Deep Learning for Tabular Data: An Empirical Study

by

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Date: .....

Abstract

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English abstract.

Uittreksel

Diepleer Tegnieke vir Gestruktrueerde Data: 'n Empiriese Studie

("Deep Learning for Tabular Data: An Empirical Study")

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Afrikaans abstract

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List of Abbreviations and/or Acronyms

ANN	Artificial Neural Network
CNN	Convolutional Neural Network
CTR	Click-through Rate
CV	Computer Vision
DL	Deep Learning
EHR	Electronic Health Records
kNN	k-Nearest Neighbour
mAP	Mean Average Precision
ML	Machine Learning
MLP	Multi-layer Perceptron
NLP	Natural Language Processing
NN	Neural Network
SGD	Stochastic Gradient Descent
SotA	State-of-the-Art

Nomenclature

N	number of observations in a dataset
p	input dimension or the number of features for an observation
K	number of labels in a dataset
$\boldsymbol{x}$	p-dimensional input vector $(x_1, x_2, \ldots, x_p)^\intercal$
λ	label
$\mathcal{L}$	complete set of labels in a dataset $\mathcal{L} = \{\lambda_1, \lambda_2, \ldots, \lambda_K\}$
Y	labelset associated with $\boldsymbol{x}$, $Y \subseteq \mathcal{L}$
$\hat{Y}$	predicted labelset associated with $\boldsymbol{x}$, $\hat{Y} \subseteq \mathcal{L}$, produced by $h(\cdot)$
$\boldsymbol{y}$	K-dimensional label indicator vector, $(y_1, y_2, \ldots, y_K)^\intercal$, associated with observation $\boldsymbol{x}$
$(\boldsymbol{x}_i, Y_i)_{i=1}^N$	multi-label dataset with N observations
D	dataset
$h(\cdot)$	multi-label classifier $h : \mathbb{R}^p \to 2^{\mathcal{L}}$, where $h(\boldsymbol{x})$ returns the set of labels for $\boldsymbol{x}$
θ	set of parameters for $h(\cdot)$
$\hat{\theta}$	set of parameters for $h(\cdot)$ that optimise the loss function
$L(\cdot, \cdot)$	loss function between predicted and true labels
$f(\cdot)$	label prediction module, $f : \mathbb{R}^p \to \mathbb{R}^K$
$t(\cdot)$	thresholding function, $t : \mathbb{R}^K \to \{0, 1\}^K$
$\mathcal{N}(\boldsymbol{x})$	points in the input space neighbourhood of $\boldsymbol{x}$

Chapter 1

Introduction

1.1 Deep Learning

This thesis is concerned with the study of *deep learning* approaches to solve *machine learning* (ML) tasks. More specifically, our interest lies in machine learning tasks that may be solved using tabular data inputs. The deep learning field is an extention of the class of machine learning algorithms called *Artifical Neural Networks* (NNs). Whereas until relatively recently, the neural network field was not a very active research field, rapid development in computing power and the growing abundance of data lead to advances in neural network optimisation and architecture. These advances constitutes the deep learning field as we know it today (Lecun *et al.*, 2015).

Currently, deep learning is receiving a remarkable amount of attention, both in research and in practice (see Figure 1.1). Much of the deep learning hype stems from the tremendous value neural networks have shown in application areas such as *computer vision* (Hu *et al.*, 2017), audio processing (Battenberg *et al.*, 2017), and *natural language processing* (NLP) (Devlin *et al.*, 2018). In these application areas, deep learning methods have reached a maturity level sufficient to be able to run these systems in a production or commercial environment. Examples of the application of deep learning in commercial applications include voice assistants like Amazon Alexa (Sarikaya, 2017), face recognition with Apple iPhones [1], and language translation with Google (Wu *et al.*, 2016).

[1] https://www.apple.com/business/site/docs/FaceID_Security_Guide.pdf
[2] https://trends.google.com/trends/explore?date=all&q=deep%20learning
[3] https://www.semanticscholar.org/search?year%5B0%5D=2000&year%5B1%5D=

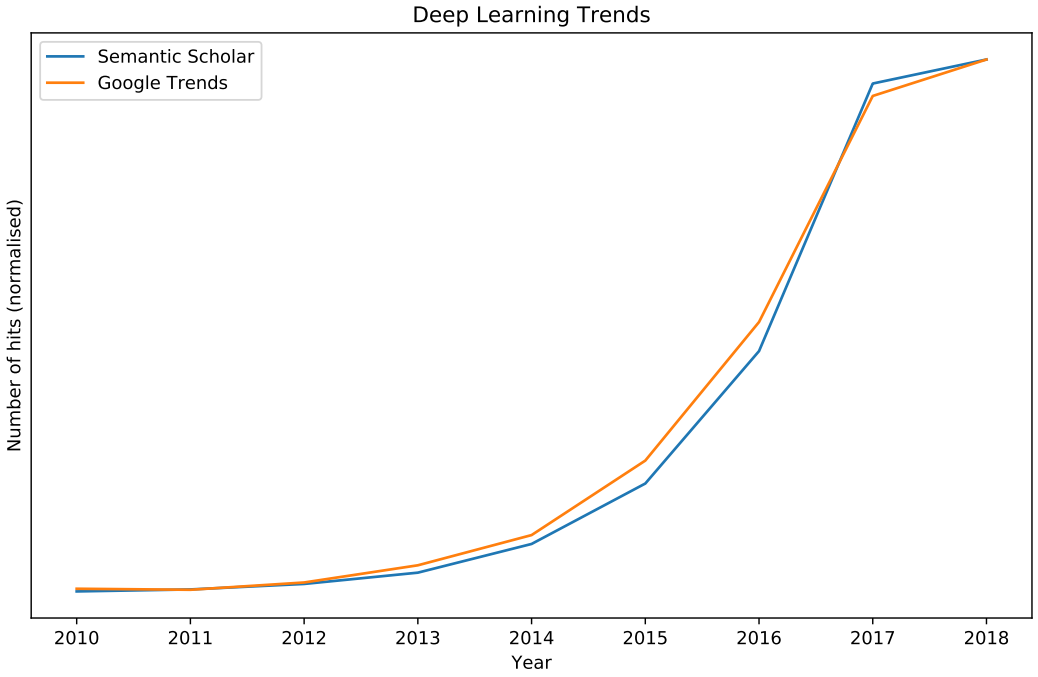


Figure 1.1: The exponential growth of published papers and Google search terms containing the term *Deep Learning*. Sources: Google Trends[2], Semantic Scholar[3]

One of the most attractive attributes of deep learning is its ability to model almost any input-output relationship. This has lead to the use of deep learning in a very wide array of applications.
For example, deep learning has been used to generate art (Gatys *et al.*, 2015) and music (Mogren, 2016), to control various modules in autonomous cars (Fridman *et al.*, 2017), to play video games (Mnih *et al.*, 2013), to recommend movies (Covington *et al.*, 2016), to improve the quality of images (Shi *et al.*, 2016), and to beat the world's best Go player (Silver *et al.*, 2017).

A common characteristic of all of the above deep learning applications, is that the data used to construct them, contain the same type of values or measurements. That is, in computer vision the data are pixel values, in NLP the data are words and in audio processing the data represent sound waves. This is not a criterion for deep learning algorithms to be successful, but may be viewed as a driver for their sucess in these application domains. It is simpler to model data consisting of the same type of measurements, since each input feature can be treated the same. Furthermore in the above deep learning

2019&q=%22deep%20learning%22&sort=relevance

applications, it is found that in each of these domains, universal patterns exist. This allows for knowledge to be transferred between tasks belonging to the same domain. The knowledge to be transferred is both knowledge aquired by humans, and that learned by a deep learning model. For example, in computer vision, advancements in classifying pictures of pets will most likely also be facilitate improved identification of tumors in X-rays. That is, patterns learned by a deep learning model when attempting one task, may also be useful in a different, but related task (see *Transfer Learning*).

A data domain in which deep learning does not flourish is that of tabular data. A *tabular dataset* can be represented by a two-dimensional table, where each of the rows of the table corresponds to one observation and where each column denotes an individual meaningful feature. We further explain the use of tabular data in Section 1.2 below.

Some research have recently been done on the use of deep learning models for tabular data (Shavitt and Segal, 2018, Song *et al.* (2018)). However, state-of-the-Art (SotA) results are reported only rarely (de Brébisson *et al.*, 2015) (and in this competition[4]). Therefore it can be said that the area is nowhere near as mature or receiving as much attention as is the case with deep learning for computer vision or for NLP. In a comprehensive study in the paper by (Fernández-Delgado *et al.*, 2014), it was found that ML tasks that make use of tabular data are typically more effectively solved using tree-based methods. This is also evident when one considers the winning solutions of relevant Kaggle competitions[5]. A possible explanation for the superior performance of tree-based metods, is the heterogeneity of tabular data (Shavitt and Segal, 2018), which forms part of the discussion in the next section.

1.2 Tabular Data

In this section, we make use of the so-called Adult[6] dataset in order to discuss the use of tabular data. The reader may refer to Table 1.1 for an extract of this dataset. The data were collected during an American census with the aim of predicting whether or not an indivdual earns more than $50,000 a year.

[4]https://www.kaggle.com/c/porto-seguro-safe-driver-prediction/discussion/44629
[5]https://www.kaggle.com
[6]http://archive.ics.uci.edu/ml/datasets/Adult

	age	occupation	education	race	sex	>=50k
1	49		Assoc-acdm	White	Female	1
2	44	Exec-managerial	Masters	White	Male	1
3	38		HS-grad	Black	Female	0
4	38	Prof-specialty	Prof-school	Asian-Pac-Islander	Male	1
5	42	Other-service	7th-8th	Black	Female	0
6	20	Handlers-cleaners	HS-grad	White	Male	0

Table 1.1: Preview of the Adult dataset.

Table 1.1 represents a typical tabular dataset, where the columns contain measurements on different features. Therefore each column may contain different data types. Some columns may consist of continuous measurements, whereas other columns contain discrete or categorical measurements. Hence the columns are heterogeneous with respect to data types. Furthermore, in tabular data, the rows and columns occur in no particular order. This of course stands in contrast to image or text data.

Many important ML applications make use of tabular data. Some of these applications are listed below:

- Various tasks that make use of Electronic Health Records. These include the prediction of in-hopsital mortality rates, and prolonged length of stay (Rajkomar *et al.*, 2018).
- Recommender systems for items like videos (Covington *et al.*, 2016) or property listings (Haldar *et al.*, 2018).
- Click-through rate (CTR) prediction in web applications, *i.e.* predicting which item a user will click on next (Song *et al.*, 2018).
- Predicting which clients are at risk of defaulting on their accounts[7].
- Predicting store sales (Guo and Berkhahn, 2016).
- Drug discovery (Klambauer *et al.*, 2017).

Tabular datasets come in all shapes and sizes. The number of rows can range from hundreds to millions, and the number of columns also has no limits. It is not unusual for tabular datasets to be noisy. A proportion of the observations may have missing features and/or incorrect values. Continuous measurements may be based upon vastly different scales, some containing outliers, whereas categorical features may have high cardinality which leads to sparse data.

[7]https://www.kaggle.com/c/loan-default-prediction

During the construction of models for tabular datasets, the most important step in terms of leading to improvements in the model performance, is pre-processing and manipulation of the input features (Rajkomar *et al.*, 2018). This includes data merging, customising, filtering and cleaning. In a process called feature engineering one strives to create new features from the original features based on some domain knowledge. The idea is that such engineered features enables a model to learn interactions between features, thereby facilitating more accurate prediction. Feature engineering is an extremely laborious process with no clear recipe to follow and therefore typically cannot succesfully be implemented without some domain expertise.

Ensemble methods based upon trees are currently viewed as the most effective machine learning models in the face of tabular datasets. As mentioned above, a possible reason for this may be their robustness to different feature scales and data types, linked with their ability to effectively model interactions among features having different data types.

Indeed, in the context of tabular data, classical neural network approaches are no match for tree ensembles. Although the deep learning field has advanced and matured a lot in recent years, it is not yet clear how to leverage these modern techniques to effectively build and train deep neural networks on tabular datasets. In this thesis we explore ways of doing so. By reviewing the most recent literature on the topic, and through empirical work, we aim to summarise best practices when using deep learning for tabular data.

1.3 Challenges of Deep Learning for Tabular Data

Some of the challenges of deep learning for tabular data have been alluded to in earlier sections of this chapter. These will form the framework for the literature review which follow later on, therefore they are summarised below, in terms of relevant questions to ask when applyting deep learning in the context of tabular data:

- **How should input features be represented numerically?**: We have mentioned that tabular data consist of mixed feature types, *i.e.* a combination of categorical and continuous features. The question here

relates to how these features should be processed and presented to the model during training.

- **How can we exploit feature interactions?**: Once we have found the optimal feature representation for all feature types, we will need a way to effectively learn the interactions between them and also a way to learn how they relate to the target. This a crucial step towards the effective application of deep learning models to tabular data.
- **How can we be more sample efficient?**: Tabular datasets are typically smaller than the datasets use in computer vision and in NLP. Moreover, no general large dataset with universal properties exists to be used by a model to learn from (as is the case in for example image classification). Thus a key challenge is to facilitate learning from less data.
- **How do we interpret model decisions?**: The use of deep learning is often restricted by its perceived lack of interpretability. Therefore we need ways of explaining the model output in order for it to be useful in many applications.

Clearly there are plenty of considerations when it comes to using deep learning for tabular data. The main objective of this thesis is to find the best ways of overcoming the above challenges. Towards this objective, the study should lead to a thorough understanding of the *status quo* of the field, and of the necessary factors in order to ensure deep learning to be as effective in other data domains as it currently is in computer vision and NLP.

The study is divided in two parts. We start by first providing an overview of the relevant literature. Subsequently, we make use of experimental work in order to compare various deep learning algorithms (and possible improvements) on relevant datasets. Here an important aim will be to ensure our experiments to be *rigorous*. The importance of rigorous research has relatively recently again been emphasised during an NIPS talk[8], during which researchers in the deep learning field have been criticised for the growing gap between the understanding of its techniques and practical successes. Currently much more emphasis is placed on the latter. The speakers urged the deep learning community to be more rigorous in their experiments where, for them, the most important part of rigor is better empiricism, not more mathematical theories. Better

[8]Talk given at NIPS2017 - https://www.youtube.com/watch?v=Qi1Yry33TQE

empiricism in classification may include, for example, practices such as using cross-validation to estimate the generalisation ability of a model, and reporting standard errors. Empirical studies should involve more than simply attempting to beat the benchmark, for example where possible, they should also involve simple experiments that facilitate understanding why some algorithms are successful, while other are not.

In addition, we want the empirical work in this study to be as reproducible as possible. This aspect is often overlooked. However it is a crucial aspect, ensuring transparent and accountable reporting of results. Reproducibility add to the value of research, since without it, researchers are not able to build on each other's work. There all code, data and necessary documentation in order to reproduce the experiments that were done in this thesis will be available [9].

Having stated the objectives of this study, we now turn to a discussion of the fundamental concepts of Statistical Learning Theory. This is followed by a more detailed summary of the thesis.

1.4 Overview of Statistical Learning Theory

Machine- or statistical learning algorithms (used interchangeably) are used to perform certain tasks that are too difficult to solve with fixed rule-based programs. Hence statistical learning algorithms are able to use data in order to learn how to perform difficult tasks. For an algorithm to learn from data means that it can improve its ability to perform an assigned *task* with respect to some *performance measure*, by processing *data*. In this section we discuss some of the important types of tasks, data and performance measures in the statistical learning field.

A learning task describes the way in which an algorithm should process an observation. An observation is a collection of features that have been measured, corresponding to some object or event that we want the system to process, for example an image. We will represent an observation by a vector $\boldsymbol{x} \in \mathbb{R}^p$, where each element x_j of the vector is an observed value of the j-th feature, $j = 1, \ldots, p$. For example, the features of an image are usually the color intensity values of the pixels in the image.

Many kinds of tasks can be solved using statistical learning. One of the most common learning tasks is that of *classification*, where it is expected of an

[9] Shared publicly at https://github.com/jandremarais/tabularLearner

algorithm to determine which of K categories an input belongs to. In order to complete the classification task, the learning algorithm is usually asked to produce a function $f : \mathbb{R}^p \to \{1, \ldots, K\}$. When $y = f(\boldsymbol{x})$, the model assigns an input described by the vector $\boldsymbol{x}$ to a category identified by the numeric code y, called the *output* or *response*. In other variants of the classification task, f may output a probability distribution over the possible classes.

Regression is another main learning task and requires the algorithm to predict a continuous value given some input. This task requires a function $f : \mathbb{R}^p \to \mathbb{R}$, where the only difference between regression and classification is the format of the output.

Learning algorithms learns such tasks by observing a relevant set of data points, *i.e.* a dataset. A dataset containing N observations of p features is commonly denoted by a data matrix $X : N \times p$, where each row represents a different observation and where each column corresponds to a different feature of the observations, *i.e.*

$$X = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1p} \\ x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \ldots & x_{Np} \end{bmatrix}.$$

Often the dataset includes annotations for each observation in the form of a label (*i.e.* in classification) or in the form of a target value (*i.e.* in regression). These N annotations are represented by the vector $\boldsymbol{y}$, where the element y_i is associated with the i-th row of X. Therefore the response vector may be denoted by

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}.$$

Note that in the case of multiple labels or targets, a matrix representation $Y : N \times K$ is required.

Statistical learning algorithms can be divided into two main categories, *viz. supervised* and *unsupervised* algorithms. This categorisation is determined by the presence (or absence) of annotations in the dataset to be analysed. Unsupervised learning algorithms learn from data consisting only of features,

X, and are used to find useful properties and structure in the dataset (see Hastie *et al.*, 2009, Ch. 14). On the other hand, superivised learning algorithms learn from datasets which consist of both features and annotations, (X, Y), with the aim to model the relationship between them. Therefore, both classification and regression are considered to be supervised learning tasks.

In order to evaluate the ability of a learning algorithm to perform its assigned task, we have to design a quantitative performance measure. For example, in a classification task we are usually interested in the accuracy of the algorithm, *i.e.* the percentage of times that the algorithm assigns the correct classification. We are mostly interested in how well the learning algorithm performs on data that it has not seen before, since this demonstrates how well it will perform in real-world situations. Thus we typically evaluate the algorithm on a *test set* of data points. This dataset is independent of the *training set* of data points that used during the learning process.

For a more concrete example of supervised learning, and keeping in mind that the linear model is one of the main building blocks of neural networks, consider the learning task underlying *linear regression*. The objective here is to construct a system which takes a vector $\boldsymbol{x} \in \mathbb{R}^p$ as input and which predicts the value of a scalar $y \in \mathbb{R}$ as response. In the case of linear regression, we assume the output be a linear function of the input. Let $\hat{y}$ be the predicted response. We define the output to be

$$\hat{y} = \hat{\boldsymbol{w}}^T \boldsymbol{x},$$

where $\hat{\boldsymbol{w}} = [w_0, w_1, \ldots, w_p]$ denotes a vector of parameters and where $\boldsymbol{x} = [1, x_1, x_2, \ldots, x_p]$. Note that an intercept is included in the model (also known as a *bias* in machine learning). The parameters are values that control the behaviour of the system. We can think of them as a set of *weights* that determine how each feature affects the prediction. Hence the learning task can be defined as predicting y from $\boldsymbol{x}$ through $\hat{y} = \hat{\boldsymbol{w}}^T \boldsymbol{x}$.

We of course need to define a performance measure to evaluate the linear predictions. For a set of observations, an evaluation metric tells us how (dis)similar the predicted output is to the actual response values. A very common measure of performance in regression is the *mean squared error* (MSE), given by

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2.$$

The process of learning from the data (or fitting a model to the data) can be reduced to the following optimisation problem: find the set of weights, $\hat{\boldsymbol{w}}$, which produces a $\hat{\boldsymbol{y}}$ that minimises the MSE. Of course this problem has a closed form solution and can quite trivially be found by means of *ordinary least squares* (OLS) (see Hastie *et al.*, 2009, p. 12). However, we have mentioned that we are more interested in the algorithm's performance evaluated on a test set. Unfortunately the least squares solution does not guarantee the solution to be optimal in terms of the MSE on a test set, rendering statistical learning to be much more than a pure optimisation problem.

The ability of a model to perform well on previously unobserved inputs is referred to as its *generalisation* ability. To be able to fit a model that generalises well to new unseen data cases is the key challenge of statistical learning. One way of improving the generalisation ability of a linear regression model is to modify the optimisation criterion J, to include a *weight decay* (or *regularisation*) term. That is, we want to minimise

$$J(\boldsymbol{w}) = MSE_{\text{train}} + \lambda \boldsymbol{w}^T \boldsymbol{w},$$

where $J(\boldsymbol{w})$ now expresses preference for smaller weights. The parameter λ is non-negative and needs to be specified ahead of time. It controls the strength of the preference by determining how much influence the penalty term, $\boldsymbol{w}^T\boldsymbol{w}$, has on the optimisation criterion. If $\lambda = 0$, no preference is imposed, and the solution is equivalent to the OLS solution. Larger values of λ force the weights to decrease, and thus referred to as a so-called *shrinkage* method ((*cf.* for example Hastie *et al.*, 2009, pp. 61-79) and (Goodfellow *et al.*, 2016).

We can further generalise linear regression to the classification scenario. First, note the different types of classification schemes. Consider $\mathcal{G}$, the discrete set of values which may be assumed by G, where G is used to denote a categorical output variable (instead of Y). Let $|\mathcal{G}| = K$ denote the number of discrete categories in the set $\mathcal{G}$. The simplest form of classification is known as binary classification and refers to scenarios where the input is associated with only one of two possible classes, *i.e.* $K = 2$. When $K > 2$, the task is known as multiclass classification. In multi-label classification an input may be associated with multiple classes (out of K available classes), where the number

of classes that each observation belongs to, is unknown. Here we start by introducing the two single label classification setups, *viz.* binary and multiclass classification.

In multiclass classification, given the input values $\boldsymbol{X}$, we would like to accurately predict the output, G, which we denote by $\hat{G}$. One approach would be to represent G by an indicator vector $\boldsymbol{Y}_G : K \times 1$, with elements all zero except in the G-th position, where it is assigned a 1, *i.e.* $Y_k = 1$ for $k = G$ and $Y_k = 0$ for $k \neq G$, $k = 1, 2, ..., K$. We may then treat each of the elements in $\boldsymbol{Y}_G$ as quantitative outputs, and predict values for them, denoted by $\hat{\boldsymbol{Y}} = [\hat{Y}_1, \ldots, \hat{Y}_K]$. The class with the highest predicted value will then be the final categorical prediction of the classifer, *i.e.* $\hat{G} = \arg\max_{k \in \{1,\ldots,K\}} \hat{Y}_k$.

Within the above framework we therefore seek a function of the inputs which is able to produce accurate predictions of the class scores, *i.e.*

$$\hat{Y}_k = \hat{f}_k(\boldsymbol{X}),$$

for $k = 1, \ldots, K$. Here $\hat{f}_k$ is an estimate of the true function, f_k, which is meant to capture the relationship between the inputs and output of class k. As with the linear regression case described above, we can use a linear model $\hat{f}_k(\boldsymbol{X}) = \hat{\boldsymbol{w}}_k^T \boldsymbol{X}$ to approximate the true function. The linear model for classification divides the input space into a collection of regions labelled according to the classification, where the division is done by linear *decision boundaries* (see Figure 1.2 for an illustration). The decision boundary between classes k and l is the set of points for which $\hat{f}_k(\boldsymbol{x}) = \hat{f}_l(\boldsymbol{x})$. These set of points form an affine set or hyperplane in the input space.

After the weights are estimated from the data, an observation represented by $\boldsymbol{x}$ (including the unit element) can be classified as follows:

- Compute $\hat{f}_k(\boldsymbol{x}) = \hat{\boldsymbol{w}}_k^T \boldsymbol{x}$ for all $k = 1, \ldots, K$.
- Identify the largest component and classify to the corresponding class, *i.e.* $\hat{G} = \arg\max_{k \in \{1,\ldots,K\}} \hat{f}_k(\boldsymbol{x})$.

One may view the predicted class scores as estimates of the conditional class probabilities (or posterior probabilities), *i.e.* $P(G = k | \boldsymbol{X} = \boldsymbol{x}) \approx \hat{f}_k(\boldsymbol{x})$. However, these values are not the best estimates of posterior probabilities. Although the values sum to 1, they do not lie in the interval [0,1]. A way to overcome this problem is to estimate posterior probabilities using the *logit*

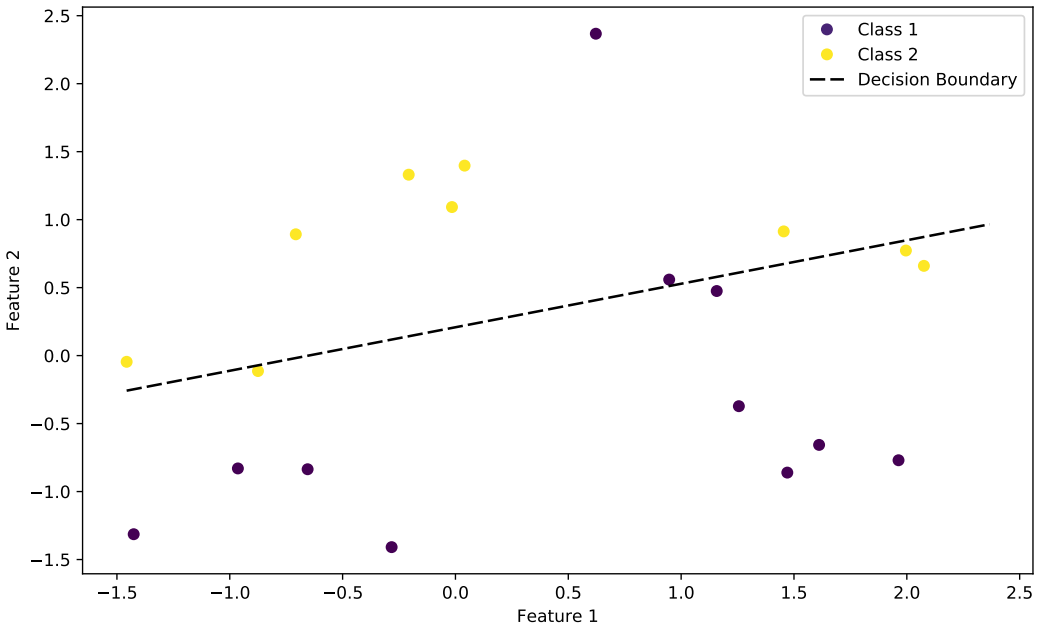


Figure 1.2: Linear model on simple binary classification dataset.

transform of $\hat{f}_k(\boldsymbol{x})$. That is,

$$P(G = k|\boldsymbol{X} = \boldsymbol{x}) \approx \frac{e^{\hat{f}_k(\boldsymbol{x})}}{\sum_{l=1} e^{\hat{f}_l(\boldsymbol{x})}}.$$

Through this transformation, the estimates of the posterior probabilities both sum to 1 and are contained in [0,1]. The above model is the well-known *logistic regression* model (Hastie *et al.*, 2009, p. 119). With this formulation there is no closed form solution for the weights. Instead, the weight estimates may be searched for by maximising the log-likelihood function. One way of doing this is by minimising the negative log-likelihood using gradient descent, which will be discussed in the next chapter.

Finally in this section, note that any supervised learning problem can also be viewed as a function approximation problem. Suppose we are trying to predict a variable Y given an input vector $\boldsymbol{X}$, where we assume the true relationship between them to be given by

$$Y = f(\boldsymbol{X}) + \epsilon,$$

where ϵ represents the part of Y that is not predictable from $\boldsymbol{X}$, because of, for example, incomplete features or noise present in the labels. Then in function approximation we are estimating f with an estimate $\hat{f}$. In parametric

function approximation, for example in linear regression, estimation of $f(\boldsymbol{X}, \theta)$ is equivalent to estimating the optimal set of weights, $\hat{\theta}$. In the remainder of the thesis, we refer to $\hat{f}$ as the *model*, *classifier* or *learner*.

1.5 Outline

This chapter provided the context, motivation, objectives and theoretical background of this study. An outline of the remainder of the thesis follows below:

In Chapter 2, the theory underlying neural networks is described. The building blocks of neural networks are discussed, thereby introducing neurons, basic layers and the way in which neural networks are trained. The important concept of regularisation is also discussed. Using the perspective of representation- and manifold learning, we then attempt to gain insight into what happens inside an neural network.

Chapter 3 continues the discussion by focusing on the key advances in neural networks in recent times. The idea is that all concepts introduced in this chapter should potentially be able to facilitate the construction of improved deep neural networks on tabular data. Improved ways of fighting overfitting, such as data augmentation, the use of dropout and transfer learning, as well as the SotA training policy called *1Cycle* are analysed here. New developments in architectural design are also highlighted. The chapter concludes with approaches towards interpretting neural networks and their predictions.

Chapter 4 may be viewed as a core chapter of this thesis. It mainly serves as a literature review of all research with regard to deep learning for tabular data. The chapter is organised according to the modelling challenges faced when using deep learning for tabular data, investigating and comparing what other researchers have done in order to overcome these challenges. It will be seen that the key concept involves finding the right representation for tabular data. This may be done through embeddings, and by means of designing architectures that can efficiently learn feature interactions. This is for example done with attention models, possibly with the help of unsupervised pretraining.

In Chapter 5 we empirically evaluate several claims made in the literature. The aim of the chapter is to evaluate and compare different approaches to tackling the various challenges. Hence the main experiments involve evaluating neural networks at various samples sizes, evaluating potential gains from

doing unsupervised pretraining and using data augmentation, and comparing attention modules with classic fully-connected layers. We also illustrate a way in which resulting neural networks may be interpreted by means of permutation importance and knowledge distillation.

The thesis concludes in Chapter 6, where we summarise the work, some highlights and the main take-home points. The limitations of this study are discussed, and promising future research directions are identified.

Chapter 2

Neural Networks

2.1 Introduction

Not unlike most supervised machine learning models, a neural network (NN) is a function which maps inputs to outputs, *i.e.* $f : \boldsymbol{x} \rightarrow y$. The structure of f is often loosely compared to the structure of the human brain. Oversimplified, the brain consists of a collection of interconnected neurons. Each neuron can generate and receive signals. A received signal may be described as an input to a neuron, whereas a sent signal may be described as an output from that neuron. If two neurons are connected, it means that the output from the one neuron serves as input to the other. In a very simple model of the brain, one may argue that a neuron receives several signals, which it weighs and combines, and if the combined value of the inputs is higher than a certain threshold, the neuron sends a output signal to the next neuron. Figure 2.1 (a) provides a schematic of a biological neuron.

An artifical neural network tries to mimic this model of the human brain - it is set up to consist of several layers of connected units (or neurons). With exception of units in the first and final layers, each unit outputs a weighted combination of its inputs, combined with a simple non-linear transformation. In each layer of the neural network, the input is passed through each of the neurons. In turn, their output is passed to the next layer.

The transformation at each neuron is controlled by a set of parameters, also known as weights. Training a neural network involves tuning these weights in order to obtain some desired output. During training, the neural network receives as input a set of training data. The neural network weights are then

learned in such a way that, when given a new set of inputs, the output predicted by the neural network matches the corresponding response of interest as closely as possible. The process of using the training data to tweak the weights is done by means of an optimisation algorithm called Stochastic Gradient Descent (SGD).

Although recently there has been plenty of excitement around neural networks, it is well known that they were invented many years ago. The development of neural networks dates back at least as far as the invention of perceptrons in (Rosenblatt, 1962). It is also interesting to compare modern neural networks with the Projection Pursuit Regression algorithm in statistics (Friedman and Stuetzle, 1981). Only recently a series of breakthroughs allowed neural networks to be more effective, leading to the renewed interest in the field.

The aim of this chapter is to provide an overview of neural networks, emphasising the basic structure (§2.2) and the way in which they are trained (§2.3). This is done with a view to discuss modern neural network structures and training policies in Chapter 3, which in turn will help us shed light on Deep Learning for tabular data. Finaly, the chapter concludes with a section on representation and manifold learning (§2.4) in an attempt to understand what a neural network is actually doing.

2.2 The Structure of a Neural Network

2.2.1 Neurons and Layers

In basic terms, a neural network processes an input $boldsymbolx$ by sending it through a series of layers. The neurons in each layer apply some transformation to their inputs, resulting in a set of outputs which are again passed on to the next layer of neurons. Eventually, the final layer produces the neural network output. In this section we provide more detail regarding the neural network structure. We start with a description of the operations inside each neuron, and follow with a discussion of the way in which the neurons may be connected in layers in order to form a complete neural network structure. Our discussion is based upon a simple regression example.

Suppose we are in pursuit of a function which is able to estimate some continuous target, y, given a p-dimensional input $\boldsymbol{x}$, *e.g.* estimating the taxi fare

from features such as distance travelled, time elapsed and number of passengers. A single neuron may act as such a function. It models y by computing a weighted average of the input features. This operation is illustrated in Figure 2.1 (b).

(a) (b)

Figure 2.1: Comparison of a biological (a) and an artificial (b) neuron[1].

In equation form, this function can be written as:

$$w_1 \cdot x_1 + w_2 \cdot x_2 + \cdots + w_p \cdot x_p + b = y,$$

where $\{w_k\}_{k=1}^p$, are the weights applied to each of the inputs $\{x_k\}_{k=1}^p$ and b the constant bias term. Clearly, this equation is simply the very common linear model and thus also can be written as:

$$\boldsymbol{w}^\intercal \boldsymbol{x} + b = y,$$

where $\boldsymbol{x} = [x_1 \quad x_2 \quad \dots \quad x_p]^\intercal$ is the input, $\boldsymbol{w} = [w_1 \quad w_2 \quad \dots \quad w_p]^\intercal$ the weights and y the output. We may compress the above equation to $\boldsymbol{w}^\intercal \boldsymbol{x} = y$, where $\boldsymbol{x}$ includes the bias term and the weight vector $\boldsymbol{w}$ a unit element, *i.e.* $\boldsymbol{x} = [1 \quad x_1 \quad \dots \quad x_p]^\intercal$ is the input, $\boldsymbol{w} = [b \quad w_1 \quad \dots \quad w_p]^\intercal$.

The weights convey the importance of each input features in predicting the target. The larger $|w_k|$ is, the greater is the contribution of x_k towards the output. If $w_k = 0$, x_k has no influence on the target. However the weights are unknown and therefore we need to estimate them.

In linear regression this is done by means of the method of ordinary least squares. Since a neural network consists of many inter-conncected neurons, an alternative estimation procedure is required. This is the topic of the next section.

Often a linear model will be too rigid to model a certain response of interest. In order to fit a more flexible model, we may add more neurons. Consider the

[1]Image credit: https://www.jeremyjordan.me/intro-to-neural-networks/

use of two neurons, where the second neuron accepts the same input as the first neuron, but uses a different set of weights. Thus we have two different outputs produced by the two neurons, *i.e.*. $z_1 = \boldsymbol{w}_1^\intercal \boldsymbol{x}$ and $z_2 = \boldsymbol{w}_2^\intercal \boldsymbol{x}$. In order to produce a final estimate from the initial two estimates, *viz.* z_1 and z_2, they are passed to a third neuron. That is, $y = \boldsymbol{w}_3^\intercal \boldsymbol{z}$, where $\boldsymbol{z} = [z_1 \quad z_2]^\intercal$. Figure 2.2 illustrates this pipepline in network form.

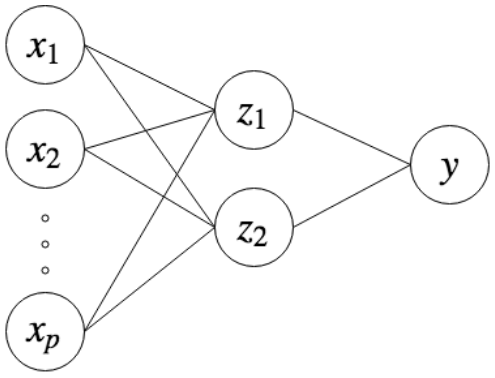


Figure 2.2: A simple neural network accepting p-sized inputs, with one hidden layer which has two neurons.

The first two neurons each received all p inputs and each produced a single output. These two outputs were received by the third neuron, and combined in order to produce the final output, *viz.* y. The operations performed by the first two neurons may be expressed as $\boldsymbol{z} = W\boldsymbol{x}^\intercal$, where

$$W = \begin{bmatrix} \boldsymbol{w}_1^\intercal \\ \boldsymbol{w}_2^\intercal \end{bmatrix} = \begin{bmatrix} w_{10} & w_{11} & w_{12} & \dots & w_{1p} \\ w_{20} & w_{21} & w_{22} & \dots & w_{2p} \end{bmatrix} \quad \text{and} \quad \boldsymbol{z} = [z_1 \quad z_2]^\intercal.$$

The collection of these two neurons is what is called a layer. Since our third neuron (which is also a layer but with a single neuron) receives the output of this layer as input, it is possible to express the complete input-output relationship in one equation, *i.e.*

$$y = \boldsymbol{w}_3^\intercal \boldsymbol{z} = \boldsymbol{w}_3^\intercal W \boldsymbol{x}.$$

Note here that the weights from the first layer, W, and the third neuron, $\boldsymbol{w}_3$, can be collapsed into a single vector $\boldsymbol{w}$, effectively reducing all of the neuron operations back into a single neuron representation and thus the fitted model is still linear. In order to fit a non-linear model, a non-linear transformation

function is applied to the output of each layer. This function is called an *activation function*.

Subsequently the neural network equation can be written as

$$y = a_2 \left(\boldsymbol{w}_3^\intercal a_1(W\boldsymbol{x}) \right),$$

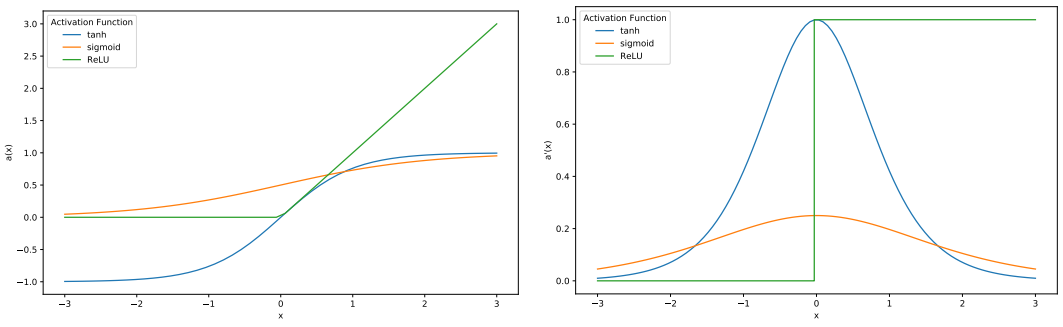
where a_1 denotes the activation function applied after the first (linear) layer, and where a_2 is the the activation function applied after the final layer.

The introduction of non-linear activation functions serves to enlarge the class of functions that can be approximated by the network *i.e.* making it possible for the network to learn complex, non-linear relationships between the inputs and the outputs. Next, we briefly discuss the various activation functions.

2.2.2 Activation Functions

There are plenty of activation functions to choose from, since any simple non-linear and differentiable function can be used. Originally, the *sigmoid* activation function was a common choice (Rumelhart *et al.*, 1988). It can be expressed as $\text{sigmoid}(x) = \frac{1}{1+e^{-x}}$. The shape of the sigmoid activation can be seen in Figure 2.3 (a). It has an S-shape and its values range between 0 and 1. The reason it fell out of favour is because of issues related to the gradient based optimisation procedure of neural networks (which we discuss in more detail in Section 2.3). One of the issues is that the values of sigmoid activations are not centered around zero. This may cause the gradient weight updates to veer too far in different directions.

The hyperbolic tangent or the *tanh* activation function, on the other hand, returns outputs centered around zero. It is expressed as $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and its shape can be seen in Figure 2.3 (a). But the problem with both the sigmoid and tanh activation functions is that they can cause the gradients to saturate during training. By observing the tails of the sigmoid and tanh functions, it is clear that the gradient tends to zero as $|x| \to \infty$. This can cause the weight updates to be very close to zero and thus resulting in the network getting stuck at a certain point in the parameter space. Furthermore, the maximum gradient of the sigmoid activation function is 0.25 (at $x = 0.5$), and because of the nature of the chain rule this causes the lower layers to train much slower than the higher layers. The tanh activation function typically have larger derivatives



(a) (b)

Figure 2.3: Plots of various activation functions (a) and their local derivatives (b).

than the sigmoid and thus it is not as susceptible to this vanishing gradient problem, however, it is still not immune to it. The local derivatives of the activation functions discussed here are plotted in Figure 2.3 (b). This will become more obvious after Section 2.3.

To date, the most popular choice in activation function is the *Rectified Linear Units* (ReLU) non-linearity. It is defined as:

$$\text{relu}(x) = \begin{cases} x & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} .$$

Again, its shape and derivative is plotted in Figure 2.3 (a) and (b), respectively. The ReLU limits the gradient vanishing problem as its derivative is always 1 when x is positive. This results in significantly shorter steps to convergence, as found by the authors in (Krizhevsky *et al.*, 2012). However, ReLUs may suffer from the "dead ReLU" problem, which is, if a ReLU neuron gets clamped to zero, then its weights will get zero gradient and may remain permanently "dead" during training. This sparsity of the activations is what some believe is the reason for the effectivenss of ReLUs (Sun *et al.*, 2014). If dead activations wants to be avoided, alternative activations functions are PReLUs (He *et al.*, 2015*a*) and Leaky ReLUs (Maas *et al.*), but they fall out of the scope of this work.

Typically, choosing the right activation function for a specific task comes down to trial and error, however, in most cases it would be sufficient to use ReLUs after each hidden layer. When doing classification, it is often useful to produce outputs between 0 and 1 for each category as estimates of the

conditional class probabilities. Therefore we may use a sigmoid activation function on the output layer. When doing (single label) multiclass classifcation it is also desirable for these ouputs to sum to 1, similar to prababilities. In that case we may use an activation function called the *softmax*, which is exactly the logit transformation introduced in §1.4: $\text{softmax}(\boldsymbol{x})_k = \frac{e^{x_k}}{\sum_{l=1}^{K} x_l}$. For regression tasks, we mostly omit an activation function on the output layer.

In our experiments we will show how the different activation functions perform on tabular data and compare it to the *Scaled Exponential Linear Units* (SELUs) (Klambauer *et al.*, 2017) activation, which is supposed to allow us to more effectively train deeper neural networks. The neural network depth refers to its number of hidden layers, whereas the width of a layer refers to the number of neurons it consists of. The choice in network depth and layer width is the topic of the next section.

2.2.3 Size of the Network

The network depth and the width of its hidden layers (*i.e.* the size of the network) are hyperparameters of the model. They control the capacity or the flexibility of a neural network; referring to its ability to model complex functions. The bigger the network, the more flexible the model is. Like with most such parameters, increasing the model size is usually benefical up to a certain point, after which its test performance starts to degrade (overfitting). In addition, more layers and more neurons adds to the time taken and hardware required to train the neural network.

Thus the challenge is to find a network size that is large enough to capture all the complexities in the data, but small enough to avoid overfitting. Currently the best way of finding the optimal size of a network for a given problem is by experimentation. Note, that this is true for many of the compoments of neural networks and deep learning. Later in this chapter, §2.3.5, we will see why tunining the network size is not necessarily the best way of controlling overfitting.

Theoretically, according to the universal approximation theorem (Cybenko, 1989), a neural network with a single hidden layer and a finite number of neurons can approximate any continuous function. Which begs the question as to why we need more hidden layers. Even though a neural network can represent any function, it does not mean that the available learning algorithms

can find these optimal weights (Ba and Caurana, 2013). It may also be that the number of neurons needed for a single hidden layer network to represent a specific function is infeasibly large. By choosing deeper networks we are assuming that the function we are trying to learn is composed of several simpler functions. Building in this prior proves to useful empirically (Goodfellow *et al.*, 2016, pp.197-198), especially for tasks of a hierarchical nature like in computer vision.

In our experiments we will see what effect the layer width and network depth have on the generalisation performance on different tabular datasets. The networks used for tabular data learning problems are typically much shallower than those used for say computer vision and NLP. We investigate why this is the case. Later in this chapter we view this problem from a representation learning perspective which will also give us some insight on the matter. But first, in the next section, we discuss the process of training a neural network.

2.3 Training a Neural Network

2.3.1 Optimisation

Statistical learning and optimisation are closely related. Optimisation refers to the task of either minimising or maximising some function $J(x)$ by altering x. The function we want to optimise is called the *objective function*. When we are minimising the objective function, we may also refer to the objective function as the *cost* or *loss function*. These terms will be used interchangeably throughout the thesis.

As mentioned in the previous chapter, parameter estimation (or optimisation) of a linear (or logistic regression) model is usually done using OLS or maximum likelihood estimation (MLE). In this section, however, we discuss an alternative parameter estimation method which is also relevant for the optimisation of neural networks.

Consider the MSE loss function:

$$\begin{aligned} L &= \sum_{i=1}^{N} L_i \\ &= \sum_{i=1}^{N} \sum_{k=1}^{K} (y_{ik} - f_k(\boldsymbol{x}_i))^2 \\ &= \sum_{i=1}^{N} \sum_{k=1}^{K} (y_{ik} - \boldsymbol{w}_k^T \boldsymbol{x}_i)^2, \end{aligned}$$

where $f_k(\cdot)$ in this case is the linear model used to predict the k-th class posterior probability. Although the MSE loss is mostly used in a regression setup and not really well suited for classification, we make use of it here for illustration purposes.

To find the weights, $\boldsymbol{w}$, that minimise L, we can follow a process of iterative refinement. That is, starting with a random initialisation of $\boldsymbol{w}$, one iteratively updates the values such that L decreases. The updating steps are repeated until the loss converges. In order to minimise L with respect to $\boldsymbol{w}$, we calculate the gradient of the loss function at the point $L(\boldsymbol{x}; \boldsymbol{w})$. The gradient (or slope) of the loss function indicates the direction in which the function has the steepest rate of increase. Therefore, once we have determined this direction, we can update the weights by a step in the opposite direction - thereby reaching a smaller value of L.

The gradient of L_i is computed by obtaining the partial derivative of L_i with respect to $\boldsymbol{w}_k$, *i.e.*:

$$\frac{\partial L_i}{\partial \boldsymbol{w_k}} = -2(y_{ik} - \boldsymbol{w}_k^T \boldsymbol{x}_i)\boldsymbol{x}_i.$$

After obtaining the above N partial derivatives, an update at the $(r+1)$-th iteration may be obtained as follows:

$$\boldsymbol{w}_k^{(r+1)} = \boldsymbol{w}_k^{(r)} - \gamma \sum_{i=1}^{n} \frac{\partial L_i}{\partial \boldsymbol{w}_k^{(r)}},$$

where γ is called the *learning rate* and determines the size of the step taken towards the optimal direction. One typically would like to set the learning rate small enough so that one does not overshoot the minimum, but large enough to limit the number of iterations before convergence. The learning rate is a crucial parameter when training neural networks; we will discuss its significance in §2.3.6.

The procedure of repeatedly evaluating the gradient of the objective function and then performing a parameter update, is called *gradient descent* (Cauchy, 1847). Gradient descent forms the basis of the optimisation procedure for neural networks.

Note that a weight update is made by evaluating the gradient over a set of observations, $\{\boldsymbol{x}_i, i = 1, \ldots, n\}$. One of the advantages of gradient descent is that at an iteration, the gradient need not be computed over the complete training dataset, *i.e.* $n \leq N$. When updates are iteratively determined by using subsets of the data, the process is called *mini-batch gradient descent*. This is extremely helpful in large-scale applications, since it obviates computation of the full loss function over the entire dataset. This leads to faster convergence, because of more frequent parameter updates, and allows processing of data sets that are too large to fit into a computer's memory. The choice regarding batch size depends on the available computation power. Typically a batch consists of 64, 128 or 256 data points, since in practice many vectorised operation implementations work faster when their inputs are sized in powers of 2. The gradient obtained using mini-batches is only an approximation of the gradient of the full loss but it seems to be sufficient in practice (Li *et al.*, 2014). Note at this point that the collection of iterations needed to make one sweep through the training data set is called an *epoch*.

The extreme case of mini-batch gradient descent is when the batch size is selected to be 1. This is called *Stochastic Gradient Descent* (SGD). Recently SGD has been used much less, since it is more efficient to calculate the gradient in larger batches compared to only using one example. However, note that it remains common to use the term SGD when actually referring to mini-batch gradient descent. Gradient descent in general has often been regarded as slow or unreliable but it works well for optimising neural networks. SGD will most probably not find even a local minimum of the objective function. It typically however finds a very low value of the cost function quickly enough to be useful.

2.3.2 Optimisation Example

To illustrate the SGD algorithm, consider the linear model in a classification context. Suppose we are given a training dataset with two-dimensional inputs and only two possible classes. Let the data be generated in the same way as described in (Hastie *et al.*, 2009, pp. 16-17).

We want to fit a linear regression model to the data such that we can classify an observation to the class with the highest predicted score. In the binary case it is only necessary to model one class probability and then assign an observation to that class if the score exceeds some threshold (usually 0.5), otherwise it is assigned to the other class. Therefore the decision boundary is given by $\{\boldsymbol{x} : \boldsymbol{x}^T\hat{\boldsymbol{w}} = 0.5\}$.

The example is illustrated in Figure 2.4. The colour shaded regions represent the parts of the input space classified to the respective classes, as determined by the decision boundary based upon OLS parameter estimates. Gradient descent was applied to the determine the optimal weights using a learning rate of 0.001. Since the total number of training observations are small, it is not necessary to use SGD. In Figure 2.4, the dashed lines represent the decision boundary defined by the gradient descent parameter estimates at different iterations. We observe that initially the estimated decision boundary is far from the OLS solution, but as the update iterations proceed, the decision boundary is rotated and translated until finally matching the OLS line. It took 29 iterations for the procedure to reach convergence.

2.3.3 Backpropogation

In Section 2.3.1 we discussed how to fit a linear model using the Stochastic Gradient Descent optimisation procedure. Currenlty, SGD is the most effective way of training deep networks. To recap, SGD optimises the parameters θ of a network to minimise the loss,

$$\theta = \arg\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\boldsymbol{x}_i, \theta).$$

With SGD the training proceeds in steps and at each step we consider a mini-batch of size $n \leq N$ training samples. The mini-batch is used to approximate the gradient of the loss function with respect to the paramaters by computing,

$$\frac{1}{n} \frac{\partial l(\boldsymbol{x}_i, \theta)}{\partial \theta}.$$

Using a mini-batch of samples instead of one at a time produces a better estimate of the gradient over the full training set and it is computationally much more efficient.

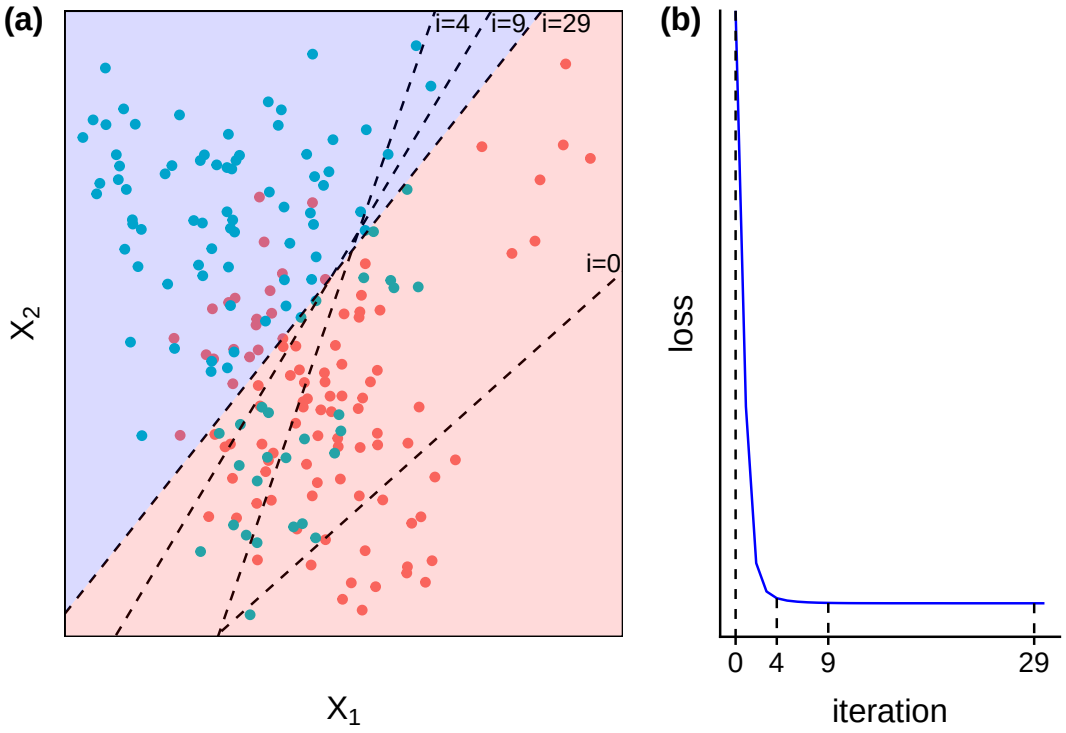


Figure 2.4: Plots of the gradient descent example. (a) The data points in input space. The shades in the background represent the class division in input space, with the decision boundary determined by linear least squares estimation. The dashed lines represent the decision boundaries learned at different iterations. (b) The loss calculated at each iteration.

This section discusses the same procedure, but applied to a simple single hidden layer neural network for multiclass classification, decomposed as:

$$f_k(\boldsymbol{x}) = g_k(\boldsymbol{\beta}_k^\intercal \boldsymbol{z}), \quad k = 1, \ldots, K$$
$$z_m = \sigma(\boldsymbol{\alpha}_m^\intercal \boldsymbol{x}), \quad m = 1, \ldots, M$$

where $\sigma(\cdot)$ is the sigmoid activation and $g(\cdot)$ the softmax activation. The neural network has a set of unknown adjustable weights that defines the input-output function of the network. They are the parameters of the linear function of the inputs, $\boldsymbol{\alpha}_m = (\alpha_{0m}, \alpha_{1m}, \ldots, \alpha_{pm})$, and the paramaters of the linear transformation of the derived features, $\boldsymbol{\beta}_k = (\beta_{0k}, \beta_{1k}, \ldots, \beta_{mk})$. Denote the complete set of parameters by θ. Then the objective function for regression can be chosen as the sum-of-squared-errors:

$$L(\theta) = \sum_{k=1}^{K} \sum_{i=1}^{N} (y_{ik} - f_k(\boldsymbol{x}_i))^2$$

and for classification, the cross-entropy:

$$L(\theta) = -\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik} \log f_k(\boldsymbol{x}_i),$$

with corresponding classifier $G(\boldsymbol{x}) = \arg\max_k f_k(\boldsymbol{x})$. Since the neural network for classification is a linear logistic regression model in the hidden units, the paramaters can be estimated by maximum likelihood. According to Hastie *et al.* (2009, p. 395), the global minimiser of $L(\theta)$ is most likely an overfit solution and we instead require regularisation techniques when minimising $L(\theta)$. Furthermore, as the network becomes larger, MLE becomes intractable.

Therefore, one rather uses gradient descent and the *backpropogation* algortihm (Rumelhart *et al.*, 1988) to minimise $L(\theta)$. This is possible because of the modular nature of a neural network, allowing the gradients to be derived by iterative application of the chain rule for differentiation. This is done by a forward and backward sweep over the network, keeping track only of quantities local to each unit.

In detail, the backpropogation algorithm for the sum-of-squared error objective function,

$$\begin{aligned} L(\theta) &= \sum_{i=1}^{N} L_i \\ &= \sum_{i=1}^{N}\sum_{k=1}^{K} (y_{ik} - f_k(\boldsymbol{x}_i))^2, \end{aligned}$$

is as follows. Following the chain-rul, the relevant derivatives for gradient descent are:

$$\begin{aligned} \frac{\partial L_i}{\partial \beta_{km}} &= -2(y_{ik} - f_k(\boldsymbol{x}_i)) g_k'(\boldsymbol{\beta}_k^T \boldsymbol{z}_i) z_{mi}, \\ \frac{\partial L_i}{\partial \alpha_{ml}} &= -\sum_{k=1}^{K} 2(y_{ik} - f_k(\boldsymbol{x}_i)) g_k'(\boldsymbol{\beta}_k^T \boldsymbol{z}_i) \beta_{km} \sigma'(\boldsymbol{\alpha}_m^T \boldsymbol{x}_i) x_{il}. \end{aligned}$$

Given these derivatives, a gradient descent update at the $(r+1)$-th iteration has the form,

$$\begin{aligned} \beta_{km}^{(r+1)} &= \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial L_i}{\partial \beta_{km}^{(r)}}, \\ \alpha_{ml}^{(r+1)} &= \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial L_i}{\partial \alpha_{ml}^{(r)}}. \end{aligned}$$

Now write the gradients as

$$\frac{\partial L_i}{\partial \beta_{km}} = \delta_{ki} z_{mi},$$
$$\frac{\partial L_i}{\partial \alpha_{ml}} = s_{mi} x_{il}.$$

The quantities, δ_{ki} and s_{mi} are errors from the current model at the output and hidden layer units respectively. From their definitions, they satify the following,

$$s_{mi} = \sigma'(\boldsymbol{\alpha}_m^T \boldsymbol{x}_i) \sum_{k=1}^{K} \beta_{km} \delta_{ki},$$

which is known as the backpropogation equations. Using this, the weight updates can be made with an algortihm consisting of a forward and a backward pass over the network. In the forward pass, the current weights are fixed and the predicted values $\hat{f}_k(\boldsymbol{x}_i)$ are computed. In the backward pass, the errors δ_{ki} are computed, and then backpropogated via the backpropogation equations to obtain s_{mi}. These are then used to update the weights. This approach extends naturally to any size network and differentiable layers (functions).

Backpropogation is simple and its local nature (each hidden unit passes only information to and from its connected units) allows it to be implented efficiently in parallel. The other advantage is that the computation of the gradient can be done on a batch (subset of the training set) of observations. This allows the network to be trained on very large datasets.

In summary, training a neural network consists of these four steps:

1. Initialise the network weights: give random set of numbers to the network parameters.
2. Forward propogation: pass the input through the network layers to produce an output.
3. Calculate the error: compare the predicted output with the true output and measure the difference using an objective function.
4. Backward propogation: calculate the gradients of the objective function with respect to the weights and update the weights accordingly.

These four steps are typically repeated until convergence of the loss function. It can take many training epochs for the objective function to converge.

2.3.4 Weight initialisation

Before one begins training a neural network, one needs to initialise its weights. We expect a well trained neural network to have an equal number of weights smaller than zero and greater than zero. If we initialise all weights to be zero, every neuron will compute the same output and therefore prodcue the same gradient and undergo the same weight update. We still want to initialise the weights as small as possible but each one unique. Sampling from zero mean and unit variance Gaussian distribution is a natural fit, however, the variance of the outputs from a randomly initialised neuron grows with increasing number of inputs. Therefore we may scale the weight vector by the square root of its number of inputs to normalise the variance to 1. This ensures that all neurons in the network initially have approximately the same output distribution and empirically improves the rate of convergence. (He *et al.*, 2015*b*) derived a weight initialisation specifically for ReLU neurons.

2.3.5 Basic Regularisation

From §2.2.3 it seems that smaller neural networks can be preferred if the data is not complex enough to prevent overfitting. However, this is untrue and there are much better ways of regularising neural networks, which we discuss shortly and in the next chapter. Smaller networks are harder to train with local methods such as gradient descent because their loss functions have poor local minima that are easy to converge to. Whereas the local minima of larger networks are much better in terms of their actual loss (Choromanska *et al.*, 2014).

One of the preferred ways of fighting overfitting in neural networks is by using L1 or L2 regularisation, *i.e.* adding a penalty term proportional to the magnitude of the weights to the objective function. This is exactly what is done in Ridge Regression and the Lasso (Hastie *et al.*, 2009, Ch. 4). In L2 regularisation we add the term $\frac{1}{2}\lambda w^2$ to the objective and in L1 regularisation the penalty term $\lambda|w|$. These penalties forces the weights to be small and the λ parameter controls the strength of the regularisation. The "$\frac{1}{2}$" in front of the L2 penalty is added for convenience to make the derivative equal to λw. This makes it then equivalent to decaying each of the weights linearly towards zero: $w' = w - \lambda w$, which is also known as *weight decay*. In practice, L2 regularisation outperforms L1 regularisaion.

Another basic way of preventing the neural network to overfit is to stop the training process "early" and to not train until the training loss converges. A converged training loss is not equivalent to an optimal test loss and therefore the test or validation loss should be observerd during training. One approach is to stop training when the validation loss stops decreasing. As mentioned before, the learning rate also plays a big part in finding the optimal weights. Next we discuss how we can tune the learning rate to train faster and to find better local minima. More advanced regularisation techniques are discussed in Chapter 3.

2.3.6 Adaptive Learning Rates and Annealing

Although the right learning rate can reduce training time and improve performance, there is no silver bullet when it comes to setting the parameter. A small learning rate slows downs the training time, but is safer against overfitting and overshooting the optimal solution. With a large learning rate, convergence may be reached quicker, but the optimal solution may not have been found. One could do a line search of a range of possible values, but this usually takes too long for bigger networks.

However, one does not need to keep the learning rate fixed throughout the training process. A popular approach is to decrease the learning rate by a fraction after a certain number of epochs or as the validation loss starts to converge, as done in (He *et al.*, 2015*a*) for example. The intuition is that larger steps can be taken when we are still far away from an optimal position on the loss surface, and then gradually take smaller steps once we get closer to not overshoot it. Note, that this means that we would also need to tune the rate of decrease and the time steps of each decrease during training. Fortunately, it is believed that the learning algorithms are not that sensitive to this choice.

In addition, there are ways of manipulating the learning rates at a local level, as opposed the aforementioned global methods. Adagrad (Duchi *et al.*, 2011) is an adaptive learning rate method which increases the learning rate at neurons with small gradients and *vice versa*. Adam (Kingma and Ba, 2014) is the most commonly used weight update approach. It also uses the magnitude of the gradient to control each weight update, in addition to the previous iteration's gradients and it combines them in a smooth fashion. This resembles the physical property of momentum (Bengio *et al.*, 2012). For more detail, the

reader can refer to the cited publications as it falls out of the scope of this work.

2.4 Representation Learning

We are now familiar with the mathematical operations of basic layers, how they are connected and how their weights are tweaked to minimise a loss function. In this section we will discuss why this works and what the neural network is actually doing to model the data. The central idea is that of a data *representation* (Bengio *et al.*, 2013) and that at each layer of the network the data is transformed into a higher-level abstraction of itself. Understanding and interpreting neural networks remains a challenge (Frosst and Hinton, 2017), but the notion of learning an optimal data representation allows us to gain a deeper intuition of the inner mechanics of neural networks.

Machine learning models are very sensitive to the form and the properties of the input given to it. Thus a large part of building machine learning models is to find the best way of representing the raw data to make it easier for the models to extract useful information. This is typically a laborious manual task of creating, analyzing, evaluating and selecting appropriate features[2] requires practitioner expertise and domain knowledge. This *feature engineering* process is more trial-and-error than a systematic recipe. Therefore if one can effectively automate this process, it will save a lot of time and raise the performance ceiling of models. Automatically learning representations of the data that make it easier to extract useful information for classifiers or other predictors is called representation learning (Bengio *et al.*, 2013).

A neural network can be viewed from the perspective of representation learning. Consider a classification task. Since the final layer of a neural network is a linear model, in order for the network to produce accuracte predictions, the previous layers should be able to project the data into a space where the classes are linearly separable. Thus the network learns a representation of the data that is optimal for classification.

Each of the simple but non-linear modules of a neural network transforms the representation at one level (starting with the raw input) into a representation at a higher, slightly more abstract level. With the composition of enough such transformations, very complex functions can be learned (Lecun *et al.*, 2015).

[2]http://blog.kaggle.com/2014/08/01/learning-from-the-best/

These transformations can emphasise (and create) features that are important for discrimination and drop those which are redundant.

Let us work through a simple example to illustrate the representations learned by a neural network. Consider a dataset with two classes; the two curves on a plane shown in Figure 2.5. Clearly, the observations from the two classes are not linearly separable in their raw form. Thus if we fit a single layer neural network (*i.e.* only an output layer) to this data, we will get an unsatisfactory decision boundary, since the decision boundary can only be linear, as shown in Figure 2.6. However, if we fit a two-layer neural network, where the hidden layer has two neurons and a sigmoid acitvation to the same dataset, the decision boundary perfectly separates the two classes. This is shown in Figure 2.7.

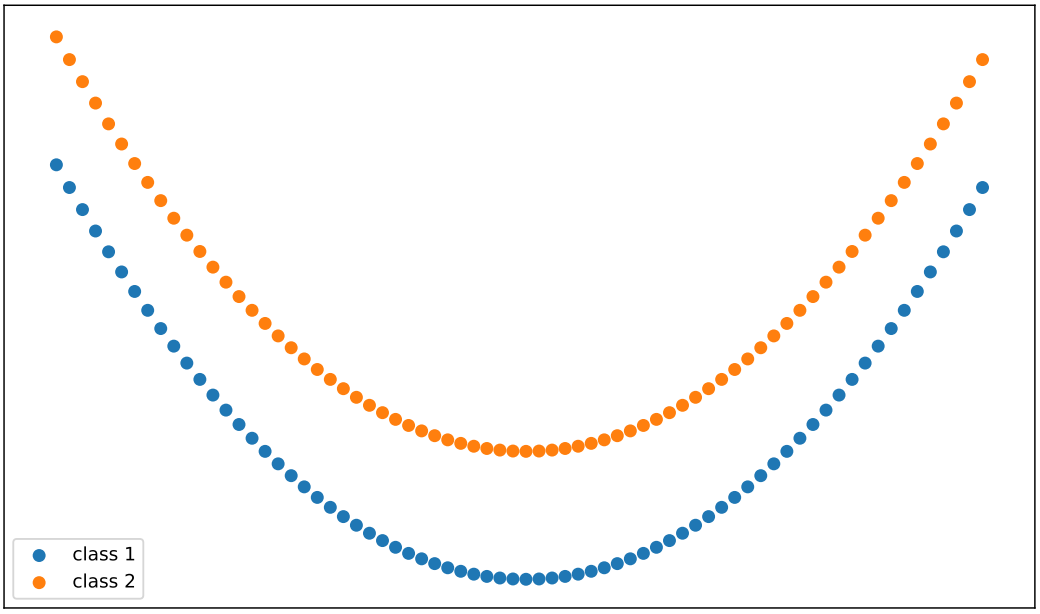


Figure 2.5: Simple dataset with two linearly inseparable classes.

Since the hidden layer consists of only two neurons, we are able to plot the output from the hidden layer after the raw data has passed through it. This is depicted in Figure 2.8. This shows how the hidden layer projected the input data into a space where the observations from the two classes are linearly separable. Which leaves it to the final layer to find the best hyperplane between them.

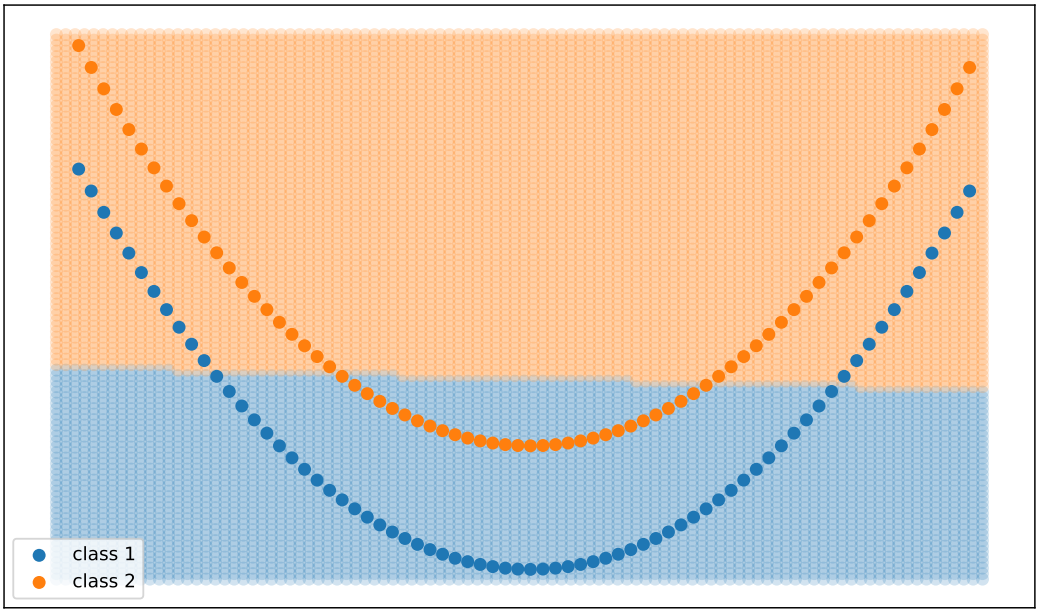


Figure 2.6: Decision boundary of 1-layer neural network.

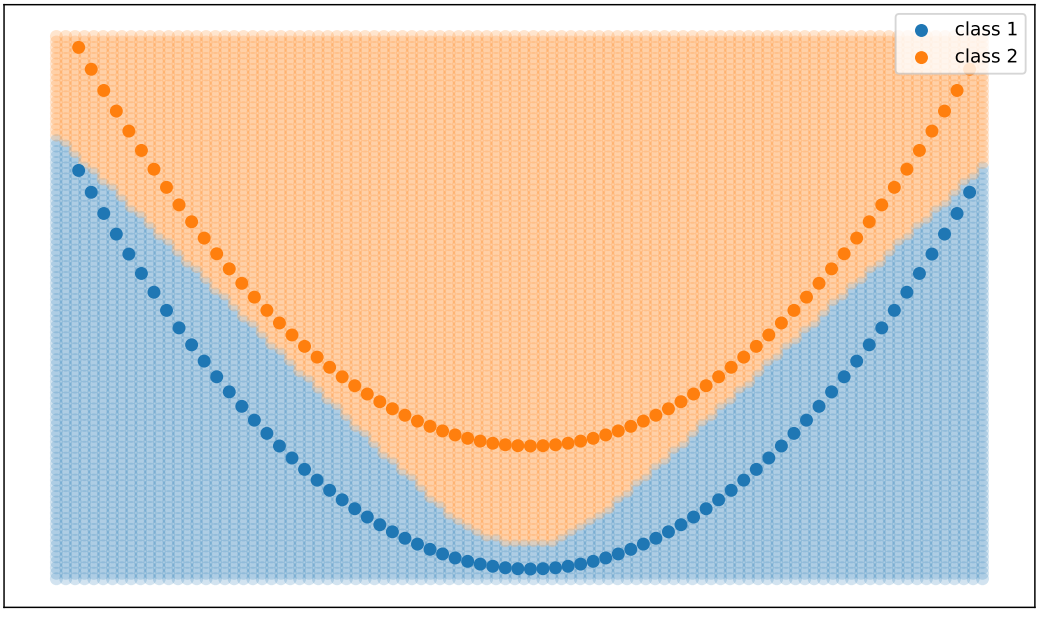


Figure 2.7: Decision boundary of 2-layer neural network.

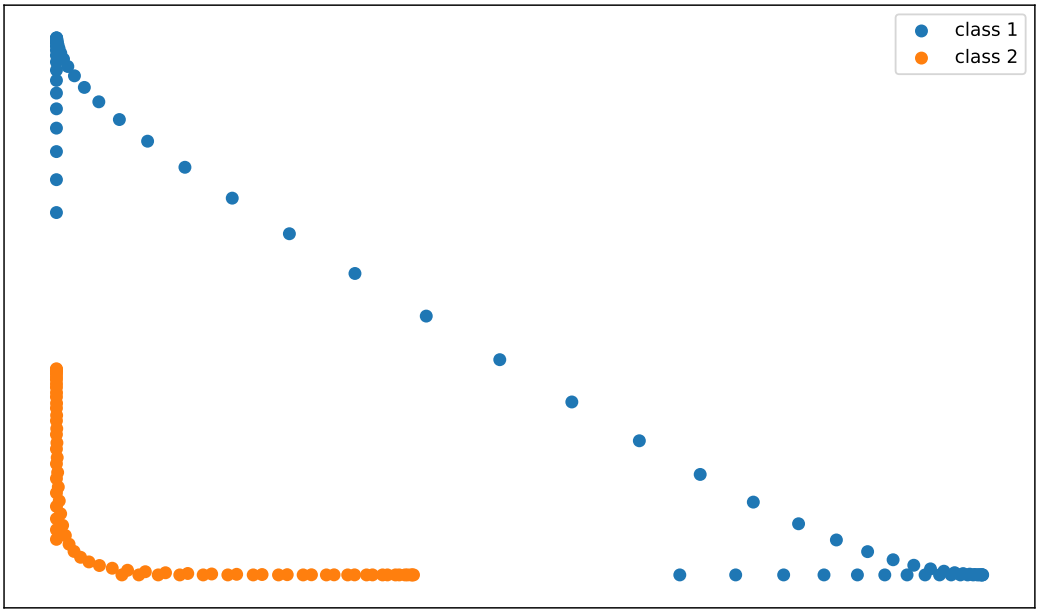


Figure 2.8: Hidden representation of 2-layer neural network.

Of course this is a very simple example, but the same concepts apply to more complicated datasets and models. However, even though it is technically possible to separate any arrangement of points with a sufficiently large network[3], in reality it can become quite challenging to find such representations. This is where the need for more data, regularisation, smarter optimsation procedures and architecture design arises. Without the aforementioned, it is likely that the network will get stuck in a sub-optimal local minima, not being able to find the optimal representation of the data. In the following chapters we explore the approaches available to find optimal represenations of tabular data for classification and regression tasks.

[3]http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

Chapter 3

Deep Learning

3.1 Introduction

Deep learning is a broadly used term. The difference between a classical neural network and a deep neural network, is merely its number of layers. Even a network with two hidden layers is sometimes referred to as deep.

In this work, we use the term deep learning to refer to modern developments in the space of neural networks. In the last decade, tons of contributions have been made to the field: new types of layers, different ways of training and novel approaches to fight overfitting. Reviewing these developments requires much more space than a chapter, therefore, for the purpose of this work, we only highlight the developments we feel are important for our next chapter on deep learning for tabular data.

Practically all deep learning developments are aimed at combatting overfitting, either explicitly or implicitly. Since neural networks can already approximate any function, but our learning algorithms cannot necassrily find these solutions, we need ways of learning more efficiently from the data. This chapter starts by introducing a different class of neural networks called *autoencoders* (§3.2). Autoencoders are mostly used as an unsupervised learning technique to help us learn more robust representations from data without labelled data, which we may then transfer to supervised learning algorithms. This process of transferring knowledge from one network to another is called transfer learning, which we discuss in §3.3.

Thereafter, we look at layers that help with regularisation: *dropout* (§3.4.1) and *batch normalisation* (§3.5.1). Data augmentation is a technique used to

artificially enlarge the training dataset and thus also helps fighting overfitting. We discuss this in §3.4.2. The other types of layers we look at in this chapter are, *skip-connections* (§3.5.2), *attention* modules (§3.5.4) and *embedding* layers (§3.5.3). They are designed to make deeper neural networks more effective, let them focus more on the important features and to process discrete input, respectively.

Then we devote a section to a training policy called the *1cycle* policy (§3.6). This method provides a way of automatically finding a good learning rate and drastically reduces the number of training iterations needed. We conclude this chapter with a discussion on the interpretability of neural networks (§3.7).

3.2 Denoising Autoeoncoders

The basic autoencoder is a neural network that is trained to attempt to reconstruct its inputs. The simplest form of an autoencoder is a neural network with with one hidden layer and an output layer the same size of the input layer (illustrated in Figure 3.1). The linear layer transforming the input to the hidden layer is referred to as the encoder, $\boldsymbol{z} = f(\boldsymbol{x})$, and the layer producing the output from the hidden layer is called the decoder, $\boldsymbol{x}' = g(\boldsymbol{z})$. The autoencoder can be trained in the same way as any other neural network, but by minimising a reconstruction loss. A reconstruction loss measures the distance between the reconstruction of the input and the actual input and thus the MSE loss function is common choice for continuous data.

Autoencoders technically belong to the self- (or semi-) supervised class of methods, although many still think of it as unsupervised. It is unsupervised in the sense that it does not require labelling, but it is stll supervised in the sense that it predicts an ouput.

In this setting, if the number of neurons in the hidden layer is greater than or equal to the number of input features, the autoencoder will be able to perfectly reconstruct $\boldsymbol{x}$ from $\boldsymbol{z}$, *i.e.* $\boldsymbol{x}' = \boldsymbol{x}$. However this is not a very useful model and instead autoencoders are usually built with some type of constraint imposed. A common option is to restrict the number of neurons in the hidden layer to be smaller than the number of input features. This forces the autoencoder to capture only the most useful properties of the data in the hidden representation and can thus effectively be used as a way of dimensionality reduction (Hinton and Salakhutdinov, 2006). When there are no non-linear activation functions

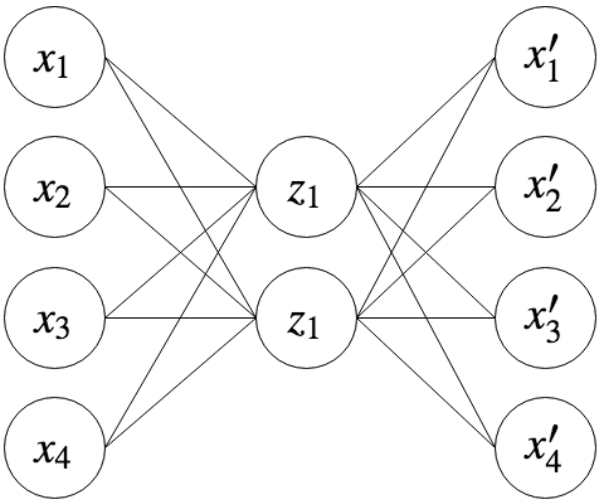


Figure 3.1: A simple single hidden layer autoencoder with 4-dimensional inputs and 2 neurons in the hidden layer.

after the linear layers, one can show that this autoencoder is equivalent to a *Principal Component Analysis* (PCA) of the inputs.

There is no restriction in the number or the size of the layers used for the encoder and decoder, and if activation functions are used, one can potentially learn a more powerful non-linear generalisation of PCA. However, if the encoder and decoder networks are allowed too much capacity, the autoencoder can learn to reconstuct the inputs without learning useful properties of the data. It is hard to tell if an autoencoder has learned a useful latent representation of the data. One way to evaluate it is to use the features extracted by the encoder for a supervised learning task and compare its performance with a model using the raw data as inputs. Autoencoders have also been used to initialise the weights of a supervised learning network, *i.e.* using the learned weight of the autoencoder as the initial weights for the supervised learning network of the same size (Larochelle *et al.*, 2009).

An autoencoder can learn to perfectly copy the input if the encoder and decoder have enough capacity, even though the latent representation is of a smaller diemsion than the inputs, and thus will not learn useful features of the data. Therefore we may want to consider other types of contraints to impose on the autoencoder.

A *denoising autoencoder* (DAE) (Vincent *et al.*, 2008) first adds noise to its inputs before it is passed to the encoder. Thus in order to minimise the reconstruction loss, the DAE should learn how to reconstruct the original input

from a corrupted version of itself. (Alain and Bengio, 2014) shows that DAEs do learn useful structures of the data.

The choice of the type of noise added to the inputs depends on the data types. One can block out inputs with zeros if zeros have no other meaning in the data or one might want to add gaussian noise to continuous outputs as long as it falls within the true range of the features. If there is too much noise in the corruption step, the DAE might not learn anything useful. The type and amount of noise to be use are things that should be experimented with.

Another type of autoencoder is a *Variational Autoencoder* (VAE) (Kingma and Welling, 2013). Instead of encoding the data into a latent vector representation, a VAE encodes the data as a Gaussian distribution. In the decoding step, observations are then sampled from the learned distribution before passing it to the fully connected layers. This is an interesting direction for future research but not in the scope of this work.

3.3 Pretraining and Transfer Learning

Unsupervised learning played a key part in the rise of deep learning (debatedly starting with (Hinton *et al.*, 2006)). It made it easier to train deeper neural networks with a process called *pretraining*. Pretraining is based on the assumption that representations learned from one task can sometimes be useful for accomplishing other tasks in the same input domain. For example, we can use a DAE to learn the structure of the data from unlabelled data and then use what it has learned as features or initialisation for a supervised learning task with the same type of inputs. We can also do supervised pretraining by first training the network to estimate one target variable and then use those weights or features when training to estimate a different target variable, for example.

Unsupervised pretraining for supervised learning is very common in NLP (Devlin *et al.*, 2018, Howard and Ruder (2018)) and supervised pretraining for supserivsed learning is very common in computer vision (Yosinski *et al.*, 2015, He *et al.* (2015*a*)). It is not yet clear theoretically why pretraining works. It may be that using the pretrained weights as initialisation to the supervised model provides a better starting position on the loss surface and thus have regulartory effects (Goodfellow *et al.*, 2016, Ch. 14). Pretraining is most effective when there is little data available for the supervised task but a lot of data available for the pretraining task.

The process of transferring what is learned doing one task (for example in pretraining) to another task (supervised learning for examples) is called *transfer learning*. When done effectively, pretraining and transfer learning can together dramatically reduce the number of training samples and computational power need to train a model.

(Zeiler and Fergus, 2014) provides an insigtful investigation of the what a CNN learns when trained on image data. From observing the types of features extracted for a trained image model (Figure 3.2) it becomes clear why they are also effective on other image datasets. The learned filters seemed to look for generic image features like edges and color gradients which are useful for most computer vision tasks.

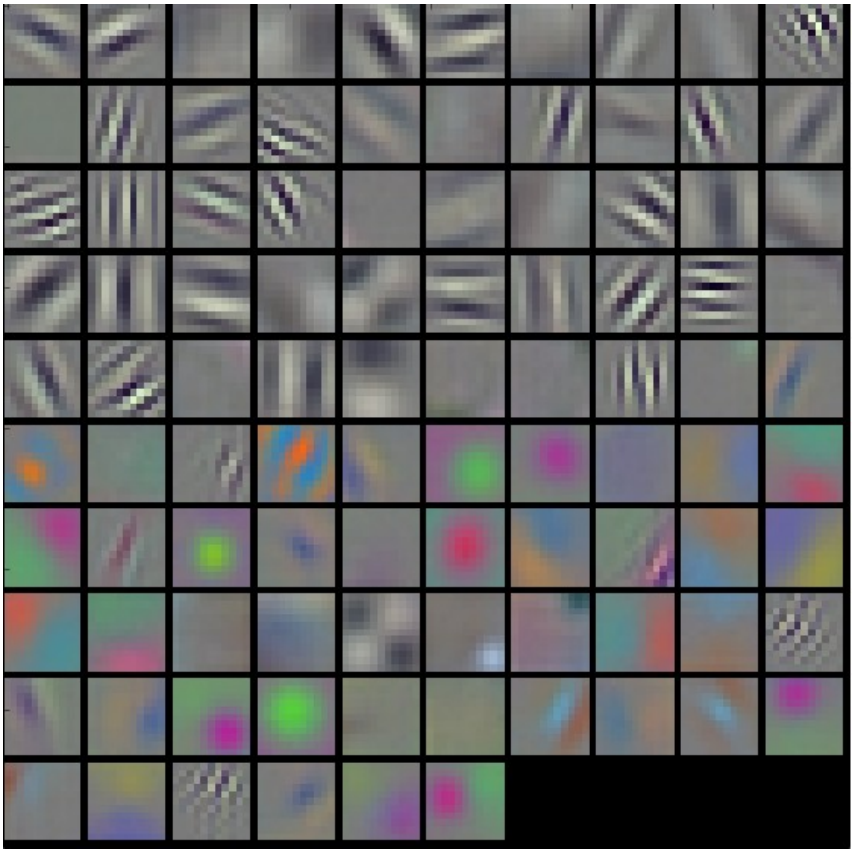


Figure 3.2: Visualising the first layer convolutional filters leared by a neural network in a large image dataset.

3.4 More Regularisation

3.4.1 Dropout

Overfitting can be reduced by using dropout (Hinton *et al.*, 2012) to prevent complex co-adaptions on the training data. Dropout consists of setting the output of a hidden unit to zero with a probability p (in the original paper they used $p = 0.5$). The units which are set to zero do not contribute to the forward pass and do not participate in backpropogation. Every time an input is presented, the neural network samples a different set of units to be dropped out.

This technique ensures that a unit does not rely on the presence of a particular set of other units. It is therefore forced to learn more robust features that are useful in conjunction with many different random subsets of the other units (Krizhevsky *et al.*, 2012).

At test time, no units are dropped out and their output is multiplied by $1-p$ (make sure) to compensate for the fact that all of the units are now active. Dropout does tremendously well to combat overfitting, but it slows down the covergence time of training.

There are also parallels to be drawn between dropout and ensembling approaches (Hinton *et al.*, 2012). Since, at each training iteration a unique set of neurons are active which may then be viewed as a unique model. During training these models are combined - similar to the process of ensembling models.

See Figure 3.3 for an illustration of how dropout effects the connections between neurons.

This shows that dropout does break up co-adaptations, which is probably the main reason why it leads to lower generalization errors.

3.4.2 Data Augmentation

As mentioned before, our aim with predictive models is to generalise well to an unseen test set. In an ideal world we would train a model on all possible variations of the data to capture all interactions and relationships. This is not possible in the real world. Such a dataset is not available and would be infinitely large.

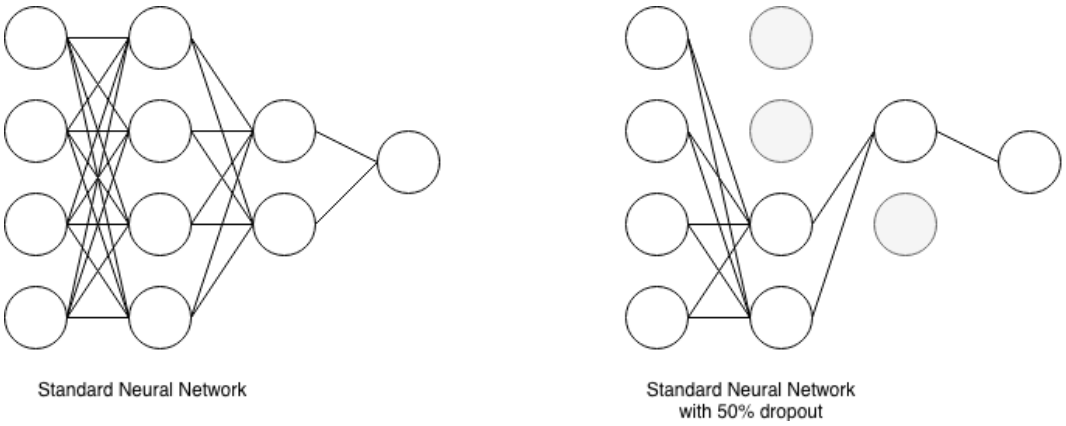


Figure 3.3: The effect dropout has on connections between neurons.

In reality we have a finite subset of the full data distribution to train on. Any new samples with unique feature combinations will likely improve the models generalisablity. If the collection of new samples is not available, we can try to artificially create more.

This is a standard approach especially in computer vision applications. For example, from a single image, we can rotate it, flip it horizontally, shift it any direction, crop it, and many other transformations without destroying the semantic content of the image. But by doing so we are artificially increasing the size of the training set to help with overfitting. Of course this is not as effective as genuine new data samples, but it is a very effective and efficient substitute (Perez and Wang, 2017).

Data augmentation consistently leads to improved generalisation.

Data augmentation can be formalised by the *Vicinal Risk Minimisation* principle (Chapelle *et al.*, 2001) where human knowledge is required to describe a vicinity around each observation in the training data so that artificial examples can be drawn from the vicinity distribution of the training sample to enlarge it. In image classification one can define the vicinity of an image as the set of its horizontal reflections and minor rotations, for example. Note that this approach is dataset dependent.

3.5 Modern Architectures

3.5.1 Normalisation

forcing the activations throughout a network to take on a unit gaussian distribution at the beginning of the training. are significantly more robust to bad initialization.

One of the things that complicate the training of neural networks is the fact that hidden layers have to adapt to the continuously changing distribution of its inputs. The inputs to each layer are affected by the paramaters of all its preceding layers and a small change in a preceding layer can lead to a much bigger difference in output as the network becomes deeper. When the input distribution to a learning system changes, it is said to experience covariate shift (Shimodaira, 2000).

Using ReLUs, carefull weight initialisation and small learning rates can help a network to deal with the internal covariate shift. However, a more effective way would be to ensure that the distribution of non-linearity inputs remains more stable while training the network. (Ioffe and Szegedy, 2015) proposed *batch normalisation* to do just that.

A batch normalisation layer normalises its inputs to a fixed mean and variance (similar to how the inputs of the network is normalised) and therefore it can be applied before any hidden layer in a network to prevent internal covariate shift. The addition of this layer dramatically accelerates the training of DNNs, also because it can be used with higher learning rates. It also helps with regularisation (Ioffe and Szegedy, 2015), therefore in some cases dropout is not necessary.

The batch normalising transform over a batch of univariate inputs, $x_1, \ldots, x_n$ is done by the following steps:

1. Calculate the mini-batch mean, μ, and variance, σ^2:

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$
$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - u)^2$$

2. Normalise the inputs,

$$\hat{x}_i = \frac{x_i - \mu}{\sqrt{\sigma^2 + \epsilon}},$$

where ϵ is a constant to ensure numerical stability.

3. Scale and shift the values,

$$y_i = \gamma \hat{x}_i + \beta,$$

where γ and β are the only two learnable paramaters of a batch normalisation layer.

The reason for the scale and shift step is to allow the layer to represent the identity transform if the normalised inputs are not suitable for the following layer, *i.e.* the scale and shift step will reverse the normalisation step if $\gamma = \sqrt{\sigma^2 + \epsilon}$ and $\beta = \mu$.

The batch normalisation layer attempts to normalise neuron activations to zero mean and unit variance (Ioffe and Szegedy, 2015). It has become the stanard when training deep CNNs. Training with normalisation techniques is perturbed by Stochastic Gradient Descent (SGD), stochastic regularisation (like dropout) and the estimation of the normalisation parameters. Both RNNs and CNNs can stabilise learning via weight sharing, therefore they are less prone to perturbations. Fully-connected NNs do not have this luxury and shows high variance in the training error when trained with normalisation techniques.

In the next chapter we will disscuss the work on Self-Normalising Neural Networks which claims to remove the need for layer normalisation. In practive, batchnorm is still very popular.

3.5.2 Skip-connections

Residual Networks became very popular after it was used to win one of the ImageNet competiions (He *et al.*, 2015*a*). The residual connection layer can simply be formalised as

$$y = F(x) + x,$$

i.e. combining the input to the layer(s) with the output of the layer(s). Here, the combination is by addition, but other ways can also be used, like multiplication or concatenation. These layers are very useful when training deeper neural networks since they encourage gradient flow through interval layers.

DenseNet is another well-known network making use of skip connections. There was also a parallel drawn between ResNet and boosting methods since both are approaches to fitting a model to the residual.

3.5.3 Embeddings

An embedding is a layer that maps a discrete input to a numeric vector representation. It was first used in NLP in order to represent words as numbers so that it can be processed by a numeric model. The goal is to map discrete inputs to a meaningful vector space where, for example, items with similar meaning exist close to eachother.

Initially the mappings were configured independenty of the neural network with approaches using co-occurence measures. The real breakthrough came when the mappings were defined as learnable layers in the network. Thus they can be tuned just like any other parameter in the network. The parameters of the embedding function (or layer) are first randomly initialised and then gets tuned along with the rest of the NN during training.

An embedding operation can either be viewed as a table lookup or a matrix multiplication of the discrete input in a one-hot encoded form.

3.5.4 Attention

Attention is one of the standout breakthroughs made in deep learning in recent times. It was first (?) proposed in neural machine translation (Bahdanau *et al.*, 2014) and now almost used ubiquitously in natural language processing applications. It was also found useful in computer vision applications, like image captioning, and also in audio processing.

The main idea of an attention module is to force a layer to only focus on a certain subset of its inputs at different stages of computation. For example, in image captioning, one may use a RNN to sequentially output words describing the image. With the use of an attention model, the network is restricted to only look at certain parts of an image at every step, avoiding having to look at the full image everytime. In an ideal world, an attention module should not be necessary and we would want the network to learn if certain parts of images are not required to look at. However, currently this built-in prior proves to be extremely helpful with current learning algorithms.

3.6 One-cycle Policy

The 1Cycle policy (Smith, 2018) reduces training time and increases performance.

Currently the process of setting the hyper-parameters, including designing the network architecture, requires expertise and extensive trial and error and is based more on serendipity than science.

Currently there are no simple and easy ways to set hyper-parameters – specifically, learning rate, batch size, momentum, and weight decay. Grid search or random search is expensive. Optimal parameters make a huge difference in training time and performance.

Look for clues of overfitting and underfitting to determine best parameters.

The experiments discussed herein indicate that the learning rate, momentum, and regularization are tightly coupled and optimal values must be determined together.

by monitoring validation/test loss early in the training, enough information is available to tune the architecture and hyper-parameters and this eliminates the necessity of running complete grid or random searches.

Underfitting is when the machine learning model is unable to reduce the error for either the test or training set. The cause of underfitting is an under capacity of the machine learning model; that is, it is not powerful enough to fit the underlying complexities of the data distributions. Overfitting happens when the machine learning model is so powerful as to fit the training set too well and the generalization error increases.

The takeaway is that achieving the horizontal part of the test loss is the goal of hyper- parameter tuning

The art of setting the network's hyper-parameters amounts to ending up at the balance point between underfitting and overfitting

If the learning rate (LR) is too small, overfitting can occur. Large learning rates help to regularize the training but if the learning rate is too large, the training will diverge.

To use CLR, one specifies minimum and maximum learning rate boundaries and a stepsize. The stepsize is the number of iterations (or epochs) used for each step and a cycle consists of two such steps – one in which the learning rate linearly increases from the minimum to the maximum and the other in which it linearly decreases.

n the LR range test, training starts with a small learning rate which is slowly increased linearly throughout a pre-training run. This single run provides valuable information on how well the net- work can be trained over a range of learning rates and what is the maximum learning rate. When starting with a small learning rate, the network begins to converge and, as the learning rate increases, it eventually becomes too large and causes the test/validation loss to increase and the accuracy to decrease. The learning rate at this extrema is the largest value that can be used as the learning rate for the maximum bound with cyclical learning rates but a smaller value will be necessary when choosing a constant learning rate or the network will not begin to converge.

the amount of regularization must be balanced for each dataset and architecture

Contrary to this early work, this Section recommends using a larger batch size when using the 1cycle learning rate schedule, which is described in the above

Weight decay is one form of regularization and it plays an important role in training so its value needs to be set properly. The important point made above applies; that is, practitioners must balance the various forms of regularization to obtain good performance. the interested reader can see kuka et al. (2017) for a review of regularization methods.

1. Learning rate (LR): Perform a learning rate range test to a "large" learning rate. The max LR depends on the architecture (for the shallow 3-layer architecture, large is 0.01 while for resnet, large is 3.0), you might try more than one maximum. Using the 1cycle LR policy with a maximum learning rate determined from an LR range test, a minimum learning rate as a tenth of the maximum appears to work well but other factors are relevant, such as the rate of learning rate increase (too fast and increase will cause instabilities).

2. Total batch size (TBS): A large batch size works well but the magnitude is typically con- strained by the GPU memory. If your server has multiple GPUs, the total batch size is the batch size on a GPU multiplied by the number of GPUs. If the architecture is small or your hardware permits very large batch sizes, then you might compare performance of different batch sizes. In addition, recall that small batch sizes add regularization while large batch sizes add less, so utilize this while balancing the proper

amount of regularization. It is often better to use a larger batch size so a larger learning rate can be used.

3. Momentum: Short runs with momentum values of 0.99, 0.97, 0.95, and 0.9 will quickly show the best value for momentum. If using the 1cycle learning rate schedule, it is better to use a cyclical momentum (CM) that starts at this maximum momentum value and decreases with increasing learning rate to a value of 0.8 or 0.85 (performance is almost independent of the minimum momentum value). Using cyclical momentum along with the LR range test stabilizes the convergence when using large learning rate values more than a constant momentum does.

4. Weight decay (WD): This requires a grid search to determine the proper magnitude but usually does not require more than one significant figure accuracy. Use your knowl- edge of the dataset and architecture to decide which values to test. For example, a more complex dataset requires less regularization so test smaller weight decay values. A shallow architecture requires more regularization so test largerweight decay values.

3.7 Model Interpretation

Although Deep Learning is now the state-of-the-art for many machine learning tasks, it is still trailing behind other algorithms in terms of model interpretability. But keep in mind this is not an unusual trade-off; between prediction performance and model interpretability. DNNs are occasionally referred to as "black boxes" since it is very difficult to interpret what is going on inside the stacks of linear and non-linear layers. This is one of deep learning's greatest criticisms and is a large reason why it cannot be used in some production environments. For example, in the clinical domain, model transparency is of utmost importance, given that predictions might be used to affect real-world medical decision-making and patient treatments (Shickel *et al.*, 2017).

Fortunately, some work has been done to gain insights from NNs.

3.7.1 Neural Network Specific

We have showed previously that it is possible to inspect activations and weights of layers at different levels of the network. If the network is small, one might

gain insight to what the network has learned or why it is making certain decisions. However, most useful neural networks are at least three layers deep, making its activations and weights more complex to interpret.

When fully convolutional networks are used, there are ways to visualise which parts of the inputs were important in making a certain decision. These visualisations are called class activation maps. But they cannot be used with fully connected layers.

Another common interpretation tool, in order to gain insight into what specific neurons are looking for, is to rank the inputs by the magnitude of their activation at that neuron. Then, if one would be able to manually spot similarities between the highest ranked inputs, one would have a potential description of the pattern that triggers that neuron. This process is manual and not guarranteed to produce useful insights, especially when there are many neurons to investigate.

- Distilling Neural Networks, i.e. training a decision tree on train neural network generated data. https://arxiv.org/pdf/1711.09784.pdf
- Mimic leanring (Che *et al.*, 2016)
- Plotting embeddings in lower dimensional space with PCA or t-sne
- evaluate which inputs get activated by a certain unit.
-

3.7.2 Model Agnostic

3.7.2.1 Permutation Importance

(Haldar *et al.*, 2018) notes that the permutation test only produces sensical results on the assumption that the features are independent. Permuting the feature independently created examples that never occurred in real life, and the importance of features in that invalid space sent us in the wrong direction. The test however is somewhat useful in determining features that were not pulling their weight. If randomly permuting a feature did not affect the model performance at all, it was a good indication that the model is probably not dependent on it.

- Partial Dependece

- SHAP

Chapter 4

Deep Learning for Tabular Data

4.1 Introduction

- core work
- combination of other work with tabular data and other domains
- not received much attention
- automate feature engineering

It is not exactly clear why DNNs are still in many cases inferior to gradient boosted trees when applied to tabular data, eventhough it outperforms all other algorithms in other application domains like text and speech. We can look for differences between tabular data and unstructured data in their properties to try and understand why this is the case. A difference between the two data types that stand out is the relative importance of each of the important features with respect to the target. In computer vision a large amount of pixels should change before an image is of something else. Whereas in tabular data a very small change in a single feature may have totally different behaviour with respect to the target (Shavitt and Segal, 2018). The same authors mention that this can be addressed by including a separate requlatisation term for each of the weights in the network. These regularisation terms are seen as additional model hyperparameters. It is easy to see that this approach is totally intractable since the only way to train these hyperpararmeters are brute force and repetitive tweaking and validatig (derivative free methods). A workaround is to make these regularisation parameters trainable like all of the other points

in the network. This is achieved by minimising the counterfactual loss, a novel loss function proposed by (Shavitt and Segal, 2018). They found that training NNs by optimising the counterfactual loss, outperform other regularisation approaches for NNs and results in NNs that are comparable to gradient boosted trees. The learned regularisation parameters can even help with interpretting feature importance.

- NNs proved to be useful for tabular data at AirBnB (**?**).

Deep Learning has set new records on various benchmarks and led to various commercial applications. Recurrent Neural Networks achieved new levels in speech and natural language processing and are already deployed on mobile devices. Their counterparts, Convolutional Neural Networks (CNNs), excel in vision tasks. CNNs are on par with human experts on detecting skin cancer. The latest self-driving cars rely on CNNs to understand video imagery. CNNs were also used in AlphaGo to evaluate board positions. (Klambauer *et al.*, 2017)

But on structured data, Deep Neural Networks have still a long way to go. Random Forests, Gradient Boosted Trees and Support Vector Machines often outperforms DNNs on structured data, both in terms of accuracy and efficiency.

DNNs on tabular data also struggle to go deeper than 3 or 4 layers.

Adopting NNs for tabular data receives far less attention and remains challenging. Fully connected model structure leads to very complex optimization hyper-planes with a high risk of falling into local optimums.

Explanation can start with the most naive DNN and then systematically add components to improve it, from architectural changes to learning changes.

4.2 Related Work

- Recommender Systems: AirBnB (Haldar *et al.*, 2018)
- Healthcare/EHR: (Rajkomar *et al.*, 2018) showed how effective NNs are for EHR data. State of the art on various predictive tasks.
- Taxi Trajectory: One of the first sucessful implementations of modern NNs for tabular data was in predicting the destination of a taxi ride based on its initial trajectory (de Brébisson *et al.*, 2015). It was hosted as a Kaggle competition and this solution outperformed all other entries by

a significant margin. **Click-through rate prediction (CTR)** (Song *et al.*, 2018). To predict the probability of a user clicking an item, critical to online applications and recommender systems.

4.3 Input Representation

It is widely held that 80% of the effort in an analytic model is preprocessing, merging, customizing, and cleaning datasets, not analysing them for insights (Rajkomar *et al.*, 2018).

The success of predictive algorithms largely depends on feature selection and data representation. The feature selection process and finding the best data representation is largely a manual and painful process.

In most machine learning tasks the greatest performance gains can be achieved by feature engineering wheras better algorithms only result inincremental boosts. In feature egineering one strives to create new features from the original features based on some domain knowledge of the data or otherwise, that makes it easier for the model to estimate the target. Although a crucial step to make the most out of the data, this can be a very laborious process. There is not formal path to follow in this stage and thus usually consists of many a trial and error, benefitted by domain knowledge of the data, only accessible in some cases. A huge advantage of using NNs on tabular data (and other data structures) is that the feature engineering process gets automated to some extent. A NN learns these optimal feature transformations implicitly during the training process. The hidden layers of a NN can be viewed as a feautre extractor that was optimised to map the inputs into the best possible features space for a model (the final layer of the network) to operate in.

4.3.1 Numerical Features

One of the things that make tree-based methods so attractive is that the numeric values of the features hardly matter, as long as their relative ordering is meaningful. On the other hand, NNs are very sensitive to the numeric value of the input. This is related to the optimisation procedure. If an abnormal feature value is fed to the network during training, large gradients can backpropogate throught the network and/or result in vanishing gradients (Clevert *et al.*, 2015).

(Haldar *et al.*, 2018) suggest to restrict the values in the range of {-1,1} and so that the median is mapped to zero. They achieved this by inspecting each of the features and if a feature looks gaussian, do the normalisation $(x - \mu)/\sigma$ and if the feature looks more like a power law distribution, transform is by $\log((1 + x)/(1 + \text{median}))$.

Another step the same authors suggest is to ensure the continuous variables follow a smooth distribution. This helps for generalisation, checking for bugs and general training efficiency. It also helps the analyst to determine whether a feature is generated by some other underlying process.

- how to normalize continuous variables
- mean subtract and error divide
- rankGauss
- scale to 0-1

http://cs231n.github.io/neural-networks-2/

It is common to standardise all inputs to have mean zero and standard deviation of one. This ensures that all input features are treated equally.

4.3.2 Categorical Features

Entity embedding not only reduces memory usage and speeds up neural networks compared with one-hot encoding, but more importantly by mapping similar values close to each other in the embedding space it reveals the intrinsic properties of the categorical variables, which you cannot obtain with one-hot encoding.

Companies like Instacart and Pinterest have reported the effective use of entity embeddings on their internal datasets. These embeddings can be reused on different machine learning tasks and do have to be relearned for each dataset.

First published work in modern times on entity embeddings was in the taxi destination prediction challenge (de Brébisson *et al.*, 2015). Another Kaggle sucess story is for predicting the total sales of a store (Guo and Berkhahn, 2016).

The embedding for discrete variables act in the exact same way. The embdding for each categorical variable gets concatenated to the continuous variables and then gets passed to the rest of the layers in the network.

In (de Brébisson *et al.*, 2015) they found that embeddings helped a lot. The embeddings can also be visualised to investigate whether make sense or to gain further insight into the data and model decision making. The weights associated with each categories projection onto the embedding space can be plotted with any dimension reduction technique like t-sne or PCA. Then we can compare the categoires based on their relative distances and positions in this reduced space.

Entity embeddings are not too different to one-hot encoding a categorical input and sending it through a standard fully connected layer. An embedding is essentailly the same operation but a separate one for each of the categorical features. Doing it this way reduces memory usage and speeds up training of a NN. This makes is incredibly useful for datasets with high cardinality features and many of them. It will also not be possible to interpret categories based on its embedding of the one-hot encoded path is followed.

We further demonstrate in this paper that entity embedding helps the neural network to generalize better when the data is sparse and statistics is unknown (Guo and Berkhahn, 2016).

As proof that these entity embeddings actually learns something useful, besides plotting the embedding matrix, one can also feed them along with the continuous features to other learning algorithms and see how it affects performance. (Guo and Berkhahn, 2016) found that the embeddings obtained from the trained neural network boosted the performance of all tested machine learning methods considerably when used as the input features.

4.3.3 Combining Features

4.3.4 Dropout

Interesetingly, (Haldar *et al.*, 2018) found that dropout was not effective in their application. They pinned it down to dropout producing invalid input scenarious that distracted the model. Therefore they opted for hand crafted noise shapes taking into account the distribution of the relevant feature.

4.4 Still to categorise

Feature engineering in general is hard and time consuming with no clear recipe to follow. But it is also very crucial to an effective learning system. The main

aim is to find a low-dimensional representation of sparse and high-dimensional raw features and their meaningful combinations. Some of the challenges of feature engineering is listed below.

Can used the Criteo[1] dataset as an example of these challenging datasets.

(Zhou *et al.*, 2017) is very similar to the rest of these citations. (Covington *et al.*, 2016) also embdding + MLP

Sparse and high-dimensional inputs. (Song *et al.*, 2018), (Wang *et al.*, 2017), (Qu *et al.*, 2016), (Cheng *et al.*, 2016), (**?**), (Covington *et al.*, 2016) Not always the case, but common. High cardinality categorical features are sparse when one-hot encoded. DNNs can easily overfit these sparse and high-dimensional datasets. One-hot encoding + fully connected layer deals with the sparse inputs and the weight matrix is bigger. Separate embeddings are also easier to interpret. Each feature is fed separately into the network so that the layers above can learn specialised representations per feature. This improves generalisation (less parameters) speeds up training and reduces memory footprint (Covington *et al.*, 2016).

Extracting high-order combinations of features. (Song *et al.*, 2018), (Wang *et al.*, 2017), (Qu *et al.*, 2016), (Guo *et al.*, 2017) They key question here is to determine which feautres to combine and how to form meaningful high-order features. Effective prediction usually relies on modelling high-order interactions between features. Majority of the time needs domain experts to help massage the data. Can follow a brute force approach but enumerating all the possible high-order features will exponentially increase the model search space which will just further increase the risk of overfitting. Can use multiple fully connected layers with non-linear activations of a NN. Fully-connected layers model all feature interactions impplicitly, but is not good enough to learn all types of interactions. These layers are inefficient in learning multiplicative feature interactions. Hard to explain which features and combinations were important. (Song *et al.*, 2018) uses a multi-head self-attention mechanism which they call the interacting layer. (Zhou *et al.*, 2017) also uses some form of attention but without the softmax layer to reserve intensity of activations. The idea comes from (Vaswani *et al.*, 2017) which itself stems from work done in (Bahdanau *et al.*, 2014). Within in the interacting layer each feature is allowed to interact with every other feature and automatically determine which of those interactions are relevant to the output. They also combine a residual

[1]http://labs.criteo.com/2014/09/kaggle-contest-dataset-now-available-academic-use/

connection between layers so that different orders of feature interactions can be combined. To explain the attention mechanism, consider feature j and the step to determine which high-order features involving feature j are meaningful. We first define the correlation between features j and k under attenion head h as:

$$\alpha_{j,k}^{(h)} = \frac{\exp\left(\phi^{(h)}(\boldsymbol{e}_j, \boldsymbol{e}_k)\right)}{\sum_{l=1}^{L} \exp\left(\phi^{(h)}(\boldsymbol{e}_j, \boldsymbol{e}_l)\right)}$$

where $\phi^{(h)}(.,.)$ is an attention function which defines the similarity between two features. It can be defined by a neural network or a simple inner product like in (Song *et al.*, 2018):

$$\phi^{(h)}(\boldsymbol{e}_j, \boldsymbol{e}_k) = \left\langle W_{\text{query}}^{(h)} \boldsymbol{e}_j, W_{\text{key}}^{(h)} \boldsymbol{e}_k \right\rangle$$

where $W_{\text{query}}^{(h)}$ and $W_{\text{key}}^{(h)}$ are transformation matrices which map the original embedding space into a new space. The representation of feature j in subspace h is then updated by combining all relevant features guided by coefficients $\alpha_{j,k}^{(h)}$:

$$\tilde{\boldsymbol{e}}_j^{(h)} = \sum_{k=1}^{K} \alpha_{j,k}^{(h)} W_{\text{value}}^{(h)} \boldsymbol{e}_k$$

$\tilde{\boldsymbol{e}}_j^{(h)}$ is a combination of feature j and its relevant features under attention head h. Therefore it is a learned combinatorial feature. Since a feature can be involved in various different combinations, we use multiple heads to extract combinations, *i.e.* $\{\tilde{\boldsymbol{e}}_j^{(h)}\}_{h=1}^{H}$. (Song *et al.*, 2018) used H=2. All of these combinatorial features are concatenated into a single vector, $\tilde{\boldsymbol{e}}_j$. Then finally the output is combined with its raw input (residual connection) and sent through a ReLU:

$$\boldsymbol{e}_j^{\text{res}} = \text{ReLU}\left(\tilde{\boldsymbol{e}}_j + W_{\text{res}} \boldsymbol{e}_j\right)$$

This mapping from $\boldsymbol{e}_j$ to $\boldsymbol{e}_j^{\text{res}}$ is done for each features to form the interacting layer. The interacting layer is thus a representation of high-order features. These interacting layers can be stacked on-top of each other to form arbitrary order combinatorial features. (Song *et al.*, 2018) shows that residual connection gives better results. (Wang *et al.*, 2017) uses the cross-network which is an automated way of building cross-features. Each layer produces higher-order interactions based on existing ones, and keeps the interactions from previous layers. The cross-network is trained jointly with a DNN. (Wang *et al.*, 2017) also used a residual connection. (Wang *et al.*, 2017) makes a case for finding a

bounded-degree feature interactions, saying that all the Kaggle competions are won with feature engineering of low-degree interactions, whereas DNNs learn highly non-linear interactions implicitly. (Wang *et al.*, 2017) cross-network consists of cross-layers that can be formalised as:

$$\boldsymbol{x}_{l+1} = \boldsymbol{x}_0 \boldsymbol{x}_l^\intercal \boldsymbol{w}_l + \boldsymbol{b}_l + \boldsymbol{x}_l$$

where $\boldsymbol{x}_l$ is the output of the l-th cross layer; $\boldsymbol{x}_0$ is the input vector; $\boldsymbol{w}_l$ and $\boldsymbol{b}_l$ are its associate weight and bias paramters respectively. Each cross layer adds back its input after feature crossing in a residual connection fashion. (Wang *et al.*, 2017) experimented with 1-6 cross layers. The degree of cross features grows with cross-network depth. The DNN trained in parallel is just a simple network with fully-connected layers and ReLUs. The output of the two streams are concatenated, send through a fully connected layer and a sigmoid layer. (Qu *et al.*, 2016) used something called a product layer, which takes pairwise inner or outer products of all feature combinations and concatenates it to all linear combinations. The output is then fed to 2 fully-connected layers. According to (Guo *et al.*, 2017) it is necessary to capture both low and high-order interactions (and wide&deep paper). They also have to parallel streams of networks, one the FM capturing the low order interactions and one the DNN captuting the high-order interactions. (Cheng *et al.*, 2016) believes it is both important to learn to memorise and generalise. Where memorise refers to recalling from known observations and generalise to predict accurately on unseen samples. They attempt to achieve this again with two streams, one linear layer (wide) and one deep network (deep). The wide stream learns to memorise and the deep network learns to generalise. Combined by a weighted sum. (**?**) Fully connected model structure leads to very complex optimization hyper-planes with a high risk of falling into local optimums. Therefore it is necessary to explicitly leverage expressive feature combinations. Furthermore it help to limit the model size to make learning more efficient. To achieve this they use automatic feature grouping, feature group reduction and recursive endocder with share embeddings. These ideas seems a little ad-hoc and not end-to-end.

Dealing with mixed input types. (Song *et al.*, 2018), (Wang *et al.*, 2017), (Qu *et al.*, 2016), (Cheng *et al.*, 2016) Processing numerical and categorical features and their combinations. (Song *et al.*, 2018) embeds both the numerical and categorical features separately into a lower-dimensional representation. By mapping both types in the same feature space faciliates more

effective learning of interactions between the mixed features. The embedding for the j-th categorical feature is obtained by (Song *et al.*, 2018), (Wang *et al.*, 2017):

$$\boldsymbol{e}_j = V_j \boldsymbol{x}_j$$

where $\boldsymbol{x}_i$ is the one-hot encoded vector representation of the j-th categorical variable and V_j is the associated embedding/weight matrix. The weights in V_j are learned along with all of the other parameters in the network. The embedding for the j-th numerical features is obtained by:

$$\boldsymbol{e}_j = \boldsymbol{v}_j x_j$$

where x_j is a scalar and $\boldsymbol{v}_j$ is the associated weight vector. Why does it help to increase the dimension of the numerical features? Is it only for balanced representation when combined with categorical features? The numerical and categorical embeddings are concatenated to form a single vector representation (Song *et al.*, 2018). (Wang *et al.*, 2017) does not embed numerical but just stack the normalised numerical features along with the categorical embeddings. (Song *et al.*, 2018) used $\log^2(z)$ if $Z > 2$ to transform numeric features to minimise its variance. But how does that work for negative values? (Wang *et al.*, 2017) used normal log transform. (Wang *et al.*, 2017) uses normalisation but dont know what yet. (Song *et al.*, 2018) experimented to find the optimal embedding size [8,16,24,32], found it depended on the dataset. (Wang *et al.*, 2017) used embedding sizes of $6 \times (\text{cardinality})^{\frac{1}{4}}$. Not a lot of work on numerical features (**?**). (Zhou *et al.*, 2017) has an intersting take on multi-hot categorical features; where a feature can have more than category associated with it. The embedding layer for that instance then outputs a list of embeddings with lenght the same as the number of categories associated with that instance and feature. The list of embeddings then gets projected back into a fixed-length representation by doing a pooling operation. (Covington *et al.*, 2016) adresses numeric feature normalisation. (Ioffe and Szegedy, 2015) shows how sensitive DNNs are to scaling and distribution. Proper normalisation of numeric features was critical for convergence (Covington *et al.*, 2016). (Covington *et al.*, 2016) does a transformation to equally distribute a numeric feature in [0,1) using the cumalitive distribution. The integral is approximated with linear interpolation on the quantiles of the feature values computed in a single pass over the data before training begins. In addition they add $\tilde{x}^2$ and $\sqrt{\tilde{x}}$ to give the network more expressive power.

Interpreting DNNs. (Song *et al.*, 2018) Model explainability is important for various reasons. Helps to know how to improve your model or where it goes wrong. Like a sanity check. If you cannot explain how a prediction is made, you cannot know how good it is. (Song *et al.*, 2018) uses the multi-head self-attention mechanism to evaluate correlations between features - globally and locally . (Zhou *et al.*, 2017) plots attention and categorical embeddings.

Small Datasets. It is well know that DNNs require a large amout of data to generalise well. Typically, tabular datasets are not as large as unstructured datasets like images and texts. There is also no large tabular dataset from which knowledge can be transferred from like ImageNet for computer vision and wikipedia for NLP. We suggest two techniques for overcoming this problem: data augmentaion and unsupervised pre-training. (Zhang *et al.*, 2016) also did pretraining with DAEs. DAEs enforce robustness to partially destroyed inputs. Can also be view from a manifold learning perspective (Vincent *et al.*, 2008). Should also consider VAE and GANS (**?**) uses output from GBDT to train an initial model and then to use it a initialisation of the actual model. They call it the transfer of structured knowledge. Data augmentation for tabular datasets is rarely studied. Can use corruption like DAEs or swap noise but then creates inputs that does not exist in the real data distribution.

Choosing DNN structural hyperparameters. Since there are no shared patterns among the diverse tabular datasets, it is hard to design a universal architecture that will fit all. Most of these parameters are very dependent on the dataset and other modeling choices and therefore the need to tune them. Structural hyperparameters are usually found using some brute search. (Song *et al.*, 2018) used a sigmoid layer for binary classification. Embedding dimension: 16 (Song *et al.*, 2018), 32 (Cheng *et al.*, 2016) Hidden layer size: 32 (Song *et al.*, 2018) Number of hidden layers: 32 Dropout: 0.5 (Song *et al.*, 2018), tuned (Zhang *et al.*, 2016) (Qu *et al.*, 2016) (Guo *et al.*, 2017) found dependent on dataset and model. Residual connections: (Song *et al.*, 2018), (Wang *et al.*, 2017) (Song *et al.*, 2018) experimented to see how many layers they should choose [1,2,3,4]. (Song *et al.*, 2018) experimented to find the optimal embedding size [8,16,24,32] (Wang *et al.*, 2017) tested number of layers [2-5] (Wang *et al.*, 2017) tested hidden layer sizes at [32-1024] (Zhang *et al.*, 2016), (Qu *et al.*, 2016), (Guo *et al.*, 2017), (Covington *et al.*, 2016) experimented for number and size of layers. Batchnorm: (Wang *et al.*, 2017) Activation functions: tanh (Zhang *et al.*, 2016), tanh vs sigmoid vs relu (tanh

and relu depending on dataset) (Qu *et al.*, 2016), relu vs tanh (relu better) (Guo *et al.*, 2017) Shapes: Diamond, constant, increasing, decreasing (Zhang *et al.*, 2016) found that Diamond shape works best. found constant to work the best (Guo *et al.*, 2017)

Choosing DNN learning hyperparameters. Loss function: logloss with L_2 penalty (Song *et al.*, 2018), (Wang *et al.*, 2017), (Zhang *et al.*, 2016), (Qu *et al.*, 2016) mini-batch aware l2 for large inputs (Zhou *et al.*, 2017), Batch size: 1024 (Song *et al.*, 2018) 512 (Wang *et al.*, 2017) Optimiser: Adam (Song *et al.*, 2018), (Wang *et al.*, 2017) Gradient clipping: (Wang *et al.*, 2017) Learning rate: 0.001-0.0001 (Wang *et al.*, 2017), [1, 0.1, . . . , 0.0001] (Zhang *et al.*, 2016) Early stopping: (Song *et al.*, 2018), (Wang *et al.*, 2017), (Zhang *et al.*, 2016) (Zhang *et al.*, 2016) compared dropout with L2 and found dropout to be better.

4.5 Learning Interactions

Automated Feature Engineering

Traditionally, input features to a machine learning algorithm must be hand-crafted from raw data, relying on practitioner expertise and domain knowledge to determine explicit patterns of prior interest. The engineering process of creating, analyzing, selecting, and evaluating appropriate features can be laborious and time consuming, and is often thought of as a "black art" requiring creativity, trial-and-error, and oftentimes luck.
In contrast, deep learning techniques learn optimal features directly from the data itself, without any human guidance, allowing for the automatic discovery of latent data relationships that might otherwise be unknown or hidden.

That being said, preprocessing of data in deep learning is not totally free of human engineering. See in the Normalisation section what measures should be taken to ensure a NN can learn effectively from tabular data.

4.5.1 Fully-Connected Layers

- how deep and how big
- architecture shape

4.5.2 Going Deeper

- Residual Connections

4.5.2.1 Self-normalising Units

Fully-connected DNNs with normalisation techniques are very sensitive to perturbations. DNNs exhibit a high variance in training error when trained using BatchNorm. This hinders the learning process. Combined with dropout just magnifies the effect. (Klambauer *et al.*, 2017) suggested the use of SeLUs which is an activation function which helps the network to maintain zero mean and unit variance activations. By using this activation, there is no need for a BatchNorm layer. SNNs do not suffer from exploding or vanishing gradients. They paper tested on 123 tabular datasets to show that on average SNNs are the best. But it is quite finicky to get the implementation right. It requires a very specific weight initialisation, one that does not really make sense for embedding matrices. And even when you get it right, the improvement is not necessarily significant. That said, it has not been tested by others on tabular data, so it is worth a try.

$$\text{selu}(x) = \lambda \begin{cases} x & \text{if} \quad x > 0 \\ \alpha e^x - \alpha & \text{if} \quad x \leq 0 \end{cases}$$

Give more detail if it is proved to be useful. Also needs a specific type of dropout.

(Klambauer *et al.*, 2017) tested SELUs on 121 classification datasets from the UCI Machine Learning repository. They compared DNNs with SELU activations to other DNNs and other classifiers like Random Forests and SVMs. They found that on the datasets with less than 1000 obervations, random forests and SVMs performed the best. However, for the datasets with more than 1000 observations, DNNs with SELU activations performed the best overall. The classifiers were compared by ranking them by their accuracy for each prediction task and doing a pairwise Wilcoxon test.

Another thing the authors found when comparing SELUs with other activations is that the model selection approach for SELU DNNs resulted in much deeper networks than DNNs with other activations.

4.5.3 Attention

4.5.4 Parallel Streams

4.6 Dealing with Small Datasets

4.6.1 Data Augmentation

- Blankout
- Swap Noise
- (Kosar and Scott, 2018) - hybrid bootstrap
- using GANS are interesting by out of scope.

Tabular data is very different to image data and the standard augmentations used in computer vision does not make sense with tabular data. You cannot rotate or scale an observation from a tabular data without losing its meaning. One transformation that does make sense for tabular input is the injection of random noise.

When working with images, we can randomly perturb the pixel intensities by a small amount so that it is still possible to make sense of its content. By adding 1 for example to all pixels and all colors in an image, will only make it slightly brighter and we will still be able to make sense of it. Bu with tabular data we can just randomly add a small amount to any feature. The input features will probably not all be on the same scale and the addition of noise might result in a feature value that is out of the true distribution. In addition, it does not make sense to add anything to a discrete variables. Thus in order to inject random noise to a tabular data sample, the noise should be scaled relative to each input feature range and the results should be a valid value for that feature. This also helps the model to be more robust to small variations in the data.

(Van Der Maaten *et al.*, 2013) suggests an augmentation approach that does this called Marginalised Corrupted Features (MCF). The MCF approach adds noise to input from some known distribution.

In the original Denoising Autoencoding papaer (Vincent *et al.*, 2008), they used a blank-out corruption procedure. Which is randomly selecting a subset of the input features and mask their values with a zero. The only conceptual problem with this approach is that for some features a zero value actually

Table 4.1: Swap Noise Example

age	occupation	education	race	sex	>=50k
Original Dataset					
49	NA	Assoc-acdm	White	Female	1
44	Exec-managerial	Masters	White	Male	1
38	NA	HS-grad	Black	Female	0
38	Prof-specialty	Prof-school	Asian-Pac-Islander	Male	1
42	Other-service	7th-8th	Black	Female	0
20	Handlers-cleaners	HS-grad	White	Male	0
Sample with swap noise					
49	Prof-specialty	Prof-school	Asian-Pac-Islander	Female	1

carries some meaning, so a suggestion is to blank-out features with a unique value not already belonging to that feature distribution.

Another input corruption approach shown to work empirically here is what is called Swap Noise (Kosar and Scott, 2018). The swap noise procedure corrupts inputs by randomly swapping input values with those of other samples in the datasets. In this way you ensure that the corrupted input at least have valid feature values. But it still might produce combinations of features that are not actually possible.

All of these methods have hyperparameters that needs to be set. I haven't gone into detail as I still need to decide what is relevant to this thesis.

Mixup. The way mixup creates artifical samples is by the following original formulation:

$$\tilde{\boldsymbol{x}} = \lambda \boldsymbol{x}_i + (1-\lambda)\boldsymbol{x}_j \tilde{\boldsymbol{y}} = \lambda \boldsymbol{y}_i + (1-\lambda)\boldsymbol{y}_j$$

where $\boldsymbol{x}$ is a input vector,$\boldsymbol{y}$ a one-hot encoded output vector and $\lambda \in [0,1]$. $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ and $(\boldsymbol{x}_j, \boldsymbol{y}_j)$ are two samples drawn at random from the training data. Thus mixup assumes that linear interpolations of input vectors lead to linear interpolations of corresponding targets.

λ controls the strength of the interpolation between input-output pairs. The closer λ is to 0 or 1, the closer the artificial sample will be to an actual training sample. The authors suggest using $\lambda \sim \text{Beta}(\alpha, \alpha)$ for $\alpha \in (0, \infty)$. They observed best performance when $\alpha \in [0.1, 0.4]$ and if α is too high, they experience underfitting.

Other ablation studies they did was to find at which stages of the network the interpolation should happen, *e.g.* raw input, after embedding, hidden layer,

etc. But the experiments are not extremely clear and therefore warrants further discussion here.

Typically data augmentation procedures are dataset dependent and therefore requires expert knowledge. It is hard to think of ways to augment tabular data, even more so a generic way of doing so. However, from this defnition it is clear that mixup can be used on any type of data, including tabular datasets.

Mixup data augmentation can be understood as a mechanism to encourage the model to behave linearly in-between training samples. (Zhang *et al.*, 2017) shows that this linear behaviour reduces the amount of undesirable variation when predicting new samples further away from the training samples. They also argue and show empirically how training with mixup is more stable in terms of model predicions and gradien norms. This is because mixup leads to decision boundaries that transition linearly between classes, resulting in smoother predictions.

The authors (Zhang *et al.*, 2017) tested mixup data augmentation on tabular datasets. They tested it on 6 classification datasets from the UCI Machine Learning repository. They used a 2-layer MLP with 128 neuros each and a batch size of 16. They found that mixup improved the performance on 4 out of the 6 datasets.

See Figure 4.1.

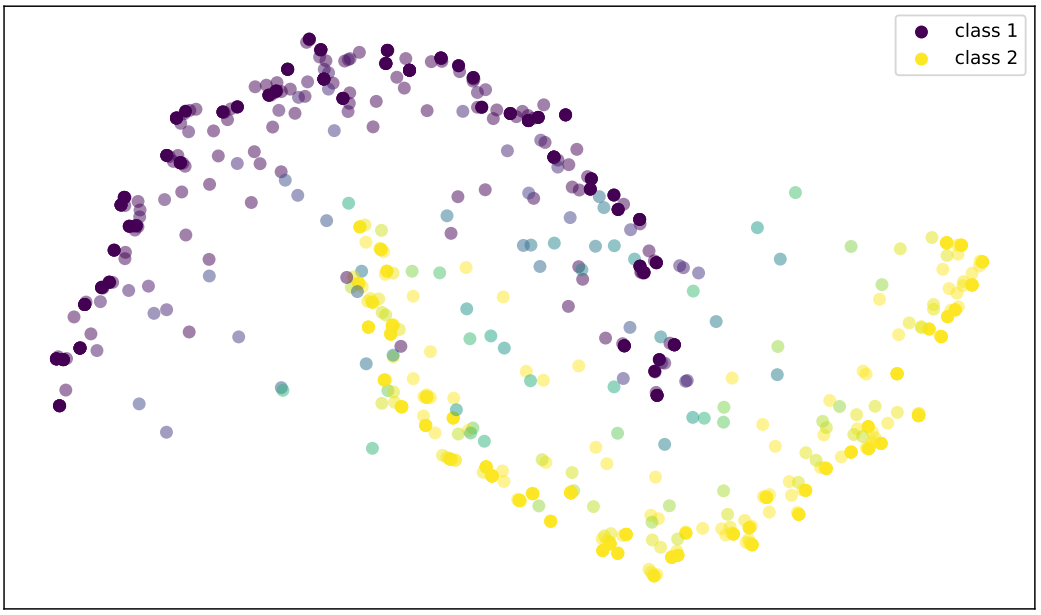


Figure 4.1: Illustration of points created by mixup augmentation.

4.6.2 Unsupervised Pretraining

(Miotto *et al.*, 2016) used a stacked denoising autoencoder to learn patient representations from EHR data. They found that these representations were useful features in predicting future health states of patients. By using these learned representations as input significantly improved the performance of predictive models compared to those only using the raw inputs.

(Miotto *et al.*, 2016) presented a novel unsupervised deep feature learning method to derive a general-purpose patient representation for EHR data that facilitates clinical predictive modelling. A stacked denoising autoencoder was used. Unsupervised feature learning attempts to overcome limitations of supervised feature space definition by automatically identifying patterns and dependencies in the data to learn a compact and general representation that make it easier to automatically extract useful information when building classifiers or other predictors (Miotto *et al.*, 2016). These techniques are very familiar and effective in text, audio and image processing, but not with tabular data. (Geras and Sutton, 2014) on gradual increasing of corruption ratio; but applied to images.

- Knowledge distillation/psuedo labelling

4.7 Other

- 1cycle not used with tabular data before
- How to interpret the model/decisions?
- other processing
- Regularisation Learning - https://arxiv.org/pdf/1805.06440.pdf

4.8 Recommended Approach

Chapter 5

Experiments

"For us, the most important part of rigor is better empiricism, not more mathematical theories."

— Ali Rahimi and Ben Recht, *NIPS 2017*

5.1 Introduction

Since theory and practice does not always go hand-in-hand, it is usually advantageous to compliment a theoretical study or literature review with empirical results. Another motivation for empirical study is that we regard the ability to implement an approach equally as important as understanding the theory behind it. We characterise a good empirical experiment as one that is *rigorous* and *reproducible*. Recently the field of DL has been criticised for the growing gap between the understanding of its techniques and its practical successes[1] where most of the recent focus was on the latter. The speakers urged the deep learning community to be more rigorous in their experiments where, for them, the most important part of rigor is better empiricism, not more mathematical theories.

In this chapter we aim for good empiricism by evaluating the models on different types of prediction tasks and datasets, exploring many hyperparamters and doing cross-validation for unbiased performance measures along with standard errors. Our work is not necessarily about beating the benchmark and consist of simple experiments that aid in the understanding of how the techniques work, as used throughout the thesis.

Furthermore, we want all our experiments to be as reproducible as possible. Therefore we provide all the code, data and necessary documentation

[1]How do I cite the talk given at NIPS2017 - https://www.youtube.com/watch?v=Qi1Yry33TQE

to reproduce the experiments that were done in this thesis[2]. This is often an overlooked feature of experiments, but is however crucial for transparent and accountable reporting and making your work useful for others to build upon.

The main aim of this chapter is to better understand the behaviours of certain models and parameters and to cross-check the literature with empirical observations. We focus on the same main issues when it comes to DL on tabular as in the previous chapter, which are:

- how to represent the inputs,
- how to learn from feature interactions, and
- how to fight overfitting.

The more general hyperparameters, like learning rate, batch size, layer size and layer depth will not receive attention here since it has already been discussed at relevant parts previously. However, since these parameters are tightly linked with each other and other model parameters, we still do a hyperparamter search where we deem appropriate and report the findings in Appendix B. The rest of the chapter continues as follows: In §5.2 an overview of the datasets used for these experiments are given and why the were chosen. We discuss our evaluation procedure and metrics in §5.3. Thereafter we start with the main experiments.

5.2 Datasets

Our experiments are done on multiple datasets. Thus we can distinguish between findings that are only true for certain datasets and tasks and findings that hold more universallt.

The criteria for selecting the datasets were: - Strong model performance baselines exist; so that we can determine how far we are from the SoTA and that is actually a relevant problem. - Entirely open source; so that anyone can access it, reproduce it and build on it. - More than 20,000 observations; since NNs are data hungry. - Does not require too much preprocessing; so that most of the energy goes into the modelling phase. - Contain a mix of continuous and categorical features.

[2]All of these are shared publicly at https://github.com/jandremarais/tabularLearner

We chose two datasets for regression, one for binary classification and one for multi(class/label) classification from the UCI machine learning repository [Dua2017]. The chosen datasets are:

The Adult dataset[3]. This dataset was collected during a census. The task here is to predict whether or a not a certain person's income exceeds $50,000 per year. The features available are things like *age*, *education*, *sex* and *race*. In total there are 14 features and 48,842 observations.

Forest Cover Type[4]: Predicting forest cover type from cartographic variables. This is a multiclass clasification task. There are 581,012 observations.

Taxi Fare Prediction: Regression task (possibly) https://www.kaggle.com/c/new-york-city-taxi-fare-prediction

- Maybe https://www.kaggle.com/c/costa-rican-household-poverty-prediction/data
- Maybe https://www.kaggle.com/c/home-credit-default-risk

Look at the datasets used by (**?**), also (Zhang *et al.*, 2017)

- Criteo (Song *et al.*, 2018), (Wang *et al.*, 2017), (Qu *et al.*, 2016), (Guo *et al.*, 2017)
- Avazu (Song *et al.*, 2018)
- KDD12 (Song *et al.*, 2018)
- MovieLens-1M (Song *et al.*, 2018)
- iPinYou (Qu *et al.*, 2016)
- Forest Cover type (Wang *et al.*, 2017)
- Higgs (Wang *et al.*, 2017)
- Tox21 (Klambauer *et al.*, 2017)
- Yahoo (**?**)
- Letor (**?**)
- Protein (**?**)
- A9A (**?**)
- Flight (**?**)

Regularisation learning paper (Shavitt and Segal, 2018) only tested their approach on one dataset.

[3]http://archive.ics.uci.edu/ml/datasets/Adult
[4]https://archive.ics.uci.edu/ml/datasets/covertype

5.3 Evaluation

(Klambauer *et al.*, 2017) did a once-off three-way split of the data into training, validation and testing datasets. Hyperparemeter decisions were made based on the valdiation dataset performace and then the selected models are compared on the test datasets. The models were compared using the pairwise Wilcoxon rank test. The problem with doing a once-off split is that it does not account for the variance of the model and the performance of the model can in fact be very sensitive to the subset of data. By doing cross-validation, we can have more robust performance metrics, including the benefit of reporting on standard errors.

The other problem with (Klambauer *et al.*, 2017) is that they only tested on classification tasks and not regression. Models can behave quite differently on the two types of tasks. (Zhang *et al.*, 2017) also only tested mixup data augmentation on tabular datasets where the task was classification.

For the regression tasks we will compare the various models using the mean squared error and for classificaion we use cross-entropy. These are the metrics directly being optimised during the training process. When comparing the results to previous work, we base it on the metrics that are commmon for the specific dataset.

5.3.1 Metrics

- loss function
- task specific
- dataset specific
- time and memory

AUC, Logloss for binary classification (Song *et al.*, 2018), (Wang *et al.*, 2017), (Zhang *et al.*, 2016), (Qu *et al.*, 2016) No cross-validation (Song *et al.*, 2018), (Zhang *et al.*, 2016) Run time per epoch (Song *et al.*, 2018), (Guo *et al.*, 2017) Model size (Song *et al.*, 2018) Think (Wang *et al.*, 2017) used CV since the report se's for hyperparameter tunings.

5.3.2 Cross-validation

For most of the experiments we will do a 5-fold cross validation (Hastie *et al.*, 2009, p. 241) to estimate the performance of a model. That is, randomly

dividing the dataset in five equal parts and then in turn, hold out one of those parts for validation purposes and train the model using the remaining four parts. Figure 5.1 visually explains how the dataset is sub-divided. The performance of the model can then be evaluated on the held-out part. This process is repeated for every one of the five segmentations of the dataset and thus five measurements of the performance of model is obtained. We can then compute the average over these five measurements to obtain a less biased estimate of the model performance. Another advantage of this approach is that we can obtain standard error for the model performance.

Cross-validation is rarely done in Deep Learning, since the models typically take very long to train and any repitition is thus more costly. However, Deep Learning is also mostly applied to large datasets and if a large test set is available, the gains from cross-validation diminishes. Fortunately, the NNs applied to tabular data are much smaller than ones used for unstructured data and for this work we have access to sufficient computing power. And therefore cross-validation makes sense.

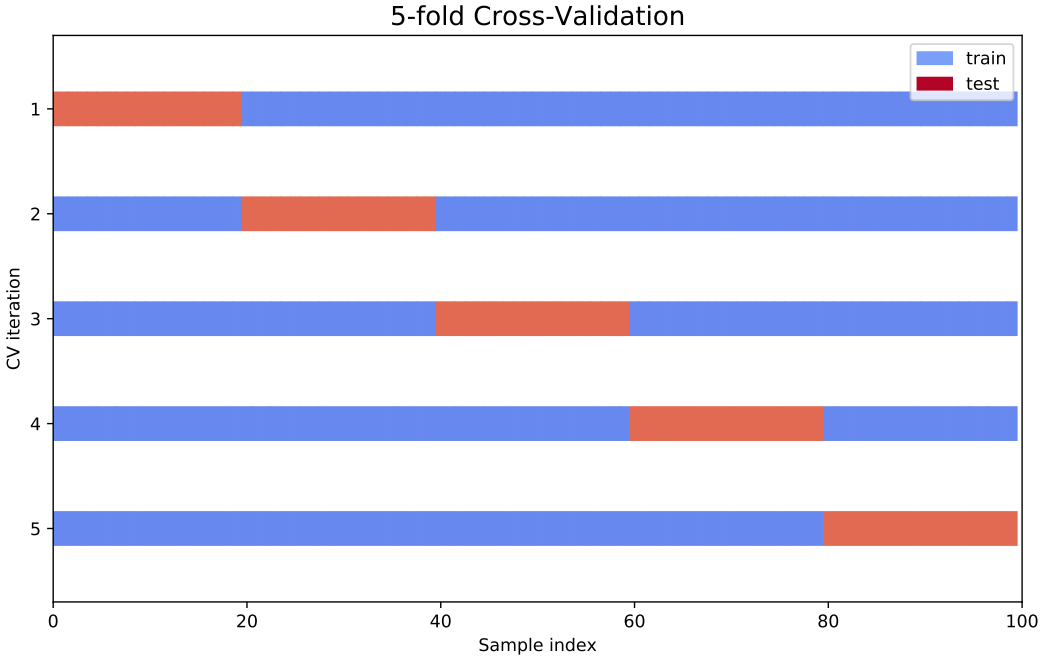


Figure 5.1: 5-Fold Cross-validation dataset split schematic.

5.4 General Approach

- which numeric normalisation
- should we embed numerics

Unfortunately, we cannot follow the hyperparameter selection process suggested by (Smith, 2018) for all the experiments. The process is too manual. Therefore we follow the approach once on each dataset to find a good selection of learning rate, number of epochs and weight decay and then use these paramters for the rest of the experiments on this dataset. If the model significantly changes over experiments, we might need to rerun the parameter selection process. Thus we will definitely not find the optimal model for each experiment but it should be sufficient to use as comparisons. According to (Smith, 2018) these parameters are also quite robust and the model is not too sensitive on these choices.

Might follow a bit of a greedy approach when selecting optimal paramters. All the hyperparameters are very dependent on each other but we cannot run experiments for every possible combination. Therefore we find optimal parameters for a certain experiment and then assume that these parameters are also good for other experiments.

Preprocessing. - Remove infrequent features (Song *et al.*, 2018) - numeric transform by $\log^2(z)$ if $Z > 2$ (Song *et al.*, 2018). - numeric features log transform (Wang *et al.*, 2017)

The idea is to do as little feature engineering as possible. So the steps we take here are generic steps that are applicable to any dataset. We do no feature selection since we would want the model to learn by itself which features are relevant.

5.5 Architectural Search

- Number of layers (vs with SeLU) (vs other activations) [1-10]
- Layer size [32-2048]
- Architecture shape [Constant, increasing, decreasingm diamond]
- Embedding sizes [proportional, fixed]
- dropout [0-1]

Recently found that the below experiments were already done by (Guo *et al.*, 2017, Qu *et al.* (2016), Zhang *et al.* (2016)). This was however only explored for Click-through rate prediction data. Thus the below experiments should be done in the light of these findings and can be compared to the their findings.

Here we investigate the effect of the size of the network on the different datasets. We compare the performance of the models at different numbers and sizes of layers. Larger networks are more flexible and therefore we expect it to act similarly to any learning model flexibility parameter. Increasing the network size will be beneficial up until a certrain point until it becomes too big and be more prone to overfitting. We hope to find a rule of thumb that might act as a good starting point and guideline to choose the network size. We also want to get a feel for how important these hyperparameters are.

- Constant size Layer sizes: 32, 64, 128, 256, 512, 1024, 2048 Number of layers: 1,2,3,4,5,6 At a constant dropout.

Suppose we choose three layers, compare the following shape at approximately equal number of parameters. Shapes: Constant, decreasing, increasing, diamond, hourglass

The aim of these experiments are to evaluate performance at different embedding sizes. We explore embedding sizes at different ratios of the cardinality of categorical variables. The ratios we look at are: 10%, 20% 30%, 40%, 50%, 60%, 70%, 80% and 90% of the cardinality of each categorical feature. Possibly explore certain max embedding sizes.

As we increase the size we will also look at the effect it has by visually inspecting the embedding layers in a 2-dimensional space.

Again, we expect there to be optimal embedding size for each variable depedning on the cardinality of the variable and how complex its relationship is with the other variables and the target. We expect the ideal embedding size to be as small as possible but still being able to capture all of the information of the variable.

Look at wide and deep models from (Cheng *et al.*, 2016). They restrics all embeddings to be of size 32.

5.6 Sample Size

- accuracy vs size of dataset

5.7 Mixup

- does it help the validation loss

5.8 Pretraining

- does it help the validation loss
- Are these features useful for tree based methods.

5.9 Attention

- with residual

5.10 Comparisons To Tree-based Methods

- Compare Neural Networks to Gradient Boosted Machines and Random Forests.

5.11 Example Interpretation

- plot embeddings
- plot attention matrices
- SHAP and permutation

Chapter 6

Conclusion

- What was done in the thesis?
- Is Deep Learning useful for tabular data?
- If it is, when?

6.1 Promising Future Directions

- Where should future work on the subject focus on?

Variational autoencoders for pretraining. Generative Adversarial Network for data augmentation (and other tab data specific augs). Feauture reuse per feature regularisation.

Appendices

Appendix A

Datasets

Details of each of the datasets used in Chapter 5 and elsewhere.

Appendix B

Hyperparameter Search

Appendix C

Software and Code

- Deep Learning Library: Pytorch and Fastai
- Hardware: GTX1080Ti
- Python and Jupyter Notebooks for programming environemnt
- github for version control
- RMarkdown for writing and compiling the thesis document

C.1 Code and Reproducibility

Note that all of the code used in the thesis, including the source documents, is made available in the tabularLearner Github repository [1]. More instructions on how to implement the code is contained in the file named `README.md`, in the repository.

[1] https://github.com/jandremarais/tabularLearner

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