FACULTY OF SCIENCE
UNIVERSITY OF COPENHAGEN

Master Thesis

Sune Andreas Dybro Debel

Deep Multi-Task Learning
For Relation Extraction

Dirk Hovy

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Abstract

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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Background

In this part, we describe the information extraction problem and the challenges it poses. Moreover, we formally describe the supervised machine learning setting. Specifically, we discuss the challenges of noise and overfitting, and show the usefulness of Vapnik-Chervonenkis analysis.

2.1 Information Extraction

In natural language processing, information extraction is the problem of extracting structured information from unstructured text. Many practical information extraction problems fall in one of two categories: **named entity recognition**, or **relation extraction** (Jurafsky and Martin, 2009). Here, we introduce each of them, and explain why they are difficult.

2.1.1 Named Entity Recognition

A named entity is roughly anything that has a proper name. The task in named entity recognition is to label mentions of entities such as people, organisations or places occurring in natural language. As an example, consider the sentence:

Jim bought 300 shares of Acme Corp. in 2006.

A named entity recognition system designed to extract the entities *person* and *organisation* should ideally assign the labels:

$[\text{Jim}]_{person}$ bought 300 shares of $[\text{Acme Corp.}]_{organisation}$ in 2006.

This is a difficult problem because of two types of ambiguity. Firstly, two distinct entities may share the same name and category, such as *Francis Bacon* the painter and *Francis Bacon* the philosopher. Secondly, two distinct entities can have the same name, but belong to different categories such as *JFK* the former American president and *JFK* the airport near New York.

Named entity recognition can be framed as a sequence labelling problem. A common approach is to apply so called tokenisation to the text, i.e finding boundaries between words and punctuation, and associate each token with a label indicating which entity it belongs to. BIO (figure 2.1) is a widely used labelling scheme in which token labels indicate whether the token is at the **B**eginning, **I**nside, or **O**utside an entity mention.

Jim	bought	300	shares	of	Acme	Corp	.	in	2006	.
`B-PER`	`O`	`O`	`O`	`O`	`B-ORG`	`I-ORG`	`I-ORG`	`O`	`O`	`O`

Figure 2.1
A sentence labeled with the BIO labels for named entity recognition.

2.1.2 Relation Extraction

Relation extraction refers to the problem of identifying relationships such as *Family* or *Employment* between entities. As an example, consider the sentence:

> Yesterday, New York based Foo Inc. announced their acquisition of Bar Corp.

Imagine we have designed a relation extraction system that recognises the relation *MergerBetween(organisation, organisation)* between two mentions of organisations. Ideally, we would like that system to extract the relation *MergerBetween(Foo Inc., Bar Corp.)* from the above sentence.

Because relation extraction is concerned with relationships between named entities, many systems that perform relation extraction applies named entity recognition first as a pre-processing step. This approach is sometimes called **pipelining**. An alternative to pipelining is **end-to-end** relation extraction, where relations and entities are extracted simultaneously. Pipeline approaches can suffer from the problem of **error propagation**, where the system erroneously assigns a label in the named entity recognition step, which later causes it to make an error in the relation extraction step.

2.1.3 Accuracy Measures

Information extraction systems are often evaluated empirically by applying them to collections of text, so called corpora, in which N mentions of named entities or relations are known. Accuracy measures used in such tests are usually defined in terms of:

True positives (tp) The number of true named entities or relations correctly labeled by the system.

True negatives (tn) The number of true non-entities or non-relations correctly labeled by the system.

False positives (fp) The number of true non-entities or relations incorrectly labeled by the system.

False negatives (fn) The number of true named entities or relations incorrectly labeled by the system.

The distribution of labels used in both named entity recognition and relation extraction is often highly imbalanced. Consider for example the BIO labelling scheme in figure 2.1. Most words will be outside a mention of a named entity, and will have the label `O`. Using simple accuracy $\frac{tp+tn}{N}$ as a performance metric is therefore not very informative, since a useless system which labels all tokens with `O` would achieve high performance.

Precision and **recall** are more appropriate performance metrics for this reason. Precision $\frac{tp}{tp+fp}$ is the fraction of true named entities or relations of all named entities or relations that were extracted by the system. This is equal to 0 when none of the information extracted by the system was correct and 1 when all of it was correct.

Recall $\frac{tp}{tp+fn}$ is the fraction of true named entities or relations that were extracted by the system. This is 0 when none of the extracted information was correct, and

1 when all of the extracted information was correct, and no true named entities or relations were incorrectly labeled.

To get a single number that summarises the performance, precision p and recall r are often combined into a single metric, the $F1$ measure, defined as the harmonic mean of precision and recall $\frac{2pr}{p+r}$.

2.2 Supervised Machine Learning

Most modern solutions to the information extraction problems in 2.1 are based on supervised machine learning techniques. In this setting, a system learns to recognise the named entities or relations between them from examples provided by a human annotator. In this section we formally describe this approach and introduce important theoretical tools for understanding supervised machine learning.

2.2.1 The Supervised Learning Problem

A set $\mathcal{D}_{train}$ of N training examples $(\mathbf{x}_i, \mathbf{y}_i)$ of inputs $\mathbf{x}_i$ and corresponding labels $\mathbf{y}_i$ is created by a human annotator. Each $\mathbf{x}_i$ belongs to an input space $\mathcal{X}$, for example the set of all english sentences. Each $\mathbf{y}_i$ belongs to a space $\mathcal{Y}$ of labels, for example the set of all sequences of BIO tags. As designers of the learning system, we specify the so called **hypothesis space** $\mathcal{H}$, a set of functions $h : \mathcal{X} \mapsto \mathcal{Y}$. We want to find a function $h \in \mathcal{H}$, sometimes called a **model** or **hypothesis**, that can automatically assign labels to a new set of un-labeled inputs $\mathcal{D}_{test} = \{\mathbf{x}_i \mid \mathbf{x}_i \in \mathcal{X}\}$ at some point in the future.

Supervised machine learning is the science of how to use an algorithm to find a function h using $\mathcal{D}_{train}$ that performs well on $\mathcal{D}_{test}$, as measured by some performance measure e. In classification problems such as named entity recognition or relation extraction where $\mathcal{Y}$ is discrete, we typically use binary error $e(\mathbf{y_1}, \mathbf{y_2}) = \mathbb{I}[\mathbf{y}_1 \neq \mathbf{y}_2]$. Importantly, we are not explicitly interested in the performance of h on $\mathcal{D}_{train}$ (Abu-Mostafa et al., 2012).

We can formalise the preference for functions h that perform well on examples outside of the training set with a quantity known as **generalisation error**.

Definition 2.2.1 (generalisation error)**.** Let $P(\mathbf{x}, \mathbf{y})$ be a joint probability distribution over inputs $\mathbf{x} \in \mathcal{X}$ and labels $\mathbf{y} \in \mathcal{Y}$. Let $e(\mathbf{y}_1, \mathbf{y_2}) = \mathbb{I}[\mathbf{y}_1 \neq \mathbf{y}_2]$ be the binary error function that measures agreement between labels $\mathbf{y}_1$ and $\mathbf{y}_2$. Then the generalisation error E of a function $h : \mathcal{X} \mapsto \mathcal{Y}$ is defined as:

$$E(h) = \mathbb{E}_{\mathbf{x},\mathbf{y} \sim P(\mathbf{x},\mathbf{y})}[e(h(\mathbf{x}), \mathbf{y})]$$

Now, formally, the objective of supervised machine learning is to find a function h^* in a space of functions $\mathcal{H}$ that minimises $E(h)$. We see the process generating the data as random, but with a behaviour describable by a distribution $P(\mathbf{x}, \mathbf{y})$. Unfortunately, this distribution is unknown, which makes E unknown. However, we can use sampled data $\mathcal{D} = \{(\mathbf{x}, \mathbf{y}) \mid \mathbf{x}, \mathbf{y} \sim P(\mathbf{x}, \mathbf{y})\}$ to estimate $E(h)$ with a quantity known as **empirical error**:

Definition 2.2.2 (empirical error)**.** Let $\mathcal{D}$ be a set of N examples $\{(\mathbf{x}_i, \mathbf{y}_i) \mid \mathbf{x}_i, \mathbf{y}_i \sim P(\mathbf{x}, \mathbf{y})\}$. Then the empirical error $\hat{E}$ is defined as:

$$\hat{E}(h, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} e(h(\mathbf{x}_i), \mathbf{y}_i)$$

Because $\mathcal{D}$ is a random quantity, it's dangerous to use $\hat{E}$ to estimate E. We risk that the samples are not representative of $P(\mathbf{x}, \mathbf{y})$, leading us to believe that h is great, when in fact it's terrible. We can bound the probability that $\hat{E}$ is a bad estimate of E if we make two assumptions:

Firstly, we assume that the samples in $\mathcal{D}$ are drawn independently from $P(\mathbf{x}, \mathbf{y})$, that is observing any one sample did not change the probability of observing any other sample.

Secondly, we assume that h is independent of $\mathcal{D}$, in other words, that h was not specifically chosen based on the sample. These assumptions enable us to apply **Hoeffding's inequality** to bound the probability that $\hat{E}$ is far away from E:

Theorem 2.2.1 (Hoeffding's inequality)**.** let $E(h)$ be defined as in definition 2.2.1, and let $E(h, \mathcal{D})$ be defined as in definition 2.2.2. Then:

$$\mathbb{P}\left(|E(h) - \hat{E}(h, \mathcal{D})| \geq \epsilon\right) \leq 2e^{-2N\epsilon^2}$$

The inequality tells us that the probability that E is more than ϵ away from $\hat{E}$ decreases exponentially in ϵ and N. In other words, the more samples in D, the less likely it is that E will be misleading.

Estimating E with a sample that is independent of h is a technique called **validation**. In validation, the sample provided by a human annotator is split into two datasets, $\mathcal{D}_{train}$, which we intend to use to search for h^*, and $\mathcal{D}_{validate}$, which we save until we're done searching. Since $\mathcal{D}_{validate}$ is independent of whichever h we selected, Hoeffding's inequality applies and $\mathcal{D}_{validate}$ can be used to estimate E.

Because $\mathcal{D}_{train}$ is used to select h, it cannot be used to estimate E by Hoeffding's inequality, and we need more sophisticated techniques to understand the relationship between $\mathcal{D}_{train}$ and E. The central question in supervised machine learning is *how can we best define $\mathcal{H}$ and use $\mathcal{D}_{train}$ to make E small?* Answering this question is the objective of a field of research known as **statistical learning theory**.

2.2.2 Statistical Learning Theory

We would like to know how best to define $\mathcal{H}$ and use $\mathcal{D}_{train}$ in order to make E small. $\mathcal{D}_{train}$ is the only information we have about $P(\mathbf{x}, \mathbf{y})$, and therefore also the only information we have about E. A straight-forward idea would be to find a function $g \in \mathcal{H}$ that minimises the **training error** $\hat{E}(g, \mathcal{D}_{train})$ in the hope that g will also minimise E.

As we argued in section 2.2, using $\hat{E}$ to estimate E can be misleading. Moreover, because D_{train} is used to specifically choose g that makes $\hat{E}$ small, the guarantees provided by Hoeffding's inequality no longer holds, and therefore it may be possible to select g such that $\hat{E}(g, \mathcal{D}_{train})$ is small and $E(g)$ is large, even when we have a large number of training examples.

The phenomena where training error is small but generalisation error is large is known as **overfitting**. As the name implies, it's caused by harmful idiosyncrasies of $\mathcal{D}_{train}$ that, when used to minimise $\hat{E}(h, \mathcal{D}_{train})$, leads us to a g with a larger E than other functions in $\mathcal{H}$. These idiosyncrasies of $\mathcal{D}_{train}$ are ultimately the product of **noise**.

In general, noise comes in two forms. The first form is known as **stochastic noise**. This type of noise is introduced by variation in the relationship between $\mathbf{x}$ and $\mathbf{y}$ that is inherently unpredictable. For example, human error is a common source of stochastic noise in information extraction, where an annotator incorrectly labels a piece of text. Selecting a g that repeats this error is a case of overfitting, because g will have lower training error but larger generalisation error than another h that doesn't predict the incorrect annotation, since presumably the error is the exception to the rule.

The second type of noise is called **deterministic noise**. This type of noise may be introduced when the relationship between $\mathbf{x}$ and $\mathbf{y}$ is deterministic, but $\mathcal{H}$ doesn't have the capacity to represent this relationship exactly.

To understand deterministic noise, imagine that even h^* can't represent the deterministic relationship $\mathbf{y} = f(\mathbf{x})$ exactly. Suppose that we get a $\mathcal{D}_{train}$ that contains a sample $(\mathbf{x}_i, \mathbf{y}_i)$ that falls outside the capacity of h^*, that is, $h^*(\mathbf{x}_i) \neq \mathbf{y}_i$. Now further imagine that in order to minimise $\hat{E}$, we select a g that predicts this sample, such that $h(\mathbf{x}_i) = \mathbf{y}_i$. This is a case of overfitting since we know that there is at least one function in $\mathcal{H}$ with lower generalisation error than g, namely h^*.

The risk of overfitting is linked to the diversity of $\mathcal{H}$. By diversity of $\mathcal{H}$, we roughly mean how different any function in $\mathcal{H}$ is from any other function in $\mathcal{H}$. The more diverse $\mathcal{H}$ is, the greater the risk that there exists a $h \in \mathcal{H}$ that will overfit $\mathcal{D}_{train}$.

A **dichotomy** is a central concept in measuring the diversity of $\mathcal{H}$. A dichotomy is a specific sequence of N labels. For example, if $\mathcal{Y} = \{0, 1\}$, and $N = 3$, then (0 1 0) is a dichotomy, and so is (1 0 0). We have listed all dichotomies for $N = 3$ in figure 2.2.

(0 0 0)
(1 0 0)
(0 1 0)
(0 0 1)
(1 1 0)
(0 1 1)
(1 0 1)
(1 1 1)

Figure 2.2
All dichotomies for $\mathcal{Y} = \{0, 1\}$ and $N = 3$. There are $2^3 = 8$ ways to choose a sequence of 3 labels from 2 possibilities.

Dichotomies allow us to group similar functions. In the rest of this section, let's assume that $\mathcal{Y} = \{0, 1\}$. By simple combinatorics the number of dichotomies for N must be smaller than or equal to 2^N. There may be infinitely many functions in $\mathcal{H}$, but on a specific $\mathcal{D}_{train}$, many of them will produce the same dichotomy since the number of training examples in $\mathcal{D}_{train}$ is finite. This allows us to quantify the diversity of $\mathcal{H}$ in terms of the number of dichotomies it's able to realise on a set of N points. This is achieved by a measure known as the **growth function**.

Definition 2.2.3 (growth function)**.** Let $\mathcal{H}(N) = \{(h(\mathbf{x}_1), \ldots, h(\mathbf{x}_N)) \mid h \in \mathcal{H}, \mathbf{x}_i \in \mathcal{X}\}$ be the set of all dichotomies generated by $\mathcal{H}$ on N points, and let $|\cdot|$ be the set cardinality function. Then the growth function m is:

$$m(N, \mathcal{H}) = \max |\mathcal{H}(N)|$$

In words, the growth function measures the maximum number of dichotomies that are realisable by $\mathcal{H}$ on N points. To compute $m(N, \mathcal{H})$, we consider any choice of N points from the whole input space $\mathcal{X}$, select the set that realises the most dichotomies and count them.

The growth function allows us to account for redundancy in $\mathcal{H}$. If two functions $h_i \in \mathcal{H}$ and $h_j \in \mathcal{H}$ realise the same dichotomy on $\mathcal{D}$, then any statement based only on $\mathcal{D}$ will be either true or false for for both h_i and h_j. This makes it possible to group the events $\hat{E}(h_i, \mathcal{D})$ *is far away from* $E(h_i)$ and $\hat{E}(h_j, \mathcal{D})$ *is far away from* $E(h_j)$, and thereby avoiding to overestimate the probability of the union of both events occurring.

If $\mathcal{H}$ is infinite, the number of redundant functions in $\mathcal{H}$ will also be infinite, since the number of dichotomies on N points is finite. If $m(N, \mathcal{H})$ is much smaller than 2^N, the number of redundant functions in $\mathcal{H}$ will be so large as to make the probability that $\hat{E}$ is far away from E very small.

This line of reasoning is the basis of the Vapnik-Chervonenkis bound, which bounds $E(h)$ in terms of $\hat{E}(h, \mathcal{D}_{train})$:

Theorem 2.2.2 (Vapnik-Chervonenkis bound)**.** Let $m(N, \mathcal{H})$ be defined as in definition 2.2.3, $E(h)$ as 2.2.1, and $\hat{E}(h, \mathcal{D})$ as in 2.2.2. Then, with probability $1 - \delta$:

$$E(h) \leq \hat{E}(h, \mathcal{D}_{train}) + \sqrt{\frac{8}{N} \ln \frac{4m(2N, \mathcal{H})}{\delta}}$$

The bound tells us that $E(h)$ will be close to $\hat{E}(h, \mathcal{D}_{train})$ if $m(N, \mathcal{H})$ is small and N is large. Intuitively, this tells us that a set $\mathcal{H}$ that contains "simple" functions will make it easier to choose g such that generalisation error will be close to training error, where simple means: functions that realise a small number of dichotomies.

On the other hand, having a set $\mathcal{H}$ that can realise a large number of dichotomies on N points, will make it easier to find a function that will make $\hat{E}(h, \mathcal{D}_{train})$ small. Using a $\mathcal{H}$ with functions that are too simple is called **underfitting**. It occurs when we search for a function in the set of functions $\mathcal{H}$, when there is another, more diverse set of functions $\mathcal{G}$ which contain a function with lower generalisation error.

This analysis tells us that an optimally diverse $\mathcal{H}$ balances the tradeoff between the risk of overfitting, represented in the bound by m, and the risk of underfitting, represented by $\hat{E}$. In practice, underfitting is less of a problem than overfitting, since modern supervised machine learning algorithms search in extremely diverse spaces of functions $\mathcal{H}$. In fact, most $\mathcal{H}$ are so diverse that steps must be taken to avoid minimising $\hat{E}$ as much as is actually possible. These techniques are known as **regularisation**, which we will see an instance of in section **??**.

2.2.3 Validation

Statistical learning theory tells us how to design $\mathcal{H}$ given a dataset of limited size by revealing the relationship between $\hat{E}(h, \mathcal{D}_{train})$ and $E(h)$. While Vapnik-Chervonenkis analysis gives us a theoretical bound on $E(h)$, we may be interested in getting a concrete empirical estimate of E, e.g in order to decide whether a system is good enough to be put in to production, or to select so called **hyper-parameters**.

In general, $\mathcal{D}_{train}$ is unsuited for this estimation because of **bias**: we use $\mathcal{D}_{train}$ to specifically select g to minimise $\hat{E}(h, \mathcal{D}_{train})$, and so the performance of g on $\mathcal{D}_{train}$ is likely an optimistic estimate of E.

In order to get an unbiased empirical estimate of E, we can split $\mathcal{D}_{train}$ into two datasets. One is used for training. Lets call this $dtrain^{-}$ to distinguish it from and one is used for estimating E. Lets cal

2.3 Summary

In this section we have seen that the purpose of named entity recognition is to identify mentions of entities such as people, organisations and places in natural language. The purpose of relation extraction systems is to identify relationships between them.

We have seen that simple accuracy is uninformative as an evaluation measure in information extraction, and described the alternative precision and recall.

We have described the formal setting of on supervised machine learning. We have discussed concepts such as overfitting and noise, diversity of the set of functions $\mathcal{H}$ from which to choose h, and its impact on training and generalisation error.

Part 3

Neural Networks

In this part we describe how to define $\mathcal{H}$ using functions called **neural networks**. These functions have the advantage of being easy to adapt to multi-task learning. We begin by describing how to design a $\mathcal{H}$ with neural networks. We then turn to the issue of how to use $\mathcal{D}_{train}$ to search this hypothesis space. Lastly, we introduce specialised neural networks that are useful for natural language processing.

3.1 Feed-Forward Neural Networks

A feed-forward neural network is a function $h : \mathcal{X} \mapsto \mathcal{Y}$. To understand how it works, it's instructive to look at each part of its name in isolation.

h is called a **network** because it's a composition of L **layers** of other functions $f^{(l)}$. Each $f^{(l)}$ receives input from $f^{(l-1)}$. For example if $L = 2$, then $h(\mathbf{x}) = f^{(2)}(f^{(1)}(\mathbf{x}))$. We denote the input to $f^{(1)}$ as $\mathbf{x}^{(0)}$, which is identical to the input vector $\mathbf{x}$, except for an added **bias** component of 1, as described later in this section. each $f^{(l)}$ outputs a vector $\mathbf{x}^{(l)}$ of dimension $d^{(l)}$ which is the input of $f^{(l+1)}$. The dimensionality of these vectors determine the **width** of the network. The number of layers L is called the **depth** of the network. $f^{(L)}$ is called the **output layer**. The remaining functions $f^{(1)}$ to $f^{(L-1)}$ are called **hidden layers**.

The functions $f^{(1)}$ to $f^{(L)}$ are ordered by their index l. By ordered, we mean that the index of the innermost functions are smaller than the index of the outermost. h is called a **feed-forward** network because each $f^{(l)}$ can receive input only from functions $f^{(i)}$ if $l > i$. In other words, it's not possible for a function $f^{(l)}$ to feed its own output into itself, or any other function that it receives input from.

Finally h is called a **neural** network since its design is loosely based on neurons in the brain (Goodfellow et al., 2016). Each component x_i of the vector $\mathbf{x}^{(l)}$ can be seen as the output of a unit similar to a neuron. Each unit in layer l receives input from units in layer $l-1$. The output $x_i^{(l-1)}$ of unit i in layer $l-1$ is multiplied by a weight $w_{ij}^{(l)}$ that gives the strength of the connection between unit i in $l-1$ and unit j in l. Unit j sums all of the input it receives from units in layer $l-1$ to obtain its **activation** $a_j^{(l)} = \sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)} x_i^{(l-1)}$. To compute its output $x_j^{(l)}$, it applies an **activation function** $\sigma(a_j^{(l)})$ to its activation.

Activation functions model the behaviour of biological neurons by outputting a signal only when the activation is above a certain threshold. To make it possible to learn this threshold for each unit using the same activation function, we introduce a special **bias** unit that always outputs 1. The index of the bias unit in layer l is 0 by convention. Figure 3.1. shows how a unit j computes its output $x_j^{(l)}$ by combining the outputs of units in layer $l-1$.

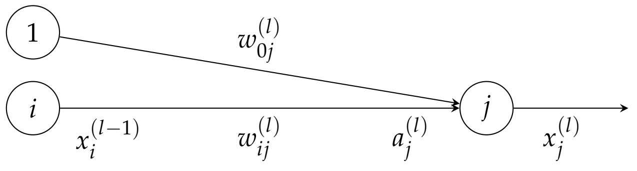
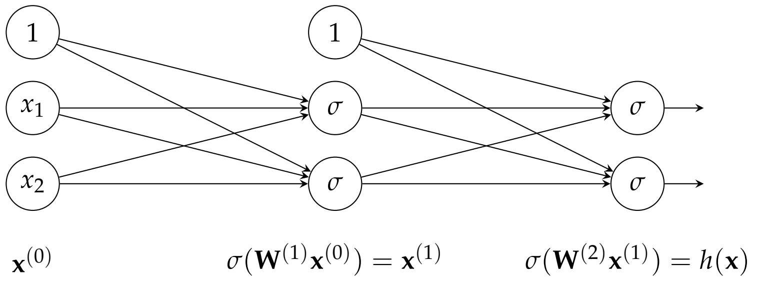


Figure 3.1
A visual representation of the connections between unit i in layer $l-1$, the bias unit in $l-1$, and unit j in layer l. The connection strength between these units is given by the weight $w_{ij}^{(l)}$ between i and j, and $w_{0j}^{(l)}$ between the bias unit and j. The activation $a_j^{(l)}$ at unit j is computed by $a_j^{(l)} = w_{ij}^{(l)} x_i^{(l)} + w_0^{(l)}$. The output $x_j^{(l)}$ of unit j is given by $x_j^{(l)} = \sigma(a_j^{(l)})$

Keeping track of the indices l, i and j quickly becomes confusing. By collecting all of the weights of connections going into unit j in layer l in a vector $\mathbf{w}_j^{(l)}$, the activation at unit j can be computed as a dot product $a_j^{(l)} = \mathbf{w}_j^{(l)} \cdot \mathbf{x}^{(l-1)}$. Moreover, we can compute the entire vector $\mathbf{a}^{(l)}$ of activations at layer l, by organising the weight vectors $\mathbf{w}_j^{(l)}$ in a matrix $\mathbf{W}^{(l)} = \begin{bmatrix} \mathbf{w}_1^{(l)} & \dots & \mathbf{w}_{d^{(l)}}^{(l)} \end{bmatrix}^T$, which leads to $\mathbf{a}^{(l)} = \mathbf{W}^{(l)} \mathbf{x}^{(l-1)}$.

By gathering the weights in matrices $\mathbf{W}^{(l)}$, we have simplified our view of h into a composition of matrix-vector products and element-wise application of activation functions. Figure 3.2 shows the parallel views of neural networks as networks of units and matrix-vector operations.



1
x_1
x_2
1
σ
σ
σ
σ
$\mathbf{x}^{(0)}$
$\sigma(\mathbf{W}^{(1)}\mathbf{x}^{(0)}) = \mathbf{x}^{(1)}$
$\sigma(\mathbf{W}^{(2)}\mathbf{x}^{(1)}) = h(\mathbf{x})$

Figure 3.2
A visual representation of $h(\mathbf{x}) = f_2(f_1(\mathbf{x}^{(0)}))$. The activation at each layer $\mathbf{a}^{(l)}$ is computed by $\mathbf{W}^{(l)}\mathbf{x}^{(l-1)}$. The output at each layer is computed by element-wise application of the activation function of $\sigma(\mathbf{a}^{(l)})$.

We now have all the components we need to specify $\mathcal{H}$ as a set of neural networks. The set is defined by the depth of the networks L, the number of units in each layer d_l , and the activation function σ. For a particular L, d_l, and σ, each $h \in \mathcal{H}$ corresponds exactly to a unique assignment of real numbers to all of its weights. We can make the dependence of h on its weights explicit by defining a vector $\mathbf{w} = \begin{bmatrix} w_{ij}^{(1)} & \dots & w_{ij}^{(L)} \end{bmatrix}$ and writing $h(\mathbf{x}, \mathbf{w})$ which means *the function h parameterised by the weight vector* $\mathbf{w}$. In the next section we discuss how to choose the activation functions at the layers of the network.

3.1.1 Activation Functions

Activation functions mimic the behaviour of neurons in the brain. A neuron emits a signal when the combined input it receives from other neurons exceeds a cer-

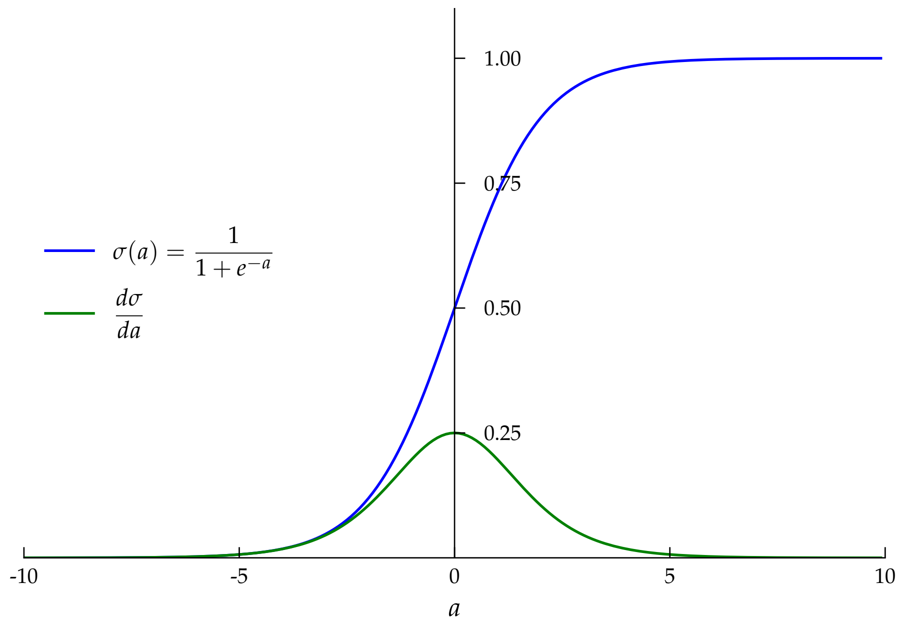


Figure 3.3
Sigmoid activation and its derivate. Sigmoid activation units have the disadvantage of ***saturating****, meaning that they become flat when a is large or small. This makes the derivative smaller than 1 everywhere, and much smaller than 1 almost everywhere.*

tain threshold. Activation functions achieve this by a variation of the step function, where an activation signal $a_j^{(l)}$ below the threshold is mapped to a value near zero, and an activation signal above the threshold is mapped to a value greater than zero. From a mathematical perspective, the role of activation functions is to introduce non-linearity in h, which allows it to approximate a much larger class of functions.

Many networks use **sigmoid** activation functions such as the classical sigmoid function $\sigma(a) = \frac{1}{1+\mathrm{e}^{-a}}$. These functions have the advantage of being differentiable everywhere. As we will see in section **??**, differential calculus is the fundamental tool for finding a good $h \in \mathcal{H}$, which makes differentiability a desirable quality. One drawback of sigmoid activation functions is that their derivates are small, as seen in figure 3.3. For example, we can show that max $\frac{d\sigma}{da} = \frac{1}{4}$. As we will see in section **??**, neural networks are trained by multiplying chains of derivatives. When these derivatives are smaller than 1, the magnitude of the derivative shrinks in the length of the chain of terms which can make learning from $\mathcal{D}_{train}$ extremely slow.

Because of this shrinking problem, the default recommendation today is to use **rectified linear units**, depicted in figure 3.4. These units use the activation function $\sigma(a) = \max(0, a)$. This function has the advantage that its derivative $\frac{d\sigma}{da} = 1$ when $a > 0$, and $\frac{d\sigma}{da} = 0$ when $a < 0$. This activation function is not strictly differentiable when $a = 0$. In practice however, this is not a big problem because a is rarely exactly 0, and we may arbitrarily choose $\sigma(0)$ to be either 0 or 1, and still successfully train our networks.

Often we would like the output of h to be a probability distribution over values in the label space $\mathcal{Y}$, since this makes it possible to design the so called **cost functions** with a principled technique **maximum likelihood**. For this reason it's common to use different activation functions in the output layer.

For example, named entity recognition can be seen as a multi-class classification

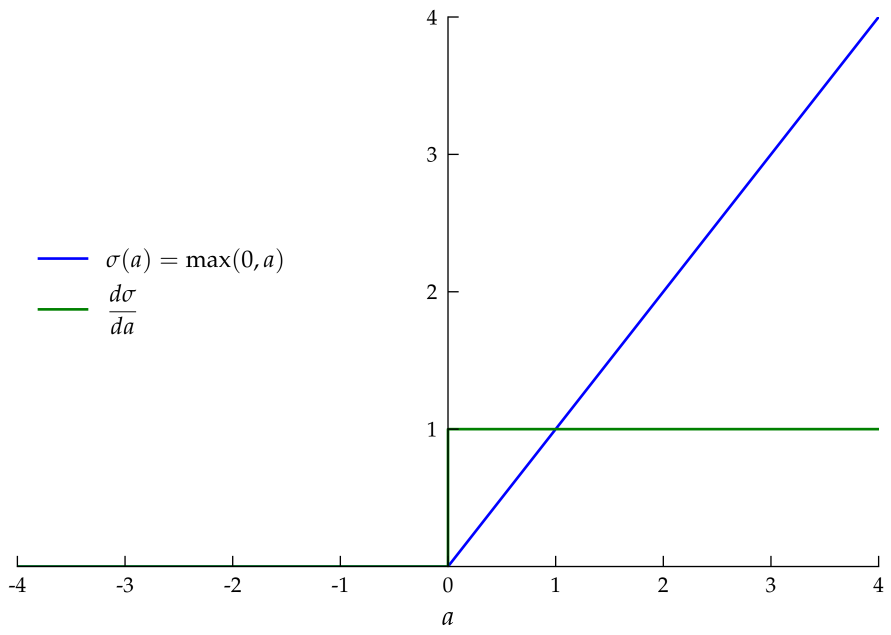


Figure 3.4
ReLU activation and its derivate. Unlike sigmoid activation, ReLU activation doesn't saturate. This means that the derivative of a unit remains large whenever that unit produces output.

problem, where each token in a sentence must be assigned one of a fixed set of C labels. To frame this as a probabilistic problem, we can encode each token label $\mathbf{y}$ as a vector of C probabilities such that component y_c of $\mathbf{y}_i \in \mathcal{D}_{train}$ is equal to 1 if $\mathbf{x}_i \in \mathcal{D}_{train}$ belongs to class c. All other components $y_{j \neq c}$ in $\mathbf{y}_i$ are equal to 0. This is known as **one-hot** encoding. $\mathbf{y}$ can be seen as a conditional probability distribution over each possible label given $\mathbf{x}_i$, that places all of the probability mass on label c.

With one hot encoding, we can design h to output vector with C components, where each component $c \in h$ gives the probability that $\mathbf{x}$ has class c. More formally, we can interpret $h(\mathbf{x})$ as conditional probability distribution $h(\mathbf{x})_c = P(y = c|\mathbf{x})$.

This type of output can be achieved by using the so-called **soft-max** activation function in the output layer. The soft-max activation is given by

$$\sigma(\mathbf{a})_c = \frac{\mathrm{e}^{a_c}}{\sum_{i=1}^{C} \mathrm{e}^{a_i}}$$

In words, the soft-max function makes sure that the output of h is a valid probability distribution, firstly by making sure that each component of $h(\mathbf{x})$ is positive by taking the exponent, and by making sure that $\sum_{c=1}^{C} h(\mathbf{x})_c = 1$ by dividing by the sum of all the exponentiated components. The last point means that unlike the other activation functions we have seen in this section, the soft-max must receive as input the vector $\mathbf{a}_L$ of all activations in layer L.

Having designed the output layer of h so that we can interpret its output as a conditional probability distribution, we can define the training error $\hat{E}(h, \mathcal{D}_{train})$, sometimes also called the **objective function** by the maximum likelihood principle, that quantifies the appropriateness of a weight vector $\mathbf{w}$ as a probability using the samples in $\mathcal{D}_{train}$. This function is crucial for finding $g \in \mathcal{H}$. We study it in the next section.

3.1.2 Objective Function

We would like a function that lets us compare functions in $\mathcal{H}$ in terms of how well they predict the samples in $\mathcal{D}_{train}$. Such a function is often called an objective function, borrowing terminology from the mathematical field of optimisation.

In section 3.1.1 we saw that the combination of one-hot encoding of the labels in $\mathcal{Y}$ and soft-max activation in the output layer of h allows us to interpret $h(\mathbf{x})$ as a conditional probability distribution. In the following, we will use a convenient rewrite of the formula given in 3.1.1:

$$P(y \mid \mathbf{x}) = \prod_{c=1}^{C} h(\mathbf{x}, \mathbf{w})_c^{y_c}$$

Where y is the true label for $\mathbf{x}_i$ and y_c is component c of the one-hot vector $\mathbf{y}$. This formulation works because $\mathbf{y}$ is a one-hot vector, which means exactly one component of $\mathbf{y}$ is equal to 1, and all other components are equal to 0. So if $\mathbf{y} = \begin{bmatrix}0 & 1 & 0\end{bmatrix}^T$ and $h(\mathbf{x}) = \begin{bmatrix}.1 & .8 & .1\end{bmatrix}^T$, then $P(y \mid \mathbf{x}) = (0.1^0)(0.8^1)(0.1^0) = 0.8$.

If we design $\mathcal{H}$ in such a way that every h outputs a probability, we can use the principle of maximum likelihood to derive a plausible objective function. Maximum likelihood estimation uses the likelihood function to compute the probability of $\mathcal{D}_{train}$ by interpreting h as a probability distribution parameterised by $\mathbf{w}$:

Definition 3.1.1 (likelihood function)**.** Let $\mathcal{D}_{train} = \{(\mathbf{x}_i, \mathbf{y}_i)\}$ be a set of N training examples, where each $\mathbf{y}_i$ is a C dimensional one-hot vector. Let $h(\mathbf{x}, \mathbf{w})$ be a neural network which outputs conditional probability distributions over the C possible classes, such that $\sum_{c=1}^{C} h(\mathbf{x}, \mathbf{w})_c = 1$ and $0 \leq c \leq 1 \, \forall c \in h(\mathbf{x}, \mathbf{w})$. Furthermore, let the notation y_{ic} denote component c of the one-hot label for example i. Then the likelihood $P(\mathcal{D}_{train} \mid \mathbf{w})$ is:

$$P(\mathcal{D}_{train} \mid \mathbf{w}) = \prod_{i=1}^{N} \prod_{c=1}^{C} h(\mathbf{x}_i, \mathbf{w})_c^{y_{ic}}$$

Informally, we can think of the likelihood function as asking the question, *assuming that $h(\mathbf{x})$ is the true distribution from which $\mathcal{D}_{train}$ was sampled, what is the probability of observing the samples in $\mathcal{D}_{train}$?* Using the likelihood function to find a good $h \in \mathcal{H}$ is a matter of finding a weight vector $\mathbf{w}$ that maximise the likelihood of observing $\mathcal{D}_{train}$.

Computing a large number of products of probabilities on a computer can be problematic because of **numerical underflow**. Since computers have limited precision, small positive numbers may be actually be represented as small negative numbers, which is bad because the likelihood function is a probability.

To avoid numerical underflow, the **log-likelihood** $\ln P(\mathcal{D}_{train} \mid \mathbf{w})$ is often used instead. The logarithm turns the products into sums, which are entirely unproblematic for computers. Since the natural logarithm is a monotonic function, applying it to the likelihood function does not change the properties we are interested in.

Finally, most other objective functions for supervised machine learning are defined in terms of training error $\hat{E}(h, \mathcal{D}_{train})$. In this view, searching for a good $h \in \mathcal{H}$ becomes a minimisation problem. For consistency, maximum likelihood estimation is often turned into a minimisation problem by using the **negative log-likelihood** $-\ln P(\mathcal{D}_{train} \mid \mathcal{W})$. In addition, most error measures are invariant to dataset size which makes it easy to compare the performance of a model on different data sets. To give the negative log-likelihood this property, it's common to divide by N, giving what is called the **average negative log-likelihood**. Minimising the average negative log-likelihood is clearly identical to maximising the likelihood, since $\max f(\mathbf{x}) = \min -f(\mathbf{x})$, and dividing by N doesn't change the optimum.

Definition 3.1.2 (average negative log-likelihood)**.** Let $\mathcal{D}_{train}$ and $h(\mathbf{x}; \mathcal{W})$ be defined as in definition 3.1.1. Then the negative log likelihood $-\ln P(\mathcal{D}_{train} \mid \mathcal{W})$ is:

$$\hat{E}(\mathbf{w}, \mathcal{D}_{train}) = -\frac{1}{N} \ln P(\mathcal{D}_{train} \mid \mathbf{w}) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{c=1}^{C} y_{ic} \ln h(\mathbf{x}_i, \mathbf{w})_c$$

This error measure is also known as **cross-entropy error**, in which the term $-\sum_{c=1}^{C} y_{ic} \ln h(\mathbf{x}_i, \mathbf{w})_c$ is taken as the error measure $e(h(\mathbf{x}_i), \mathbf{y}_i)$, which allows us to write $\hat{E}$ in the familiar form used in section 2.2.2: $\hat{E}(h, \mathcal{D}_{train}) = \frac{1}{N} \sum_{i=1}^{N} e(h(\mathbf{x}_i), \mathbf{y}_i)$.

In the next section, we will see how to use the average negative log-likelihood to find a good $h \in \mathcal{H}$.

3.2 Learning Algorithm

Finding a function $h \in \mathcal{H}$ that maximises the likelihood of $\mathcal{D}_{train}$ is an optimisation problem. Optimisation is solved by answering the question: *how does $\hat{E}$ change when we change h?* We answer questions of this type with differential calculus. Sadly, finding the h which maximises the likelihood by analytical differentiation is impossible. Neural network optimisation is therefore solved using an iterative algorithm called **gradient descent**, which we describe in this section. We then explore an algorithm for computing the gradient of $\hat{E}$ called **backpropagation**. Finally, we look into **regularisation** which are tools for constraining the learning algorithm in order to avoid overfitting. Lastly, we describe a specific learning algorithm called **Adam**, an efficient variation on gradient descent.

3.2.1 Gradient Descent

We want to find a $h \in \mathcal{H}$ that minimises $\hat{E}$ as described in section 3.1.2. Each h is defined exactly by the weight vector $\mathbf{w}$. $\hat{E}$ can't be minimised analytically, since its derivative with respect to $\mathbf{w}$ is a system of non-linear equations, which in general does not have an analytical solution. We therefore look for h by choosing an initial weight vector $\mathbf{w}_0$, and iteratively reduce $\hat{E}$: In iteration i, the weight vector $\mathbf{w}_i$ is found by taking a small step η in a direction given by a vector $\mathbf{v}$, or more formally: $\mathbf{w}_i = \mathbf{w}_{i-1} + \eta\mathbf{v}$. The main question is, which direction should we choose?

$\hat{E}$'s direction of steepest descent at each $\mathbf{w}_i$ is given by the gradient $\nabla\hat{E}$. $\nabla\hat{E}$ is a vector where each component is a partial derivative $\frac{\partial}{\partial w}\hat{E}$ with respect to a weight $w \in \mathbf{w}$:

Definition 3.2.1 (gradient)**.** Let $w_{ij}^{(l)} \in \mathbf{w}$ be every weight in h, and let $\hat{E}$ be defined as in definition 3.1.2. Then the gradient $\nabla\hat{E}$ is:

$$\nabla\hat{E} = \begin{bmatrix} \frac{\partial}{\partial w_{ij}^{(1)}}\hat{E} \\ \vdots \\ \frac{\partial}{\partial w_{ij}^{(L)}}\hat{E} \end{bmatrix}$$

The gradient can be used for computing the rate of change of $\hat{E}$ in the direction of a unit vector $\mathbf{u}$ by taking the dot product $\mathbf{u}^T\nabla\hat{E}$. We would like to know in which direction $\mathbf{u}$ we should change $\mathbf{w}_i$ in order to make $\hat{E}$ as small as possible. The dot product of $\mathbf{u}^T \nabla \hat{E}$ is equal to $|\nabla \hat{E}||\mathbf{u}| \cos \theta$ where θ is the angle between $\nabla \hat{E}$ and $\mathbf{u}$. The direction $\mathbf{u}$ with the greatest positive rate of change of $\hat{E}$ is the direction in which $\theta = 0°$, in other words, the same direction as $\nabla \hat{E}$. The direction with the greatest negative rate of change of $\hat{E}$ is the direction in which $\theta = 180°$, in other words, the direction $-\nabla \hat{E}$. This means that we can make $\hat{E}$ smaller by taking a small step η in the direction $-\nabla \hat{E}$, such that $\mathbf{w}_i = \mathbf{w}_{i-1} - \eta \nabla \hat{E}$. A small example is given in figure 3.5 and 3.6.

One challenge of gradient descent is that $\nabla \hat{E} = \frac{1}{N} \sum_{i=1}^{N} \nabla e(h(\mathbf{x}_i, \mathbf{y}_i)$ is based on all the examples in $\mathcal{D}_{train}$. This means that computing $\nabla \hat{E}$ requires one full iteration over the training set. If the training set is large, this means that every update to the weights $\mathbf{w}$ takes a long time, which makes learning slow. **Stochastic gradient descent** is a common variation of gradient descent which addresses this problem. In stochastic gradient descent, a single training example $(\mathbf{x}_i, \mathbf{y}_i)$ is sampled from $\mathcal{D}_{train}$. Instead updating $\mathbf{w}_i$ by the gradient $-\nabla \hat{E}$ over all the training examples, we update the weights based on the gradient of a single example $\mathbf{w}_i = \mathbf{w}_{i-1} - \eta \nabla e(h(\mathbf{x}_i, \mathbf{y}_i)$. Since each sample in $\mathcal{D}_{train}$ can be drawn with probability $\frac{1}{N}$, stochastic gradient descent is identical to gradient descent in expectation:

$$\mathbb{E}(-\nabla e(h(\mathbf{x}_i), \mathbf{y}_i)) = \frac{1}{N} \sum_{i=1}^{N} -\nabla e(h(\mathbf{x}_i), \mathbf{y}_i) = -\nabla \hat{E}$$

Another practical issue of using gradient descent is how to choose the learning rate η. We investigate a method called Adam that uses a heuristic to select η dynamically in each iteration in section 3.2.4.

Gradient descent gives us an algorithm for minimising $\hat{E}$ using $\nabla \hat{E}$. In the next section we explore an algorithm for computing $\nabla \hat{E}$ called backpropagation.

3.2.2 Backpropagation

We want to compute $\nabla \hat{E}$ in order to use gradient descent to make $\hat{E}$ small. Because of the sum and product rules of differential calculus, we can simplify our analysis by computing $\nabla \hat{E}$ of a single example $(\mathbf{x}, \mathbf{y})$:

$$\nabla \hat{E} = \nabla \frac{1}{N} \sum e(h(\mathbf{x}_i), \mathbf{y}_i) = \frac{1}{N} \sum \nabla e(h(\mathbf{x}_i), \mathbf{y}_i)$$

In our explanation we will use the cross-entropy error $e(h(\mathbf{x}), \mathbf{y}) = -\sum_{c=1}^{C} y_c \ln h(\mathbf{x})_c$ as an example.

If we can derive a generic formula for a single element $\frac{\partial e}{\partial w_{ij}^{(l)}}$ of ∇e, we can compute all of ∇e. The partial derivative is asking the question *how does e change if we change $w_{ij}^{(l)}$?* The weight $w_{ij}^{(l)}$ influences e only through the activation $a_j^{(l)}$. We can therefore decompose the derivative using the chain rule of calculus:

$$\frac{\partial e}{\partial w_{ij}^{(l)}} = \frac{\partial e}{\partial a_j^{(l)}} \frac{\partial a_j^{(l)}}{\partial w_{ij}^{(l)}}$$

The term $\frac{\partial a_j^{(l)}}{\partial w_{ij}^{(l)}}$ is easy to compute, because $a_j^{(l)}$ depends directly on $w_{ij}^{(l)}$ in a simple sum:

$$\frac{\partial a_j^{(l)}}{\partial w_{ij}^{(l)}} = \frac{\partial}{\partial w_{ij}^{(l)}} \sum_{k=0}^{d^{(l-1)}} w_{kj}^{(l)} x_k^{(l-1)} = x_i^{l-1}$$

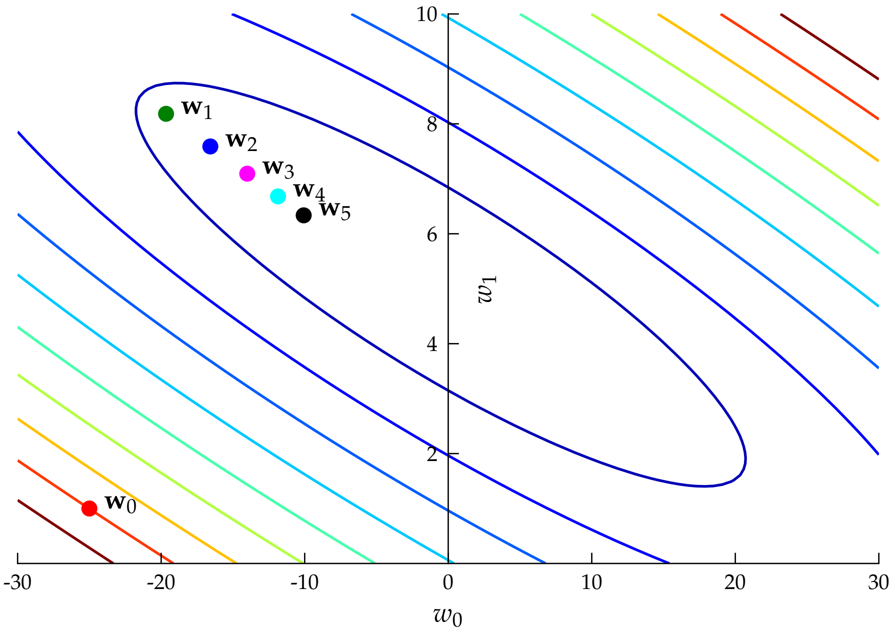


Figure 3.5
Level curves of squared training error $\hat{E}(h, \mathcal{D}_{train}) = \frac{1}{N}\sum_{i=1}^{N}(h(\mathbf{x}_i) - y_i)^2$ *for a toy* $\mathcal{D}_{train}$ *shown in 3.6, and the simple* $\mathcal{H} = \{h = \mathbf{w}^T\mathbf{x}^{(0)} \mid \mathbf{w} \in \mathbb{R}^2\}$*.* $\hat{E}$ *has its minimum at* $(0, 5)$*. Each colored dot corresponds to a step* $\mathbf{w}_i$ *in gradient descent using a fixed learning rate* η*. The first step from* $\mathbf{w}_0$ *to* $\mathbf{w}_1$ *makes a lot of progress towards the minimum, and each subsequent update to* $\mathbf{w}_i$ *is much less dramatic.*

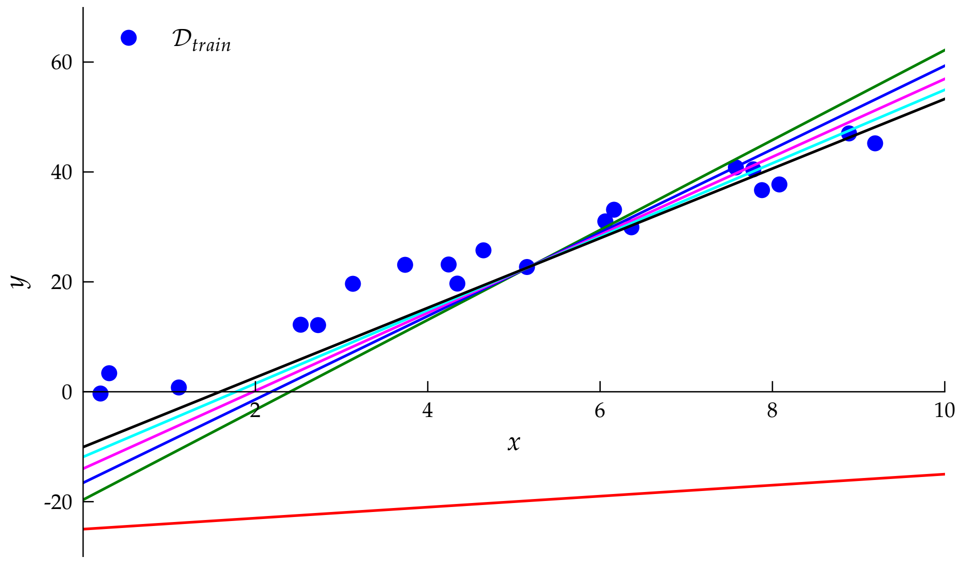


Figure 3.6
The training data $\mathcal{D}_{train}$ *used in figure 3.5. The colored lines correspond to* $h(\mathbf{x}, \mathbf{w}_i) = 0$ *for each weight vector* $\mathbf{w}_i$ *found by gradient descent in figure 3.5, such that for example* $h(\mathbf{x}, \mathbf{w}_0) = 0$ *is given by the red line. We see as gradient descent makes* $\hat{E}$ *smaller, the lines fit* $\mathcal{D}_{train}$ *better.*

The term $\frac{\partial e}{\partial a_j^{(l)}}$ is more involved since $a_j^{(l)}$ influences e through units in layers $m > l$ that directly or indirectly receives input from unit j in layer l. Computing $\frac{\partial e}{\partial a_j^{(l)}}$ therefore requires a number of applications of the chain rule that depend on the number of layers between $a_j^{(l)}$ and the output. The backpropagation algorithm solves this problem by defining $\delta_j^{(l)} = \frac{\partial e}{\partial a_j^{(l)}}$, and deriving a recursive formula for $\delta_j^{(l)}$ that relates it to $\delta_j^{(l-1)}$.

We start by computing $\delta_j^{(L)}$, since the activation in the output layer $a_j^{(L)}$ influences e directly and can therefore be used as a base case for the recursion, that doesn't depend on any other $\delta_j^{(l)}$

Lets start by rewriting e in terms of the output of layer L:

$$e(h(\mathbf{x}), \mathbf{y}) = -\sum_{c=0}^{C} y_c \ln x_c^{(L)}$$

Where $x_c^{(L)}$ is the output of unit c in the output layer. When using soft-max activation in the output layer would mean that $x_c^{(L)} = \sigma(\mathbf{a}^{(L)})_c = \frac{e^{a_c^{(l)}}}{\sum_{i=1}^{C} e^{a_i^{(l)}}}$.

Since $a_j^{(L)}$ affects e through the soft-max activation, we will need to compute the derivative of the soft-max activation with respect to the activation $\frac{\partial x_i^{(L)}}{\partial a_j^{(L)}}$ in order to compute $\delta_j^{(L)}$. This derivative is different depending on which output $x_i^{(L)}$, and which activation $a_j^{(L)}$ we consider.

If $i = j$, that is, we are taking the derivative of the output of a unit with respect to its activation, we get:

$$\begin{aligned}
\frac{\partial x_i^{(L)}}{\partial a_i^{(L)}} &= \frac{\partial}{\partial a_i^{(L)}} \frac{e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} = \frac{e^{a_i^{(L)}} \sum_{c=1}^{C} e^{a_c^{(L)}} - e^{a_i^{(L)}} e^{a_i^{(L)}}}{\left(\sum_{c=1}^{C} e^{a_c^{(L)}}\right)^2} = \frac{e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} \frac{\left(\sum_{c=1}^{C} e^{a_c^{(L)}}\right) - e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} \\
&= \frac{e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} \left(1 - \frac{e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}}\right) \\
&= x_i^{(L)}(1 - x_i^{(L)})
\end{aligned}$$

If $i \neq j$, in other words, if we are taking the derivative of the output of a unit with respect to the activation of another unit, we get:

$$\frac{\partial x_i^{(L)}}{\partial a_j^{(L)}} = \frac{0 - e^{a_i^{(L)}} e^{a_j^{(L)}}}{\left(\sum_{c=1}^{C} e^{a_c^{(L)}}\right)^2} = -\frac{e^{a_i^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} \frac{e^{a_j^{(L)}}}{\sum_{c=1}^{C} e^{a_c^{(L)}}} = -x_i^{(L)} x_j^{(L)}$$

Armed with $\frac{\partial x_i^{(L)}}{\partial a_j^{(L)}}$, we can go on to compute $\delta_j^{(L)}$:

$$\begin{aligned}
\delta_j^{(L)} &= \frac{\partial e}{\partial a_j^L} = -\sum_{c=1}^{C} y_c \frac{\partial}{\partial a_j^L} \ln x_c^{(L)} = -\sum_{c=1}^{C} y_c \frac{1}{x_c^{(L)}} \frac{\partial x_c^{(L)}}{\partial a_j^{(L)}} = -\frac{y_j}{x_j^{(L)}} \frac{\partial x_j^{(L)}}{\partial a_j^{(L)}} - \sum_{c \neq j}^{C} \frac{y_c}{x_c^{(L)}} \frac{\partial x_c^{(L)}}{\partial a_j^{(L)}} \\
&= -\frac{y_j}{x_j^{(L)}} x_j^{(L)}(1 - x_j^{(L)}) - \sum_{c \neq j}^{C} \frac{y_c}{x_c^{(L)}}(-x_c^{(L)} x_j^{(L)}) = -y_j + y_j x_j^{(L)} + \sum_{c \neq j}^{C} y_c x_j^{(L)} \\
&= -y_j + \sum_{c=1}^{C} y_c x_j^{(L)} = -y_j + x_j^{(L)} \sum_{c=1}^{C} y_c \\
&= x_j^{(L)} - y_j
\end{aligned}$$

Finally, we see that the derivative of the error with respect to the activation of unit j in the output layer is simply $x_j^{(L)} - y_j$.

Having derived a formula for $\delta_j^{(L)}$, we can go on to recursively derive $\delta_i^{(l-1)}$. Since e depends on $a_i^{(l-1)}$ only through $x_i^{(l-1)}$, we can use the chain rule to decompose $\delta_i^{(l-1)}$:

$$\delta_i^{(l-1)} = \frac{\partial e}{\partial a_i^{(l-1)}} = \frac{\partial e}{\partial x_i^{(l-1)}} \frac{\partial x_i^{(l-1)}}{\partial a_i^{(l-1)}}$$

The derivative of the output of unit i with respect to its input is simply the derivative of the activation function σ. We leave this generic here:

$$\frac{\partial x_i^{(l-1)}}{\partial a_i^{(l-1)}} = \sigma'(a_i^{(l-1)})$$

Since e depends on $x_i^{(l-1)}$ through the activation of every unit j that i is connected to, the chain rule tells us that we must sum the effects on e of changing $x_i^{(l-1)}$:

$$\frac{\partial e}{\partial x_i^{(l-1)}} = \sum_{i=1}^{d^{(l)}} \frac{\partial a_j^{(l)}}{\partial x_i^{(l-1)}} \frac{\partial e}{\partial a_j^{(l)}} = \sum_{i=1}^{d^{(l)}} w_{ij}^{(l)} \delta_j^{(l)}$$

We now finally have a recursive formula for $\delta_i^{(l-1)}$:

$$\delta_i^{(l-1)} = \frac{\partial e}{\partial a_i^{(l-1)}} = \sigma'(a_i^{(l-1)}) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)} \delta_j^{(l)}$$

To summarise, we now have a recursive formula for every weight component of the gradient $\frac{\partial e}{\partial w_{ij}^{(l)}}$ given by:

$$\frac{\partial e}{\partial w_{ij}^{(l)}} = x_i^{(l-1)} \delta_j^{(l)}, \quad \delta_j^{(l)} = \sigma'(a_i^{(l)}) \sum_{i=1}^{d^{(l+1)}} w_{ij}^{(l+1)} \delta_j^{(l+1)}$$

3.2.3 Regularisation

In section 2.2.2 we saw that the distance between E and $\hat{E}(h, \mathcal{D}_{train})$ is bounded by a function that's roughly a measure of the diversity of $\mathcal{H}$. In this section we discuss techniques for restricting the learning algorithm to search only in subsets of $\mathcal{H}$, with the aim of reducing E. These techniques are collectively known as regularisation.

For a $\mathcal{H}$ thats parameterized by a weight vector $\mathbf{w}$, such as the hypothesis space given by a particular neural network architecture, we can limit the region of weight space that our learning algorithm is allowed to consider by imposing the constraint that the norm of $\mathbf{w}$ must be smaller than some constant C. This has the effect that the weights can be selected only from a limited spherical region around the origin. This reduces the effective number of different hypotheses available during learning, and the Vapnik-Chervonenkis bound gives us confidence that this should improve generalisation.

If the weights $\mathbf{w}^*$ that minimises the unconstrained training error $\hat{E}(\mathbf{w}, \mathcal{D}_{train})$ lie outside this ball, then the weights $\bar{\mathbf{w}}$ that minimises $\hat{E}$ while still satisfying the constraint $\bar{\mathbf{w}}^T\bar{\mathbf{w}} \leq C$, must have norm equal to C, in other words lie on the surface of the sphere with radius C. The normal vector to this surface at any $\mathbf{w}$ is $\mathbf{w}$ itself. At $\bar{\mathbf{w}}$, the normal vector must point in the exact opposite direction of $\nabla\hat{E}$, since otherwise $\nabla\hat{E}$ would have a component in along the border of the constraint sphere, and we could decrease $\hat{E}$ by moving along the border of the sphere in the direction of $\nabla\hat{E}$ and still satisfy the constraint. In other words, the following equality holds for $\bar{\mathbf{w}}$:

$$\nabla\hat{E}(\bar{\mathbf{w}}, \mathcal{D}_{train}) = -2\lambda\bar{\mathbf{w}}$$

Where λ is some proportionality constant. Equivalently, $\bar{\mathbf{w}}$ satisfy:

$$\nabla(\hat{E}(\bar{\mathbf{w}}, \mathcal{D}_{train}) + \lambda\bar{\mathbf{w}}^T\bar{\mathbf{w}}) = \mathbf{0}$$

Because $\nabla(\bar{\mathbf{w}}^T\bar{\mathbf{w}}) = 2\bar{\mathbf{w}}$. In other words, for some $\lambda > 0$, $\bar{\mathbf{w}}$ minimises a new error function which we will call **augmented error** $\bar{E}(\mathbf{w}, \mathcal{D}_{train})$:

$$\bar{E}(\mathbf{w}, \mathcal{D}_{train}) = \hat{E}(\mathbf{w}, \mathcal{D}_{train}) + \lambda\mathbf{w}^T\mathbf{w}$$

This means that the problem of minimising $\hat{E}(\mathbf{w}, \mathcal{D}_{train})$ constrained by $\mathbf{w}^T\mathbf{w} \leq C$ is equivalent of minimising $\bar{E}(\mathbf{w}, \mathcal{D}_{train})$. This is useful because minimising $\bar{E}(\mathbf{w}, \mathcal{D}_{train})$ can be done by gradient descent, which makes it a useful regularisation scheme for neural networks where analytical solutions are not possible in general.

This particular form of regularisation, where a penalty on the norm of the weight vector is added to the minimisation objective, is called **weight decay**. To see why, lets consider a single step of the gradient descent algorithm when minimising $\bar{E}(\mathbf{w}, \mathcal{D}_{train})$. In iteration i, the weight vector $\mathbf{w}_i$ is given by:

$$\mathbf{w}_i = \mathbf{w}_{i-1} - \eta\nabla\bar{E}(\mathbf{w}, \mathcal{D}_{train}) = \mathbf{w}_{i-1}(1 - 2\eta\lambda) - \eta\nabla\hat{E}(\mathbf{w}_{i-1}, \mathcal{D}_{train})$$

In words, the added norm penalty of $\bar{E}(\mathbf{w}, \mathcal{D}_{train})$ has the effect of pulling the vector $\mathbf{w}_i$ towards $\mathbf{0}$, by multiplying by $1 - 2\eta\lambda$ in each iteration. In this way, weight decay is limiting the region that gradient descent can explore in a finite number of iterations, and is therefore limiting the diversity of $\mathcal{H}$.

3.2.4 Adam

3.3 Convolutional Neural Networks

A convolution is a mathematical operation that takes as input two functions f and k, commonly written as $f * k$.

Definition 3.3.1 (convolution). Let $f(x) \in \mathbb{R}$ and $k(x) \in \mathbb{R}$ be two real-valued functions defined for the entire real number line. Then the convolution $f * k$ is defined as

$$(f * k)(x) = \int f(y)k(x - y)dy$$

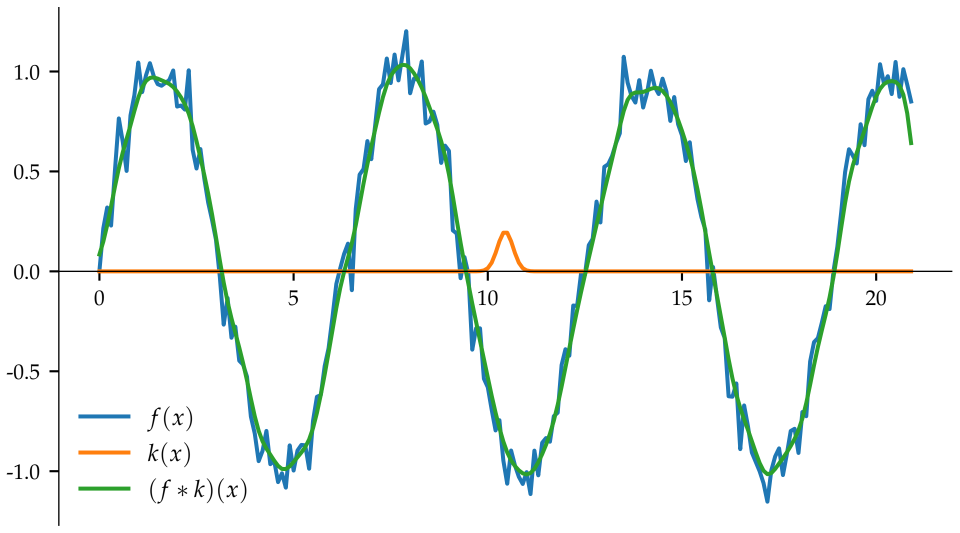


Figure 3.7
Visualisation of a noisy signal f convolved with a small Gaussian kernel k. The output of the convolution $f * k$ captures the general trend of f by averaging the outputs of f at every x, such values of f of inputs close to x contribute more to the output of the convolution, than inputs far away from x thanks to the weights of the Gaussian kernel.

In practical applications involving computers, f and k are discrete, and the integral turns into a sum:

$$(f * k)(x) = \sum_{y=-\infty}^{\infty} f(y)k(x-y)$$

Most functions in practical applications of convolutions represent signals such as images, sound or text, which are only defined over a limited range of indices x. In these cases it's assumed that whenever x is beyond the domain of f or k, the output of either function is 0.

We can think of a convolution as a weighted sum of the output of f where the output of k acts as the weights. This view of convolution is used heavily in signal processing applications, where k is chosen to produce certain properties in the convolution output, such as reducing noise in f. In this setting k is often referred to as a **kernel**. As an example consider the noisy signal convolved with a gaussian kernel in figure 3.7.

The kernel k can also act as a **feature detector**. When the output of f is closely correlated with the output of k, the output of the convolution spikes. See for example figure 3.8.

Convolutional neural networks are neural networks that take advantage of convolutions as feature detectors. By arranging the layers and weights in the network in specific ways, we can construct a network such that the output of each layer l is the output of layer $l-1$ convolved with a kernel k, where the weights of k are exactly the neural network weights connecting the units in layer l and $l-1$.

Specifically, the weights connecting layers l and $l-1$ in a convolutional neural network should be arranged such that they are:

sparse each unit in layer l receives input from a small number of units layer $l-1$.

shared the weights connecting units in layer l and $l-1$ are shared across the layer, in the same way that the same kernel weights are used at every index x in the convolution operation. See figure 3.9.

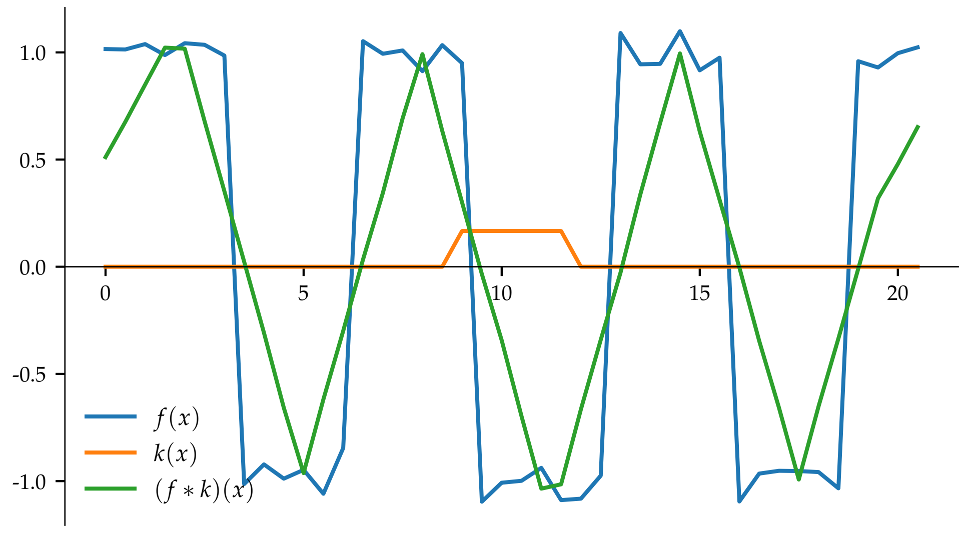


Figure 3.8
Visualisation of convolutional kernel as feature detector. When the signal f is similar to the kernel, the output of the convolution is maximally positive.

These restrictions on the network architecture reduces the number of unique weights of the model. This has the effect of reducing both the memory requirements of storing the network, but also limits the number of operations required to compute the output of the network for a given input.

Intuitively, the output at each unit u in l in a convolutional layer indicates how strongly the feature detected by the kernel given by its connecting weights is present in the output of units that u connects to in layer $l-1$. Since the weights are learned by gradient descent, the feature detected by units in layer l is learnt as well.

Often, the simple presence or absence of a feature in the output of layer $l-1$ is very informative for the classification task the convolutional network was built to solve. The exact position of a detected feature in layer $l-1$ is often less informative however. For this reason, convolutional layers are often interleaved with so called **pooling layers**. The output of a pooling layer can be thought of as a summary how strongly a feature is detected in layer l, that discards information about the exact position at which the features was detected. Very commonly, max-pooling is used which simply outputs the maximum value over all outputs of units in layer l.

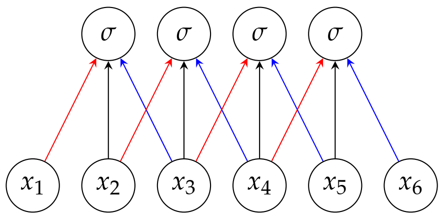


Figure 3.9
Visual representation of a one-dimensional convolution implemented as the first layer of a convolutional neural network. The connections between the input layer and the convolutional layer are sparse in that each unit is connected only to three of six inputs. The colors of the connections indicate how the weights are shared.

3.4 Word Vectors

The way text is represented in a computer doesn't in general encode any information about semantic similarities between words or sentences. Instead, text is most often represented as sequences of discrete symbols. Learning a h that maps from discrete features without any concept of distance, such as words, to a prediction, such as the presence of a named entity, may be more difficult than learning a mapping from continuous features to a prediction, since a continuous function can be expected to have some smoothness properties, i.e similar inputs should have similar outputs (Bengio et al., 2003).

For this reason some effort has been devoted to designing real-valued vector representation of words, so called **word vectors**, that encode semantic similarities, such that words with similar meaning are close to each other in word-vector space. The notion of "meaning" of a word is a philosophically challenging one. A simple definition which leads to simple but useful algorithms is that words have similar meaning if they are used in similar contexts.

This leads to the idea of representing words as vectors of co-occurrence counts. Two words w_i and w_j co-occur in a context of c words, if w_j appears somewhere in a window of c words from w_i in some piece of text. By representing w_i as a vector $\mathbf{w}_i \in \mathbb{R}^V$ of co-occurrence counts for the V words in some vocabulary, words that occur in similar contexts will be close to each other in co-occurrence vector space.

The main problems with this representation is that V may be very large, and $\mathbf{w}_i$ may be very sparse, that is, most of its components are 0 since most words never co-occur together. Recent solutions to this problem learn lower dimensional word vectors using co-occurrence statistics. **GloVe** is a recent and successful technique for learning word vectors that encode much useful syntactic and semantic information (Pennington et al., 2014). In GloVe, each word w_i is represented by a word vectors $\mathbf{w}_i$, and a context word vector $\tilde{\mathbf{w}}_i$. The vectors are initialised randomly

Glove vectors are learned by minimising the objective function:

$$\sum_{i=1}^{V}\sum_{i=1}^{V} f(\mathbf{X}_{ij})(\mathbf{w}_i^T\tilde{\mathbf{w}}_j + b_i + \tilde{b}_j - \ln \mathbf{X}_{ij})^2$$

Where $\mathbf{X}_{ij}$ is the co-occurrence count for word w_i and w_j, and b_i and $\tilde{b}_j$ are bias terms. f is a weighting function that gives low weight to infrequent terms and caps extremely frequent terms, defined as:

$$f(x) = \begin{cases} (x/x_{max})^{3/4} & \text{when } x < x_{max} \\ 1 & \text{otherwise} \end{cases}$$

Minimising this objective leads to word vectors whose dot products are close to log-co-occurrence counts for the words they represent. It can be shown that this has the effect that word vector differences encode information about ratios of log-co-occurrence probabilities which are highly informative of semantic similarity.

It is now common practice to incorporate word vectors in neural network models for natural language processing tasks in a so called embedding layer. In this scheme, the components of the word vectors are parameters that can be trained by back propagation to yield word vector representations that are informative for a given task. These word embedding vectors, or simply word embeddings, can be initialised with small random components as any other neural network parameter, or they can be initialised with pre-learned word vectors, for example GloVe vectors.

Part 4

Multi-Task Learning

Part 5

Experiment

5.1 Target Task

5.2 Auxiliary Tasks

5.3 Network Architecture

Part 6

Results

Part 7

Discussion

Part 8

Conclusion

Bibliography

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Appendix A

Appendix

A.1 First