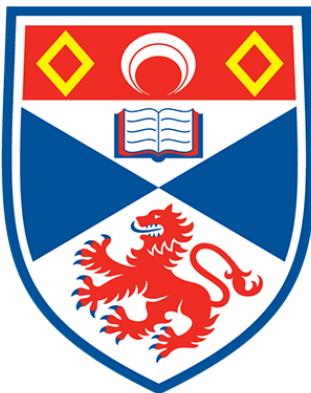


SENIOR HONOURS PROJECT



University of
St Andrews

Freeing Neural Training Through Surfing

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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 13986 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

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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**

1.1 Context survey

1.1.1 Artificial neural networks

The first mathematical model representing neurons in the human brain, so-called *perceptrons*, was formulated by McCulloch and Pitts [1943] (see Section 2.2). In 1958, the psychologist Frank Rosenblatt published the first perceptron learning algorithm [Rosenblatt 1958], but this type of network lacked the ability to learn mappings that were not *linearly separable*. It was not until the 1980s with the introduction of the backpropagation algorithm capable of training networks with hidden layers, that neural networks experienced a substantial rise in popularity.

Backpropagation To this date, the backpropagation (BP) algorithm, attributed to Rumelhart et al. [1986], remains the prominent method of training neural networks. It involves computing the gradient of the loss function with respect to the weights and then using some gradient-based optimisation technique such as gradient descent to update the weights. With the rise in popularity of deep neural networks, methods have been developed to increase the speed of converging to a minimum. The two main approaches are parallelising the computation and using adaptive learning rates like in the ‘Adam optimizer’ [Kingma and Ba 2014]. It is well-established that BP, provided a suitable choice of hyperparameters, is guaranteed to converge to a local (but likely not global) minimum. A common technique to subdue the effect of this issue is to run BP multiple times with different random initialisations.

Derivative-free optimisation The class of derivative-free optimisation (DFO) algorithms are optimisation techniques that attempt to find a global optimum, requiring only an objective function, but no gradient information. One example of such an algorithm is simulated annealing (SA), proposed by Kirkpatrick et al., that mimics the motion of atoms in the physical process of a slowly cooling material [1983]. Originally employed in discrete optimisation problems such as the combinatorial travelling salesman problem [Černý 1985], it was later generalized and applied to problems with continuous domains [Bélisle et al. 1993]. However, in a comparative study of derivative-free optimisation algorithms, Rios and Sahinidis found that SA performed relatively poorly in comparison to more modern DFOs on general optimisation problems¹ [2009].

The concept of applying DFO as a means of training neural networks is not unique to this project. In the 1990s, several training regimes for neural networks were proposed that did not rely on derivative calculations, employing variants of random and local search [Battiti and Tecchiolli 1995; Hirasawa et al. 1998]. These approaches seemed to find better minima and did not get stuck in local minima as BP did. More recently, a particular random search approach was affirmed in outperforming BP in the context of deep neural networks for reinforcement learning, although a different family of DFO algorithms, so-called genetic algorithms were proposed as a superior alternative [Such et al. 2017].

A very recent work presents a DFO technique for neural networks that uses a variant of local search belonging in the family of random search algorithms [Aly et al. 2019]. This technique parallels the finding from other works that DFOs are often able to escape some² local minima and thus produce better training results; however, they require more iterations and computational resources than BP.

Aly et al., Such et al., and similar works studied the performance of their respective DFO algorithms for training neural networks with a large parameter space (in the order of 10^6 parameters) which, while providing valuable practical insight, made it impossible to examine the structure of the loss surface analytically in order to assess issues such as severely suboptimal local minima.

The local minimum problem The local minimum problem, which arises when an algorithm converges to a suboptimal local minimum with a comparatively high loss value, has been extensively studied as a phenomenon in optimisation problems. However, with regards to neural networks, there seems to be differing opinions on the severity of this issue. One frequently cited article claims that “In practice, poor local minima are rarely a problem with large networks” [LeCun et al. 2015]. This is underpinned in theory by other works which proved the nonexistence of suboptimal local minima, although they make varying assumptions on the structure of the underlying neural networks [Kawaguchi

¹It is important to note that Rios and Sahinidis did not assess DFOs for the purpose of neural network optimisation, but rather compared their performances on general convex and non-convex optimisation problems.

²Guaranteed convergence to a global minimum in every scenario is not asserted, although the results indicate that the local minima are not as ‘poor’.

2016; Laurent and von Brecht 2018; Nguyen et al. 2018]. On the other hand, a recent article asserts that “The apparent scarcity of poor local minima has lead practitioners to develop the intuition that bad local minima [...] are practically non-existent” [Goldblum et al. 2019]. Therefore, it can be said that the local minimum problem is still an active area of research.

The local minimum problems as it relates to neural training has been investigated extensively here in St Andrews. One particularly promising approach seems to be setting subgoals on the goal path. However, setting these subgoals requires some finesse. Lewis and Weir [1999] show that simply employing a linear chain of subgoals (such as in Gorse et al. [1997]) does not suffice in reliably finding the global minimum, but instead a non-linear chain of subgoals is required. A technique of setting and achieving subgoals that does not rely on BP has been explored in Weir et al. [2000].

1.1.2 Implementation tools

In both academia and industry, Python is the de facto standard programming language for machine learning. A 2019 analysis on the world-leading software development platform GitHub found that Python is the most popular language for open source machine learning repositories [Elliott 2019]. Python is a simple yet versatile language that natively supports different programming paradigms (imperative, functional, object-oriented, and more). It is often called an interpreted language³ because it is dynamically typed and performs automatic memory management (garbage collection) which generally facilitates shorter code than compiled languages such as C or Java, but also means that pure-Python implementations of data-intensive algorithms will usually not be as efficient. One of the most fundamental packages, NumPy, implements very efficient array manipulation operations that, although specified in Python, are carried out at a lower level for performance.

NumPy is just one piece of Python’s rich ecosystem of packages that are maintained by open-source contributors in the scientific and engineering community. The two main frameworks for machine learning are TensorFlow by Google and PyTorch by Facebook. At their core, both frameworks facilitate the computation of mathematical operations on tensors, offering support for hardware acceleration via *graphics processing units* (GPUs) and providing parallelisation strategies for distributed computing which is especially potent in the context of machine learning where many operations fit the *single instruction, multiple data* (SIMD) pattern. A TensorFlow program is specified as a directed *computational graph* where nodes represent operations and edges represent their inputs and outputs (data tensors) [Martín Abadi et al. 2015]. In the new TensorFlow 2, this graph does not need to be explicitly constructed anymore but is created on the fly which is known as *eager execution*, thereby providing the user with a simpler API similar to NumPy. The slightly younger PyTorch framework provided dynamic computation graphs and a NumPy-like interface since

³There is nuance associated with this statement, but Python certainly exhibits more traits of an interpreted than a compiled language.

its initial release in 2016, and more recently added support for static computational graphs. Hence the newest versions of both frameworks provide similar computational capabilities. They also facilitate the automatic computation of gradients which is useful for training neural networks. TensorFlow is one of the most popular repositories on GitHub, and PyTorch’s popularity is rapidly growing [GitHub 2019].

Keras is a neural network library for Python which is conceived as a high-level interface rather than a framework. It provides implementations of, and abstractions over, common components of neural networks such as layers, optimisers, and activation functions. TensorFlow 2 adopted Keras as part of its core library so that the abstractions provided by Keras can easily be used with the TensorFlow backend.

One should not overlook the concept of interactive notebooks made possible by Python’s interpreted nature – that is, mixing rich text (markdown), Python code, and its output. Not only does this allow the programmer to make changes to the code without having to rerun the program, but it also provides a means of presenting Python code in a more engaging way than just comments. Any type of Python output, including data visualisations, can be presented in such notebooks which makes it attractive for machine learning. These notebooks can be created using the Jupyter package or even run online in the cloud using for example Google Colab.

1.2 Requirements specification

TODO

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. Design and implement the neural surfing technique.
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.

1.3 Software engineering process

TODO

1.4 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.

Chapter 2

Neural network theory

2.1 Supervised learning

Definition 1 (Regression model). In machine learning, a regression model R is defined as a mathematical function of the form $R : \mathbb{R}^D \rightarrow \mathbb{R}$ given by

$$R(\mathbf{x}) = \hat{y} = y + \epsilon \quad (2.1)$$

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 (Input space). The input space \mathcal{I}_R of a regression model R is the set of all possible assignments to the feature vector \mathbf{x} . For a feature vector of D dimensions,

$$\mathcal{I}_A = \mathbb{R}^D. \quad (2.2)$$

Definition 3 (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

$$\mathbf{y} = [y_1 \ y_2 \ \cdots \ y_N]^T \quad (2.3)$$

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

$$\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_N]^T \quad (2.4)$$

for representing the corresponding feature vectors.

Definition 4 (Supervised learning). A supervised learning algorithm for a regression task infers the function f given in Equation (2.1) from a set of *labelled training data* of the form explained previously. We use the vector

$$\hat{\mathbf{y}} = [\hat{y}_1 \ \hat{y}_2 \ \cdots \ \hat{y}_N]^T \quad (2.5)$$

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

2.2 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 z_i , is calculated as the weighted sum

$$z_i = \sum_{j=1}^n w_{j,i} a_j + b_i \quad (2.6)$$

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

$$a_i = g(z_i) = g\left(\sum_{j=1}^n w_{j,i} a_j + b_i\right). \quad (2.7)$$

Activation functions In its original form, McCulloch and Pitts defined the neuron as having only binary activation [1943]. This means that in our model from Equation (2.7), 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 defined⁴ as

$$g_{\text{thres}}(x) = \begin{cases} 0 & x < 0 \\ 1 & x \geq 0 \end{cases}. \quad (2.8)$$

Commonly used activation functions in modern neural networks include the sigmoid

$$g_{\text{sig}}(x) = \frac{1}{1 + e^{-x}} \quad (2.9)$$

and the rectified linear unit (ReLU)

$$g_{\text{ReLU}} = \begin{cases} 0 & x < 0 \\ x & x \geq 0 \end{cases} \quad (2.10)$$

which are depicted in Figure 2.1. 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

⁴In 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.

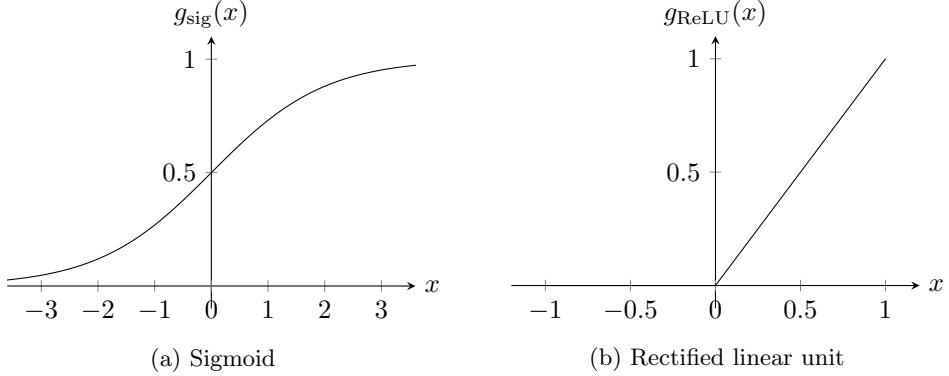


Figure 2.1: Plots of the the two most common activation functions.

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 prevelant in shallow⁵ networks so the sigmoid function still remains popular [Neal 1992].

Particularly in deep neural networks, different neurons (grouped in *layers*, see Section 2.2.2) 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 Equation (2.1). 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 Equation (2.7) 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].

⁵Shallow networks refer to ANNs with few layers.

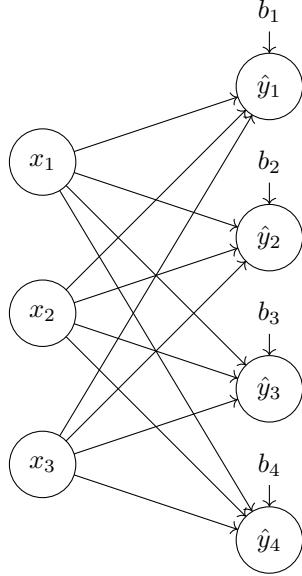


Figure 2.2: A single-layer perceptron with three input and four output neurons.

2.2.1 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 2.2. 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 Equation (2.8) [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 Equation (2.7) to give the activation of a particular output neuron \$i\$ as

$$a_i = y_i = g(z_i) = g\left(\sum_{j=1}^m w_{j,i}x_j + b_i\right) = g(\mathbf{w}_i^\top \mathbf{x}_i + b_i) \quad (2.11)$$

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

$$\mathbf{S}(\mathbf{x}; \mathbf{W}, \mathbf{b}) = \mathbf{g}(\mathbf{W}^\top \mathbf{x} + \mathbf{b}) \quad (2.12)$$

where the $m \times n$ matrix

$$\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \cdots \ \mathbf{w}_n] = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,1} & w_{m,2} & \cdots & w_{m,n} \end{bmatrix} \quad (2.13)$$

captures all weights and the vector

$$\mathbf{b} = [b_1 \ b_2 \ \cdots \ b_n]^\top \quad (2.14)$$

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 Equation (2.1). Moreover, if we additionally use the threshold activation function from Equation (2.8), we arrive at the SLP model given by Rosenblatt [1958].

2.2.2 Multi-layer perceptron

A multi-layer perceptron⁶ (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 6 (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

$$M(\mathbf{x}; \mathcal{P}) = \hat{y} = f_L(f_{L-1}(\dots(f_1(\mathbf{x})))) \quad (2.15)$$

for the trainable parameters $\mathcal{P} = \langle \mathcal{W}, \mathcal{B} \rangle$ consisting of the weight matrices $\mathcal{W} = \mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_L$ and bias vectors $\mathcal{B} = \mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_L$ 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 $f_L(\mathbf{x}) = S(\mathbf{x}; \mathbf{W}_L, \mathbf{b}_L)$.

⁶Unlike 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 2.2 [Burkov 2019; Hastie et al. 2017]. Hence we can use the term ‘multi-layer perceptron’.

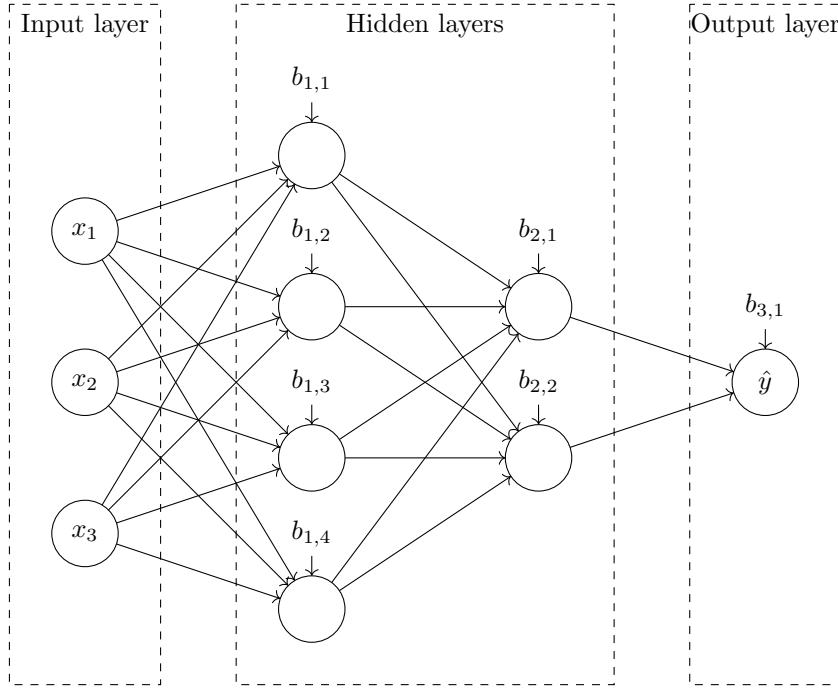


Figure 2.3: A multi-layer perceptron with three inputs and two hidden layers.

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 2.3. 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 Equation (2.12).

2.3 The decision boundary in input space

We will briefly introduce the concept of binary classification and show how it fits in the framework of the already defined regression model. This will allow us to examine the so-called decision boundary in input space which will be useful for formulating the stripe problem (Section 5.2).

Definition 7 (Binary classification model). A binary classification model C is defined as a mathematical function of the form

$$C(\mathbf{x}) = \hat{y} = y + \epsilon \quad (2.16)$$

with the same notation as in Definition 1 except that we impose the additional restriction that $y, \hat{y} \in \{0, 1\}$ such that the signature of the function becomes $C : \mathbb{R}^D \rightarrow \{0, 1\}$.

Definition 8 (Decision boundary). Given a binary classification model C , the decision boundary is the hypersurface⁷ in input space \mathcal{I}_C that separates the two output classes [Russell and Norvig 2010, p. 723]. We will also use the term ‘hyperplane’ to loosely refer to the decision boundary if it is flat/linear.

Lemma 1. *Given a decision threshold t , we can use a regression model R to solve any binary classification problem.*

Proof. We are looking define an equivalent classification model C that outputs 0 if $R(\mathbf{x}) < t$ and 1 otherwise. This can be achieved using the threshold activation function g_{thres} from Equation (2.8) in the form

$$C(\mathbf{x}) = g_{\text{thres}}(R(\mathbf{x}) - t). \quad (2.17)$$

□

Remark. What we have shown is that we can repurpose any regression model for a binary classification task, including for example MLPs. When using a MLP, the sigmoid activation function Equation (2.9) naturally lends itself to be used on the output unit because its range, the interval $(0, 1)$, can be interpreted as a probability. In this case we would set the decision threshold $t = \frac{1}{2}$.

Lemma 2 (Single-layer sigmoidal decision boundary). *A single-layer sigmoidal MLP with a decision threshold $t \in (0, 1)$ will have only one hyperplane in input space.*

Proof. Consider a single-layer MLP M with m inputs. By Definition 6, this is equivalent to SLN S with m inputs and one output as shown in Figure 2.4. The equation of decision boundary can be obtained by setting the output equal to the decision threshold, so $t = S(\mathbf{x})$ for the input feature vector $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_m]^T$. We have

$$\begin{aligned} t &= S(\mathbf{x}) \\ &= g_{\text{sig}}(\mathbf{w}^T \mathbf{x} + b) \\ &= \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x} - b}} \\ \frac{1}{t} - 1 &= e^{-\mathbf{w}^T \mathbf{x} - b} \\ \ln\left(\frac{1}{t} - 1\right) &= -\mathbf{w}^T \mathbf{x} - b. \end{aligned}$$

⁷A hypersurface is a manifold with one fewer dimension. Since the input space is D -dimensional, the hypersurface representing the decision boundary will have $D - 1$ dimensions.

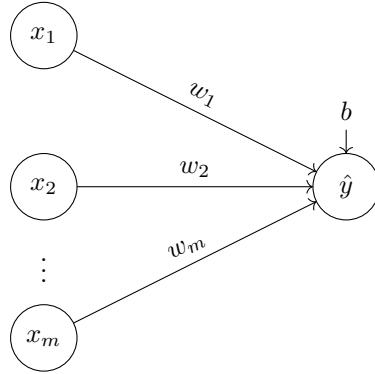


Figure 2.4: The DAG representing a SLN with m inputs and one output unit.

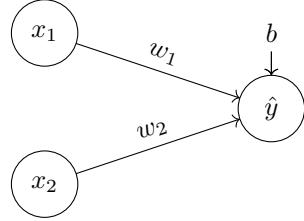


Figure 2.5: A simple MLP with one layer and two inputs (equivalently, a SLN with two inputs and one output).

For $\ln\left(\frac{1}{t} - 1\right)$ to be real-valued, we must ensure that $\frac{1}{t} - 1 > 0$ which is the case because $0 < t < 1$.

We obtain only one linear equation of the form

$$0 = w_1 x_2 + w_2 x_2 + \dots + w_m x_m + b + \ln\left(\frac{1}{t} - 1\right) \quad (2.18)$$

which means that there is only one hyperplane. \square

Example 1. Let us consider a MLP M with only one layer and two inputs, as depicted in Figure 2.5. We will consider the configuration where $w_1 = w_2 = 1$ and $b = 0$. The output unit will have the sigmoid activation function, and we will choose the decision threshold $t = \frac{1}{2}$.

The decision boundary will be a line because \mathcal{I}_M has two dimensions, and a hyperplane in a two-dimensional space is simply a line. The equation of this

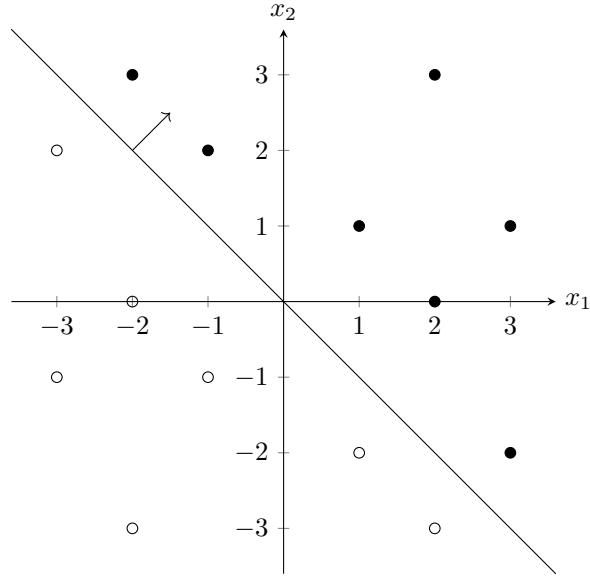


Figure 2.6: Plot of the input space of the MLP from Figure 2.5 with sigmoid activation where $w_1 = w_2 = 1$, $b = 0$, and some sample data. Filled in dots represent a prediction of $\hat{y} > \frac{1}{2}$ whereas the empty circular dots represent $\hat{y} < \frac{1}{2}$.

line can be obtained from Equation (2.18) as

$$\begin{aligned}
0 &= w_1x_1 + w_2x_2 + b + \ln\left(\frac{1}{(\frac{1}{2})} - 1\right) \\
&= x_1 + x_2 + \ln 1 \\
x_2 &= -x_1.
\end{aligned}$$

Figure 2.6 depicts this hyperplane along with some samples in input space to show how they would be classified. The arrow on the hyperplane shows the direction of increasing output, i.e. what would be classified as 1.

Chapter 3

Neural network training

This chapter will introduce two methods of training neural networks to provide an intuition on how this can be achieved. Later in this report, we will look at some issues related to these methods as a means of setting the scene for the neural surfing technique.

In this context, *training* refers to the process of changing the network's weights and biases with the goal of achieving an optimal configuration that reduces the error of the predictions, i.e. how far they are 'off'. We will use a simple loss function that uses mean squared error for this purpose.

Definition 9 (Mean squared error). Let $\{\langle \mathbf{x}_i, y_i \rangle\}_{i=1}^N$ be a labelled dataset (see Definition 3). The mean squared error of a set of predictions $\hat{\mathbf{y}}$ is given as an average over the sum of squared differences,

$$E(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2. \quad (3.1)$$

Definition 10 (Loss function). Given an MLP M with P trainable parameters (weights and biases), the loss function $L : \mathbb{R}^P \rightarrow \mathbb{R}$ is a function that maps weight (and bias) configurations to their associated error values. Let $\mathbf{y} \in \mathbb{R}^N$ be the target outputs for training. Then the loss function is defined as

$$L(\mathbf{p}) = \sum_{i=1}^N (M(\mathbf{x}_i; \mathbf{p}) - y_i)^2. \quad (3.2)$$

Notice the similarity to Equation (3.1). However, we have omitted the factor $\frac{1}{N}$ since the actual loss values are not as important as their relationship to each other, and multiplying by N will retain that relationship. We use the term *error-weight surface* to refer to the graph of this function.

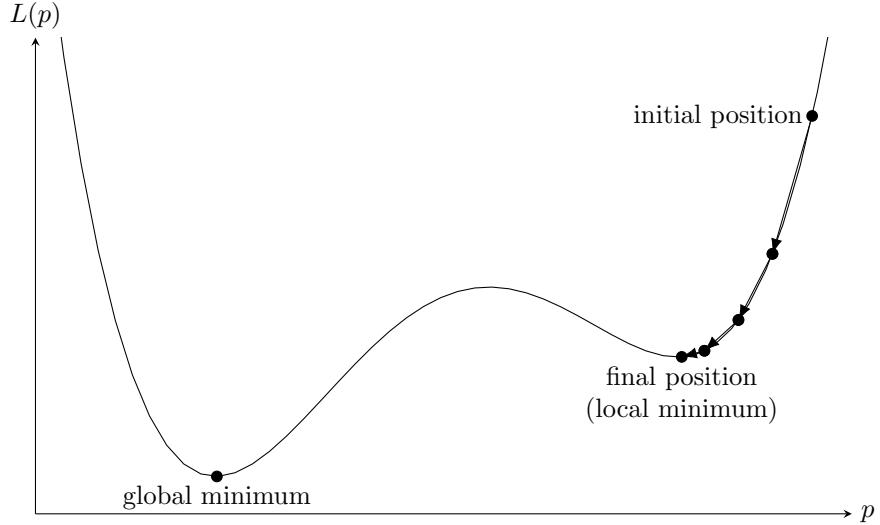


Figure 3.1: An illustration gradient descent training on an error-weight surface with only one parameter (not drawn to scale).

3.1 Backpropagation via gradient descent

Backpropagation (BP) via gradient descent is an iterative algorithm for training neural networks that, provided a suitable learning rate α , is guaranteed to converge to a *local minimum* (see Chapter 5). The main idea is as follows:

1. Calculate the derivative of the loss function with respect to the current trainable parameters \mathbf{p} as $\Delta\mathbf{p} = \frac{\delta L}{\delta \mathbf{p}}(\mathbf{p})$.
2. Take a step in the negative direction of this gradient, i.e. update the trainable parameters $\mathbf{p} \leftarrow \mathbf{p} - \alpha \Delta\mathbf{p}$ where $\alpha \in \mathbb{R}$ is the learning rate.
3. Repeat steps 1 and 2 until a predefined convergence criterion is met.

Figure 3.1 shows the steps that this algorithm would make on a simple error-weight surface with only one parameter.

Calculating the derivative of the loss function with respect to each of the trainable parameters is a core part of the gradient descent algorithm. Let us look at calculating this gradient for the example of a single-layer MLP. We will come back to these results in Section 5.2.

Example 2 (Gradient in a single-layer MLP). Let us revisit the SLN with m inputs and one output from Figure 2.4. The loss function will be in terms of

the trainable parameters, i.e. the weights \mathbf{w} and bias b , so

$$\begin{aligned} L = L(\mathbf{w}, b) &= \sum_{i=1}^N (S(\mathbf{x}_i; \mathbf{w}, b) - y_i)^2 \\ &= \sum_{i=1}^N (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i)^2. \end{aligned} \quad (3.3)$$

We obtain the partial derivative of the loss with respect to the bias as

$$\begin{aligned} \frac{\delta L}{\delta b} &= 2 \sum_{i=1}^N (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) \frac{\delta}{\delta b} (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) \\ &= 2 \sum_{i=1}^N (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) g'(\mathbf{w}^\top \mathbf{x}_i + b), \end{aligned} \quad (3.4)$$

and similarly we can differentiate with respect to the weights

$$\begin{aligned} \frac{\delta L}{\delta \mathbf{w}} &= 2 \sum_{i=1}^N (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) \frac{\delta}{\delta \mathbf{w}} (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) \\ &= 2 \sum_{i=1}^N (g(\mathbf{w}^\top \mathbf{x}_i + b) - y_i) g'(\mathbf{w}^\top \mathbf{x}_i + b) \mathbf{x}_i. \end{aligned} \quad (3.5)$$

Now we would denote the gradient of the loss with respect to the trainable parameters \mathbf{p} as the row vector

$$\frac{\delta L}{\delta \mathbf{p}} = \left[\frac{\delta L}{\delta w_1} \quad \frac{\delta L}{\delta w_2} \quad \cdots \quad \frac{\delta L}{\delta w_m} \quad \frac{\delta L}{\delta b} \right].$$

3.2 Greedy probing

Unlike BP, greedy probing is a simple derivative-free optimisation (DFO) technique. At each iteration, the algorithm will sample a predefined number of configurations in the local neighbourhood of the current parameter configuration \mathbf{p} . The loss is calculated at each of these samples, and the best (i.e. lowest value) is chosen as the new parameter configuration. In this sense, greedy probing is similar to gradient descent, except that the gradient is manually calculated instead of using the partial derivative. As a result, greedy probing will suffer similar issues as gradient descent, but depending on the sampling radius $r \in \mathbb{R}$ it is conjectured that it might be less sensitive to local perturbations ('noise') on the error-weight surface.

The sampling technique may either be *exhaustive* or *random*. In the exhaustive case, the samples around point \mathbf{p}_i are given by

$$\left\{ \mathbf{p}_i + r \frac{\begin{bmatrix} p_1 & p_2 & \cdots & p_P \end{bmatrix}^\top}{\| \begin{bmatrix} p_1 & p_2 & \cdots & p_P \end{bmatrix} \|} : p_1, p_2, \dots, p_P \in \{-1, 0, 1\} \text{ and } \left\| \begin{bmatrix} p_1 & p_2 & \cdots & p_P \end{bmatrix} \right\| \neq 0 \right\} \quad (3.6)$$

which means that $3^P - 1$ samples are generated at each iteration. On the other hand, the random sampling technique will generate a predefined number of random samples in weight space with the condition that given the current configuration \mathbf{p}_i , for every candidate sample $\hat{\mathbf{p}}$, it must be true that $\|\mathbf{p}_i - \hat{\mathbf{p}}\| = r$.

3.3 Simulated annealing

The rationale of the simulated annealing (SA) algorithm lies in its analogy to the behaviour that atoms exhibit in a substance that is slowly cooling down [Kirkpatrick et al. 1983]. At high temperatures, the atoms move around with high kinetic energy, but as the temperature cools down, they begin to move more slowly until completely losing thermal mobility. When this process is carried out sufficiently slowly, the atoms will settle in a perfectly aligned crystal structure with minimum energy. However, if the cooling process is too fast, the final structure will be chaotic and hence not be at the minimum energy state [Press et al. 1992, p. 444].

At each iteration, the algorithm will explore random sample points one after another in the local neighbourhood of the current configuration \mathbf{p}_i until one is accepted. The probability of accepting a candidate sample point $\hat{\mathbf{p}}$ at the i th iteration is given by the probability distribution

$$P(\hat{\mathbf{p}}|\mathbf{p}_i) = \begin{cases} \exp\left(-\frac{k}{T_i}(L(\hat{\mathbf{p}}) - L(\mathbf{p}_i))\right) & L(\hat{\mathbf{p}}) > L(\mathbf{p}_i) \\ 1 & L(\hat{\mathbf{p}}) \leq L(\mathbf{p}_i) \end{cases} \quad (3.7)$$

for an energy coefficient $k \in \mathbb{R}$ [Rios and Sahinidis 2009]. This means that the SA algorithm will always accept a better location, but, with a certain probability, might take a suboptimal step.

The temperature at the i iteration is determined according to a *cooling schedule*. We will employ a simple approach as a proof of concept that calculates T_i as the geometric sequence

$$T_i = (1 - c) T_{i-1} = (1 - c)^i T_0 \quad (3.8)$$

where c is a cooling rate typically of the order of 10^{-1} or 10^{-2} . Already, this simple SA algorithm has three hyperparameters: the energy coefficient k , the initial temperature T_0 , and the cooling rate c . More sophisticated implementations will require even more hyperparameters (such as the algorithm proposed by Press et al. [1992] which will be remarked upon in Section 9.3.3) that makes it increasingly difficult to design SA in a generic fashion to suit the training of neural networks.

3.4 Issues

Suboptimal local minima One prevalent problem such optimisation techniques face is that of suboptimal local minima (also known simply as the ‘local

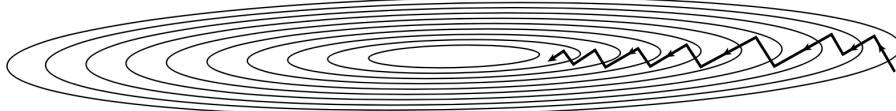


Figure 3.2: Contour plot of the method of steepest gradient descent in a long, narrow valley [Press et al. 1992, p. 421]. Travel proceeds in near right angles due to the gradients.

minimum problem') which was introduced in Section 1.1.1 and will be explored in great detail in Chapter 5. Figure 3.1 provides a simple example where gradient descent via BP fails to find the global minimum in favour of a local minimum. However, this issue is not unique to BP: greedy probing, being in effect a form of gradient descent itself, suffers from the same problem as the evidence suggests in Section 5.3.2. SA tries to circumvent the local minimum problem by allowing intermediate states that are worse than their predecessors, but even this technique is not guaranteed to find the global minimum in a finite amount of time.

Efficiency In the context of computation time per epoch, BP will outperform the derivative-free techniques because it computes only the gradient of the loss function (along with the loss value itself). Both of these computations are in the order of the complexity of computing a forward pass. On the other hand, derivative-free techniques rely on probing, so they must compute as many forward passes as samples they require per epoch. In that sense, the DFO algorithms will be slower.

However, BP has other efficiency drawbacks as a result of relying solely on derivatives: it is more sensitive to local ‘noise’ in the loss function, and it becomes quite slow in long, narrow valleys [Press et al. 1992] as explained in Figure 3.2. Per contra, DFO algorithms are not as sensitive to local noise, and their probing approach will facilitate more efficient progress along narrow valleys.

Chapter 4

Neural surfing theory

The main idea behind the neural surfing technique lies in viewing the neural training problem from a different perspective. Instead of only considering the error-weight space, the neural surfing technique looks at the so-called output space as well. This chapter will discuss the concepts of weight and output space, as well as issues related to these concepts such as unrealisable regions and what is meant by a goal-connecting path.

4.1 Weight and output spaces

In Definition 6 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. These parameters will be useful for defining the weight and output spaces.

Definition 11 (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

$$\mathcal{W}_A = \mathbb{R}^P. \quad (4.1)$$

Definition 12 (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 Equation (2.5), 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

$$\mathcal{O}_A = \mathbb{R}^N. \quad (4.2)$$

Lemma 3. *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 Equation (2.13) and bias vector $\mathbf{b} \in \mathbb{R}^n$ from Equation (2.14). By Definition 11, 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 4. 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 6, 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 3,

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

By splitting off 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

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

□

Remark. The significance of Lemma 4 is that we obtain a formula for the number of trainable parameters P in a MLP. By Definition 11, P determines the dimensionality of the weight space. On other other hand, Definition 12 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} .

4.1.1 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].

Definition 13 (Weight-output mapping). Given an artifical 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 $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_N]^T \in \mathbb{R}^{N \times m}$ is

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

Note that we use the term ‘weight-output mapping’ to refer to the ‘weight-to-output-space mapping’ which should be confused with the mapping from weight space to a particular output prediction.

Theorem 5. 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 2.4. Modifying the formula for a SLN given in Definition 5 Equation (2.12) for the case where there is only one output unit, we obtain $\hat{y} = f_{\text{SLP}}(\mathbf{x}; \mathbf{w}^T, b) = g(\mathbf{w}\mathbf{x} + b)$ where $\mathbf{x} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_m]^T$ is the input feature vector.

We will consider a dataset with N samples where the input is given by the $N \times m$ matrix $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_N]^T$ as in Equation (2.4). By Definition 13, the mapping from weight to output space $h_S : \mathcal{W}_S \rightarrow \mathcal{O}_S$ is

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

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

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

leaving

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

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 equation⁸, 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 5.1. *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 5 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 4.1.

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

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

⁸Cauchy'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].

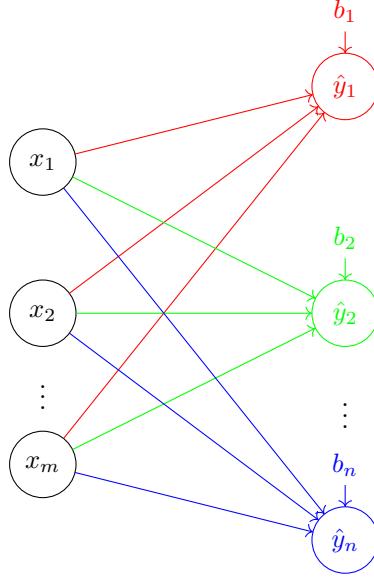


Figure 4.1: The DAGs representing the constructions of n SLNs with one output from a SLN with m inputs and n outputs. Each color represents one of the constructed smaller SLNs.

By Theorem Theorem 5, each S_i does not have a linear mapping from weight space to output space, so S cannot have a linear mapping either. \square

Corollary 5.2 (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 6, M is a nested function of L SLNs. Corollary Corollary 5.1 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

Remark. The findings from Corollary Corollary 5.2 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 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.

4.1.2 Gradient descent from the perspective of weight and output space

Gradient descent with mean squared error is classically viewed from the perspective of the error-weight surface. In this regard, its objective is to descend the error-weight surface. Now that we have examined the relationship between the weight and output spaces, it follows naturally to determine how gradient descent fits in this frame of reference. It becomes apparent that in output space, MSE can be thought of as greedily trying to reduce the Euclidean distance from $\hat{\mathbf{y}}$ to \mathbf{y} , i.e. from the prediction to the target. To see this, recall Definition 9 and substitute

$$\|\hat{\mathbf{y}} - \mathbf{y}\| = \sqrt{\sum_{i=1}^N (\hat{y}_i - y_i)^2}$$

in Equation (3.1) to obtain $E(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N} \|\hat{\mathbf{y}} - \mathbf{y}\|^2$. Since the number of samples N is constant during training, there exists a linear relationship between the mean squared error and the Euclidean distance of the current output to the target output (goal).

4.2 Unrealisable regions

Definition 14 (Strongly unrealisable point). Given an artificial neural network A , a point $\mathbf{p} \in \mathcal{O}_A$ in output space is *strongly unrealisable* 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 15 (Strongly unrealisable region). Given an artificial neural network A , a *strongly unrealisable* region $\mathcal{U} \subset \mathcal{O}_A$ is a subspace of the output space where every point $\mathbf{p} \in \mathcal{U}$ is strongly unrealisable.

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 unrealisable region in output space. Hence we define a *weakly unrealisable* region for a particular neural learning algorithm as a region in output space that cannot be attained by a particular algorithm.

Lemma 6. *A strongly unrealisable region cannot encompass the whole output space.*

Proof. Let us consider an artificial neural network A . We will show that for every unrealisable region, $\mathcal{U} \subsetneq \mathcal{O}_A$. By Definition 15, $\mathcal{U} \subset \mathcal{O}_A$, so it remains to prove that every unrealisable 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 unrealisable because \mathbf{w} achieves \mathbf{p} . Hence no unrealisable 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 unrealisable regions.

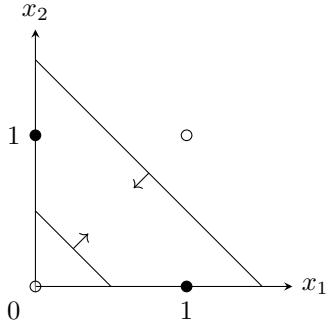


Figure 4.2: The locations of the two hyperplanes in input space acting as decision boundaries required to learn an XOR mapping. The filled-in dot represents an activation of 1 (true) and the circle represents 0 activation (false).

Example 3. A trivial example of an unrealisable region is predicting two different outputs for the same training sample. Consider again an MLP M with one layer and two inputs, as shown in Figure 2.5. Let $\mathbf{x} \in \mathbb{R}^2$ be any point in input space. For this example, let the training data be the matrix $\mathbf{X} = [\mathbf{x} \ \mathbf{x}]^\top$. Now we can define an unrealisable 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 4 (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 4.2. We will consider the same single-layer architecture from Figure 2.5 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 unrealisable. So $\mathcal{U} = \{\mathbf{p}\}$ is an example of an unrealisable region.

Remark. Example 3 demonstrate that unrealisable regions can arise even in very simple scenarios, so it is vital to take this phenomenon into account when designing a path-finding technique in output space, such as the neural surfer. Furthermore, one must also consider what happens if the target \mathbf{y} lies in an unrealisable region (which means that \mathbf{y} itself is unrealisable). In this case, the global minimum of the error-weight surface (using mean squared error) would be the weight configuration that produces the point closest to \mathbf{y} (in terms of Euclidean distance) which is realisable.

4.3 Goal-connecting paths

Definition 16 (Goal-connecting path). For an artificial neural network A with current weight configuration $\mathbf{w}_0 \in \mathcal{W}_A$, a goal-connecting path in output space to the goal $\mathbf{g} \in \mathcal{O}_A$ is a sequence of points $\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_S \in \mathcal{O}_A$ where the initial state $\mathbf{s}_0 = h_A(\mathbf{w}_0)$ and final state $\mathbf{s}_S = \mathbf{g}$. The points $\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_S$ are referred to as *subgoals*, hence S is the number of subgoals in the goal-connecting path.

The goal-connecting path is *realizable* if and only if no subgoal is a strongly unrealisable point (Definition 14). This means that a realizable goal-connecting path can equivalently be defined by the weight configurations $\mathbf{w}_0, \mathbf{w}_1, \dots, \mathbf{w}_S \in \mathcal{W}_A$ such that $h_A(\mathbf{w}_i) = \mathbf{s}_i$ for $i \leq S$.

Definition 17 (Ideal goal-connecting path). The ideal goal-connecting path of S subgoals for an artifical neural network A is, in terms of weight space, the *shortest* realizable goal-connecting path with equidistant subgoals.

Lemma 7. Given \mathbf{w}_0 and \mathbf{w}_S , the i th subgoal of the ideal goal-connecting path in weight space is given by $\mathbf{w}_i = \mathbf{w}_0 + \frac{i}{S} (\mathbf{w}_S - \mathbf{w}_0)$.

Proof. First, we will show that the points are equidistant, i.e. $\|\mathbf{w}_0 - \mathbf{w}_1\| = \|\mathbf{w}_1 - \mathbf{w}_2\| = \dots = \|\mathbf{w}_{S-1} - \mathbf{w}_S\|$. This is equivalent to asserting that $\|\mathbf{w}_{i-1} - \mathbf{w}_i\| = \|\mathbf{w}_i - \mathbf{w}_{i+1}\|$ for $0 < i < S$. Substituting on the LHS,

$$\begin{aligned} \|\mathbf{w}_{i-1} - \mathbf{w}_i\| &= \left\| \mathbf{w}_0 + \frac{i-1}{S} (\mathbf{w}_S - \mathbf{w}_0) - \mathbf{w}_0 - \frac{i}{S} (\mathbf{w}_S - \mathbf{w}_0) \right\| \\ &= \left\| -\frac{1}{S} (\mathbf{w}_S - \mathbf{w}_0) \right\|, \end{aligned}$$

and on the RHS,

$$\begin{aligned} \|\mathbf{w}_i - \mathbf{w}_{i+1}\| &= \left\| \mathbf{w}_0 + \frac{i}{S} (\mathbf{w}_S - \mathbf{w}_0) - \mathbf{w}_0 - \frac{i+1}{S} (\mathbf{w}_S - \mathbf{w}_0) \right\| \\ &= \left\| -\frac{1}{S} (\mathbf{w}_S - \mathbf{w}_0) \right\|. \end{aligned}$$

The shortest path between two points is a straight line, so the ideal goal-connecting path in weight space must form a straight line from \mathbf{w}_0 to \mathbf{w}_S , and all subgoals must lie on this line. The equation of the line $l : \mathbb{R} \rightarrow \mathcal{W}_A$ from \mathbf{w}_0 to \mathbf{w}_S is $l(\lambda) = \mathbf{w}_0 + \lambda(\mathbf{w}_S - \mathbf{w}_0)$. It is easy to see that $l\left(\frac{i}{S}\right) = \mathbf{w}_i$ for $0 \leq i \leq S$, so the subgoals are collinear. \square

Remark. Lemma 7 shows a construction for achieving the ideal goal-connecting path, given knowledge of the target weight configuration \mathbf{w}_S . Of course, this is not known to the neural learning algorithm while it is learning, only once it finished and was able to actually achieve the goal. However, we can use the ideal goal-connecting path in retrospect to evaluate the performance of the neural learning algorithm in comparison to the ideal path. Furthermore, we can plot the ideal goal-connecting path in output space in order to find unrealisable regions.

4.4 A ‘cheat’ technique for evaluating subgoal trajectories

The neural surfer must be able to perform two main tasks: (i) set the subgoals in output space; and (ii) achieve these subgoals. This ‘cheat’ technique pertains only to the latter task, ignoring the former. It can be used in order to determine whether and to what extent a training regime⁹ is *capable* of realising each subgoal. The idea is that splitting the problem into two parts will facilitate a better analysis of the neural surfing technique by isolating pain points and performance issues. Two main questions can be evaluated:

- How well is the approach getting to the subgoals?
- How good is the state the approach ends up in when it achieves the subgoal?

Achieving a subgoal One important question that must be answered is what constitutes realising a subgoal. For the purpose of this technique, we will assume that achieving some fraction $\mu \in (0, 1)$ of the distance to the subgoal constitutes as ‘achieving’ it. In more sophisticated scenarios, this technique could be extended to use functions that give a specific threshold for each subgoal.

Procedure The steps below explain the methodology of this technique, for S subgoals (where the last subgoal represents the goal). Figure 4.3 illustrates this technique in output space.

1. Determine the point in weight space \mathbf{w}_S that corresponds to the target in output space (i.e. the global minimum on the error-weight surface).

⁹This technique can be used for *any* regime that provides a mechanism for achieving (sub)goals. As such, this technique not only provides a means of testing the neural surfing algorithm, but also provides a means of using gradient to realise a subgoal trajectory.

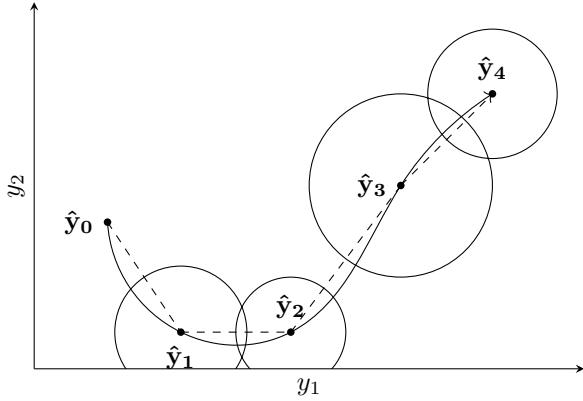


Figure 4.3: Output space for the ‘cheat’ technique for $S = 4$ subgoals and $\mu = \frac{1}{2}$. The circles around each point indicate the threshold that constitutes ‘achieving’ a particular point. The radius of the circle around point $\hat{\mathbf{y}}_i$ is $(1-\mu) \|\hat{\mathbf{y}}_i - \hat{\mathbf{y}}_{i-1}\|$ for $i = 1, \dots, S$; hence the circles are not necessarily identical in size. While the weight configurations $\mathbf{w}_0, \dots, \mathbf{w}_S$ are equidistant and collinear in weight space, it is important to note that the corresponding points in output space $\mathbf{y}_1, \dots, \mathbf{y}_{n+1}$ will usually neither be collinear nor equidistant due to the inherent non-linearity of the network. In practice, μ will be set to a larger value such as 0.9 (which will decrease the circles’ radii) to ensure that enough progress was made in achieving a subgoal before proceeding to the next.

This can be done either by (i) analytically finding the global minimum of the error-weight space if the network architecture is simple enough (see Theorem 14); or (ii) running gradient descent from many random initial configurations in order to find the (likely) global minimum.

2. Determine the ideal goal line $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_S$ in weight space using Lemma 7 and the corresponding goal-connecting path $\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \dots, \hat{\mathbf{y}}_S$ in output space.
3. Let $i = 0$. Starting at weight configuration \mathbf{w}_i , perform the particular neural network training technique until achieving a point \mathbf{p} in output space where $\|\mathbf{p} - \hat{\mathbf{y}}_{i+1}\| \leq (1 - \mu) \|\hat{\mathbf{y}}_i - \hat{\mathbf{y}}_{i+1}\|$, i.e. at least a fraction μ of the distance to the next subgoal is achieved.
4. Repeat the previous step for $i = 1, 2, \dots, S$.

We will employ this technique in Sections 5.3.3 and 5.3.4 to evaluate the feasibility of the ideal goal line in a suboptimal local minimum setting using both gradient-based and derivative-free optimisation regimes.

Chapter 5

The local minimum problem

5.1 The mathematics of local and global minima

Before analysing an instance of the local minimum problem, we must define what is meant by ‘local’ and ‘global’ minima. We will further introduce a theorem that we can later use as a tool to prove their existence.

Definition 18 (Global minimum). The function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ has a *global minimum* at point $\mathbf{p} \in \mathbb{R}^n$ if and only if for all $\mathbf{x} \in \mathbb{R}^n$ it is true that $f(\mathbf{p}) \leq f(\mathbf{x})$.

Definition 19 (Local minimum). The function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ has a *local minimum* at point $\mathbf{p} \in \mathbb{R}^n$ if there exists a ball with centre \mathbf{p} where $f(\mathbf{p}) \leq f(\mathbf{x})$ for all points \mathbf{x} in that ball. A *suboptimal local minimum* is a local minimum that is not a global minimum.

Definition 20 (Jacobian). Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a continuously differentiable function of the form $f = f(\mathbf{x})$ where $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_n]^\top$. The Jacobian of f (or simply *derivative* of f) is a row vector of its first-order partial derivatives,

$$\mathbf{J}_f = \frac{\delta f}{\delta \mathbf{x}} = \left[\frac{\delta f}{\delta x_1} \quad \frac{\delta f}{\delta x_2} \quad \dots \quad \frac{\delta f}{\delta x_n} \right].$$

Definition 21 (Hessian). Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function of the form $f = f(\mathbf{x})$ where $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_n]^\top$ for which all second partial derivatives exist and are continuous over \mathbb{R}^n . The Hessian of f is a $n \times n$ matrix of the second-order partial derivatives, given by

$$\mathbf{H}_f = \begin{bmatrix} \frac{\delta^2 f}{\delta x_1^2} & \frac{\delta^2 f}{\delta x_1 x_2} & \dots & \frac{\delta^2 f}{\delta x_1 x_n} \\ \frac{\delta^2 f}{\delta x_2 x_1} & \frac{\delta^2 f}{\delta x_2^2} & \dots & \frac{\delta^2 f}{\delta x_2 x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\delta^2 f}{\delta x_n x_1} & \frac{\delta^2 f}{\delta x_n x_2} & \dots & \frac{\delta^2 f}{\delta x_n^2} \end{bmatrix}.$$

Definition 22 (Positive definite matrix). A symmetric $n \times n$ matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$ is said to be *positive definite* if and only if $\mathbf{x}^\top \mathbf{M} \mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^n \setminus \mathbf{0}$.

We will prove a simple technique for showing that a 2×2 matrix is positive definite, as this will help us prove the existence of local minima later.

Theorem 8 (2×2 positive definite matrix). *The matrix $\mathbf{M} = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ is positive definite if $a > 0$ and $ac - b^2 > 0$.*

Proof. Let $\mathbf{x} = [x_1 \ x_2]^\top$ and $f(x_1, x_2) = \mathbf{x}^\top \mathbf{M} \mathbf{x}$. Performing the multiplication,

$$\begin{aligned} f(x_1, x_2) &= [x_1 \ x_2] \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= [x_1 a + x_2 b \ x_1 b + x_2 c] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= x_1^2 a + 2x_1 x_2 b + x_2^2 c. \end{aligned}$$

We will now discuss under what conditions $f(x_1, x_2) > 0$ holds. When $x_2 = 0$, it must necessarily be the case that $a > 0$. Otherwise, dividing by x_2^2 , we can write

$$\left(\frac{x_1}{x_2}\right)^2 a + \frac{2x_1 b}{x_2} + c > 0,$$

and substituting $p = \frac{x_1}{x_2}$ we get

$$p^2 a + 2pb + c > 0.$$

Treating this as a quadratic function in terms of p , we realise that since $a > 0$, the parabola opens up. The discriminant $D = 4b^2 - 4ac$ is negative if $ac - b^2 > 0$ which means that the parabola has no roots. Thus its range is positive.

We have shown that $f(x_1, x_2) > 0$ if $a > 0$ and $ac - b^2 > 0$ for all $x_1, x_2 \in \mathbb{R}$ except $x_1 = x_2 = 0$. By Definition 22, \mathbf{M} must be positive definite. \square

Theorem 9 (Local minimum). *Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a continuously differentiable function, and let the point $\mathbf{p} \in \mathbb{R}^n$ be such that $\mathbf{J}_f(\mathbf{p}) = \mathbf{0}$ and $\mathbf{H}_f(\mathbf{p})$ is positive definite. Then \mathbf{p} is a local minimum of f .*

We will require this theorem to prove that training converges to a local minimum in Section 5.2. However, the proof of this theorem exceeds the scope of this report. The interested reader may consult Loomis and Sternberg [1990, p. 190].

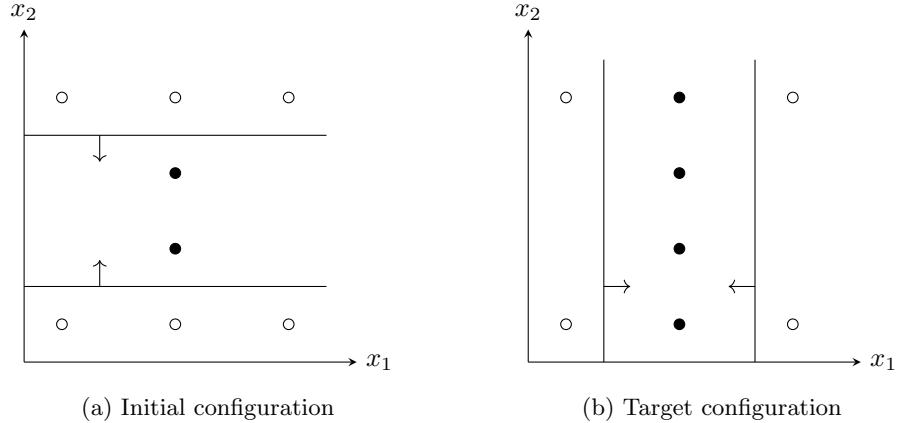


Figure 5.1: Hyperplanes in input space for the stripe problem with eight samples (adapted from Weir [2019]).

5.2 The stripe problem

The stripe problem provides a practical example of the local minimum problem. We will consider a two-dimensional input space with two (initially) parallel hyperplanes that form a stripe. The initial configuration will have the hyperplanes arranged horizontally and misclassify some of the samples. Changing the weights in the neural network will allow the hyperplanes to rotate, but when they do so, they are forced to misclassify even more samples (thereby increasing the mean squared error) until eventually reaching the target configuration with zero error.

The stripe problem can be achieved by a 2-2-1 sigmoidal MLP [Weir 2019]. Figure 5.1 shows the initial and target configurations of the hyperplanes for this type of network. The hidden layer is required because without it, the sigmoid activation function will produce only one hyperplane, as proved in Lemma 2.

In this section, we will formulate a version of the stripe problem that requires no hidden layers and fewer input samples by using a different kind of activation function. The reduced number of parameters will lend itself better for analysis.

5.2.1 Radial basis activation functions

We will first introduce the concept of radial basis functions. When used as the activation function, they exhibit some advantageous properties that will aid us to contrive a simple version of the stripe problem.

Definition 23 (Radial basis function). A radial basis function (RBF) is a smooth continuous real-valued¹⁰ function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ that satisfies the property

¹⁰We define RBFs as having a scalar domain and range because this suffices for our purposes. In actual fact, RBFs are defined more generally to map between suitable vector spaces

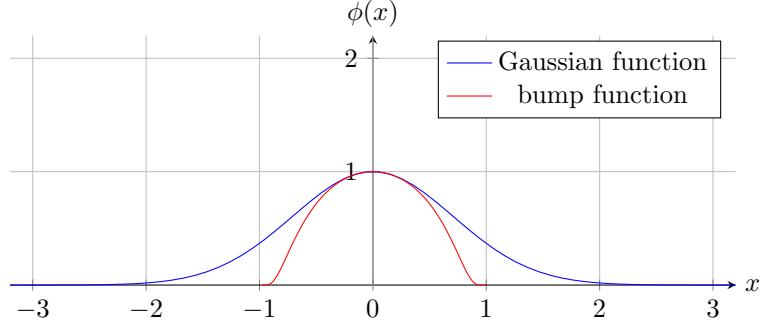


Figure 5.2: Plots of the two most common radial basis functions.

$\phi(x) = \phi(\|x\|)$ [Buhmann 2000]. For RBFs to be useful activation functions, we have three additional restrictions: (i) $\phi(0) = 1$; (ii) $\phi(x)$ is strictly decreasing for the domain $[0, \infty)$ when $\phi(x) \neq 0$; and (iii) that

$$\lim_{x \rightarrow -\infty} \phi(x) = \lim_{x \rightarrow \infty} \phi(x) = 0.$$

Two commonly used RBFs, both infinitely differentiable, are the Gaussian function

$$\phi(x) = e^{-x^2} \quad (5.1)$$

and the bump function¹¹

$$\phi(x) = \begin{cases} e^{1-\frac{1}{1-x^2}} & \text{for } -1 < x < 1 \\ 0 & \text{otherwise} \end{cases}. \quad (5.2)$$

These functions, graphed in Figure 5.2, exhibit slightly different properties. The Gaussian function never actually reaches zero and its derivative is never zero (except at the peak, i.e. $x = 0$). On the other hand, for the bump function, we have $\phi(x) = 0$ and $\frac{d\phi}{dx} = 0$ for $x \notin (-1, 1)$.

Lemma 10 (Single-layer RBF decision boundaries). *A single-layer Gaussian RBF MLP with decision threshold $t \in (0, 1)$ will have two hyperplanes in input space.*

Proof. The proof is similar in method as in Lemma 2. Consider an equivalent SLN S with m inputs and one output as shown in Figure 2.4. To obtain the

[Buhmann 2000].

¹¹We give a slightly modified version of the well-known C_∞ ‘‘bump’’ function [Johnson 2015] that is vertically scaled such that $\phi(0) = 1$ for convenience.

decision boundaries, we set the output equal to the decision threshold, so

$$\begin{aligned} t &= S(\mathbf{x}) \\ &= \phi(\mathbf{w}^\top \mathbf{x} + b) \\ &= e^{-(\mathbf{w}^\top \mathbf{x} + b)^2} \\ -\ln t &= (\mathbf{w}^\top \mathbf{x} + b)^2 \\ \pm \sqrt{-\ln t} &= \mathbf{w}^\top \mathbf{x} + b. \end{aligned}$$

Since $t \in (0, 1)$, it follows that

$$\begin{aligned} 0 < t < 1 \\ \ln t < \ln 1 \\ -\ln t > 0 \\ \sqrt{-\ln t} > 0 \end{aligned}$$

which means that $\sqrt{-\ln t} \neq 0$. Hence

$$\mathbf{w}^\top \mathbf{x} + b \pm \sqrt{-\ln t} = 0 \quad (5.3)$$

has two distinct solutions, no matter the values of \mathbf{w} , \mathbf{x} , and b . Thus there will always be two hyperplanes. \square

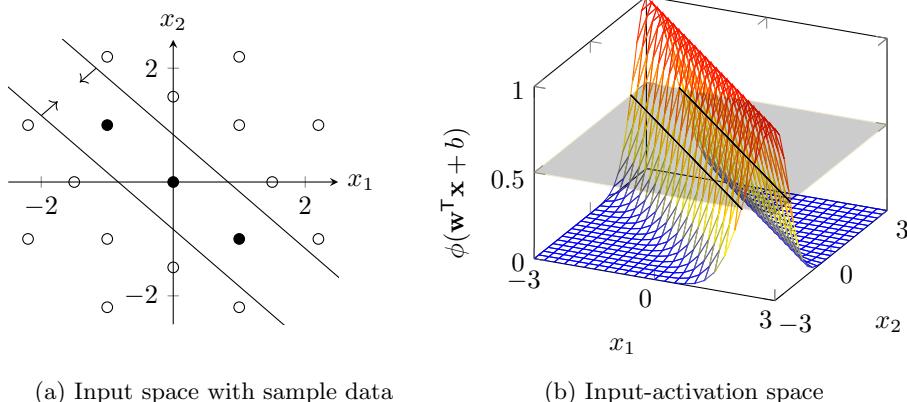
Remark. Although Lemma 10 proves the existence of two hyperplane decision boundaries for Gaussian RBFs, it is trivial to modify this proof for any other type of RBF, such as the bump function. As a consequence, we know that unlike single-layer sigmoidal networks (see Lemma 2), we can use single-layer RBF networks to generate a decision boundary in the form of a stripe which will allow us to use this type of network to provide a more simple example of the stripe problem.

Example 5. Like in Example 1, let us consider once more a single-layered MLP M with two inputs, depicted in Figure 2.5, where $w_1 = w_2 = 1$ and $b = 0$. Let the threshold be $t = \frac{1}{2}$ again, but this time, we will use the Gaussian RBF as the activation function.

From Equation (5.3), we obtain the equations of the hyperplanes as

$$\begin{aligned} \mathbf{w}^\top \mathbf{x} + b \pm \sqrt{-\ln \frac{1}{2}} &= 0 \\ w_1 x_1 + w_2 x_2 + b &= \pm \sqrt{-\ln \frac{1}{2}} \\ x_1 + x_2 &= \pm \sqrt{-\ln \frac{1}{2}}, \end{aligned}$$

so the hyperplanes are at $x_2 = -x_1 - 0.8325\dots$ and $x_2 = -x_1 + 0.8325\dots$, as shown in Figure 5.3.



(a) Input space with sample data

(b) Input-activation space

Figure 5.3: Plots of the hyperplanes of the MLP from Figure 2.5 with Gaussian RBF activation where $w_1 = w_2 = 1$, $b = 0$.

Remark. One key realisation is that when w_1 is fixed, changing the value of w_2 will result in both hyperplanes being rotated around their respective x_1 -intercepts (the hyperplanes remain parallel). The same is true vice-versa, except that the hyperplanes are rotated around their x_2 -intercepts. Changing the value of b simply translates the hyperplanes linearly in input space.

5.2.2 Formulating the problem

Example 5 showed that a simple 2-1 network with radial basis activation constructs a scenario where the hyperplanes form a stripe that can be rotated by adjusting the weights. This means that we could easily contrive the stripe problem from Figure 5.1. However, since we established that the hyperplanes will always remain parallel in our RBF network and since they rotate around the origin¹² when b is fixed, we can create a much simplified version of the stripe problem using only four samples.

Figure 5.4 depicts the initial and target configurations of this simplified version. It is obvious that whichever direction the stripe rotates, it will need to misclassify one of the samples before achieving the target configuration. On the other hand, the zero-excitation line must always pass through the origin (because we have no bias term) which means that the sample at the origin will always have maximal activation. Hence we can discard this sample, leaving only three samples to consider. This will lend itself comfortably for analysis later, as the output space can be visualised in a three-dimensional plot.

We give the dataset for the stripe problem in Table 5.1. Notice that the second and third samples do not have a target output of zero, but rather $\phi(2)$

¹²More precisely, when changing w_1 , the hyperplanes rotate around their respective x_2 intercepts, and similarly when altering w_2 the centre of rotation are the x_1 -intercepts in input space.

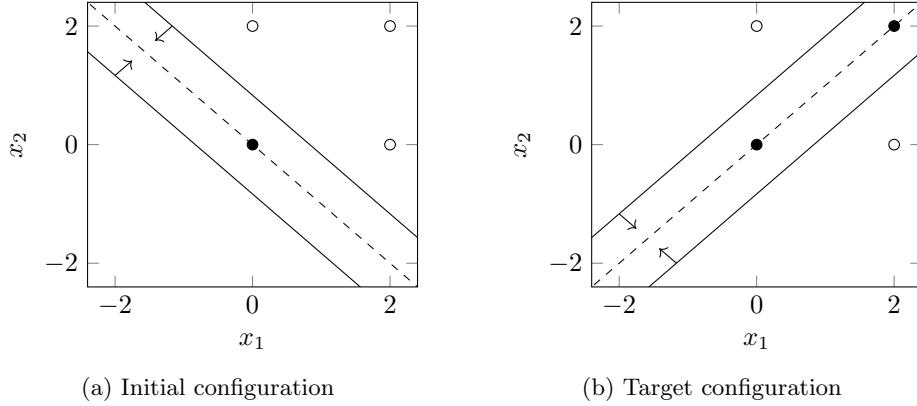


Figure 5.4: The hyperplanes in the initial and target configurations of the RBF stripe problem. The dashed line represents the zero-excitation line.

input (\mathbf{x})	target output (y)	initial output (\hat{y})
$\begin{bmatrix} 2 & 2 \end{bmatrix}$	1	$\phi(4)$
$\begin{bmatrix} 0 & 2 \end{bmatrix}$	$\phi(2)$	$\phi(2)$
$\begin{bmatrix} 2 & 0 \end{bmatrix}$	$\phi(2)$	$\phi(2)$

Table 5.1: The dataset for the RBF stripe problem.

which is close to zero (for the Gaussian RBF, $\phi(2) \approx 0.018$, and for the bump function $\phi(2) = 0$). This will make some calculations later more convenient because it guarantees that there exists at least one weight configuration with a MSE of zero.

Let us examine the error-weight surface of the stripe problem. It is depicted in Figures 5.5 and 5.6 for the Gaussian and bump activation functions, respectively. The graphs are quite similar, showing that the initial weight configuration \mathbf{w}_0 has a MSE of around 1. Most importantly, we see that in order to get to any of the goal weight states \mathbf{w}_S in the region where the MSE is close to zero, we must first overcome a ‘hill’.

For the remainder of this project, we will consider only the Gaussian RBF function, but let it be noted that in principle, any type of RBF that satisfies the criteria given in Definition 23 is suitable. The Gaussian RBF, however, lends itself better for the purposes of analysis because it is not a piecewise defined function, and it does not have a derivative of zero anywhere except at $x = 0$. In addition, gradient descent fails immediately with the bump function because the initial weight configuration is at an area where the gradient is exactly zero. Henceforth the term ‘stripe problem’ shall be used to refer to the Gaussian RBF version of the stripe problem.

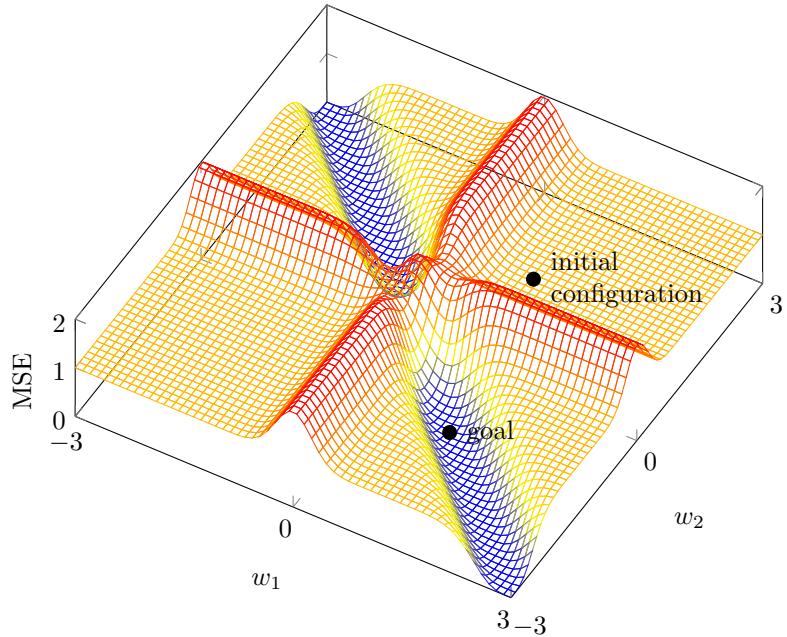


Figure 5.5: Error-weight surface of the stripe problem with Gaussian activation.

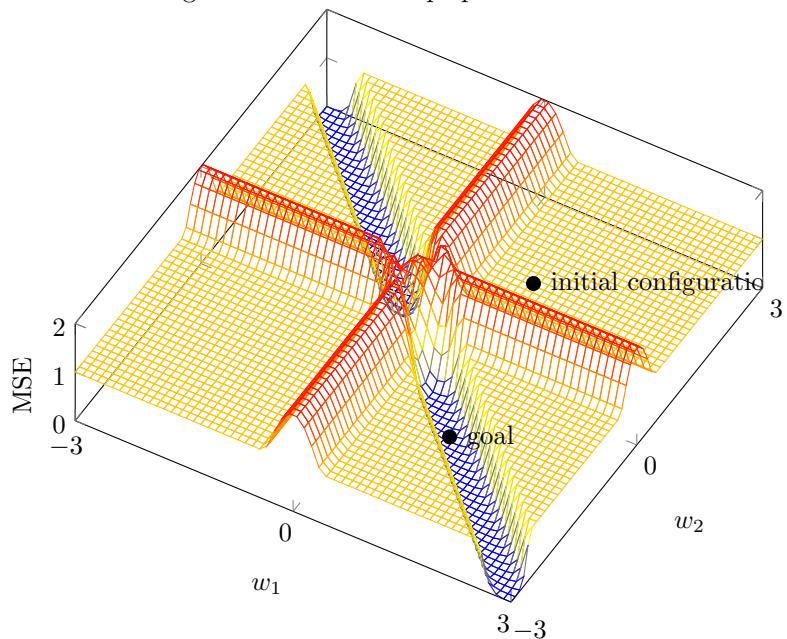


Figure 5.6: Error-weight surface of the stripe problem with bump activation.

5.2.3 Critical points

We will now attempt to find the critical of the error-weight surface analytically, so we can subsequently determine the local minima in the next step. From Table 5.1 we obtain the input matrix

$$\mathbf{X} = \begin{bmatrix} 2 & 2 \\ 0 & 2 \\ 2 & 0 \end{bmatrix}$$

and target output vector $\mathbf{y} = [1 \ \phi(2) \ \phi(2)]^\top$. Modifying the SLN function from Definition 5 for the case of our 2-1 RBF network without bias, we have $S(\mathbf{x}) = \phi(\mathbf{w}^\top \mathbf{x})$. This means that our loss function is given by

$$\begin{aligned} L(\mathbf{w}) = L &= \sum_{i=1}^3 (\phi(\mathbf{w}^\top \mathbf{x}_i) - y_i)^2 \\ &= (\phi(\mathbf{w}^\top \mathbf{x}_1) - 1)^2 + (\phi(\mathbf{w}^\top \mathbf{x}_2) - \phi(2))^2 + (\phi(\mathbf{w}^\top \mathbf{x}_3) - \phi(2))^2 \\ &= (\phi(2w_1 + 2w_2) - 1)^2 + (\phi(2w_2) - \phi(2))^2 + (\phi(2w_1) - \phi(2))^2. \end{aligned}$$

Substituting Equation (5.1), we obtain

$$L = (e^{-4(w_1+w_2)^2} - 1)^2 + (e^{-4w_2^2} - e^{-4})^2 + (e^{-4w_1^2} - e^{-4})^2. \quad (5.4)$$

We will now identify and examine the critical points of this function.

Lemma 11. *Three critical points of the error-weight surface given by L are $\mathbf{p}_1 = [-1 \ 1]^\top$, $\mathbf{p}_2 = [1 \ -1]^\top$, and $\mathbf{p}_3 = [0 \ 0]^\top$.*

Proof. We need to find the Jacobian, \mathbf{J}_L like in Example 2. Differentiating L with respect to w_1 gives

$$\begin{aligned} \frac{\delta L}{\delta w_1} &= 2(e^{-4(w_1+w_2)^2} - 1) \frac{\delta}{\delta w_1} e^{-4(w_1+w_2)^2} \\ &\quad + 2(e^{-4w_2^2} - e^{-4}) \frac{\delta}{\delta w_1} e^{-4w_2^2} \\ &= -16(e^{-(2w_1+2w_2)^2} - 1)(w_1 + w_2)e^{-4(w_1+w_2)^2} \\ &\quad - 16w_1(e^{-4w_1^2} - e^{-4})e^{-4w_1^2}, \end{aligned}$$

and for w_2 we have

$$\begin{aligned} \frac{\delta L}{\delta w_2} &= 2(e^{-4(w_1+w_2)^2} - 1) \frac{\delta}{\delta w_2} e^{-4(w_1+w_2)^2} \\ &\quad + 2(e^{-4w_2^2} - e^{-4}) \frac{\delta}{\delta w_2} e^{-4w_2^2} \\ &= -16(e^{-4(w_1+w_2)^2} - 1)(w_1 + w_2)e^{-4(w_1+w_2)^2} \\ &\quad - 16w_2(e^{-4w_2^2} - e^{-4})e^{-4w_2^2}. \end{aligned}$$

This allows us to express the Jacobian as

$$\begin{aligned}\mathbf{J}_L &= \begin{bmatrix} \frac{\delta L}{\delta w_1} & \frac{\delta L}{\delta w_2} \end{bmatrix} \\ &= -16 \left(e^{-4(w_1+w_2)^2} - 1 \right) (w_1 + w_2) e^{-4(w_1+w_2)^2} \\ &\quad - 16 \begin{bmatrix} w_1 \left(e^{-4w_1^2} - e^{-4} \right) e^{-4w_1^2} \\ w_2 \left(e^{-4w_2^2} - e^{-4} \right) e^{-4w_2^2} \end{bmatrix}^\top.\end{aligned}\tag{5.5}$$

To find the critical points, we set $\mathbf{J}_L = \mathbf{0}$. It is trivial to see that \mathbf{p}_1 , \mathbf{p}_2 , and \mathbf{p}_3 are solutions to this equation. \square

At first, it seems like these three points are the only solutions to $\mathbf{J}_L = \mathbf{0}$. However, upon examining some trial runs of gradient descent, there seemed to be two more local minima around $[1 \ 1]^\top$ and $[-1 \ -1]^\top$.

Lemma 12. *Two more critical points are at $\mathbf{p}_4 = [\eta \ \eta]^\top$ and $\mathbf{p}_5 = [-\eta \ -\eta]^\top$ where η can be numerically approximated to 0.999916 (6 s.f.).*

Proof. We can find these critical points by setting $w_1 = w_2$ in the Jacobian; due to the symmetry of the Jacobian this results in both components becoming. Setting $\mathbf{J}_L = 0$ with $w_1 = w_2$, we obtain

$$\begin{aligned}-32 \left(e^{-16w_1^2} - 1 \right) w_1 e^{-16w_1^2} - 16w_1 \left(e^{-4w_1^2} - e^{-4} \right) e^{-4w_1^2} &= 0 \\ 2 \left(e^{-16w_1^2} - 1 \right) w_1 e^{-16w_1^2} + w_1 \left(e^{-4w_1^2} - e^{-4} \right) e^{-4w_1^2} &= 0.\end{aligned}$$

Noting that $w_1 = 0$ is a solution (which we have already found in Lemma 11), we can divide by w_1 to obtain

$$\begin{aligned}0 &= e^{-32w_1^2} \left(2 + e^{28w_1^2} \right) - 2e^{-16w_1^2} - e^{-4} \\ &= 2e^{-32w_1^2} + e^{-4w_1^2} - 2e^{-16w_1^2} - e^{-4}.\end{aligned}$$

Substituting $x = e^{-4w_1^2}$, we get the equation

$$2x^8 - 2x^4 + x - e^{-4} = 0$$

which cannot be simplified further. Using a numerical solver, we can find the two roots of this equation and then find the value of $w_1 = \pm \frac{1}{2} \sqrt{-\log x}$ (discarding the non-real solutions) as $w_1 \approx 0.999916$ and $w_1 \approx -0.999916$. Since $w_1 = w_2$ we get the solutions \mathbf{p}_4 and \mathbf{p}_5 . \square

For the remainder of this project, we will assume that these five critical points are the only ones. Analysing the graph from Figure 5.5 does suggest so.

5.2.4 Local minima

Lemma 13. *The local minima on the error-weight surface given by L are \mathbf{p}_1 , \mathbf{p}_2 , \mathbf{p}_3 .*

Proof. We have previously shown that $\mathbf{J}_L = \mathbf{0}$ for the three critical points \mathbf{p}_1 , \mathbf{p}_2 , and \mathbf{p}_3 . Let us now compute the Hessian. We will express the Jacobian from Equation (5.5) as

$$\mathbf{J}_L = -16 \left(r + \begin{bmatrix} s(w_1) \\ s(w_2) \end{bmatrix}^\top \right) \quad (5.6)$$

where

$$\begin{aligned} q &= e^{-4(w_1+w_2)^2} \\ r &= (q^2 - q)(w_1 + w_2) \\ s(x) &= x \left(e^{-8x^2} - e^{-4-4x^2} \right). \end{aligned}$$

Let us first compute the derivatives of q with respect to w_1 and w_2 , which, interestingly enough, are equal:

$$\frac{\delta q}{\delta w_1} = \frac{\delta q}{\delta w_2} = -8q(w_1 + w_2).$$

The derivative of r with respect to w_1 is

$$\begin{aligned} \frac{\delta r}{\delta w_1} &= q^2 - q + (w_1 + w_2) \frac{\delta}{\delta w_1} (q^2 - q) \\ &= q^2 - q + (w_1 + w_2)(2q - 1) \frac{\delta q}{\delta w_1} \\ &= q^2 - q - 8q(w_1 + w_2)^2(2q - 1). \end{aligned}$$

Here, it can be shown that $\frac{\delta r}{\delta w_1} = \frac{\delta r}{\delta w_2}$. The exact derivation is left as an exercise to the reader.

It remains to find the derivative of s ,

$$\begin{aligned} s'(x) &= e^{-8x^2} - e^{-4-4x^2} + x \frac{\delta}{\delta x} \left(e^{-8x^2} - e^{-4-4x^2} \right) \\ &= e^{-8x^2} - e^{-4-4x^2} - 8x^2 \left(2e^{-8x^2} - e^{-4-4x^2} \right). \end{aligned}$$

Calculating all the second derivatives of Equation (5.6), we get

$$\begin{aligned} \frac{\delta^2 L}{\delta w_1^2} &= -16 \frac{\delta}{\delta w_1} (r + s(w_1)) \\ &= -16 \left(\frac{\delta r}{\delta w_1} + s'(w_1) \right), \end{aligned}$$

$$\begin{aligned}\frac{\delta^2 L}{\delta w_1 \delta w_2} &= -16 \frac{\delta}{\delta w_2} (r + s(w_1)) \\ &= -16 \frac{\delta r}{\delta w_2} = -16 \frac{\delta r}{\delta w_1},\end{aligned}$$

$$\begin{aligned}\frac{\delta^2 L}{\delta w_2 \delta w_1} &= -16 \frac{\delta}{\delta w_1} (r + s(w_2)) \\ &= -16 \frac{\delta r}{\delta w_1},\end{aligned}$$

and

$$\begin{aligned}\frac{\delta^2 L}{\delta w_2^2} &= -16 \frac{\delta}{\delta w_2} (r + s(w_2)) \\ &= -16 \left(\frac{\delta r}{\delta w_2} + s'(w_2) \right) = -16 \left(\frac{\delta r}{\delta w_1} + s'(w_2) \right).\end{aligned}$$

This allows us to write an expression for the Hessian matrix in the form

$$\mathbf{H}_L = \begin{bmatrix} -16s'(w_1) & 0 \\ 0 & -16s'(w_2) \end{bmatrix} - 16 \frac{\delta r}{\delta w_1}. \quad (5.7)$$

First critical point ($w_1 = -1, w_2 = 1$) By Theorem Theorem 8, \mathbf{H}_L is positive definite if and only if $a > 0$ and $ac - b^2 > 0$ when expressing the matrix in the form $\mathbf{H}_L = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$. We will begin by showing $a = \frac{\delta^2 L}{\delta w_1^2} > 0$. To do that, we must first evaluate $q, s'(w_1)$, and $\frac{\delta r}{\delta w_1}$ for the current weight configuration.

$$\begin{aligned}q &= e^{-4(w_1+w_2)^2} = 1 \\ s'(w_1) &= e^{-8w_1^2} - e^{-4-4w_1^2} - 8w_1^2 \left(2e^{-8w_1^2} - e^{-4-4w_1^2} \right) = -8e^{-8} \\ \frac{\delta r}{\delta w_1} &= q^2 - q - 8q(w_1 + w_2)^2(2q - 1) = 0.\end{aligned}$$

We get

$$\begin{aligned}a &= -16s'(w_1) - 16 \frac{\delta r}{\delta w_1} \\ &= 128e^{-8} > 0.\end{aligned}$$

It remains to show that $ac - b^2 > 0$. Noticing that $s'(1) = s'(-1)$, we realise that in fact $a = c$. So,

$$\begin{aligned}ac - b^2 &= a^2 - b^2 \\ &= 128^2 e^{-16} - \left(-16 \frac{\delta r}{\delta w_1} \right)^2 \\ &= 128^2 e^{-16} > 0.\end{aligned}$$

Hence, we showed that the point \mathbf{p}_1 forms a local minimum.

Second critical point ($w_1 = 1, w_2 = -1$) Notice that this point can be obtained simply by switching w_1 and w_2 from the previous critical point. We have showed previously that $s'(-1) = s'(1)$ and furthermore we established earlier that $\frac{\delta r}{\delta w_1} = \frac{\delta r}{\delta w_2}$. Hence the Hessian from Equation (5.7) will be positive definite too, thus proving that the second critical point is a local minimum.

Third critical point ($w_1 = w_2 = 0$) Using the same notation as Equation (5.7), we evaluate $q, s'(w_1)$, and $\frac{\delta r}{\delta w_1}$ for this weight configuration.

$$\begin{aligned} q &= e^{-4(w_1+w_2)^2} = 1 \\ s'(w_1) &= e^{-8w_1^2} - e^{-4-4w_1^2} - 8w_1^2 \left(2e^{-8w_1^2} - e^{-4-4w_1^2} \right) = 1 - e^{-4} \\ \frac{\delta r}{\delta w_1} &= q^2 - q - 8q(w_1 + w_2)^2(2q - 1) = 0. \end{aligned}$$

We get

$$\begin{aligned} a &= -16s'(w_1) - 16 \frac{\delta r}{\delta w_1} \\ &= 16e^{-4} - 16 \not> 0. \end{aligned}$$

This violates the first condition of Theorem Theorem 8, so this point is not a local minimum.

Fourth critical point ($w_1 = w_2 \approx 0.999916$) Calculating the Hessian for \mathbf{p}_4 numerically, we obtain

$$\mathbf{H}_L \approx \begin{bmatrix} 0.04295905890 & -0.00005595797825 \\ -0.00005595797825 & 0.04295905890 \end{bmatrix}$$

and it is easy to see that the determinant of \mathbf{H}_L as well as its top left cell are positive, so we have a local minimum.

Fifth critical point ($w_1 = w_2 \approx -0.999916$) The Hessian obtained at \mathbf{p}_5 is equal to the Hessian at \mathbf{p}_4 . It follows that this point is a local minimum as well. In summary, we have shown that $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_4, \mathbf{p}_5$ are local minima, but not \mathbf{p}_3 . \square

5.2.5 Global minima

In Section 5.2.3 we identified five critical points on the error-weight surface for the stripe problem, and in Section 5.2.4 we have shown that all but one of these points are local minima. Now we will determine which of these local minima are also global minima. Figure 5.7 shows the critical points which allows the hypothesis that if we have identified all local minima, then \mathbf{p}_1 and \mathbf{p}_2 should be the global minima. While we were not able to prove that the five critical points we identified are the only ones, we *can* prove that \mathbf{p}_1 and \mathbf{p}_2 are in fact global minima because their loss values minimal.

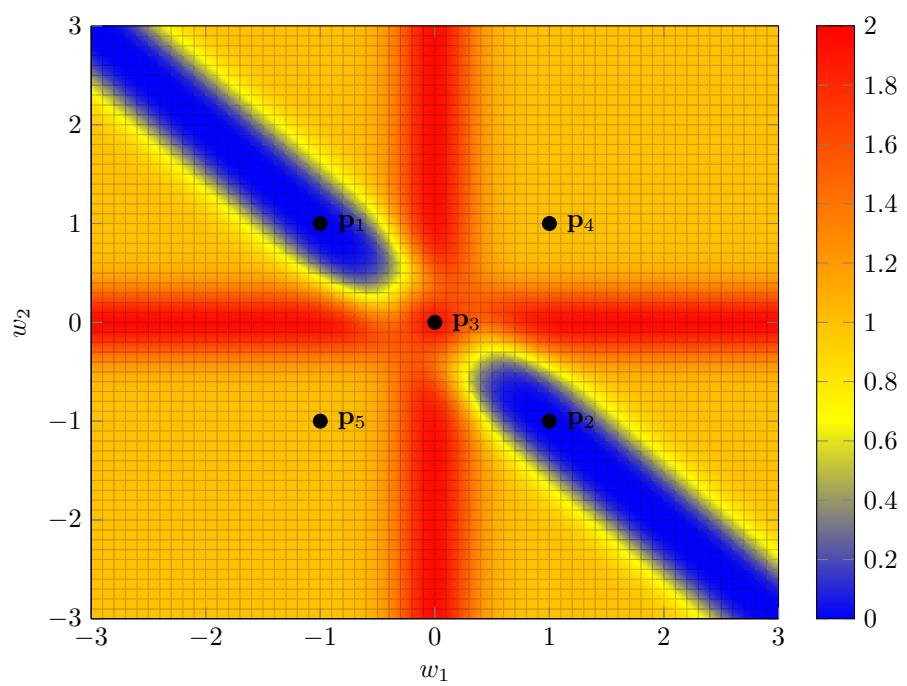


Figure 5.7: Heat map of the stripe problem’s error-weight surface showing the critical points. It provides a birds-eye perspective of Figure 5.5.

Theorem 14. *The points $\mathbf{p}_1 = [-1 \ 1]^\top$ and $\mathbf{p}_2 = [1 \ -1]^\top$ are global minima of the stripe problem's error-weight surface $L(\mathbf{w})$.*

Proof. The loss function $L(\mathbf{w})$ from Equation (5.4) is a sum of squared terms whose arguments are real-valued. This means that if we can show that $L(\mathbf{w}) = 0$ for some \mathbf{w} , then we have proved, by Definition 18 that L has a global minimum at \mathbf{w} . Let us look at the value of the loss function at \mathbf{p}_1 ,

$$\begin{aligned} L(\mathbf{p}_1) &= \left(e^{-4(w_1+w_2)^2} - 1\right)^2 + \left(e^{-4w_2^2} - e^{-4}\right)^2 + \left(e^{-4w_1^2} - e^{-4}\right)^2 \\ &= (e^0 - 1)^2 + (e^{-4} - e^{-4})^2 + (e^{-4} - e^{-4})^2 = 0. \end{aligned}$$

Similarly, we obtain $L(\mathbf{p}_2) = 0$. It follows that both \mathbf{p}_1 and \mathbf{p}_2 are global minima. \square

Corollary 14.1. *The points \mathbf{p}_4 and \mathbf{p}_5 are suboptimal local minima.*

Proof. We have already shown in Lemma 13 that \mathbf{p}_4 and \mathbf{p}_5 are local minima. Let us look at the loss values at \mathbf{p}_4 .

$$L(\mathbf{p}_4) = \left(e^{-16\eta^2} - 1\right)^2 + \left(e^{-4\eta^2} - e^{-4}\right)^2 + \left(e^{-4\eta^2} - e^{-4}\right)^2$$

Since $\eta > 0$, we conclude that $L(\mathbf{p}_4) > 0$. In Theorem 14 we have shown that the minimum of $L(\mathbf{w})$ is zero. Thus, by Definition 18, it follows that \mathbf{p}_4 is *not* a global minimum, so it is a suboptimal local minimum. By extension, since $L(\mathbf{w}) = L(-\mathbf{w})$ and $\mathbf{p}_4 = -\mathbf{p}_5$, it must be the case that \mathbf{p}_5 represents a suboptimal local minimum as well. \square

5.2.6 On the convergence of gradient descent

Theorem 14 and Corollary 14.1 allow us to characterise the nature of the error-weight space and provide a rigorous argument that the stripe problem indeed has suboptimal local minima. In fact, if w_1 and w_2 are either both positive or both negative, gradient descent will converge to a suboptimal local minimum, whereas if w_1 and w_2 have different signs, gradient descent training will converge to a global minimum. To see this, consider the vector field of the directions of the negative gradients depicted in Figure 5.8. When starting at a point with $w_1 > 0$, $w_2 > 0$ and following the arrows, one will end up at the suboptimal local minimum \mathbf{p}_4 eventually. On the other hand, when starting at a point $w_1 < 0$, $w_2 > 0$, it is easy to see that travel will converge to \mathbf{p}_1 . The same logic can be applied to the other two points due to symmetry. Note that would be possible to formally prove this observation by considering the directions of the Jacobian in different regions of the plot. However, this proof would be very long and exceed the scope of this report. Furthermore, the experimental evidence in Section 5.3.1 verifies this claim empirically.

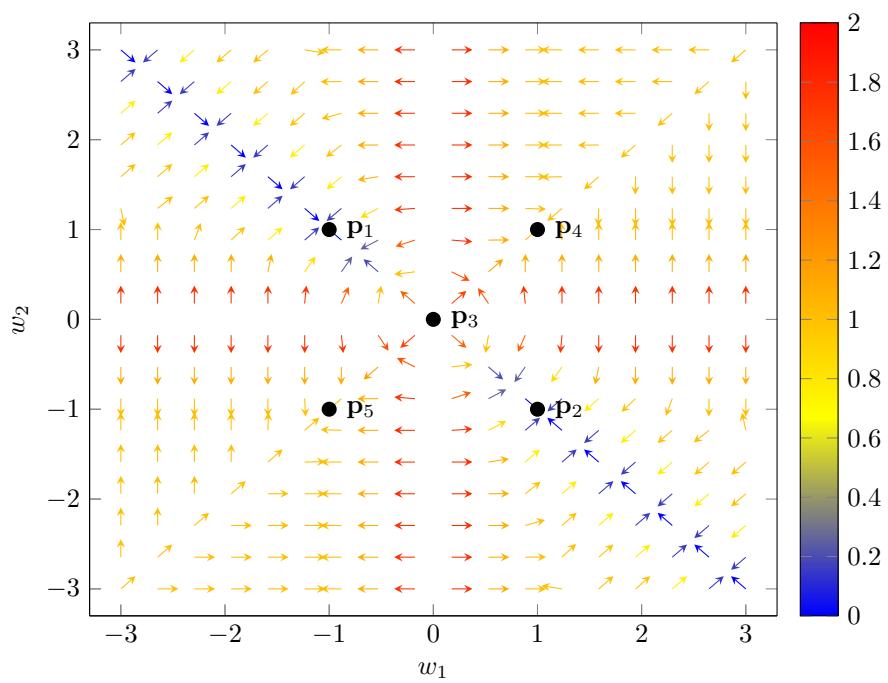


Figure 5.8: Vector field of the negative gradients of the error-weight function. The vectors' magnitudes are normalised and their colour represents the loss values at their respective origins.

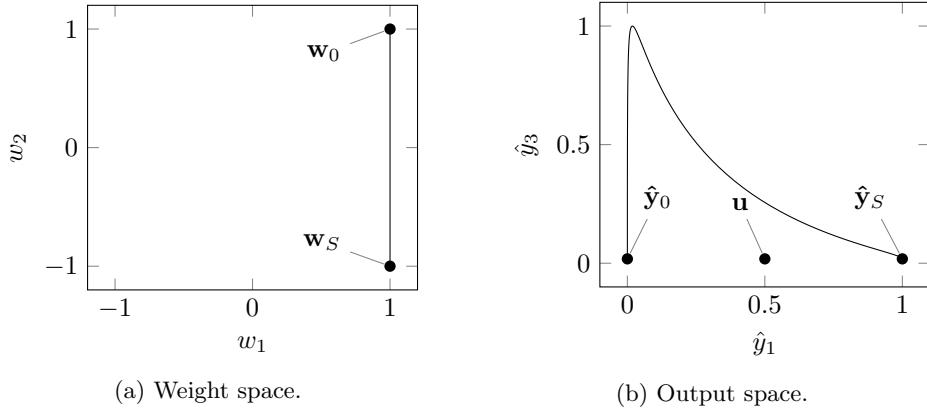


Figure 5.9: Ideal goal-connecting path in weight and output spaces. It suffices to show the first and third samples of the output space as the second stays constant. Note also that $\hat{\mathbf{y}}_S = \mathbf{y}$ because the target is in fact realisable. The point labelled \mathbf{u} is the example of an unrealisable point referred to in Section 5.2.7.

5.2.7 Ideal goal-connecting path

In Lemma 7 we showed that the ideal goal-connecting path is a straight line in weight space that starts at the initial configuration \mathbf{w}_0 and ends at the goal \mathbf{w}_S . We established that the initial weight configuration is $\mathbf{w}_0 = [1 \ 1]^\top$ which is near a suboptimal local minimum (see Corollary 14.1) and the target is $\mathbf{w}_S = [1 \ -1]^\top$ which we proved in Theorem 14 is a global minimum.

Figure 5.9 depicts the ideal goal line in weight space as well as how this line corresponds to output space. It is interesting to see the extreme deformation of this path in output space. In fact, a straight line from $\hat{\mathbf{y}}_0$ to $\hat{\mathbf{y}}_S$ would *not* be a valid goal-connecting path because it would pass through an unrealisable region. To see this, consider for example the point \mathbf{u} lying midway on the straight line between the initial and target configurations,

$$\mathbf{u} = \frac{\mathbf{y} - \hat{\mathbf{y}}_0}{2} = \left[\frac{1-\phi(4)}{2} \quad \phi(2) \quad \phi(2) \right]^\top.$$

Lemma 15. *The point \mathbf{u} is strongly unrealisable.*

Proof. We need to find a weight configuration $\mathbf{w} = [w_1 \ w_2]^\top$ that satisfies $\phi(\mathbf{w}^\top \mathbf{x}_i) = u_i$ for $i = 1, 2, 3$ where u_i is the i th component of \mathbf{u} . The first input

\mathbf{x}_1 is given by $\mathbf{x}_1 = [2 \ 2]^\top$ and so we obtain the following equation:

$$\begin{aligned}\phi(\mathbf{w}^\top \mathbf{x}_1) &= \frac{1 - \phi(4)}{2} \\ e^{-4(w_1 + w_2)^2} &= \frac{1 - e^{-16}}{2} \\ w_1 + w_2 &= \pm \frac{1}{2} \sqrt{-\ln \frac{1 - e^{-16}}{2}}.\end{aligned}\tag{5.8}$$

Similarly, for the second input $\mathbf{x}_2 = [0 \ 2]^\top$ we obtain

$$\begin{aligned}\phi(\mathbf{w}^\top \mathbf{x}_2) &= \phi(2) \\ e^{-4w_2^2} &= e^{-4} \\ w_2 &= \pm 1,\end{aligned}\tag{5.9}$$

and finally for $\mathbf{x}_3 = [2 \ 0]^\top$ we get

$$\begin{aligned}\phi(\mathbf{w}^\top \mathbf{x}_3) &= \phi(2) \\ e^{-4w_1^2} &= e^{-4} \\ w_1 &= \pm 1.\end{aligned}\tag{5.10}$$

There exist no solutions for w_1 and w_2 that satisfy Equations (5.8) to (5.10). Thus, by Definition 14, we conclude that \mathbf{u} is a strongly unrealisable point. \square

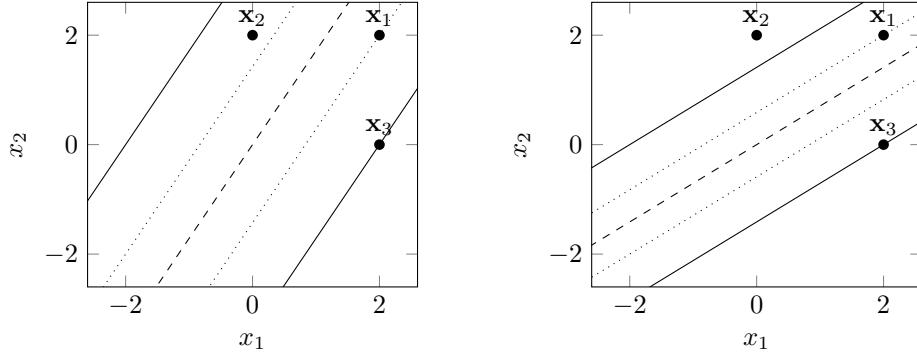
Remark. Lemma 15 proves the existence of one specific unrealisable point, but this methodology could be repeated for other points in order to prove that there is actually a larger unrealisable region consisting of more than that one point on the goal line. Although this will not be carried in this report, it is an important aspect of the stripe problem to keep in mind. The intuition in this scenario with three outputs is that it will often be possible to satisfy two of the three output targets, but not the third. Figure 5.10 illustrates this point by considering the hyperplanes of the target output values for the point \mathbf{u} discussed above.

5.3 Experimental results and analysis

A variety of experiments have been carried out on the stripe problem using the different optimisation techniques from Chapter 3 with and without subgoals. This section will summarise the findings from some of these experiments.

5.3.1 Gradient descent

In order to test the theoretical findings from Section 5.2.6, gradient descent was used to train on the stripe problem from a dozen different starting configurations. When considering w_1 and w_2 as the x and y axes of the Cartesian plane, a total of three initial weight configurations per quadrant were tested.



(a) Input space for $w_1 = 1$ and $w_2 = \frac{1}{2} \sqrt{-\ln \frac{1-e^{-16}}{2}} - 1$.

(b) Input space for $w_1 = 1$ and $w_2 = -\frac{1}{2} \sqrt{-\ln \frac{1-e^{-16}}{2}} - 1$.

Figure 5.10: Input space with hyperplanes at zero excitation (dashed), $\frac{1-e^{-16}}{2}$ activation (dotted) and $\phi(2)$ activation (solid) for two possible input configurations. It can be seen that although \mathbf{x}_1 always intersects with the dotted line, only one of the two other input points will intersect with the solid line.

trial	initial weights \mathbf{w}_0	learning rate α	momentum β
1	[1.8 1.5]	10	0.9
2	[1.5 1.8]	10	0.9
3	[2.0 2.0]	100	0.7
4	[1.8 -1.5]	1	0.9
5	[1.5 -1.8]	1	0.9
6	[2.0 -2.0]	100	0.7
7	[-1.8 -1.5]	10	0.9
8	[-1.5 -1.8]	10	0.9
9	[-2.0 -2.0]	100	0.7
10	[-1.8 1.5]	1	0.9
11	[-1.5 1.8]	1	0.9
12	[-2.0 2.0]	100	0.7

Table 5.2: The dataset for the RBF stripe problem.

Table 5.2 shows the initial configurations along with the learning rate α and momentum¹³ β of the BP via gradient descent algorithm. For each trial, training

¹³As explained in Section 3.1, the learning rate α controls the step size. However, due to the fact that training using only a specific step size took too long, it was decided to use BP with momentum. Essentially, instead of determining the weight update based solely on the magnitude of the gradient and value of α , we additionally take into account an exponentially weighted average of the past gradients where the hyperparameter $\beta \in [0, 1]$ determines the degree of that weighting. Introducing the momentum term is common practice in this type of scenario, so it will not be explained in further detail. It should not adversely affect the performance of gradient descent, so it is fair to use this technique to aid the speed of the

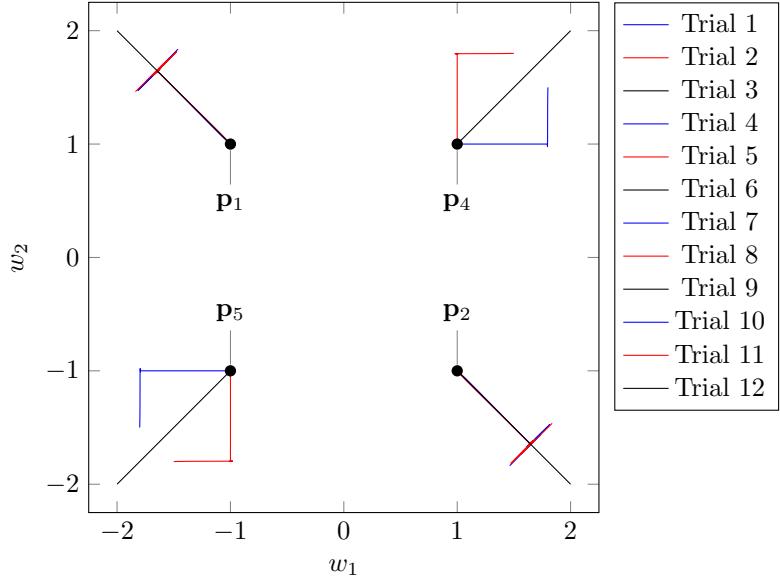


Figure 5.11: Some gradient descent trajectories in weight space. Trials in the same quadrant have different colours to differentiate between them. Trials 1-3 are in the first quadrant (Q1), 4-6 in Q2, 7-9 in Q3 and 10-12 in Q3.

was carried out for 10000 epochs. The hyperparameters had to be adjusted depending on the initial weight configuration in order to ensure convergence within the epoch limit. In Figure 5.11, the trajectories of each of the trials in weight space is shown. It is evident that each trial converges to the local minimum point in the quadrant of its initial weight configuration. This means that trials 1-3 and 7-9 converge to a suboptimal local minimum (Q1 and Q3), whereas trials 4-6 and 10-12 converge to a global minimum (Q2 and Q4), thus empirically affirming the claim made in Section 5.2.6.

Even with a relatively large learning rate and despite the use of momentum, the fact that training requires around 10000 epochs to converge highlights one of the core issues of gradient descent. As discussed in Section 3.4, specifically Figure 3.2, the classical BP algorithm becomes quite slow in “long, narrow valleys” [Press et al. 1992, p. 421] due to the gradient alternating in near right-angle directions. Although the motivation of the stripe problem is to highlight another issue (that of suboptimal local minima), it is noteworthy that this example is quite potent in highlighting other issues as well. The error-weight surface in Figure 5.5 shows examples of this phenomenon quite convincingly because the area marked in blue is a long, narrow valley.

experiments.

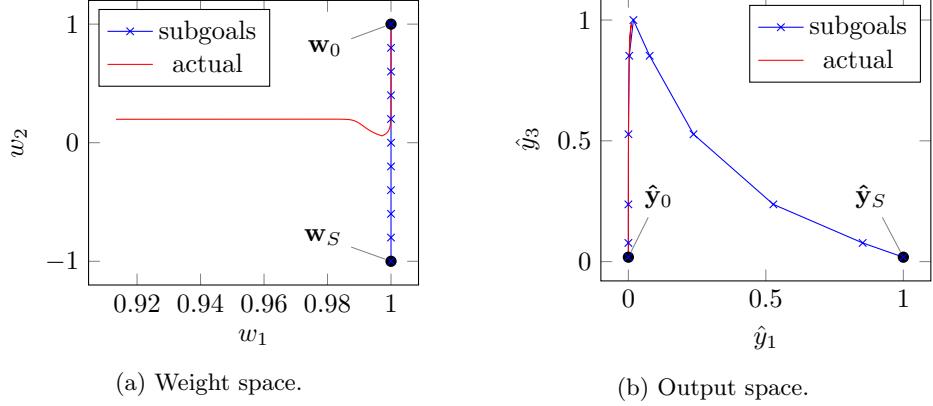


Figure 5.12: Gradient descent with $S = 10$ subgoals on the ideal goal-connecting path.

5.3.2 Derivative-free techniques

Other techniques, namely greedy probing and simulated annealing have been evaluated in the context of the stripe problem, too. They parallel the findings of Section 5.3.1 insofar as initial weight configurations in Q1 and Q3 converging to suboptimal local minima. In fact, the trajectories in weight space are quite similar to Figure 5.11 with the notable difference that training using these derivative-free techniques found the local or global minimum (depending on the quadrant of initialisation) requiring only around 100 epochs where BP required 100000. These findings can be reproduced using the framework (see Chapter 8).

5.3.3 Gradient descent with subgoals

After empirically verifying in Section 5.3.1 that the classical BP algorithm fails to converge to a global minimum with a weight initialisation in Q1 or Q3, we will now employ the ‘cheating’ technique introduced in Section 4.4 using gradient descent as a means to test if neural training techniques in general can realise the ideal goal line (or some trajectory close to it).

Recall the inputs and target outputs of the stripe problem presented in Table 5.1. Figure 5.12 shows the ideal goal line from the initial configuration $\mathbf{w}_0 = [1 \ 1]^T$ to the target $\mathbf{w}_S = [1 \ -1]^T$ along with the $S = 10$ equidistant subgoals on that line. The red line represents the actual weight and output trajectories achieved by the ‘cheat’ technique in conjunction with gradient descent for the parameter¹⁴ $\mu = 0.9$. It can be seen in Figure 5.12b that although the fifth subgoal was achieved, the approach failed to realise the sixth subgoal, and

¹⁴Recall from Section 4.4 that μ is the minimum fractional progress that needs to be attained towards the next subgoal before that subgoal is considered ‘realised’. The value of $\mu = 0.9$ was chosen after experiments with different values showed that when μ is too low, the path deformation in output space from the ideal goal line can become very extreme.

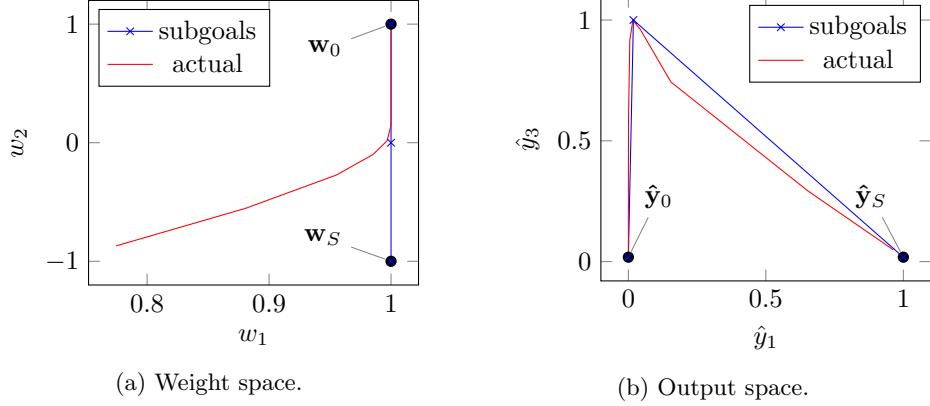


Figure 5.13: Gradient descent ($\alpha = 0.1$, $\beta = 0$) with $S = 2$ subgoals on the ideal goal-connecting path.

hence the remaining path to the goal. The training regime achieves the first four subgoals in weight space (see Figure 5.12a) perfectly, but just shy of achieving the fifth subgoal, w_2 is altered such that the subgoal can never be reached.

Notice that the goal line in weight space keeps the weight w_1 constant, whereas the actual trajectory violates this principle. Upon achieving the third subgoal, the technique fails to simply continue to decreasing the value of w_2 such that it becomes negative. This is due to the nature of the radial basis activation function. As shown in Figure 5.2, the RBF outputs its maximum value when the input is zero, and its output decreases as the absolute value of the input increases. The gradient descent approach is almost at the maximum of the RBF when en route to achieving the fourth subgoal, but it does not know that the function would decrease again if it continued further. Essentially, there is a ‘blind spot’ [Karayannidis 1998] because the algorithm cannot ‘see’ the other side of the hump. Furthermore, the gradient of the RBF is flat when the input is zero ($\phi'(0) = 0$) which is another reason why gradient descent might have difficulties mounting the top of the hump.

It was conjectured that in order to mitigate the problem of the ‘blind spot’, it might be necessary to increase the step size at the region where the gradient is near-zero, as this would increase the likelihood of the technique ‘jumping’ over the hump. One method of ensuring a greater step size in that region is introducing momentum. Experiments were conducted with different numbers of subgoals, and different learning rates. The most important finding is that the target could be achieved using only a minimal number of subgoals ($S = 2$, so using only one subgoal and the actual goal) by keeping the learning rate $\alpha = 0.1$ (like in Figure 5.12) but using momentum with $\beta = 0.9$. The relevant trajectories are depicted in Figure 5.13. While the subgoal is achieved reasonably well in the two dimensions of output space portrayed in Figure 5.13b, the final prediction of \hat{y}_2 changes by around 0.07 albeit it should stay constant. This

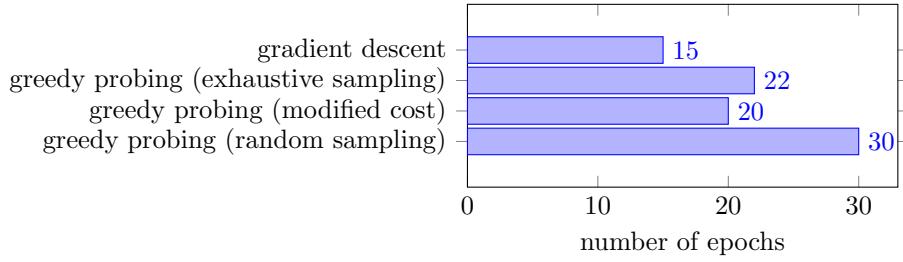


Figure 5.14: Number of epochs until achieving the final subgoal by training regime.

is because the step size due to momentum increased too much after overcoming the ‘hump’. One mechanism to mitigate this problem would be to increase a learning rate schedule; since the final weight configuration is already in the right quadrant, gradient descent is guaranteed to converge to the target (as discussed theoretically in Section 5.2.6 and confirmed empirically in Section 5.3.1), given an adequate learning rate.

5.3.4 Derivative-free techniques with subgoals

The greedy probing approach was also tested with $S = 2$ subgoals using a sampling radius of $r = 0.1$. To ensure that the trajectory in output space gets close enough to the first subgoal such that it passes the ‘hump’, the fractional progress parameter μ had to be increased to 0.99.

One of the drawbacks of the greedy probing technique is that per epoch, it needs to compute the forward pass of the network for every weight sample and every output sample. Hence if the sampling technique generates s samples per epoch and the dataset contains N records, a total of sN forward passes must be computed¹⁵. In the case of the exhaustive sampling technique, Section 3.2 explains that $s = 3^P - 1$ samples are generated for a P -dimensional weight space. So, for the stripe problem, the exhaustive sampling technique will generate 8 weight samples which means that a total of 24 forward passes must be carried out per epoch. Note that gradient descent must only perform one derivative calculation which is comparable in computational complexity to a forward pass (assuming the loss value itself is not calculated, only its derivative). The advantage of the random sampling technique is twofold: the user may specify the number of samples to calculate, and the directions are not as constrained in weight space. We chose a value of $s = 6$ for the random sampling

¹⁵In practice, since the weights are the same for each sample, the forward passes are batched for each sample which means that s forward passes are computed, each with a batch dimension of N . This is possible because the neural layers in essence just represent a matrix multiplication (see Equation (2.12)), but keep in mind that this can only achieve a speedup if the matrix multiplication is parallelised (on a GPU for example), and even then, this argument only applies to large values of N , whereas for the stripe problem $N = 3$. Therefore, let us just say for argument’s sake that sN forward passes must be computed.

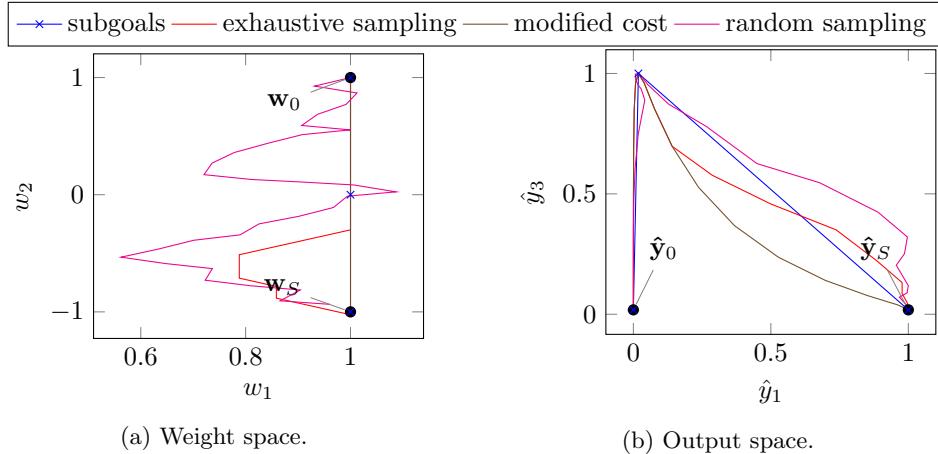


Figure 5.15: Greedy probing ($r = 0.1$) with $S = 2$ subgoals on the ideal goal-connecting path.

technique which means that it only requires 18 forward passes per epoch. However, in Figure 5.15 it becomes apparent that there is a drawback: the random sampling technique needs more epochs to achieve the final goal. In this regard, gradient descent actually outperformed all of the tested derivative-free schemes because it requires fewer epochs and fewer forward passes per epoch. However, it must be noted that finding the optimal hyperparameters that actually allowed gradient descent to converge with only one subgoal was not easy and required a lot of trial and error, so these results are highly customised towards the stripe problem and will likely perform poorly in other settings.

An alternative cost function was also tested for the greedy probing approach, calculating the cost as the sum of the trajectory's strain in both weight space and output space in order to penalise large turns in both spaces. Figure 5.15 provides a comparison of the trajectories of all three approaches. It can be seen that the modified cost function exactly produces the ideal goal line in weight space; however, this is only because the initial direction of the trajectory in weight space was correct. If this were not the case, this modified cost function would fail, so in that regard it is not fair to claim that the modified cost function is superior. Another observation is that due to the randomness of the random sampling technique, its trajectory is chaotic in both the weight and output spaces. For the exhaustive sampling technique, it is interesting to see that like gradient descent (Figure 5.13), the trajectory in weight space begins to deviate from the goal line in weight space after achieving the subgoal, but unlike gradient descent, it is actually able to find back to the goal line. A possible explanation for this could be the increased value of μ used for greedy probing.

Chapter 6

The neural surfing technique

6.1 Clothoids

Consider a scenario in two-dimensional output space, as is shown in Figure 6.1. The current weight configuration produces a point C in output space. How do we evaluate the effectiveness of a candidate sample point B in achieving the goal (or subgoal), A ? We would like to analyse the properties of a curve that originates at C , passes through B , and ends at A . This curve should undergo a linear decrease in curvature until reaching a curvature of zero at the goal. We call this type of curve *clothoid*, and there can only be one clothoid that passes through all three points and has a curvature of zero at A . In fact, this clothoid will be a segment of the *Euler spiral* (up to some affine transformation).

For the purposes of the neural surfer, we are interested in two specific properties of that clothoid: the angle that the goal line makes with the tangent of

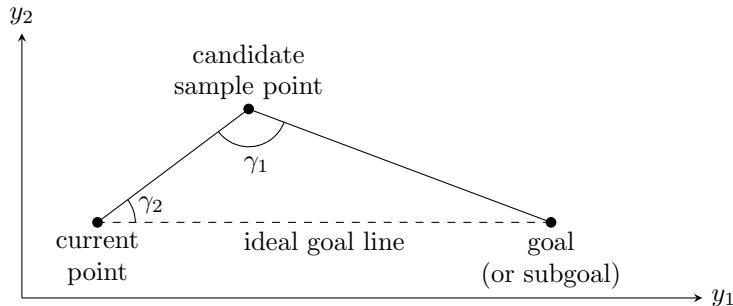


Figure 6.1: A scenario in two-dimensional output space. Note that the ideal goal line need not be parallel to the y_1 axis.

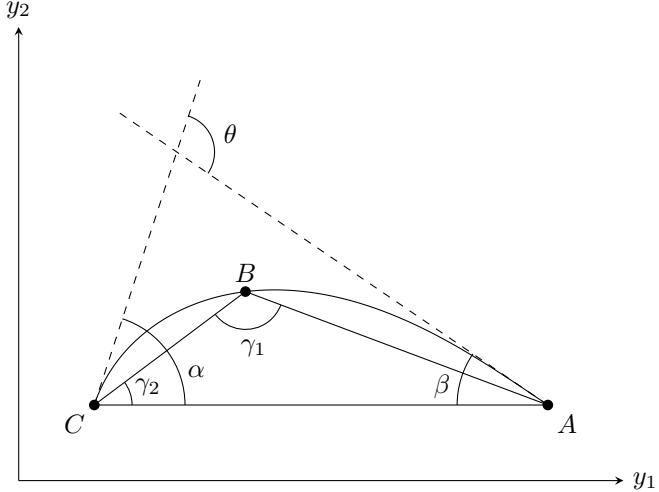


Figure 6.2: The scenario from Figure 6.1 with the goal-connecting clothoid.

the clothoid at C , and that angle at A . In Figure 6.4, these angles are marked α and β , respectively. This leads to the following problem which we will discuss in this section:

Problem 1 (Clothoid construction). Given the angles γ_1 and γ_2 , determine the angles α and β of the resulting clothoid, i.e. find a function that evaluates the mapping $\langle \gamma_1, \gamma_2 \rangle \rightarrow \langle \alpha, \beta \rangle$.

6.1.1 Euler spiral

The Euler spiral is a special curve with an interesting property: its curvature increases linearly with the curve length from the origin. As a consequence, the Euler spiral never forms a complete loop (or circle), a trait that will become useful for the neural surfing technique. Figure 6.3 depicts the normalised Euler spiral. It can be defined using the Fresnel sine and cosine integrals

$$F_S(t) = \int_0^t \sin \frac{\pi s^2}{2} ds \quad (6.1)$$

and

$$F_C(t) = \int_0^t \cos \frac{\pi s^2}{2} ds \quad (6.2)$$

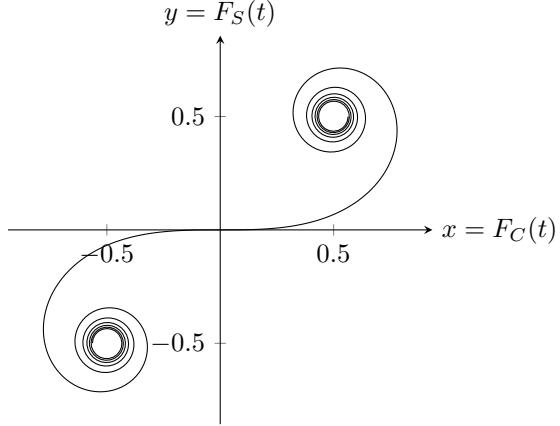


Figure 6.3: Plot of the Euler spiral.

with the parametric equations $x = F_C(t)$ and $y = F_S(t)$. The derivative at a specific point (x, y) in terms of t is calculated as

$$\frac{dy}{dx} = \frac{\left(\frac{dy}{dt}\right)}{\left(\frac{dx}{dt}\right)} = \frac{\sin \frac{\pi t^2}{2}}{\cos \frac{\pi t^2}{2}} = \tan \frac{\pi t^2}{2},$$

so the angle ω of the clothoid's tangent at $(F_C(t), F_S(t))$ can be expressed in terms of t as

$$\omega(t) = \tan^{-1} \left(\tan \frac{\pi t^2}{2} \right) = \frac{\pi t^2}{2}. \quad (6.3)$$

6.1.2 Construction

Figure 6.4 shows how the three points A, B, C from the scenario in Figure 6.1 can be mapped to the Euler spiral. Let us use the notation $\mathcal{A}, \mathcal{B}, \mathcal{C}$ to denote the corresponding points in two-dimensional Cartesian coordinate plane of the Euler spiral. \mathcal{A} must be at the origin of the spiral in order to ensure that the curvature is zero at the goal point. Then the two points \mathcal{B} and \mathcal{C} must be found along the curve such that the triangle formed by these points, $\triangle \mathcal{ABC}$, has angles $\angle \mathcal{ABC} = \gamma_1$ and $\angle \mathcal{ACB} = \gamma_2$.

The problem of finding $\triangle \mathcal{ABC}$ is equivalent to finding the values $t_{\mathcal{A}}, t_{\mathcal{B}}, t_{\mathcal{C}}$ that produce the points $\mathcal{A}, \mathcal{B}, \mathcal{C}$ when plugged into Equations (6.1) and (6.2). We have established previously that $\mathcal{A} = (0, 0)$; thus $t_{\mathcal{A}} = 0$ but it remains to find $t_{\mathcal{B}}$ and $t_{\mathcal{C}}$.

Let us constrain $t_{\mathcal{A}}$ and $t_{\mathcal{B}}$ to be in the interval $(0, \sqrt{3}]$ to ensure that the resulting clothoid will not wind too tight¹⁶. Furthermore, it must be the case

¹⁶In fact, the clothoid from Figure 6.4 was plotted for $0 \leq t \leq \sqrt{3}$. At $t = \sqrt{3}$, the clothoid

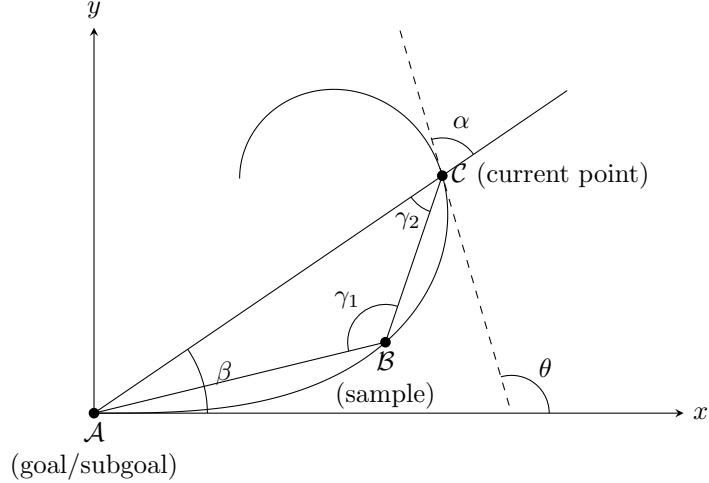


Figure 6.4: Plot of a clothoid segment with three points of interest: \mathcal{C} is the initial point, \mathcal{B} is the sample point and \mathcal{A} is the goal/subgoal (at the origin of the clothoid). The dashed line is tangential to the clothoid at \mathcal{C} .

that $t_{\mathcal{A}} < t_{\mathcal{B}} < t_{\mathcal{C}}$ which is also why the interval above does not include zero. The steps below can be used to find $t_{\mathcal{B}}$ and $t_{\mathcal{C}}$.

1. Create a sequence of n sample values of t such that $t_i = \frac{i}{n}\sqrt{3}$ for $i = 1, 2, \dots, n$.
2. Calculate the points P_1, P_2, \dots, P_n along the Euler spiral where the i th point is given by $P_i = (F_C(t_i), F_S(t_i))$.
3. For $b, c \in \mathbb{Z}^+$ subject to $b < c \leq n$, find the pair of values b, c that minimises

$$(\angle AP_bP_c - \gamma_1)^2 + (\angle AP_cP_b - \gamma_2)^2. \quad (6.4)$$

In other words, find the triangle formed by the points P_b , P_c , and \mathcal{A} which is the most similar¹⁷ to $\triangle ABC$. When $n \rightarrow \infty$, we find $t_b = t_{\mathcal{B}}$ and $t_c = t_{\mathcal{C}}$ (equivalently, $P_b = \mathcal{B}$ and $P_c = \mathcal{C}$), but values of n in the order of 1000 will be suitable for practical purposes.

Once we have determined $t_{\mathcal{B}}$ and $t_{\mathcal{C}}$ and thus know the coordinates of \mathcal{B} and \mathcal{C} , we can find β as the angle that \mathcal{C} makes with the x -axis, giving

$$\beta = \tan^{-1} \left(\frac{\mathcal{C}_y}{\mathcal{C}_x} \right). \quad (6.5)$$

'points' downwards.

¹⁷Two triangles are *similar* if their side lengths are proportional and hence angles are identical.

Since θ is the angle of the tangent at \mathcal{C} , we obtain from Equation (6.3) that $\theta = \frac{\pi}{2} (t_c)^2$. Furthermore, we can deduce from Figure 6.4 that $\theta = \alpha + \beta$, so

$$\alpha = \theta - \beta = \frac{\pi}{2} (t_c)^2 - \beta. \quad (6.6)$$

This completes the construction of the clothoid; we have found a naïve algorithm for computing Problem 1.

6.1.3 Lookup table

A disadvantage of the algorithm from Section 6.1.2 is that it must compute n points on the Euler spiral and then perform the angle calculations for $\mathcal{O}(n^2)$ triangles, *for each sample point* and this is carried out *at every training step*. Instead, we could sample n points along the Euler spiral for values of t in the interval $(0, \sqrt{3}]$, use these to construct the triangles as explained in step 2 of the algorithm, compute the angles $\gamma_1, \gamma_2, \alpha, \beta$ for each triangle and record these values in a table. This table will only need to be constructed once, thus the expensive calculations are not repeated. Treating $\langle \gamma_1, \gamma_2 \rangle$ as the (multi-dimensional) index to the table, our table will represent exactly the mapping $\langle \gamma_1, \gamma_2 \rangle \rightarrow \langle \alpha, \beta \rangle$ from Problem 1.

However, this table will only have a total of $(n - 1)(n - 2)$ entries which means that the mapping would only be defined for certain values of $\langle \gamma_1, \gamma_2 \rangle$. When querying using some pair $\langle \bar{\gamma}_1, \bar{\gamma}_2 \rangle$ that is not in the table, we will find the pair $\langle \gamma_1, \gamma_2 \rangle$ in the table which is closest in terms of Euclidean distance (its *nearest neighbour*) and return that entry's $\langle \alpha, \beta \rangle$. In fact, this is equivalent to minimising Equation (6.4) when setting $\bar{\gamma}_1 = \angle AP_b P_c$ and $\bar{\gamma}_2 = \angle AP_c P_b$.

The nearest neighbour can be found quite efficiently using a so-called k -d tree data structure with an average time complexity logarithmic to the number of points [Friedman et al. 1977]. Hence, using this technique, we can find the clothoid parameters for Problem 1 in $\mathcal{O}(\log n)$ time¹⁸ on average.

6.2 Scaling sample points

TODO : explain how sample points are scaled to be at roughly the same radius in output space

6.3 Adaptive clothoid technique

TODO

¹⁸This is because we have n^2 points and $\mathcal{O}(\log n^2) = \mathcal{O}(\log n)$.

Chapter 7

Generalising neural surfing

TODO : generalize to classification as regression with multiple output variables
(this can be done by concatenating all output variables' dimensions into the output vector/space)

Chapter 8

The framework

8.1 Design

TODO

8.2 Implementation

TODO

8.3 Experimental results

TODO

Chapter 9

Evaluation and critical appraisal

9.1 Error and weight space

9.2 Local minimum problem

9.3 Optimisation techniques

9.3.1 Gradient descent

9.3.2 Greedy probing

also talk about sampling techniques

9.3.3 Simulated annealing

More complex implementations of SA may combine the so-called downhill simplex algorithm [Nelder and Mead 1965] with SA such as in Press et al. [1992, p. 444-455], thereby introducing three additional hyperparameters. In fact, Press et al. remark that “there can be quite a lot of problem-dependent subtlety” in choosing the hyperparameters, and that “success or failure is quite often determined by the choice of annealing schedule” [1992, p. 452].

TODO : generic framework, so could not implement custom annealing schedules with restarts, etc. Furthermore, at what point is the algorithm ‘adjusted too much’ to the problem?

9.4 The framework

compare with `scipy.optimize` and `nevergrad`; also explain that they do not specifically target neural networks

Chapter 10

Conclusions and future work

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