine Learning Research*, pages 315–323, Fort Lauderdale, FL, USA. PMLR.
- Hastie, T., Friedman, J., and Tibshirani, R. (2017). *The Elements of statistical learning: data mining, inference, and prediction*. Springer, 2nd edition.
- McCulloch, W. S. and Pitts, W. (1943). A logical calculus of the ideas immanent in nervous activity. *The Bulletin of Mathematical Biophysics*, 5(4):115–133.
- Neal, R. M. (1992). Connectionist learning of belief networks. *Artificial Intelligence*, 56(1):71–113.
- Reem, D. (2017). Remarks on the cauchy functional equation and variations of it. *Aequationes mathematicae*, 91(2):237–264.
- Rosenblatt, F. (1958). The perceptron: A probabilistic model for information storage and organization in the brain. *Psychological Review*, 65(6):386–408.
- Rudin, W. (2006). *Functional Analysis*. International series in pure and applied mathematics. McGraw-Hill.
- Russell, S. and Norvig, P. (2010). *Artificial Intelligence: A Modern Approach*. Pearson, 3rd edition.