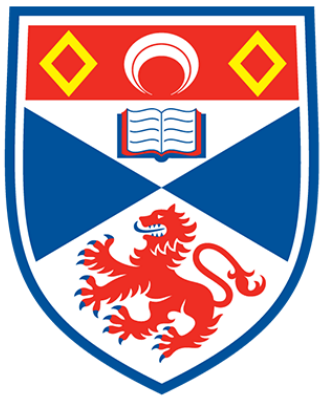
Senior Honours Project



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St Andrews

Freeing Neural Training Through Surfing

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Abstract

TODO

Declaration

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Georg Wölflein

Contents

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

Regression model In machine learning, a regression model f is defined as a mathematical function of the form

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

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 $\hat{y}$.

Labelled dataset A dataset consists of N tuples of the form $\langle \mathbf{x}_i, y_i \rangle$ for $i = 1, \ldots, N$. 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

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_N \end{bmatrix}^\mathsf{T} \tag{4.2}$$

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

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_N \end{bmatrix}^\mathsf{T} \tag{4.3}$$

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

$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 & \hat{y}_2 & \cdots & \hat{y}_N \end{bmatrix}^\mathsf{T} \tag{4.4}$$

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

4.2 Artifical neural networks

Artifical 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 ex_i, is calculated as the weighted sum

$$ex_i = \sum_{j=1}^{n} w_{j,i} a_j + b_i \tag{4.5}$$

where $a_j \in \mathbb{R}$ is another unit j's *activation* and $b_i \in \mathbb{R}$ is the ith unit's *bias*. Notice that 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_i. We have

$$a_i = g_i\left(ex_i\right) = g_i\left(\sum_{j=1}^{n} w_{j,i} a_j + b_i\right). \tag{4.6}$$

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 $g_{\text{thres}} : \mathbb{R} \to \{0, 1\}$ which would be defined[1] as

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

Commonly used activation functions in modern neural networks include the sigmoid

$$S(x) = \frac{1}{1 + e^{-x}} \tag{4.8}$$

and the rectified linear unit (ReLU)

$$g_{\text{ReLU}} = \begin{cases} 0 & x < 0 \\ x & x \geq 0 \end{cases}. \tag{4.9}$$

Rectified units do not suffer from the *vanishing gradient effect* [Glorot et al., 2011]. This phenomenon occurs with sigmoid activation functions when they 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 prevelant in shallow[2] networks so the sigmoid function still remains popular [Neal, 1992].

[1] In 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.

[2] Shallow networks refer to ANNs with few layers.

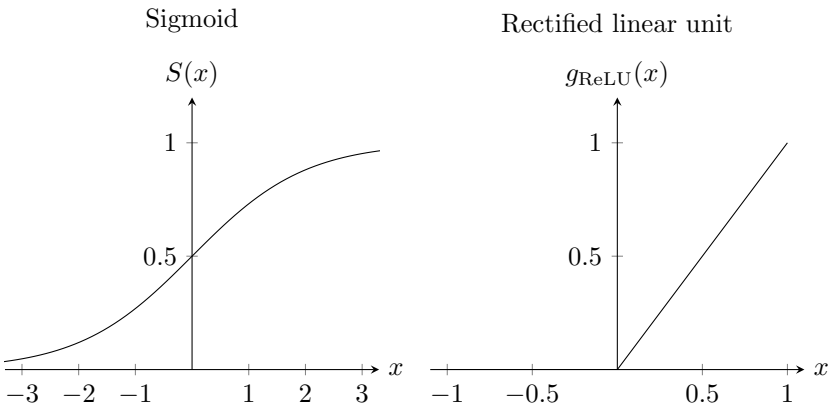

Figure 4.1: Plots of the the two most common activation functions.

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 ith unit to the value the ith element in $\mathbf{x}$ for $i = 1, \ldots, D$. 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* [Russell and Norvig, 2010].

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.

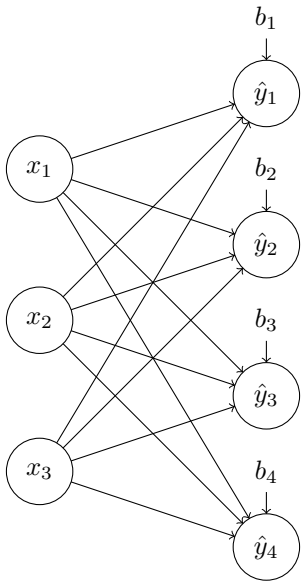

Figure 4.2: A single-layer perceptron with three input and four output neurons.

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

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

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

Definition 1 (Single-layer network)**.** A SLN with m inputs and m outputs is the mathematical formula

$$\mathbf{f}_{\text{SLN}}(\mathbf{x}; \mathbf{W}, \mathbf{b}, \mathbf{g}) = \mathbf{g}\left(\mathbf{W}^{\mathsf{T}}\mathbf{x} + \mathbf{b}\right) \tag{4.11}$$

where the $m \times n$ matrix

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

captures all weights, the vector $\mathbf{b} = \begin{bmatrix} b_1 & b_2 & \cdots & b_n \end{bmatrix}^{\mathsf{T}}$ represents the biases, and $\mathbf{g}$ is the vector-valued activation function.

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 perceptron[3] (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 2 (Multi-layer perceptron)**.** A MLP with L layers is the mathematical function

$$f_{\text{MLP}}(\mathbf{x}) = \hat{y} = f_L\left(\mathbf{f}_{L-1}\left(\ldots\left(\mathbf{f}_1\left(\mathbf{x}\right)\right)\right)\right) \tag{4.13}$$

where $\mathbf{f}_l(\mathbf{x}) = \mathbf{f}_{\text{SLN}}(\mathbf{x}; \mathbf{W}_l, \mathbf{b}_l, \mathbf{g}_l)$ for $l = 1, \ldots, L-1$. The outermost function f_L represents a SLN with only one output unit and is hence the scalar-valued function $f_L(\mathbf{x}) = f_{\text{SLN}}(\mathbf{x}; \mathbf{W}_L, \mathbf{b}_L, \mathbf{g}_L)$. This means that we can fully define the parameters of a MLP with the three-tuple

$$\langle \mathscr{W}, \mathscr{B}, \mathscr{G} \rangle \tag{4.14}$$

where $\mathscr{W} = \mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_L$ are the weight matrices, $\mathscr{B} = \mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_L$ the bias vectors, and $\mathscr{G} = \mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_L$ the vector-valued activation functions.

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 esnure 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).

[3]Unlike 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 **??** [Hastie et al., 2017; Burkov, 2019]. Hence we can use the term 'multi-layer perceptron'.

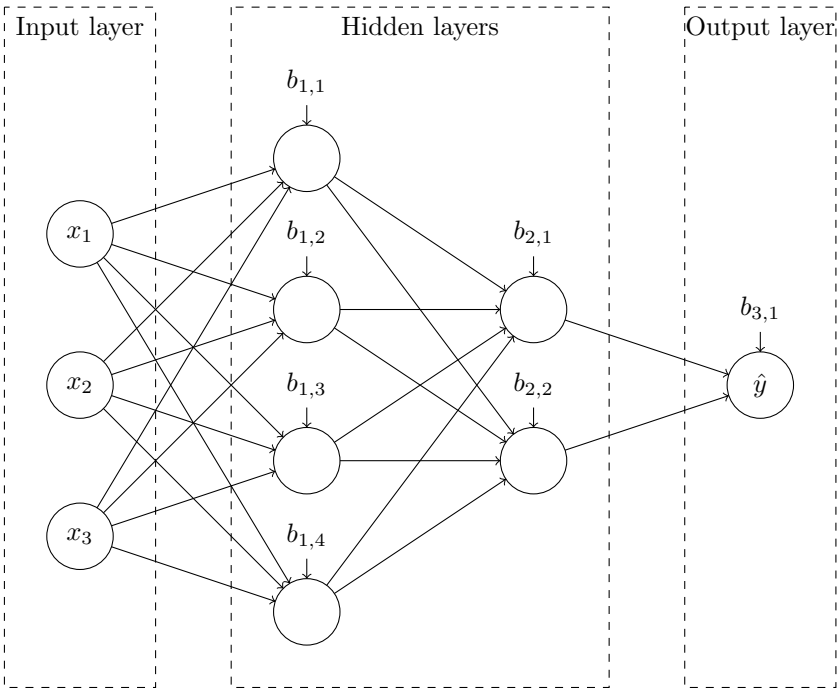

Figure 4.3: A multi-layer perceptron with three inputs and two hidden layers.

Chapter 5

Neural network learning

Chapter 6

Neural surfing theory

6.1 Weight and output spaces

In Definition 2 we established that the three-tuple from (4.14) is sufficient to fully define a MLP. Most importantly, we have $\mathscr{W} = \mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_L$ and $\mathscr{B} = \mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_L$ representing each layer's weight matrices and bias vectors, respectively.

Definition 3 (Weight space)**.** We define the weight space $\mathcal{W}$ of a MLP as the set of all possible assignments to its *trainable parameters*. The trainable parameters are its weights and biases, so the weight space encompasses all possible configurations of $\mathscr{W}$ and $\mathscr{B}$. Hence the weight space for a network with P trainable parameters is defined as

$$\mathcal{W} = \mathbb{R}^P. \tag{6.1}$$

Lemma 1. *A MLP with L layers where the number of inputs to layer l is given as m_l will have a total of $P = \sum_{l=1}^{L-1} (m_{l+1}(m_l + 1)) + m_L + 1$ trainable parameters.*

Proof. A SLN with m inputs and n outputs will have $m \times n$ weights and n biases, totalling $n(m + 1)$ trainable parameters. Now consider a MLP with L layers, where $m_1, m_2, \ldots, m_L$ is the number of inputs to each layer. For any layer l, the number of outputs $n_l = m_{l+1}$ except for the last layer where $n_L = 1$. It follows that the total number of trainable parameters in the network is

$$\begin{aligned} P &= \sum_{l=1}^{L} (n_l(m_l + 1)) \\ &= \sum_{l=1}^{L-1} (n_l(m_l + 1)) + n_L(m_L + 1) \\ &= \sum_{l=1}^{L-1} (m_{l+1}(m_l + 1)) + m_L + 1. \end{aligned}$$

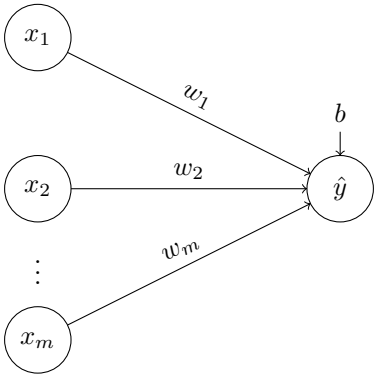

Figure 6.1: The DAG representing a SLN with m inputs and one output unit.

□

Definition 4 (Output space)**.** The output space $\mathcal{O}$ spans the space of all possible output predictions on the training set. In Definition 2, it states that the network must only have one output node and thus the prediction $\hat{y}$ is a scalar. From (4.4), the vector $\hat{\mathbf{y}}$ represents the prediction $\hat{y}$ for all N training samples. This means that the output space spans all possible assignments of $\hat{\mathbf{y}}$, so

$$\mathcal{O} = \mathbb{R}^N. \tag{6.2}$$

Theorem 2 (Relationship between $\mathcal{W}$ and $\mathcal{O}$)**.** *For any SLN with one output unit, the function $h : \mathcal{W} \to \mathcal{O}$ mapping the weights to outputs is not a linear mapping.*

Proof. Let us consider a SLN with m inputs and one output, as depicted in Figure 6.1. Modifying the formula for a SLN given in Definition 1 (4.11) for the case where there is only one output unit, we obtain $\hat{y} = f_{\text{SLP}}(\mathbf{x}; \mathbf{w}^\mathsf{T}, b, g) = g\left(\mathbf{w}^\mathsf{T}\mathbf{x} + b\right)$ where $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix}^\mathsf{T}$ is the input feature vector.

We will consider a dataset with N samples where the input is given by a $N \times m$ matrix $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_N \end{bmatrix}^\mathsf{T}$ as in (4.3) and the labelled outputs $\hat{\mathbf{y}}$ are defined as in (4.4). For our SLN, the function $h : \mathcal{W} \to \mathcal{O}$ is defined as applying the SLN to each input sample, so

$$h\left(\mathbf{w}\right) = \hat{\mathbf{y}} = \begin{bmatrix} g\left(\mathbf{w}^\mathsf{T}\mathbf{x}_1 + b\right) \\ g\left(\mathbf{w}^\mathsf{T}\mathbf{x}_2 + b\right) \\ \vdots \\ g\left(\mathbf{w}^\mathsf{T}\mathbf{x}_N + b\right) \end{bmatrix}.$$

We will assume 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 $\mathbf{u}, \mathbf{v} \in \mathcal{W}$ [Rudin,

2006]. On the LHS we have

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

and on the RHS we get

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

We obtain

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

Let $\alpha_i=\mathbf{u}^{\mathsf{T}}\mathbf{x}_i$ and $\beta_i=\mathbf{v}^{\mathsf{T}}\mathbf{x}_i$ 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 equation[1], 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. □

TODO : Significance of this proof

[1] Cauchy'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].

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

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