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Master Thesis

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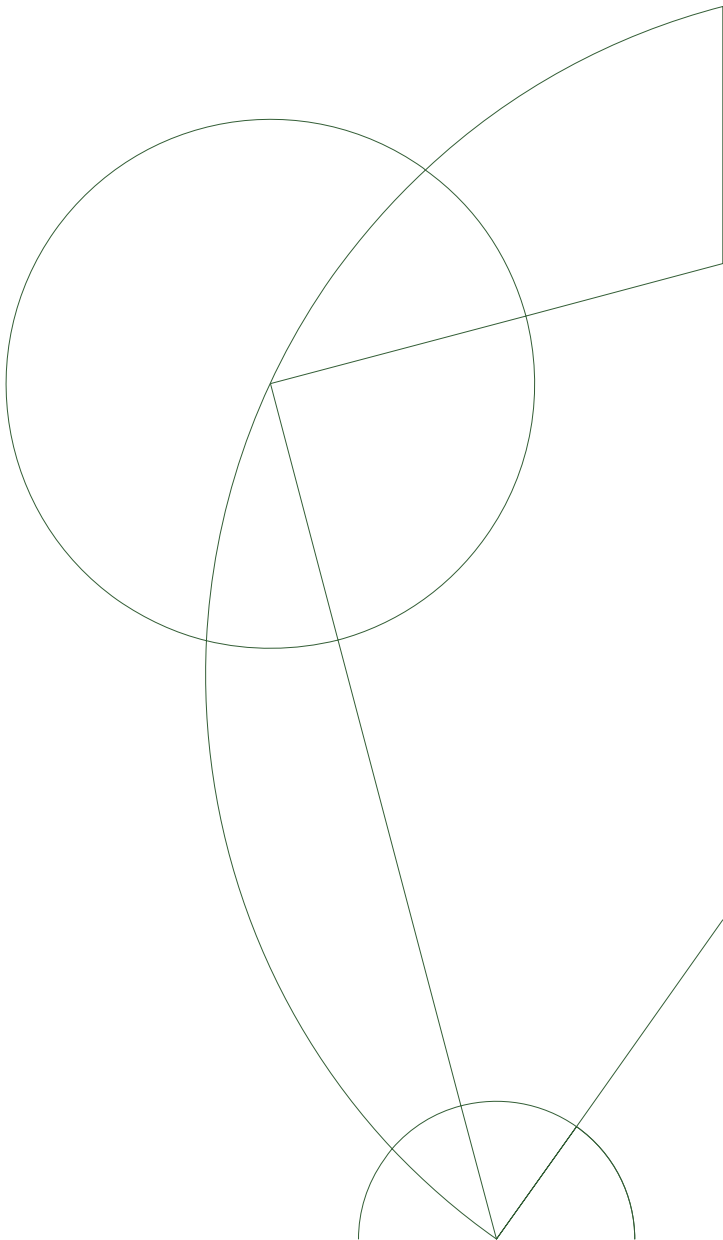
Deep Multi-Task Learning

For Relation Extraction



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Abstract

In this thesis we investigate the usefulness of a multi-task, convolutional neural network architecture for relation classification. We review the relevant theoretical and practical research literature for relation classification, supervised machine learning, convolutional neural networks, and deep multi-task learning. We test a state-of-the-art multi-task convolutional neural network architecture designed for relation classification on the SemEval 2010 Task 8 dataset using several hard weight sharing strategies. We investigate the sample complexity dynamics of learning SemEval 2010 Task 8 simultaneously with other natural language processing tasks. We find that only one of the proposed weight sharing strategies lead to improvements in generalization performance of this target task. We identify potential causes for this difference in generalization performance across weight sharing strategies, and make recommendations for further experimentation in this direction.

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Part 1

Introduction

1.1 Motivation

The volume of digital text that exists in the world is rapidly increasing: The number of active science journals is growing with an annual rate of approximately 2.5%. The total number of published articles in these journals grew from 1.8 in 2009 to 2.5 million in 2015 (Mabe and Ware, 2009; Ware and Mabe, 2015). Similar staggering growth rates can be cited for content produced by online newspapers, social media and digital documents generated by businesses (Perrin, 2015; Mitchell and Rosenstiel, 2015).

Finding the right information at the right time in the face of this data volume is challenging. A significant reason is that information contained in digital text is in the form of natural language which is often cited as being **unstructured** (despite the fact that natural language is actually highly structured). Unstructured data can be understood as being essentially the opposite of the kind of data we find in relational databases where every data item is associated with metadata such as column names and column types. This metadata makes the structured data easy to search and analyze with computers. In contrast, unstructured data such as text, images, sound and video is not.

This problem has driven the development of so called **information extraction** techniques. The goal of these is to assign metadata to unstructured data, thereby giving some structure to it. This is an ambitious goal since in many cases it involves developing computer systems that perform tasks such as recognizing objects in images, converting speech to text or building data structures that capture the semantics of natural language, tasks we don't fully understand how humans are able to perform.

Relation extraction is an information extraction task the goal of which is to automatically identify a fixed set of semantic relationships of interest such as *Father-Son(Luke Skywalker, Darth Vader)* when they occur in natural language. Identifying these relations can significantly improve the quality of applications such as information retrieval or question answering systems (Jurafsky and Martin, 2009).

Like most other natural language processing problems, relation extraction is extremely challenging because of the high degree of variation and ambiguity of natural language. Relation extraction systems are therefore usually composed of sub-

systems that each solve a sub-problem of relation extraction. Specifically, most relation extraction systems proceed by first identifying the potential arguments such as *Luke Skywalker* and *Darth Vader* in our example for any relation of interest. The system then detects whether or not a relation does in fact exist between them, and finally classifies the relation if it exists.

Supervised machine learning in general, and **deep learning** in particular, are very successful techniques for solving information extraction problems. These approaches are based on the idea of supplying examples of inputs such as text and corresponding correct outputs, so called labels, that we would like the system to reproduce given the input. The goal is to teach the system to give approximately correct output for new inputs that it hasn't seen before.

The conditions under which supervised machine learning systems can be expected to give approximately correct answers are fairly well understood. Theoretical analysis shows that the number of training examples provided for the learning system is one of the main ingredients in this guarantee. Producing these examples can be costly however: It often requires a human annotator with specialized skills to provide the correct labels. This means there is significant motivation for reusing labeled training data to reduce the need to create large new collections of data for each new supervised machine learning problem.

Multi-task learning is a technique for reusing labeled data (Caruana, 1997). In essence, it relies on the idea that it may be easier to learn related tasks simultaneously than in isolation, or in other words, that a learning system that learns from previously annotated data may require fewer examples for learning a new task, thereby reducing the cost of data annotation.

1.2 Problem Statement

In this thesis we investigate multi-task learning for relation extraction. We focus on the relation classification sub-problem using deep learning techniques. Our goal is to investigate how the performance of a deep learning system trained on an auxiliary and target task simultaneously compares to a system trained only on the target task when the available data for this task is limited. Specifically:

1. We survey the relevant research literature in order to formally answer questions such as *when is multi-task learning beneficial? How can we evaluate the usefulness of an auxiliary task?*
2. We implement a deep multi-task learning relation classification system based on our research.
3. We apply our theoretical understanding by analyzing our deep multi-task learning system for relation classification in order to make predictions about its performance.
4. We empirically test our predictions about the system's performance using appropriate accuracy measures.

Part 2

Background

In this part we describe the information extraction problem and the challenges it poses. Moreover, we formally describe the supervised machine learning setting: We discuss the challenges of noise and overfitting, and show the usefulness of Vapnik-Chervonenkis analysis. We also cover validation techniques for supervised machine learning systems and appropriate accuracy measures for evaluating information extraction systems.

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). We introduce each of them in this section, and explain the challenges they pose.

2.1.1 Named Entity Recognition

A named entity is roughly anything that has a proper name. The goal of named entity recognition (NER) is to label mentions of entities such as people, organizations or places occurring in natural language. The list of things these systems are tasked with recognizing is often extended to include things that aren't technically named entities such as amounts of money or calendar dates.

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 *organization* should ideally assign the labels:

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

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

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 BIO labels for named entity recognition.

and *JFK* the airport near New York. This means that named entity recognition systems need to have some model of the context in which these entities appear in order to produce correct output.

Named entity recognition can be framed as a sequence labeling problem. A common approach is to apply so called tokenization 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-labeling (figure 2.1) is a widely used labeling scheme in which token labels indicate whether the token is at the **B**eginning, **I**nside, or **O**utside an entity mention.

2.1.2 Relation Extraction

The goal of relation extraction is to identify relationships such as *Family* or *Employment* in natural language. The set of relations we would like a relation extraction system to recognize is commonly referred to as the **inventory**. Most often, the inventory is limited to relations between named entities. In some relation extraction tasks however, the goal is to more generally recognize relations between nominal expressions that include nouns and pronouns. (Hendrickx et al., 2009). In both cases, the words between which a relation exists are referred to as the **arguments** of the relation.

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 recognizes the relation *MergerBetween(organization, organization)* between two mentions of organizations. Ideally, we would like that system to extract the relation *MergerBetween(Foo Inc., Bar Corp.)* from the above sentence.

To simplify the relation extraction problem, it's often solved in three steps:

1. **Named entity recognition** Identify the named entities in the input text.
2. **Relation detection** For each pair of named entities in the input text, determine if a relation exists between them. This is a binary classification problem where the input is the text and the named entities detected in step 1, and the output is yes/no.
3. **Relation classification** Classify each of the detected relations in the previous step. This a multi-label classification problem where the input is the input text and the named entities for which a relation was detected in step 2, and the output is a relation label.

In this thesis we focus on step 3: assigning labels to detected relations. This is a difficult problem because of the high degree of ambiguity of natural language. As an example, consider the sentence

> *Susan left JFK.*

Imagine that we want to design a relation extraction system that can detect the relations *Physical(person, location): a person has a physical relation to a location* and *Personal-Social(person, person): two persons have a social relation*. Both can reasonably be assigned to the previous sentence, depending on whether *JFK* refers to the airport near New York, or the former American president. Just as in named entity recognition, providing the correct label in this situation depends on context information.

Early relation extraction systems relied on hand-crafted lexical and syntactic rules for detecting relations. Hearst (1992) is perhaps the earliest example of this approach. She considers the following sentence:

> *Agar is a substance prepared from a mixture of red algae such as Gelidium for laboratory or industrial use.*

Most people won't know what *Gelidium* is. From the context we can infer that it's a type of algae however. She suggests that the following lexico-syntactic pattern between two noun phrases NP_1 and NP_2:

$$NP_1 \text{ such as } NP_2$$

implies the relation $Hyponym(NP_1, NP_2)$. By performing a syntactic parse of the input sentence we can try to extract hyponym relations between noun phrases using such manually created rules. Because of the huge amount of variation found in natural languages, this is of course a cumbersome yet brittle approach.

More recent solutions rely on supervised machine learning techniques to solve relation extraction problems. In this setting, a system learns to recognize relations in the inventory from annotated examples. The earliest examples of such systems relied on hand-crafted features of words in the neighborhood of the relation arguments, for example: *the words separating the relation arguments are "such as"* (Jurafsky and Martin, 2009). As we will see in part 3, the major attraction of solutions based on deep learning is the promise of avoiding complicated hand-crafted features of the sentence, but having the system learn useful lexico-syntactic features on its own.

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. In these tests, accuracy measures for each class c of information we wish to extract are usually defined in terms of how many times the system correctly predicted class c. Most metrics use the following terminology:

	predicted as c	**predicted as not** c
c	True positives (tp)	False negatives (fn)
not c	False positives (fp)	True negatives (tn)

Where for example tp is the number of true positives produced for class c.

The distribution of labels used in both named entity recognition and relation extraction is often highly imbalanced. Consider for example the BIO labelling scheme for named entity recognition in figure 2.1. Most words will be outside a mention of a named entity, and will have the label O. Using simple accuracy $\frac{tp+tn}{tp+tn+fn+fp}$ as a performance metric for a system that outputs bio labels for each token in the text 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 information items for which the system predicted class c that actually belonged to class c. Recall $\frac{tp}{tp+fn}$ on the other hand is the fraction of information items in the corpora of class c that the system correctly extracted.

In a multi-class classification problem we are forced to decide how to average these metrics across classes. Specifically, there are two ways of averaging an accuracy measure across C different classes: micro and macro averaging (Sokolova and Lapalme, 2009). In macro averaging, an accuracy measure is computed for each class c separately, and then averaged across all C classes. For example macro-precision p_M:

$$p_M = \frac{1}{C}\sum_{c=1}^{C} p_c$$

Where p_c is the precision of the system for class c. Micro averaging on the other hand, averages an accuracy measure by accumulating tp, tn, fp and fn across all C classes. For example micro-precision p_μ:

$$p_\mu = \frac{\sum_{c=1}^{C} tp_c}{\sum_{c=1}^{C} tp_c + fp_c}$$

Where for example tp_c is the true positives a system produces for class c.

The main difference between macro and micro averages of accuracy measures is that micro averaging gives more weight to more frequent classes. In other words, micro averaging encodes the bias that infrequent classes are unimportant, and a misclassification of an example of such a class should not penalize the accuracy measure as much as a misclassification of a more frequent class. Whether or not this a reasonable bias depends on the problem. In order to be agnostic about the frequency of semantic relations we use macro averaging for all our reporting in this thesis.

To get a single number that summarizes the performance, precision p and recall r are often combined into a single metric: the $F1$ measure. $F1$ is defined as the harmonic mean of precision and recall $\frac{2pr}{p+r}$. Variations that use the micro and macro versions of precision and recall can naturally be computed as the harmonic mean of the micro or macro precision and recall respectively.

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 recognize 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 it's limitations.

2.2.1 The Supervised Learning Problem

A training set $\mathcal{D}$ of N 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 an output space $\mathcal{Y}$ of labels, for example the set of all sequences of BIO tags. As designers of the learning system we specify a set of functions $h : \mathcal{X} \mapsto \mathcal{Y}$, the so called **hypothesis space** $\mathcal{H}$. 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 $\mathcal{D}$ that performs well on $\mathcal{D}_{test}$ as measured by some performance measure e. In theoretical analyses of 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 only interested in the performance of h on $\mathcal{D}$ to the extent that it informs us how the system will perform on future data (Abu-Mostafa et al., 2012).

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

Definition 2.2.1 (generalization 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 $e(\mathbf{y}_1, \mathbf{y_2})$ be an error function that measures agreement between labels $\mathbf{y}_1$ and $\mathbf{y}_2$. Then the generalization error E of a function $h : \mathcal{X} \mapsto \mathcal{Y}$ is defined as:

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

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

Definition 2.2.2 (empirical error)**.** Let $\mathcal{S}$ 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:

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

Because $\mathcal{S}$ 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:

1. The samples in $\mathcal{S}$ are drawn independently from $P(\mathbf{x}, \mathbf{y})$. In other words, observing any one sample did not change the probability of observing any other sample.

2. h is independent of $\mathcal{S}$. In other words, 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 $E(h, \mathcal{S})$ be defined as in definition 2.2.2. Then:

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

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 $\mathcal{S}$, the less likely it is that $\hat{E}$ will be misleading. Estimating E with a sample that's independent of h is a technique called **validation** and will be discussed in section 2.2.3

Because $\mathcal{D}$ is used to select h, Hoeffding's inequality doesn't hold and we need more sophisticated techniques to understand the relationship between $\hat{E}$ and E. The central question in supervised machine learning is: *how can we best define $\mathcal{H}$ and use $\mathcal{D}$ 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

$\mathcal{D}$ is the only information we have about $P(\mathbf{x}, \mathbf{y})$, and therefore also the only information we have about E. If our goal is to minimize E, a straight-forward idea would be to find a function $g \in \mathcal{H}$ that minimizes the **training error** $\hat{E}(h, \mathcal{D})$ in the hope that g will also minimize E.

As we argued in section 2.2, using $\hat{E}$ to estimate E can be misleading. Moreover, because D 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 $\hat{E}(g, \mathcal{D})$ 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 generalization error is large is known as **overfitting** (Abu-Mostafa et al., 2012). As the name implies, it's caused by harmful idiosyncrasies of $\mathcal{D}$ that causes us to select a g with a larger E than other functions in $\mathcal{H}$. These idiosyncrasies of $\mathcal{D}$ 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 irrelevant to the problem we are trying to solve. For example, human error where a human annotator incorrectly labels a piece of text is a common source of stochastic noise in information extraction. Selecting a g that repeats this error is a case of overfitting because g will have lower training error but larger generalization error than

another h that doesn't predict the incorrect annotation.

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 the training data is generated by a deterministic function f such that $\mathbf{y}_i = f(\mathbf{x}_i)$. Deterministic noise is present when even h^* can't represent the deterministic relationship exactly. Suppose that we get a $\mathcal{D}$ 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 minimize $\hat{E}$, we select a g that predicts this sample, such that $g(\mathbf{x}_i) = \mathbf{y}_i$. This is a case of overfitting since we know that there is at least one function in $\mathcal{H}$ with lower generalization error than g, namely h^*.

The risk of overfitting is linked to the diversity of $\mathcal{H}$. When we say that $\mathcal{H}$ is diverse, we roughly mean that the functions $h \in \mathcal{H}$ are very different from each other. The more diverse $\mathcal{H}$ is, the greater the risk that there exists a $h \in \mathcal{H}$ that will overfit $\mathcal{D}$.

A **dichotomy** is a central concept in measuring the diversity of $\mathcal{H}$. A dichotomy is a specific sequence of N labels. For simplicity, most theoretical analyses of $\mathcal{H}$ assume a binary output space $\mathcal{Y} = \{0, 1\}$ and we will too. In that case, if $N = 3$ 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. By simple combinatorics the number of dichotomies for N must be smaller than or equal to 2^N if $\mathcal{Y}$ is binary. There may be infinitely many functions in $\mathcal{H}$, but on a specific $\mathcal{D}$, many of them will produce the same dichotomy since the number of training examples in $\mathcal{D}$ is finite. This allows us to quantify the diversity of $\mathcal{H}$ in terms of the number of dichotomies it's able to realize 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 realizable 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 realizes 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 $\hat{E}(h, \mathcal{D})$ (Vapnik and Chervonenkis, 1971):

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

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

The bound tells us that $E(h)$ will be close to $\hat{E}(h, \mathcal{D})$ 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 generalization error will be close to training error, where simple means: functions that realize a small number of dichotomies. Using a small hypothesis space means we require fewer training examples in order to guarantee that $\hat{E}$ is close to E.

On the other hand, having a set $\mathcal{H}$ that can realize a large number of dichotomies on N points, will make it easier to find a function that will make $\hat{E}(h, \mathcal{D})$ 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 generalization 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 using all of $\mathcal{H}$ when learning from it. These techniques are known as **regularization**, which we will see an instance of in section 3.2.4.

A simple rewrite of theorem 2.2.2 leads to a very popular equivalent formulation: a **sample complexity** bound. Sample complexity denotes the number of training examples required for a certain level of generalization performance. Exercising a bit of algebra on the Vapnik-Chervonenkis bound leads to the insight that in order for E to

be no more than ϵ away from $\hat{E}$ with probability $1 - \delta$, it requires:

$$N \geq \frac{1}{\epsilon^2} \ln \frac{4m(2N, \mathcal{H})}{\delta}$$

As we will see in part 4, sample complexity bounds will prove to be valuable tools for understanding how multi-task learning can help reduce the annotation burden for new supervised machine learning problems.

2.2.3 Validation

Statistical learning theory tells us how to design $\mathcal{H}$ given a dataset by revealing the relationship between $\hat{E}(h, \mathcal{D})$ 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, for example in order to decide whether a system is good enough to be put in to production.

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

In order to get an unbiased empirical estimate of E we can split $\mathcal{D}$ into two datasets: $\mathcal{D}_{val}$ containing V samples and $\mathcal{D}_{train}$ containing $N - V$ samples. $\mathcal{D}_{train}$ is used by the learning system to find a function $g^- \in \mathcal{H}$. The minus superscript indicates that the function was selected using only a subset of $\mathcal{D}$. $\mathcal{D}_{val}$ is used to compute $\hat{E}(g^-, \mathcal{D}_{val})$ as an unbiased estimate of E.

We can use Vapnik-Chervonenkis analysis to bound the error of $\hat{E}(g^-, \mathcal{D}_{val})$ as an estimate of $E(g^-)$ (Abu-Mostafa et al., 2012). We can view $\mathcal{D}_{val}$ as a training set, which we use to search a hypothesis space containing just g^-. This leads to:

$$E(g^-) \leq \hat{E}(g^-, \mathcal{D}_{val}) + O(\frac{1}{\sqrt{V}})$$

The inequality tells us that V should be large in order for $\hat{E}(g^-, \mathcal{D}_{val})$ to be close to $E(g^-)$. This presents a problem since increasing the size of V decreases the number of examples available for training. Though hard to prove theoretically, it's empirically well documented that more training data lead to lower generalization error (Abu-Mostafa et al., 2012). In other words, making V large will lead to a very accurate estimate of a very poor hypothesis.

Cross validation is a technique that may be used to overcome this dilemma. In this setting, $\mathcal{D}$ is split into K parts called **folds** containing $\frac{N}{K}$ samples each. $\mathcal{D}_{train}$ is then composed of $K - 1$ folds, and the remaining fold is used as $\mathcal{D}_{val}$. This leads to K iterations of the learning procedure yielding K hypotheses g_k^- and K estimates of generalization error $e_k = \hat{E}(g_k^-, \mathcal{D}_{val})$. We define the cross-validation error as the average of these estimates:

$$E_{cv} = \frac{1}{K} \sum_{k=1}^{K} e_k$$

We want to know E, but it would be almost as useful to know the expected E of our learning system when trained on any dataset $\mathcal{D}$ drawn from $P(\mathbf{x}, \mathbf{y})$ of size N. For

this purpose, we can define

$$\tilde{E}(N) = \mathbb{E}_{\mathcal{D}}[E(g)]$$

In words, the expected generalization error with respect to datasets of size N. The expected value of E_{cv} is $\tilde{E}(N - \frac{N}{K})$. To see why, consider the expected value of a single estimate e_k:

$$\mathbb{E}[e_k] = \mathbb{E}_{\mathcal{D}_{train}}\mathbb{E}_{\mathcal{D}_{val}}[\hat{E}(g_k^-, \mathcal{D}_{val})] = \mathbb{E}_{\mathcal{D}_{train}}[E(g_k^-)] = \tilde{E}(N - \frac{N}{K})$$

Since the equality holds for a single estimate, it also holds for the average E_{cv} (Abu-Mostafa et al., 2012).

In words, the cross validation error estimates the expected generalization error of the learning system when trained on $N - \frac{N}{K}$ samples. We can control the number of samples available for finding each function g_k^- by increasing K, at no cost of estimation accuracy. However, increasing K increases computation time since we have to search the hypothesis space K times.

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, organizations and places in natural language. The purpose of relation extraction systems is to identify relationships between them. We described how the ambiguity of natural language makes information extraction problems difficult.

We have seen that simple accuracy is uninformative as an evaluation measure in information extraction. We have introduced precision, recall and $F1$ as alternative metrics that mitigate the problems of simple accuracy.

We have described the formal setting of 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 generalization error. Finally we have discussed validation as a technique for estimating E empirically, and cross-validation as a technique to overcome the dilemma of setting aside too much vs. too little data for validation.

In the coming sections we present a concrete hypothesis space that has some convenient properties for multi-task learning: neural networks.

Part 3

Neural Networks

In this part we describe how to define $\mathcal{H}$ using functions called **neural networks**. One advantage of these functions is that they're easy to adapt to multi-task learning. We begin by describing how to design $\mathcal{H}$ using neural networks. We then turn to the issue of how to use $\mathcal{D}$ to search this hypothesis space. We then cover regularization techniques the purpose of which is to prevent overfitting. Lastly, we introduce convolutional neural networks which are specialized functions often used for text classification problems such as relation extraction.

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 function $f^{(l)}$ receives input from $f^{(l-1)}$. For example if $L = 2$, then $h(\mathbf{x}) = f^{(2)}(f^{(1)}(\mathbf{x}))$. Each $f^{(l)}$ outputs a vector $\mathbf{x}^{(l)}$ of dimension $d^{(l)}$. We denote the input to $f^{(1)}$ as $\mathbf{x}^{(0)}$ which is identical to the input vector $\mathbf{x}$ with an added **bias** component as described later in this section. 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 such that the index of the layers increase as we move from the input to the output layer. 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 the sum of its weighted input.

Activation functions model the behavior 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 $l-1$.

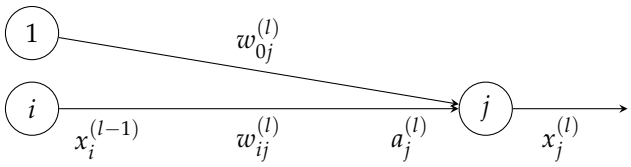


Figure 3.1
A visual representation of the connections between unit i in layer $l-1$, the bias unit in $l-1$, and unit j in layer l. The connection strength between these units is given by the weight $w_{ij}^{(l)}$ between i and j, and $w_{0j}^{(l)}$ between the bias unit and j. The activation $a_j^{(l)}$ 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 organizing 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.

We can think of each neuron in a neural network as a feature detector of sorts: each neuron learns to detect the presence of a pattern implicitly defined by it's incoming weights (Goodfellow et al., 2016). In this view, each hidden layer is tasked with learning a **representation** thats useful for the task the neural network meant to learn. As we will see in section 4.5, the intuition of neural networks as representation learners forms the foundation for their adaptation to multi-task learning.

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 practice, it's common to use different activation functions at different layers of the network. In the next section we discuss how to choose these activation functions.

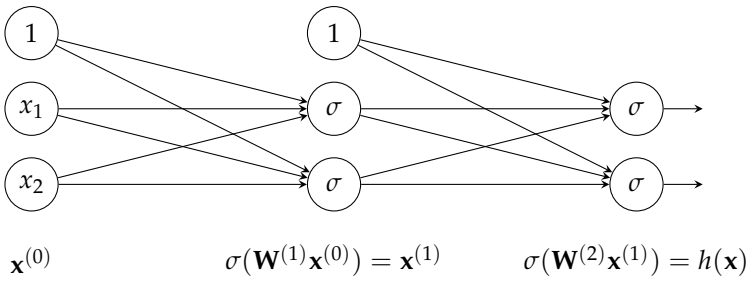


Figure 3.2
A visual representation of $h = f_2(f_1(\mathbf{x}^{(0)}))$. The activation at each layer $\mathbf{a}^{(l)}$ is computed by $\mathbf{W}^{(l)}\mathbf{x}^{(l-1)}$. The output at each layer is computed by element-wise application of the activation function of $\sigma(\mathbf{a}^{(l)})$.

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 certain 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 $\mathcal{H}$ to model a larger class of functions (Goodfellow et al., 2016).

Many networks use **sigmoidal** activation functions such as the classical sigmoid function $\sigma(a) = 1/(1 + \mathrm{e}^{-a})$. These functions have the advantage of being differentiable everywhere. As we will see in section 3.2, differential calculus is the fundamental tool for finding a good $h \in \mathcal{H}$ which makes differentiability a desirable quality. One drawback of sigmoidal activation functions is that their derivates are small as seen in figure 3.3. As we will see in section 3.2, 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 $\mathcal{D}$ extremely slow (Goodfellow et al., 2016).

Because of this shrinking problem, the default recommendation today is to use **rectified linear units**. These units use the rectified linear activation function $\sigma(a) = \max(0, a)$ depicted in figure 3.4. The rectified linear activation function has the advantage that its derivative $\frac{d\sigma}{da} = 1$ when $a > 0$, and $\frac{d\sigma}{da} = 0$ when $a < 0$. The function is not strictly differentiable when $a = 0$. In practice however, this is not a big problem because a is rarely exactly 0 and since neural networks are trained through an iterative process as described in section 3.2.1 in which we can skip iterations where

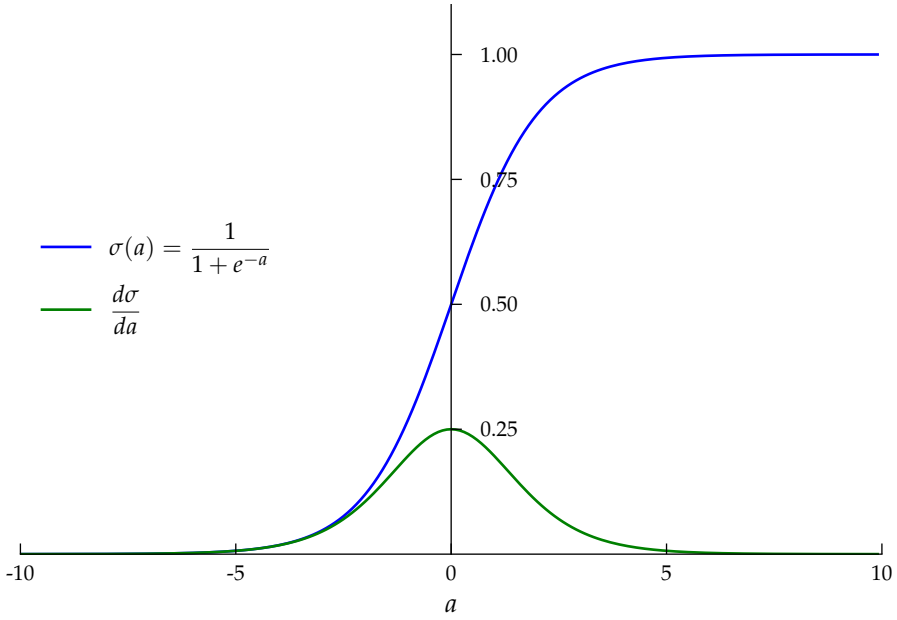


Figure 3.3
*Sigmoid activation and its derivate. Sigmoid activation units have the disadvantage of **saturating**, meaning that they become flat when a is large or small. This makes the derivative smaller than 1 everywhere, and much smaller than 1 almost everywhere.*

units have zero activation.

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 learning algorithm with a principled technique called **maximum likelihood** in which the appropriateness of h is measured by the probability it assigns to the training data. For this reason, it's common to use different activation functions in the output layer that enables us to interpret the output of h as a probability distribution.

For example, named entity recognition can be seen as a multi-class classification 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 $\mathbf{y}_i$ is equal to 1 if example $\mathbf{x}_i$ 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. $\mathbf{y}_i$ 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.

Using one hot encoding we can design h to output a vector with C components where each component $h_c \in h(\mathbf{x}_i, \mathbf{w})$ gives the probability that $\mathbf{x}_i$ has class c when h is parameterized by $\mathbf{w}$. More formally, we can interpret $h(\mathbf{x}, \mathbf{w})$ as conditional probability distribution such that $h(\mathbf{x}, \mathbf{w})_c = P(Y = c \mid X = \mathbf{x}, W = \mathbf{w})$ where X and Y are random variables over $\mathcal{X}$ and $\mathcal{Y}$ and W is a random variable over the possible weights for h.

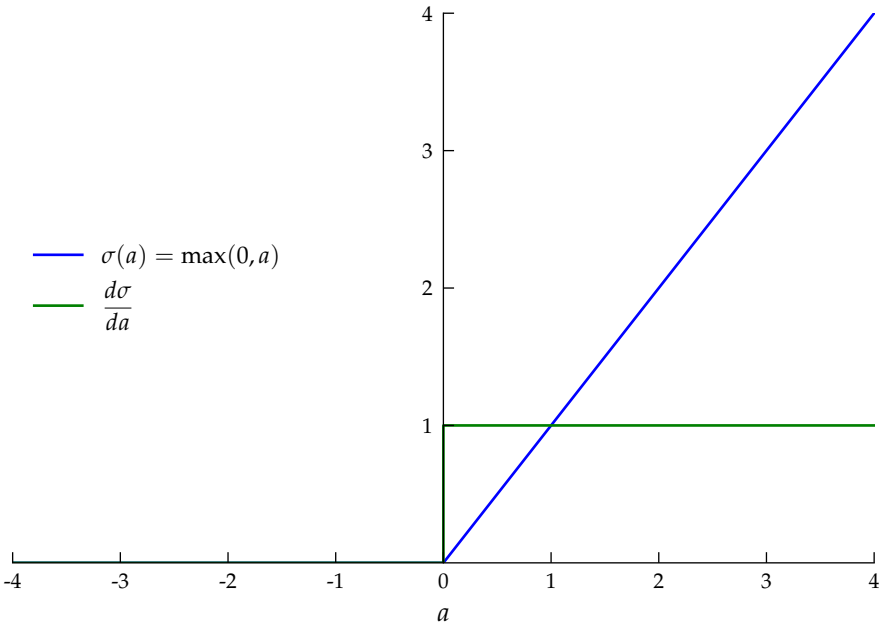


Figure 3.4
ReLU activation and its derivate. Unlike sigmoid activation, ReLU activation doesn't saturate. This means that the derivative of a unit remains large whenever it produces output.

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

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

Where the notation $\mathbf{a}_c$ denotes the c'th component of the vector $\mathbf{a}$. In words, the soft-max function ensures that the output of h is a valid probability distribution 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 latter 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 so called **objective function** by the maximum likelihood principle that quantifies the appropriateness of a weight vector $\mathbf{w}$ as a probability using the samples in $\mathcal{D}$. This function is crucial for finding $g \in \mathcal{H}$ as we explain 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 $\mathcal{D}$. Such a function is often called an **objective function**

borrowing terminology from the mathematical field of optimization. Minimizing the straight-forward binary error function $\hat{E}(h, \mathcal{D}) = 1/N \sum_{i=1}^{N} \mathbb{I}[h(\mathbf{x}_i) \neq \mathbf{y}_i]$ unfortunately leads to an intractable minimization problem (Marcotte and Savard, 1992). It's therefore common to use a **surrogate error function** that captures properties we are interested and approximates binary error well (Goodfellow et al., 2016). In this section, we discuss how using the maximum likelihood framework leads to a useful surrogate error function for neural networks.

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:

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

Where $y \in \mathcal{Y}$ and $\mathbf{y}_c$ 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 $h(\mathbf{x}, \mathbf{w}) = \begin{bmatrix} .1 & .8 & .1 \end{bmatrix}^T$, then $P(Y = y \mid X = \mathbf{x}, W = \mathbf{w}) = (0.1^0)(0.8^1)(0.1^0) = 0.8$.

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 $\mathcal{D}$ by interpreting h as a probability distribution parameterized by $\mathbf{w}$:

Definition 3.1.1 (likelihood function)**.** Let $\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}$ 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 $\mathbf{y}_{ic}$ denote component c of the one-hot label for example i. Then the likelihood $P(\mathcal{D} \mid \mathbf{w})$ is:

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

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

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 may lead to problems because the likelihood function must be interpreted as a probability in neural network training.

To avoid numerical underflow, the **log-likelihood** $\ln P(\mathcal{D} \mid \mathbf{w})$ 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, namely it's maximum.

Finally, many objective functions for supervised machine learning are defined in terms of training *error* $\hat{E}(h, \mathcal{D})$ and not *probability*. In this view, searching for a good $h \in \mathcal{H}$ becomes a minimization 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**. Minimizing the average negative log-likelihood is clearly identical to maximizing the likelihood, since $\max f(\mathbf{x}) = \min -f(\mathbf{x})$, and dividing by N doesn't change the optimum (Goodfellow et al., 2016).

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

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

We use the notation $\hat{E}(\mathbf{w}, \mathcal{D})$ interchangeably with the average negative log likelihood in the following sections. 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: $\hat{E}(h, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} e(h(\mathbf{x}_i), \mathbf{y}_i)$.

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 maximizes the likelihood of $\mathcal{D}$ is an optimization problem. Optimization is solved by answering the question: *how does* $\hat{E}$ *change when we change* $\mathbf{w}$*?* We answer questions of this type with differential calculus. Sadly, there is no known method for finding the $\mathbf{w}$ which maximizes the likelihood by analytical differentiation. Neural network optimization is therefore solved using an iterative algorithm called **gradient descent**, which we describe in this section. We go on to explore an algorithm for computing the gradient of $\hat{E}$ called **backpropagation**. Finally, we look into **regularization** 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 minimizes $\hat{E}$ as described in section 3.1.2. Each h is defined exactly by the weight vector $\mathbf{w}$. $\hat{E}$ can't be minimized 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 (Goodfellow et al., 2016). We therefore look for h by choosing an initial weight vector $\mathbf{w}_0$ close to the origin, 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 ascent at each $\mathbf{w}_i$ is given by the gradient $\nabla\hat{E}$ (Abu-Mostafa et al., 2012). $\nabla\hat{E}$ 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 $\nabla\hat{E}(\mathbf{w}, \mathcal{D})$ is:

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

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 $\mathcal{D}$. 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 on gradient descent which addresses this problem (Abu-Mostafa et al., 2012).

In stochastic gradient descent, a single training example $(\mathbf{x}_i, \mathbf{y}_i)$ is sampled uniformly from $\mathcal{D}$. Instead of 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 $\mathcal{D}$ can be drawn with probability $\frac{1}{N}$, stochastic gradient descent is identical to gradient descent in expectation:

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

In traditional gradient descent, $\nabla\hat{E}$ approaches $\mathbf{0}$ when $\mathbf{w}_i$ approaches a local or global minimum for $\hat{E}$. This prevents the algorithm from stepping far away from this minimum once it's close to a solution. When using stochastic gradient descent

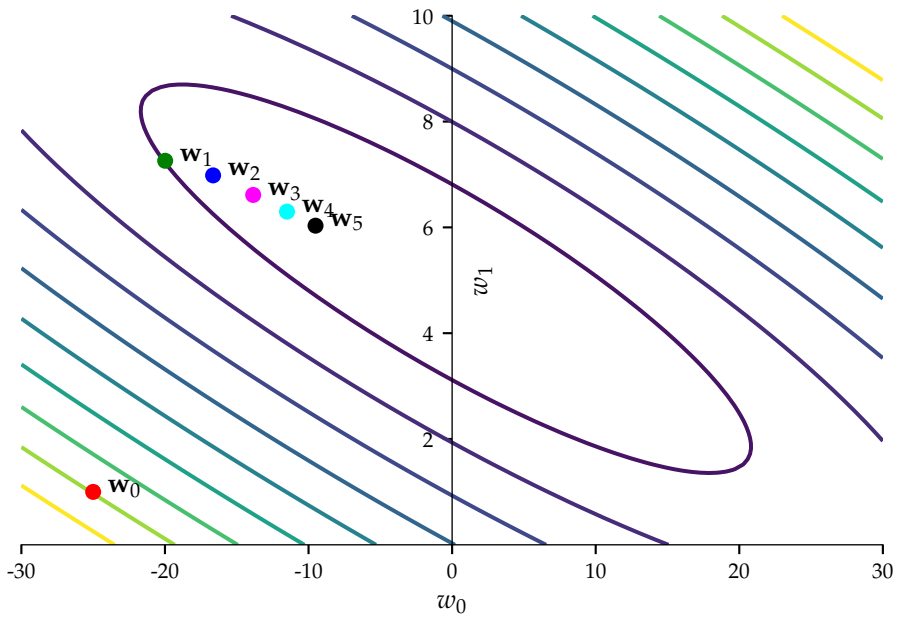


Figure 3.5
Level curves of squared training error $\hat{E}(h, \mathcal{D}) = \frac{1}{N}\sum_{i=1}^{N}(h(\mathbf{x}_i) - y_i)^2$ for a toy $\mathcal{D}$ shown in 3.6, and the simple $\mathcal{H} = \{h = \mathbf{w}^T\mathbf{x}^{(0)} \mid \mathbf{w} \in \mathbb{R}^2\}$. $\hat{E}$ has its minimum at $(0, 5)$. 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.

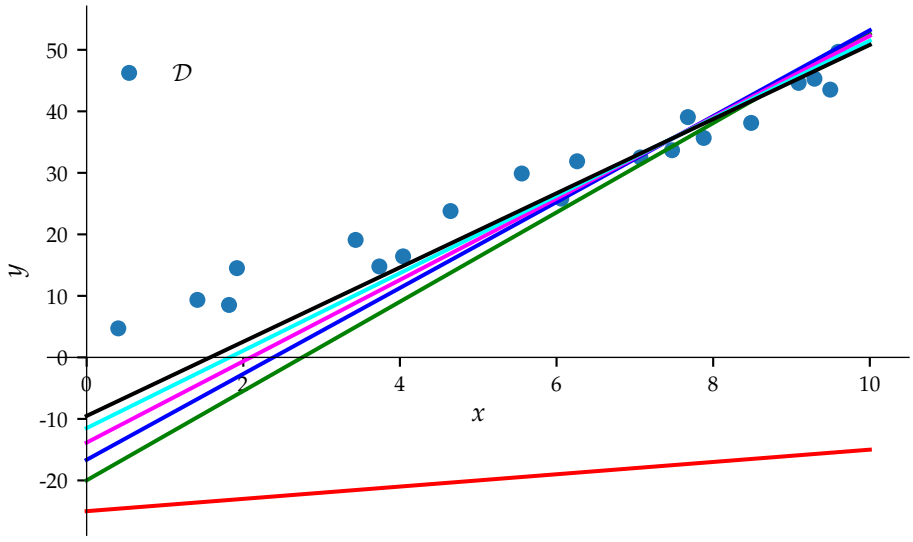


Figure 3.6
The training data $\mathcal{D}$ used in figure 3.5. The colored lines correspond to $h(\mathbf{x}, \mathbf{w}_i) = 0$ for each weight vector $\mathbf{w}_i$ found by gradient descent in figure 3.5, such that for example $h(\mathbf{x}, \mathbf{w}_0) = 0$ is given by the red line. We see as gradient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

however, each update to the weights is based on just a single example and is therefore noisy which means that $\nabla e(h(\mathbf{x}_i, \mathbf{y}_i)$ may be large even if $\mathbf{w}_i$ is close to a value that minimizes $\hat{E}$.

To reduce the noise in the gradient estimate, it's common to sample a small mini-batch $\mathcal{B}$ of b examples from $\mathcal{D}$ and perform gradient descent on that. In addition, its common to shrink the learning rate η as the algorithm progresses to avoid stepping away from a minimum due to the noise in the gradient estimate. We will see a strategy for shrinking η systematically in the next section.

3.2.2 Adam

The Adam algorithm is a variation on stochastic gradient descent that attempts to shrink the learning rate η automatically in each iteration (Kingma and Ba, 2014). Since the learning rate varies from iteration to iteration, we will denote the learning rate in iteration i as η_i. Moreover, Adam adapts the learning rate for each parameter $w \in \mathbf{w}$ individually by using a learning rate vector $\boldsymbol{\eta}$ instead of a scalar in the update rule, such that $\mathbf{w}_i = \mathbf{w}_{i-1} - \boldsymbol{\eta}_i \nabla e(h(\mathbf{x}_i), \mathbf{y}_i)$

Adam uses the following heuristic: the learning rate for parameters w for which $\frac{\partial}{\partial w} e(h(\mathbf{x}_i), \mathbf{y}_i)$ is frequently large should decrease more quickly than parameters that consistently have small derivatives. To achieve this, Adam scales η by $\mathbf{v}_i$ such that:

$$\mathbf{v}_i = \beta_1 \mathbf{v}_{i-1} + (1 - \beta_1)(\nabla e(h(\mathbf{x}_i, \mathbf{y}_i))^2$$

Where $\mathbf{v}_0 = \mathbf{0}$. In words, $\mathbf{v}_i$ is an exponentially decaying average of past squared gradients where β_1 is the decay rate usually set to a value near .9. To cancel the bias introduced by initialising $\mathbf{v}_i$ to $\mathbf{0}$, a bias corrected value $\hat{\mathbf{v}}_i = \mathbf{v}_i / (1 - \beta_1^i)$ is computed. The learning rate is then computed as:

$$\boldsymbol{\eta}_i = \frac{\eta}{\sqrt{\hat{\mathbf{v}}_i} + \epsilon}$$

Where ϵ is small value introduced to prevent division by 0.

In addition to scaling the learning rate, Adam uses the idea of **momentum** to speed up stochastic gradient descent. Momentum is designed to make stochastic gradient descent more robust to high curvature in $e(h(\mathbf{x}_i), \mathbf{y}_i)$ and noisy gradients. This is achieved by changing the update rule, such that the parameters $\mathbf{w}_i$ are updated not in the direction of $-\nabla e(h(\mathbf{x}_i), \mathbf{y}_i)$, but in the direction of an exponentially decaying average of past gradients $\mathbf{m}_i$:

$$\mathbf{m}_i = \beta_2 \mathbf{m}_{i-1} + (1 - \beta_2) \nabla e(h(\mathbf{x}_i), \mathbf{y}_i)$$

where $\mathbf{m}_0 = 0$ and β_2 is the decay rate. Just as before, the initialisation bias is corrected by computing $\hat{\mathbf{m}}_i = \mathbf{m}_i / (1 - \beta_2^i)$.

The full update rule for Adam is thus:

$$\mathbf{w}_i = \mathbf{w}_{i-1} - \frac{\eta}{\sqrt{\hat{\mathbf{v}}_i} + \epsilon} \hat{\mathbf{m}}_i$$

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

3.2.3 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 consider a neural network h that uses soft-max activation in its output layer and 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 component $\frac{\partial e}{\partial w_{ij}^{(l)}}$ 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 (Abu-Mostafa et al., 2012):

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

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:

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

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

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

This allows us to compute $\nabla \hat{E}$ and use it to search $\mathcal{H}$ iteratively for a function h that minimizes $\hat{E}$. In the next section, we consider regularization techniques that restrict gradient descent in ways that prevent overfitting.

3.2.4 Regularization

In section 2.2.2 we saw that the distance between $E(h)$ and $\hat{E}(h, \mathcal{D})$ is bounded by, among other things, a function of the diversity of $\mathcal{H}$. In this section we discuss techniques for restricting the learning algorithm to search only in a subset of $\mathcal{H}$ with the aim of reducing E. These techniques are collectively known as regularization.

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 generalization.

If the weights $\mathbf{w}^*$ that minimize the unconstrained training error $\hat{E}(\mathbf{w}, \mathcal{D}_{train})$ lie outside this ball, then the weights $\bar{\mathbf{w}}$ that minimize $\hat{E}$ while still satisfying the constraint $\bar{\mathbf{w}}^T\bar{\mathbf{w}} \leq C$ must have norm equal to C. In other words, these weights 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 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 (Abu-Mostafa et al., 2012).

In other words, the following equality holds for $\bar{\mathbf{w}}$:

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

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

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

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

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

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

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

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

In words, the added norm penalty of $\bar{E}(\mathbf{w}, \mathcal{D})$ 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 effective diversity of $\mathcal{H}$.

Early stopping is a form of regularization for iterative optimization methods that is particularly straight-forward to implement, and as an added bonus gives a reasonable stopping criterion for gradient descent. It works very similarly to weight decay: by limiting the region of $\mathcal{H}$ that can be explored in a finite number of iterations.

For a single iteration i of gradient descent with step size η, gradient descent explores all weights in a radius of η around $\mathbf{w}_i$ since a step in the direction of the

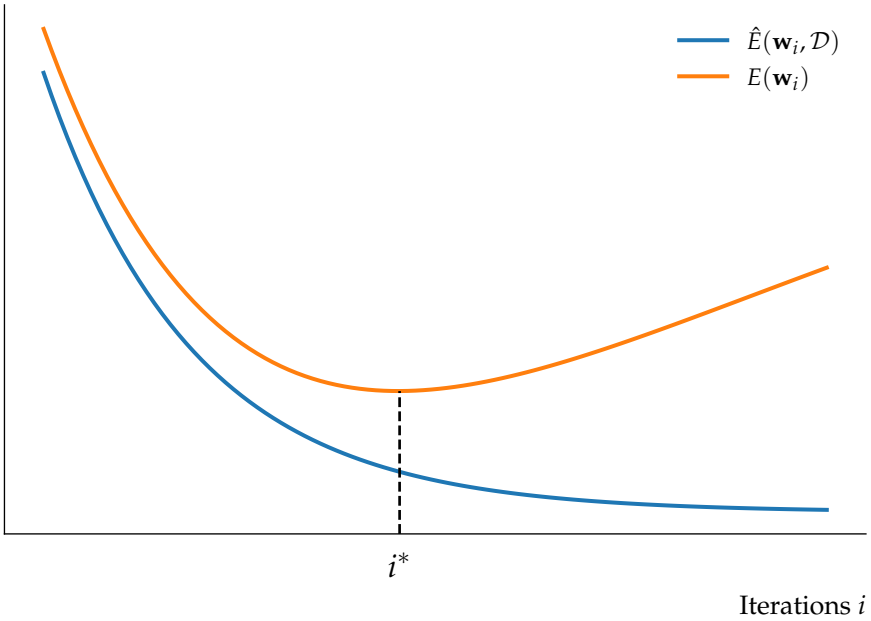


Figure 3.7
Typical behavior of E and $\hat{E}$ as a function of the number of iterations i of gradient descent. Both errors are reduced until a point i^* beyond which the training error is reduced, but generalization error increases.

negative gradient minimizes $\hat{E}(\mathbf{w}, \mathcal{D})$ among all weights with $||\mathbf{w} - \mathbf{w}_i|| \leq \eta$ (Abu-Mostafa et al., 2012). In other words, we can think of an effective hypothesis space $\mathcal{H}_i$ for each iteration thats limited by η:

$$\mathcal{H}_i = \{\mathbf{w} \mid ||\mathbf{w} - \mathbf{w}_i|| \leq \eta\}$$

We can think of the hypothesis space $\mathcal{H}$ explored by gradient descent in a finite number of steps I as the union of these sets:

$$\mathcal{H} = \bigcup_{i=1}^{I} \mathcal{H}_i$$

As I increases, $\mathcal{H}$ becomes more diverse, and Vapnik-Chervonenkis theory tells us that the risk of selecting $\mathbf{w} \in \mathcal{H}$ that fits the noise in $\mathcal{D}$ increases. In practice, it is consistently observed that both $E(\mathbf{w_i})$ and $\hat{E}(\mathbf{w}_i, \mathcal{D})$ is decreased as a function of i until a certain point i^* after which only $\hat{E}(\mathbf{w}_i, \mathcal{D})$ is decreased as a consequence of fitting the noise in $\mathcal{D}$ which causes $E(\mathbf{w}_i)$ to increase. See figure 3.7 for a visualization.

When using early stopping, we treat the optimal number of iterations of gradient descent i^* as a parameter we want to estimate. This is done through validation as described in section 2.2.3. Specifically, after each gradient descent iteration $\hat{E}(\mathbf{w}_i, \mathcal{D}_{val})$ is computed as an estimate of E. When this quantity is no longer improved, gradient descent is halted and the the parameters $\mathbf{w}_{i^*}$ are returned.

When using stochastic gradient descent, $\hat{E}(\mathbf{w}_i, \mathcal{D}_{val})$ may vary slightly from iteration to iteration due to the noise introduced by the stochastic gradient. This means that the simple heuristic stopping criterion described above may fail when using stochastic gradient descent. A so called **patience** parameter is a simple solution to this problem. When using patience p, stochastic gradient descent is only halted when no improvement on $\hat{E}(\mathbf{w}_i, \mathcal{D}_{val})$ has been observed for p iterations.

3.3 Convolutional Neural Networks

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

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

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

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

Many 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** or **convolutional filter**. As an example, consider the noisy signal convolved with a gaussian kernel in figure 3.8.

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 3.9.

Convolutional neural networks are neural networks that take advantage of convolutions as feature detectors (LeCun et al., 1989). 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 re-used around every index of f. See figure 3.10.

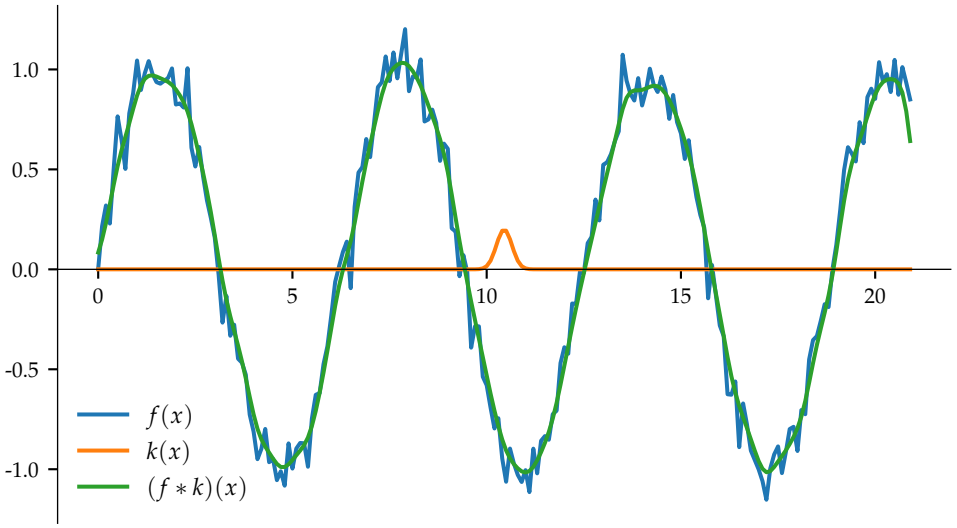


Figure 3.8
Visualisation of a noisy signal f convolved with a small Gaussian kernel k. The output of the convolution $f * k$ captures the general trend of f by averaging the outputs of f at every x, such values of f of inputs close to x contribute more to the output of the convolution, than inputs far away from x thanks to the weights of the Gaussian kernel.

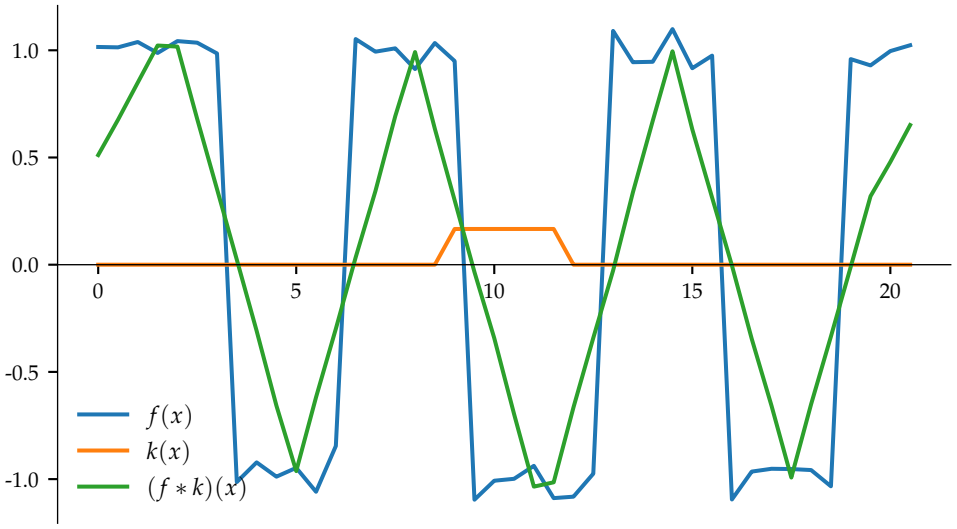


Figure 3.9
Visualisation of convolutional kernel as feature detector. When the signal f is similar to the kernel, the output of the convolution is maximally positive.

These restrictions on the network architecture reduces the number of unique weights of the model. This improves the statistical efficiency of these types of models, i.e reduces the complexity of the induced hypothesis space (Goodfellow et al., 2016). Moreover, the reduction in the effective number of parameters 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**. A pooling layer performs an aggregation function over the output of a neural network layer $f^{(l)}$ such as taking the mean or max across the output units.

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 feature was detected. Very commonly, max-pooling is used which simply outputs the maximum value over all outputs of units in layer l.

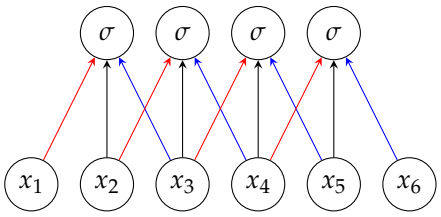


Figure 3.10
Visual representation of a one-dimensional convolution implemented as the first layer of a convolutional neural network. The connections between the input layer and the convolutional layer are sparse in that each unit is connected only to three of six inputs. The colors of the connections 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 a discrete input space where distances between points don't encode similarity, such as words, to a prediction, such as the presence of a named entity, may be more difficult than learning a mapping from a continuous input space 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 (Jurafsky and Martin, 2009).

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 $\tilde{\mathbf{w}}_i$.

Glove vectors are learned by initializing each vector $\mathbf{w}_i$ and $\tilde{\mathbf{w}}_i$ randomly and then minimizing 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:

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

Minimizing this objective leads to word vectors whose dot products are close to log-co-occurrence counts for the words they represent. Pennington et al. (2014) argue that word vectors with this property 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 particular, words are mapped to word vectors through a word-embedding matrix such that column i in this matrix corresponds to word i in the vocabulary. The weights of the word embedding matrix is then optimized through gradient descent just as any other weight of the network.

In this scheme, the components of the word vectors are weights that can be trained by backpropagation to yield word vector representations that are informative for a given task. These word embedding vectors can be initialized with small random components as any other neural network weight, or they can be initialized with pre-learned word vectors, for example GloVe vectors which often leads to great improvements on a host of language processing tasks (Collobert and Weston, 2008;

Collobert et al., 2011; Nguyen and Grishman, 2015; Kim, 2014; Zhang and Wang, 2015)

3.5 Summary

In this section we have seen how to define $\mathcal{H}$ with neural networks, and we have seen how to search this space using backpropagation and gradient descent. We have presented the Adam algorithm as a useful extension to stochastic gradient descent that incorporates ideas of learning rate scaling and momentum.

Moreover, we have discussed regularization techniques that restrict the learning algorithm to a limited region of $\mathcal{H}$ in order to reduce the risk of overfitting. In particular, we have presented early stopping as a simple yet effective regularization technique. Finally, we have introduced convolutional neural networks that take advantage of convolutions as feature detectors. As we will discuss in part 5, convolutional neural networks are often used to solve sentence classification problems such as relation classification.

In the next part, we introduce the multi-task learning framework as an extension to Vapnik-Chervonenkis analysis presented in section 2.2.2.

Part 4

Multi-Task Learning

In this section we introduce an extension to the supervised machine learning framework called multi-task learning. We first cover the main ideas and motivation for multi-task learning. We then summarize different variations on statistical learning theory to gain an intuition of how and when multi-task learning works. Finally, we describe how to implement multi-task learning with neural networks.

4.1 Multi-Task and Single-Task Learning

In our description of supervised machine learning so far we have assumed that the input for the learning system was an annotated dataset $\mathcal{D}$ in which all samples $(\mathbf{x}_i, \mathbf{y}_i) \in \mathcal{D}$ are drawn independently from the same distribution $P(\mathbf{x}, \mathbf{y})$. In the real world however, it's often possible to combine data from disparate sources if we relax this assumption: We may have access to a set $\mathcal{D}_M$ of M datasets $\mathcal{D}_m \in \mathcal{D}_M$, drawn from a set $\mathcal{P}$ of M different distributions $P_m(\mathbf{x}, \mathbf{y}) \in \mathcal{P}$. Since creating new labels for a machine learning task is often both cumbersome and costly, it would be desirable if re-using previously labeled data could reduce the need for data annotation

In many cases, we are not interested in implementing a learning system that performs well on all M learning tasks. We really only care about one **target** task defined by a distribution $P_t \in \mathcal{P}$ and $\mathcal{D}_t \in \mathcal{D}_M$ in which case we consider the other datasets $\mathcal{D}_A = \{\mathcal{D}_m \mid \mathcal{D}_m \in \mathcal{D}_M, m \neq t\}$ to be **auxiliary**. Since we are dealing with more than one probability distribution, it becomes useful to think of generalization error with respect to a particular distribution. Thus, we extend our notation for generalization error from E to E_m to mean:

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

We can speculate that if $\mathcal{D}_t$ and $\mathcal{D}_A$ are related somehow, and if the learning system is able to share what is learnt between the learning tasks, learning the tasks simultaneously may improve generalization for the target task relative to learning from $\mathcal{D}_t$ in isolation (Caruana, 1997). To distinguish the two approaches, the traditional approach to supervised machine learning as described in section 2.2 is called **single-task learning**, and the new approach in which the learning system uses all of $\mathcal{D}_M$ is called **multi-task learning**.

In the following sections we introduce contributions from statistical learning theory that shed some light on when and how learning from $\mathcal{D}_M$ is beneficial.

4.2 Bias Learning

Selecting the hypothesis space $\mathcal{H}$, sometimes referred to as **biasing** the hypothesis space, is often the hardest problem in supervised machine learning (Baxter, 2000). Vapnik-Chervonenkis analysis tells us that $\mathcal{H}$ must be large enough to contain a good solution to the learning problem of interest, yet small enough that the selected model can generalize from a small sample. This motivates developing techniques that can learn a good $\mathcal{H}$ from the data.

Baxter (2000) formalizes this idea by introducing a model of **bias learning** in which the learning system is tasked with learning a hypothesis space $\mathcal{H}$ from a family of hypothesis spaces $\mathbb{H} = \{\mathcal{H}\}$. The system is supplied with M datasets $\mathcal{D}_m$ each drawn from M distributions P_m over $\mathcal{X} \times \mathcal{Y}$. The goal of the system is then to first select a good hypothesis space $\mathcal{H} \in \mathbb{H}$, and then to select a vector $\mathbf{h}$ of M hypothesis $h_m \in \mathcal{H}$. In his framework, the goal of the learning system is to minimize the multi-task generalization error defined as the average generalization error over the M learning problems:

$$E(\mathbf{h}) = \frac{1}{M} \sum_{m=1}^{M} E_m(h_m)$$

Similarly, we can generalize the empirical single-task error to an average multi-task empirical error $\hat{E}(\mathbf{h}, \mathcal{D}_M)$:

$$\hat{E}(\mathbf{h}, \mathcal{D}_M) = \frac{1}{M} \sum_{m=1}^{M} \hat{E}(h_m, \mathcal{D}_m)$$

The bias learning model of Baxter (2000) extends Vapnik-Chervonenkis analysis to the multi-task learning problem. To this end, he defines $\mathcal{H}(N, M)$ to be the set of all matrices of dichotomies, that can be formed from selecting M hypothesis from $\mathcal{H}$ and applying them to the to the N samples of the M datasets in $\mathcal{D}_M$:

$$\mathcal{H}(N, M) = \left\{ \begin{bmatrix} h_1(\mathbf{x}_{11}) & \cdots & h_1(\mathbf{x}_{1N}) \\ \vdots & \ddots & \vdots \\ h_M(\mathbf{x}_{M1}) & \cdots & h_M(\mathbf{x}_{MN}) \end{bmatrix} : h_1, \ldots, h_M \in \mathcal{H} \right\}$$

This allows him to define a concept of dichotomies on multi-task samples $\mathcal{D}_M$ for hypothesis space families, $\mathbb{H}(N, M)$:

$$\mathbb{H}(N, M) = \bigcup_{\mathcal{H} \in \mathbb{H}} \mathcal{H}(N, M)$$

And extend the growth function m to the multi-task setting:

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

With a binary label space, the maximum size of $\mathbb{H}(N, M)$ is 2^{NM}. Baxter uses this to define the Vapnik-Chervonenkis dimension $d(M, \mathbb{H})$ of the hypothesis space family $\mathbb{H}$:

$$d(M, \mathbb{H}) = \max\{N : m(N, M, \mathbb{H}) = 2^{NM}\}$$

In words, the Vapnik-Chervonenkis dimension of the hypothesis space family $\mathbb{H}$ is the largest number of samples N for M tasks for which the family can generate all possible binary dichotomy matrices.

Using the same reasoning as is the basis of the original Vapnik-Chervonenkis bound, Baxter is able to show that in order for the average true error $E(\mathbf{h})$, to be within ϵ of the average empirical error $\hat{E}(\mathbf{h}, \mathcal{D}_M)$ with probability $1 - \delta$, it requires that the number of samples N for each task is:

$$N \geq O\left(\frac{1}{\epsilon^2}\left(d(M, \mathbb{H}) \log \frac{1}{\epsilon} + \frac{1}{M} \log \frac{1}{\delta}\right)\right)$$

Ignoring the confidence parameters ϵ and δ, we see that the number of examples N depends inversely on the number of tasks M. This means that we can reduce the number of samples required to keep E close to $\hat{E}$ if we can increase the number of learning tasks. This is an important result since it shows that multi-task bias learning can improve our confidence that E_m is close to $\hat{E}(h_m, \mathcal{D}_m)$ at least on average.

On the other hand, it's also a limited result in the sense that it doesn't tell us anything about how $\hat{E}(h_m, \mathcal{D}_m)$ behaves in multi-task learning relative to single-task learning. In other words, it may be possible that bias learning leads to a hypothesis space $\mathcal{H}$ where $\hat{E}(\mathbf{h}, \mathcal{D}_M)$ is close to $E(\mathbf{h})$, but $E(\mathbf{h})$ is much larger than would have been possible to achieve if the learning algorithm applied to each task was not restricted to the same hypothesis space.

4.3 Representation Learning

Representation learning is a special case of bias learning that's especially relevant for deep learning techniques. In this view, the bias is modeled specifically as a transformation of the input data, a representation, that is shared across the M learning tasks.

Baxter (1995) provides a basic framework for formally understanding the mechanics of representation learning. To enable the learning system to take advantage of the disperse datasets, the hypothesis space $\mathcal{H}$ is split into two parts $\mathcal{F} = \{f \mid f : \mathcal{X} \to \mathcal{V}\}$ and $\mathcal{G} = \{g \mid g : \mathcal{V} \to \mathcal{Y}\}$ where $\mathcal{V}$ is an arbitrary set. We achieve this by defining each function $h \in \mathcal{H}$ as a composition of two functions, i.e $h = g \circ f$ where $f \in \mathcal{F}$ and $g \in \mathcal{G}$. $\mathcal{F}$ is called the **representation space**, and $\mathcal{G}$ is called the **output space**.

According to Baxter (2000), the objective of representation learning is to find a good representation $f \in \mathcal{F}$ which is shared between each of the output functions g_1 to g_M. To formalize this, he introduces the notation $\mathbf{g} \circ f$ which denotes the composition of a vector $\mathbf{g}$ of M output functions with the representation function f as $\mathbf{g} \circ f = [g_1 \circ f, \ldots, g_M \circ f)]$. A good representation f is then a function which re-

duces the generalization error $E(\mathbf{g} \circ f)$:

$$E(\mathbf{g} \circ f) = \frac{1}{M} \sum_{m=1}^{M} E_m(g_m \circ f)$$

In words, the generalization error of f is the average single task generalization error over the M tasks when the tasks share a common representation f.

Since $\mathcal{P}$ is unknown we can only estimate the true generalization by an empirical error measure, $\hat{E}(\mathbf{g} \circ f, \mathcal{D}_M)$:

$$\hat{E}(\mathbf{g} \circ f, \mathcal{D}_M) = \frac{1}{M} \sum_{m=1}^{M} \hat{E}(g_m \circ f, \mathcal{D}_m)$$

In words, the average empirical error over each task and each training sample for each task, using a common representation for all tasks.

Baxter (1995) is able to show that if the tasks are learnt by minimizing $\hat{E}$ with a common representation f, we can decrease the number of examples N for each task required to ensure that $\hat{E}$ will be close to E with high probability by increasing the number of tasks M. In other words, learning with a common representation reduces the gap between training error and generalization error.

As is the case with the bound presented in Baxter (1995) however, this result only bounds the average distance between $\hat{E}$ and E. In other words, it doesn't tell us when multi-task representation learning is beneficial in an absolute sense: if representation learning can reduce the complexity of $\mathcal{H}$ and $\hat{E}$ simultaneously as compared to single task learning.

As we will see in section 4.5, the potential advantages of multi-task learning with neural networks are enabled precisely by a shared representation. This makes the contribution of Baxter (1995) important since it provides a theoretical basis for deep multi-task learning.

4.4 Task Relatedness

Our presentation of multi-task learning so far has been limited to the statistical properties of learning multiple tasks simultaneously without consideration as to how the tasks are related to one another. Intuitively, we expect that learning related tasks should yield better results than learning unrelated tasks.

Ben-David et al. (2003) attempts to quantify this intuition by extending the work of Baxter (2000) with a notion of task "relatedness". They focus on modeling similarity between the M distributions P_1 to P_M from which the M datasets $D_m \in \mathcal{D}_M$ are drawn.

Specifically, they consider two learning tasks, defined by the probability distributions P_1 and P_2 on the input space $\mathcal{X}$, to be related if P_1 and P_2 are identical up to

a transformation $f : \mathcal{X} \to \mathcal{X}$. To formalize this, they define a set of such transformations $\mathcal{F}$, and say that two learning tasks are $\mathcal{F}$-related if for some fixed probability distribution, the data in each of these tasks are generated by applying some $f \in \mathcal{F}$ to that distribution.

Formally, let $\mathcal{F}$ be a set of transformations $f : \mathcal{X} \to \mathcal{X}$, and P_1, P_2 be probability distributions over $\mathcal{X} \times \mathcal{Y}$ where $\mathcal{Y} = \{0, 1\}$. P_1 and P_2 are $\mathcal{F}$-related if there exists some $f \in \mathcal{F}$ such that for any $T \subseteq \mathcal{X} \times \mathcal{Y}$, T is P_1-measurable iff $f[T] = \{(f(\mathbf{x}), \mathbf{y}) \mid (\mathbf{x}, \mathbf{y}) \in T\}$ is P_2-measurable and $P_1(T) = P_2(f[T])$. Two samples are $\mathcal{F}$-related if they are sampled from $\mathcal{F}$-related distributions (Ben-David et al., 2003).

In the framework of Ben-David et al. (2003) they assume that the learning system knows the set $\mathcal{F}$ but doesn't know which function $f \in \mathcal{F}$ relates the distributions the system is learning from. Therefore, the ease with which the learner can transfer information about the underlying distributions from one learning task to another depends on the size of $\mathcal{F}$. The larger this set is, the looser the notion of relatedness between the learning tasks.

In order to let the learning system take advantage of the multiple datasets $\mathcal{D}_M$, Ben-David et al. (2003) uses their notion of task relatedness to reduce the complexity of the hypothesis space $\mathcal{H}$ by first using all the data $\mathcal{D}_M$ to select a subspace of $\mathcal{H}$ which is likely to contain good solutions to the set of learning problems. After this initial biasing of $\mathcal{H}$, M functions h_m are selected from this subspace for each learning problem. Specifically, from the hypothesis space $\mathcal{H}$, create a family of hypothesis spaces $\mathbb{H}$ of sets of hypotheses $h \in \mathcal{H}$ that are equivalent up to transformations in $\mathcal{F}$, assuming that for each $f \in \mathcal{F}$ and $h \in \mathcal{H}$, we have $h \circ f \in \mathcal{H}$.

To formalize this, Ben-David et al. (2003) define an equivalence relation $\sim \mathcal{F}$ on $\mathcal{H}$. This means that h_1 and h_2 are equivalent if there exists $f \in \mathcal{F}$ such that $h_2 = h_1 \circ f$. They use the notation $[h]_{\sim \mathcal{F}}$ to mean the equivalence class of h under $\mathcal{F}$.

Ben-David et al. (2003) uses the notion of equivalence classes to partition $\mathcal{H}$ into the family $\mathbb{H}$ of equivalence classes of $\mathcal{H}$ under $\mathcal{F}$, i.e $\mathbb{H} = \mathcal{H} \backslash \sim \mathcal{F}$

Note that if two learning tasks defined by the distributions P_1 and P_2 are $\mathcal{F}$-related, then there exists $f \in \mathcal{F}$ such that the generalization errors of any function $h \in \mathcal{H}$ on both tasks are equal. In other words, there exists $f \in \mathcal{F}$ such that:

$$E_1(h) = E_2(h \circ f)$$

This means that the equivalence classes of $\mathcal{H}$ perform equally well on the different tasks, when measured by:

$$E_m(H) = \inf_{h \in \mathbb{H}} E(h)$$

Ben-David et al. (2003) uses this fact of equivalence classes to build on Baxter (2000) and shows that if the number of examples N in each learning task satisfy:

$$N \geq O\left(\frac{1}{\epsilon^2}\left(d(M, \mathbb{H}) \log \frac{1}{\epsilon} + \frac{1}{M} \log \frac{1}{\delta}\right)\right)$$

Then, with probability $1 - \delta$, for any $1 \leq i \leq M$:

$$\left| E_i([h]_{\sim_{\mathcal{F}}}) - \inf_{h_1,\ldots,h_M \in [h]_{\sim_{\mathcal{F}}}} \frac{1}{M} \sum_{m=1}^{M} \hat{E}(h_m, \mathcal{D}_m) \right| \leq \epsilon$$

The main difference between this result and the one obtained by Baxter (2000) is that Ben-David et al. (2003) bounds the distance between $E_m([h]_{\sim_{\mathcal{F}}})$, i.e the generalization error of the equivalent functions $[h]_{\sim_{\mathcal{F}}}$ for *any* task m, and the functions that minimizes the training errors for each $\mathcal{D}_m$, whereas Baxter (2000) bounds the distance between the *average* generalization error and training error.

This is an important result because it gives credence to our intuition that learning related tasks improves the guarantees that can be made on the distance between training and generalization error over learning unrelated tasks. However, just as the bound provided by Baxter (2000), this bound does not reveal anything about how learning from $\mathcal{D}_M$ might improve $E_m(h_m)$ in an absolute sense. Moreover, the range of domains where tasks are $\mathcal{F}$-related are limited. Specifically, the notion of $\mathcal{F}$-relatedness is limited to domains where two tasks are essentially two different views of the same data, for example video footage of the same scenery from two different perspectives. This may not be an appropriate assumption for natural language processing tasks.

The intuition that learning related tasks is more appropriate than learning unrelated tasks is supported by experimental results that indicate that some auxiliary tasks do not lead to gains in target task generalization (Bingel and Søgaard, 2017; Luong et al., 2015; Mou et al., 2016; Alonso and Plank, 2016; Benton et al., 2017). Since investigating which auxiliary tasks are useful by training a multi-task learning system and experimentally comparing generalization dynamics across tasks is impractical, finding target and auxiliary dataset characteristics that indicate gains in target task generalization has received a fair amount of attention.

For example, Luong et al. (2015) finds that auxiliary datasets which outsize the target dataset lead to worse target task generalization than datasets that are smaller than the target dataset. Bingel and Søgaard (2017) finds that auxiliary tasks for which generalization error plateaus more slowly as a function of training examples compared to the target task are the most beneficial. Mou et al. (2016) finds that using an auxiliary tasks that's similar to the target task, for example a target and auxiliary relation classification task, leads to better results than learning two different tasks simultaneously, for example an auxiliary named entity recognition task and a target relation classification task. Alonso and Plank (2016) finds that properties of the label distribution of the auxiliary dataset such as skewness and kurtosis are good predictors of generalization performance.

However, these results are obtained by investigating statistical correlation between dataset characteristics and target task generalization for a relatively small number of tasks. Since correlation famously does not imply causation, in the absence of an over-arching theory of multi-task learning that fully describes when and how an auxiliary task is beneficial, the only reliable way to determine the usefulness of an auxiliary task is by training a multi-task learning system and testing it empirically.

4.5 Deep Multi-Task Learning

Neural networks have the advantage of being easy to adapt from single-task learning to multi-task learning. The simplest way of turning two single task learning problems into a multi-task learning problem using neural networks is by hard weight sharing of a subset of the weights of the networks for the learning tasks and learning them simultaneously (Caruana, 1997). As an example, consider figure 4.1 and 4.2.

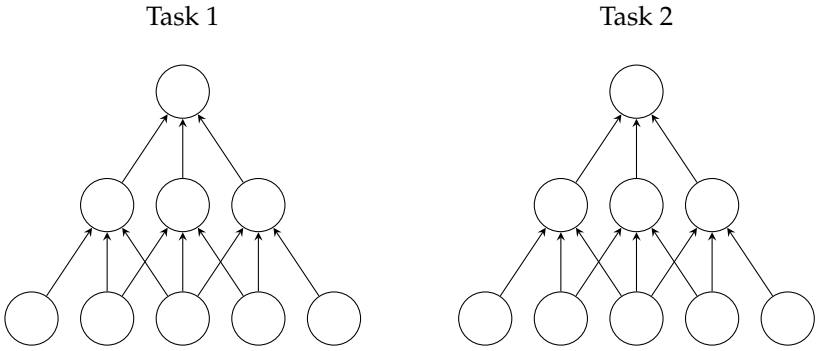


Figure 4.1
Visual representation of single-task learning with neural networks. A set of neural network weights are learnt separately for Task 1 and Task 2.

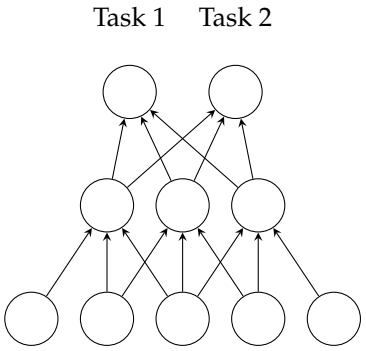


Figure 4.2
Visual representation multi-task learning with neural networks. The weights of the hidden layer is shared between the two tasks.

Multi-task learning techniques that are based on sharing neural network weights between tasks are collectively known as **deep multi-task learning**. Deep multi-task learning is closely associated with the idea of representation learning presented in section 4.3 and the more general framework of bias learning presented in section 4.2. The shared layers, often the early layers of the network, constitute a shared representation f. The full networks for each learning task are built from the shared representation f and hypotheses $h_1 = (g_1 \circ f)(\mathbf{x})$ to $h_M = (g_M \circ f)(\mathbf{x})$, where g_m is $L - S$ neural network layers specific to each task.

The exact circumstances under which deep multi-task learning leads to lower overall generalization error compared to deep single-task learning are not yet theoretically well understood. Caruana (1997) lists 3 suggestions for how multi-task learning can reduce generalization error:

Statistical Data Amplification The effective number of training examples available to a deep multi-task learning system is increased due to the examples in the auxiliary data. The extensions to the Vapnik-Chervonenkis bound seen in the preceding sections gives us confidence that this reduces the risk that generalization error is far away from training error.

Eavesdropping If a hidden layer feature is useful to both Task 1 and Task 2, but much easier to learn when learning Task 2, sharing the hidden layer between the two tasks is likely to reduce generalization error for Task 1.

Representation Bias If Task 1 and Task 2 share a common minimum in weight-space, learning the tasks with weight sharing biases the learning system to choose the shared minimum. This is effectively a form of regularization that forces the learning system to search for a good hypothesis in a hypothesis space that is restricted to hypotheses that are useful for more than one task.

Baxter (2000) applies his bias learning framework to the case where the hypothesis space family $\mathbb{H}$ is constructed of neural networks where the first two layers are shared between tasks.

Specifically, a feature map $\phi_{\mathbf{w}} : \mathbb{R}^d \mapsto \mathbb{R}^{d^{(2)}}$ is a two layer neural network parameterized by $\mathbf{w}$ that maps an input vector $\mathbf{x} \in \mathbb{R}^d$ to feature vector $\phi_{\mathbf{w}}(\mathbf{x})$. Each feature $\phi_{\mathbf{w},j} \in \phi_{\mathbf{w}}$ is defined by:

$$\phi_{\mathbf{w},j}(\mathbf{x}) = \sigma\left(w_{0j} + \sum_{i=1}^{d^{(1)}} w_{ij} h_i(\mathbf{x})\right)$$

h_i is the output of unit i in the first layer, w_{ij} is the weight connecting unit $\phi_{\mathbf{w},j}$ and i and w_{0j} is the bias weight. For simplicity, Baxter (2000) considers only the binary threshold activation function:

$$\sigma(a) = \begin{cases} +1 & \text{when } a \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

The output of each unit in the first layer h_j is computed as

$$h_j(\mathbf{x}) = \sigma\left(v_{0j} + \sum_{i=1}^{d} v_{ij} x_i\right)$$

where v_{ij} is the weight connecting the input feature x_i to unit j in the first layer and v_{0j} is a bias weight. The total number of weights W in these two layers is thus $W = d^{(1)}(d^{(0)} + 1) + d^{(0)}(d + 1)$. The space of all such feature maps $\{\phi_{\mathbf{w}} \mid \mathbf{w} \in \mathbb{R}^W\}$ can be thought of as the representation space $\mathcal{F}$ in the representation learning framework of Baxter (1995).

Baxter (2000) defines a hypothesis space $\mathcal{H}_{\mathbf{w}}$ as a set of binary decision functions on top of the feature maps. Specifically:

$$\mathcal{H}_{\mathbf{w}} = \left\{ \sigma \left(a_0 + \sum_{i=1}^{d^{(2)}} a_i \phi_{\mathbf{w},i} \right) \;\middle|\; a_0, \ldots, a_{d^{(2)}} \in \mathbb{R} \right\}$$

where a_i is the weight connecting feature $\phi_{\mathbf{w},i}$ and the output unit and a_0 is a bias weight. The set of all such hypothesis spaces can be considered a hypothesis space $\mathbb{H}$ family such that:

$$\mathbb{H} = \{\mathcal{H}_{\mathbf{w}} \mid \mathbf{w} \in \mathbb{R}^W\}$$

Recall that the goal in bias learning is to select a vector $\mathbf{h}$ of M hypotheses h_m that minimizes the average generalization error $E(\mathbf{h}) = \frac{1}{M} \sum_{m=1}^{M} E_m(h_m)$. With the limitations described above, Baxter (2000) is able to show that in order for the average empirical error $\hat{E}(\mathbf{h}, \mathcal{D}_M)$ to be within ϵ of the average generalization error $E(\mathbf{h})$ with probability $1 - \delta$, it suffices that the number of examples N per task satisfies:

$$N \geq O\left(\frac{1}{\epsilon^2} \left(\frac{W}{M} + d^{(2)} + 1 \right) \log \frac{1}{\epsilon} + \frac{1}{M} \log \frac{1}{\delta} \right)$$

Ignoring the confidence parameters ϵ and δ, the sample complexity bound tells us that learning complicated neural network representations where $d^{(1)}$ and $d^{(2)}$ and therefore also W are large, is harder than learning simple representations in the sense that it requires more samples to succeed. The benefit gained by multi-task learning is that we can reduce N by increasing M, an option we don't have in the single task learning setting. This means we can afford to learn more complicated representations in the hope that this can lead to lower training error for one or more tasks and still have high confidence that generalization is possible by increasing M.

4.6 Summary

In this section we have introduced important contributions to statistical learning theory that shed light on some of the possible benefits of multi-task learning. Specifically, we have seen how multi-task learning can be seen as a form of bias learning that automatically learns a hypothesis space from a family of hypothesis spaces $\mathbb{H}$. Vapnik-Chervonkis style analysis of this view of multi-task learning shows that the distance between generalization and training error depends inversely on the number of tasks M. This means that multi-task learning is a feasible approach of re-using annotated data.

We have discussed representation learning as a specific instance of bias learning. We have cited a result that shows that representation learning leads to much the same sample complexity dynamics as bias learning.

Moreover, we have discussed the impact of learning related vs. unrelated tasks. We have seen that Vapnik-Chervonenkis analysis confirms our intuition that learning related tasks can provide stronger guarantees on the potential benefits for generalization error. We have also discussed efforts towards finding characteristics of target and auxiliary tasks that are good predictors of gains in generalization performance

for multi-task learning. We have argued that despite these efforts, the most reliable approach for determining if multi-task learning is appropriate for a particular problem is through trial and error.

Finally, we have discussed how to adapt neural networks for multi-task learning using hard weight sharing. We have presented a Vapnik-Chervonkenkis style analysis of deep multi-task learning that shows that the difficulty of learning a good representations for a set of tasks using hard neural network weight sharing is governed by the amount of target and auxiliary data and the the number of weights in the shared layers.

In the next section we explain how we have applied this understanding of deep multi-task learning to implement an experiment that tests it's effectiveness in the context of relation classification.

Part 5

Experiment

In this section we explain our experimentation with deep multi-task learning for relation classification. We begin by describing related work on deep multi-task learning for natural language processing tasks and relation extraction. We focus on papers that have had a direct impact on architectural and algorithmic choices in our own experimentation. We then describe in some detail the benchmark relation classification dataset which will act as our target task. We continue by describing each auxiliary task used in our experiments. Finally, we describe the target and auxiliary neural network architecture and algorithm used to jointly train and probe generalization performance.

5.1 Related Work

To our knowledge, there hasn't been any experimental work done on deep multi-task learning for relation classification despite the popularity of these techniques in natural language processing in general. The work of Jiang (2009) is perhaps most closely related to our own. She demonstrates a technique for sharing weights between logistic regression classifiers trained for binary classification of a target relation and auxiliary relation when there is only a small number of seed training instances available for the target task.

The input to these binary classifiers are hand-crafted linguistic features based on syntactic and dependency parse trees. She finds that sharing components of the weight vectors for each of these classifiers improves the F1 score on a validation set compared to learning the weight vectors in a single-task fashion.

Moreover, she finds that the benefit of weight sharing decreases as the number of seed instances is increased. In particular, she finds that when the number of target examples exceed a 1000 samples single task learning produces better results than multi-task learning.

The work of Alonso and Plank (2016) is also closely related to our own. They test the effect of multi-task learning with on a number of tasks that also involve extracting data structures that capture the semantics of sentences such as predicting semantic frames from FrameNet Baker et al. (1998). To this end, they use a recurrent neural network where parameters of a single recurrent layer is shared between a target se-

mantic and auxiliary syntactic task. They find that multi-task learning in this setting is beneficial with statistical significance for only one target semantic task.

Collobert et al. (2011) is one of the earliest works that detail how to solve natural language processing tasks with neural networks. They focus on neural networks for sequence prediction problems. Specifically, they use two different convolutional neural network architectures for predicting tags for words by considering a window of neighboring words around the target word, transform this window into a matrix of concatenated word-vectors and feed this into a convolutional neural network. The major contribution of this technique was to show that state-of-the-art performance was possible for these tagging tasks without manual feature engineering, but simply by learning word vectors and convolutional filters directly from the words.

Collobert et al. (2011) also experimented with deep multi-task learning through hard weight sharing and found that weight sharing in general increased performance on most of the tasks they considered.

Bingel and Søgaard (2017) performs a thorough experiment on deep multi-task learning using recurrent neural networks for sequence prediction problems in natural language processing. They run experiments of 90 different configurations of target and auxiliary task and compare generalization error for the target task when compared to single-task learning. Their goal is to investigate correlation between dataset statistics and characteristics in single-task learning that are good predictors for gains in multi-task learning.

They find that the best predictor for multi-task learning gains is single-task learning curves over gradient descent iterations. Specifically, if the target task generalization error quickly plateaus, learning it simultaneously with an auxiliary task that doesn't plateau is likely to improve generalization. They speculate this happens because the inclusion of an auxiliary task can move neural network weights out of local minima during training.

Neural networks have also been tested for sentence classification problems such as relation classification. Kim (2014) designs a convolutional neural network for sentence classification and tests it on a number of sentence classification tasks such as sentiment analysis and semantic category prediction in a single-task learning setting. His architecture achieves state-of-the-art performance on a number of these tasks without any manual feature engineering.

Nguyen and Grishman (2015) adapts the work of Kim (2014) to the relation classification problem. Their addition to the architecture is a mechanism for marking the relation arguments in the input. This leads to state-of-the-art performance. They do not consider multi-task learning.

Zhang and Wang (2015) investigate the performance of recurrent neural networks on the relation extraction problem. They suggest a simple bi-directional recurrent architecture where the relation arguments are marked simply by special tokens that indicate the beginning and end of each argument. With this architecture they achieve almost state-of-the-art results close to the results of Nguyen and Grishman (2015). They find that for sentences where the relation arguments are far apart, the recurrent architecture outperforms the convolutional architecture.

5.2 Target Task

We have chosen a target relation classification dataset which will act as a benchmark across our experiments in order to empirically investigate the dynamics of sample complexity for multi-task relation classification. The SemEval 2010 Task 8 dataset has arguably become somewhat of a standard for relation classification papers, and so is a reasonable choice for the role of target task in this context (Hendrickx et al., 2009).

The SemEval 2010 Task 8 dataset consists of 10,717 English sentences. Each sentence is annotated with exactly one of the following semantic relations:

> **Cause-Effect** An event or object leads to an effect. Example: *those [cancers] were caused by radiation [exposures].*
>
> **Instrument-Agency** An agent uses an instrument. Example: *[phone] [operator].*
>
> **Product-Producer** A producer causes a product to exist. Example: *a [factory] manufactures [suits].*
>
> **Content-Container** An object is physically stored in a delineated area of space. Example: *a [bottle] full of [honey] was weighed*
>
> **Entity-Origin** An entity is coming or is derived from an origin (e.g., position or material). Example: *[letters] from foreign [countries].*
>
> **Entity-Destination** An entity is moving towards a destination. Example: *the [boy] went to [bed].*
>
> **Component-Whole** An object is a component of a larger whole. Example: *my [apartment] has a large [kitchen].*
>
> **Member-Collection** A member forms a nonfunctional part of a collection. Example: *there are many [trees] in the [forest].*
>
> **Message-Topic** A message, written or spoken, is about a topic. Example: *the [lecture] was about [semantics].*
>
> **Other** Any other relation.

SemEval 2010 Task 8 is not a traditional relation classification task. In particular, the objective of traditional relation extraction is to identify semantic relationships between named entities. In the SemEval dataset however, the annotated relationships are between head words of nominal phrases, for example *Message-Topic(lecture, semantics)* in the sentence *the lecture was about semantics* where neither *lecture* nor *semantics* are named entities.

Moreover, the annotation process for the SemEval dataset includes some restrictions which are designed to make the resulting learning problem easier. Firstly, the annotators exclude sentences where relationships depend on discourse knowledge, for example when one of the arguments are pronouns. Secondly, sentences where the relation arguments occur in different sentential clauses are excluded. For example,

we could argue that the relationship *Instrument-Agency(man, unicycle)* exists in the sentence *the man, who rides a unicycle, came to see me.*, but since the arguments occur in different sentential clauses it would be excluded from the SemEval dataset.

The annotators aimed for a uniform distribution of relations in the SemEval dataset. To this end, they initially collected approximately 1200 sentences for each relation category by pattern based web search. This ultimately led to the distribution shown in figure 5.1. One consequence of this selection procedure is that the label distribution does not follow the distribution of relations found in natural language data in the wild.

Ideally, we'd like to be able to make conclusions about the usefulness of multi-task learning for relation classification in general and not just on SemEval 2010 Task 8 based on the results in this thesis. This is possible to the extent that the SemEval data is a realistic sample and that the target relations are general enough that they are useful for a wide range of domains. As discussed above, both of these qualities can be called into question.

Handschuh et al. (2016) provides a brief discussion of the generality of SemEval 2010 Task 8. In addition to the limitations we have already pointed out, they highlight that the relations in the SemEval dataset are mainly concerned with relations between concrete, physical objects. Taken together, the limitations of SemEval 2010 Task 8 could indicate that a need exists for authoring a more general relation classification task that is more appropriate as a benchmark task. At this time however, we use the SemEval dataset as target task in our experiments because of its prevalence in the research literature despite these points of criticism.

5.3 Auxiliary Tasks

Here we describe each of the datasets used as auxiliary tasks in our multi-task learning experiment. We focus on auxiliary tasks for which there exists well documented neural network architectures that don't require bespoke components which may make deep multi-task learning by hard weight sharing impractical. We describe the goal of each task in some detail in order to reason about its potential benefit as an auxiliary task for SemEval 2010 Task 8.

5.3.1 ACE 2005 Relations

Intuitively, we expect that a feature transformation in the early layers of a neural network that's useful for one relation classification task should also be useful to another, assuming the relations of interest in one task are semantically related to the relations in another.

We therefore test the usefulness of incorporating an auxiliary relation classification task as measured by generalization error on the SemEval dataset. Next to SemEval, the ACE 2005 relation classification dataset is the most widely used in contemporary literature (Walker et al., 2006). Unlike the SemEval 2010 dataset, the stated goal of the ACE 2005 relation classification task is to identify relations between named entities. Specifically, the relations in the ACE 2005 dataset are defined be-

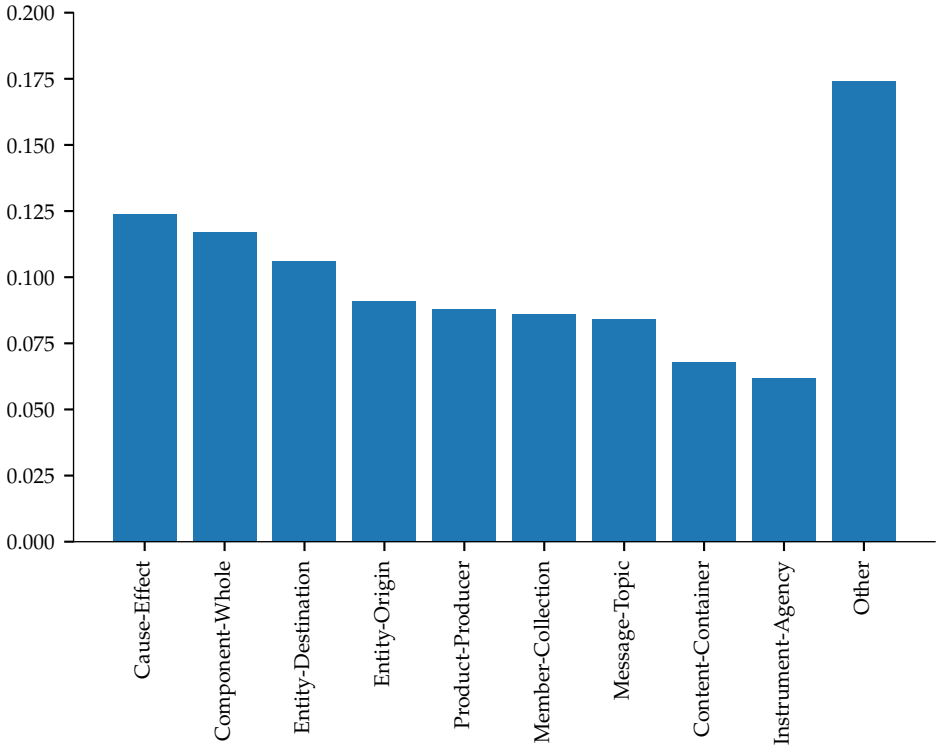


Figure 5.1
Label distribution of SemEval 2010 Task 8.

tween the entity types: person, organization, location, facility, weapon, vehicle and geo-political entity. Unlike the SemEval annotation process, the annotation guide for ACE 2005 contains no restrictions on the complexity of the sentences in terms of dependence on discourse knowledge or sentential clauses.

The ACE 2005 relation classification dataset contains 8,365 english sentences collected from various sources such as transcribed news broadcasts and phone conversations, as well as Usenet discussion forums and Newswire. Each sentence is annotated with exactly one of the following relations:

> **Physical** Two entities are physically related. Example: *[Donald Trump] lives in [The White House].*
>
> **Part-Whole** One entity constitutes part of another. Example: *[Gibraltar] is territory of the [UK].*
>
> **Personal-Social** Entities are people with a social relation. Example: *[Darth Vader] is the father of [Luke Skywalker].*
>
> **Organization-Affiliation** A person is affiliated with an organization. Example: *[Ray Kroc] founded [McDonald's].*
>
> **Agent-Artifact** An entity is the agent of an artifact. Example: *[James Bond] drives an [Aston Martin DB5].*
>
> **Gen-Affiliation** Affiliation between a person and a political or religious entity and ethnic affiliation. Example: *[Mitt Romney] is a member of [the Mormon church].*

In truth, each of the relations above are further sub-categorized in the ACE 2005 corpus. For example, the *Person-Social* relation is further subcategorized into *Family*, *Business* and *Lasting-Personal* relations. For simplicity, we pursue the task of prediction only the top level relation classes enumerated above.

There is clear semantic overlap between the relation categories of the SemEval dataset and the ACE dataset, for example for the categories *Agent-Artifact* and *Physical* in the ACE corpus and *Instrument-Agency* and *Entity-Origin* in the SemEval corpus. We can speculate that a neural network representation that's useful for one task may be useful for the other which may lead to improved generalization error on the target task.

5.3.2 CONLL2000 Part-of-Speech

Part-of-speech (POS) tagging is the task of assigning part-of-speech tags such as noun, verb etc. to word tokens (Jurafsky and Martin, 2009). Part-of-speech tags are known to be a useful input feature for a number of other supervised machine learning systems for natural language processing tasks, here-among named entity recognition and relation extraction. This is believed to be the case since word classes are highly informative of a word's semantic role in a sentence (Jurafsky and Martin, 2009).

Several part-of-speech tagging schemes exists. The universal tag-set is a simple and commonly used scheme which contains 12 different tags:

VERB Verbs (all tenses and modes)

NOUN Nouns (common and proper)

PRON Pronouns

ADJ Adjectives

ADV Adverbs

ADP Adpositions (prepositions and postpositions)

CONJ Conjunctions

DET Determiners

NUM Cardinal numbers

PRT Particles or other function words

X Other - foreign words, typos, abbreviations.

. Punctuation

Part-of-speech tagging can be seen as sequence labeling problem. The goal is to assign a tag to each token in a sentence. See for example figure 5.2.

I	saw	the	man	with	the	telescope	.
PRON	VERB	DET	NOUN	ADP	DET	NOUN	.

Figure 5.2
A sentence tagged with universal part-of-speech tags.

The CONLL2000 dataset was produced as a shared task for the year 2000 Conference on Computational Natural Language Learning (Tjong Kim Sang and Buchholz, 2000). It contains 10,948 sentences with 259,104 tokens from the Wall Street Journal section of the Penn Treebank (et al., 1999). The part-of-speech tag for each token is supplied not by a human annotator, but from an automatic tagging system called the Brill tagger (Brill, 1992).

We speculate that a neural network representation that's useful for part-of-speech tagging will also be useful for relation classification. In particular, if word vectors or neural network features encode information about part-of-speech-tags it may help to resolve ambiguity for words that are crucial for identifying semantic relations, such as words that are verbs in some contexts but nouns in others.

5.3.3 CONLL2000 Chunking

Assigning structure to a sentence is generally known as parsing. Syntactic parsing is a fundamental task in natural language processing which involves segmenting a sentence into a hierarchical structure that captures its syntactic elements (Jurafsky and Martin, 2009). Consider figure 5.3 as an example.

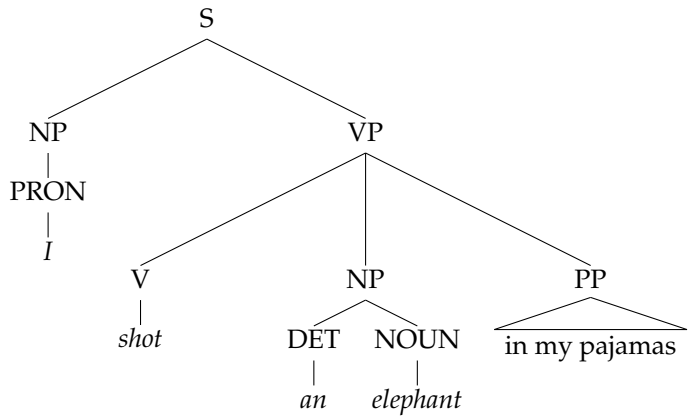


Figure 5.3
Syntactic parse tree for the sentence: I shot an elephant in my pajamas. *The parse tree captures the fact that the sentence is composed from a noun phrase (NP) followed by a verb phrase (VP) followed by a prepositional phrase (PP).*

I	shot	an	elephant	in	my	pajamas	.
B-NP	B-VP	B-NP	I-NP	B-PP	I-PP	I-PP	O

Figure 5.4
Chunks of the sentence: I shot an elephant in my pajamas*, annotated with BIO-labelling.*

Many practical applications do not require full syntactic parses. **Chunking** is a simpler partial parsing technique that can often be used as an alternative (Jurafsky and Martin, 2009). The goal of chunking is to identify the flat, non-overlapping parts of a sentence that constitute its major non-recursive phrase structures. Se for example figure 5.4.

The CONLL2000 dataset is annotated with chunking information in the BIO-labelling scheme introduced in section 2.1.1 in addition to part-of-speech tags.

A neural network representation that's useful for predicting syntactic chunks may benefit a relation classification task since the syntactic structure of a sentence is highly informative for how nominals are semantically related to each other. For example, in order to determine whether the relationship between *The Ford Motor Company* and *Dearborn, Michigan* in the sentence

The Ford Motor Company produces cars in Dearborn, Michigan

is *Entity-Origin* and not for example *Product-Producer*, it's useful to know that *cars* is a noun-phrase whereas *Dearborn, Michigan* is a prepositional phrase, and therefore not the object of *produces*.

5.3.4 GMB Named Entity Recognition

We described the named entity recognition problem in section 2.1.1. Groningen Meaning Bank is a corpus annotated with various semantic information such as named entity information developed at University of Groningen (Basile et al., 2012).

The corpus contains 62,010 sentences annotated with the following named entity types:

Person Individuals that are human or have human characteristics, such as divine entities.

Location Geographical entities such as geographical areas and landmasses, bodies of water, and geological formations.

Organization Corporations, agencies, and other groups of people defined by an established organizational structure.

Geo-Political Entity Geographical regions defined by political and/or social groups. A GPE entity subsumes and does not distinguish between a city, a nation, its region, its government, or its people.

Artifact Manmade objects, structures and abstract entities, including buildings, facilities, art and scientific theories.

Natural Object Entities that occur naturally and are not manmade, such as diseases, biological entities and other living things.

Event Incidents and occasions that occur during a particular time.

Time References to certain temporal entities that have a name, such as the days of the week and months of a year.

Even though SemEval 2010 Task 8 is not explicitly concerned with classifying relationships between named entities, we can speculate that neural network features that are useful for predicting named entity types is also useful for predicting semantic relations for the SemEval task. For example, learning a named entity task leads to neural network features that are useful for discriminating between people and locations. We can speculate that although *forest* is not a named entity in the sentence:

there are many trees in the forest

the features learned for a named entity task could non the less indicate that *forest* is more likely to be a location than, say, a person. If the model is able to learn that locations are more likely arguments for *Member-Collection* than, say, *Component-Whole*, this may improve the target systems confidence for the correct relation.

5.4 Neural Network Architecture

Our neural network architecture for relation classification is based on Nguyen and Grishman (2015). We chose this architecture since it achieves the best results that we've encountered in contemporary research literature on SemEval 2010 Task 8, which would make our findings relevant to state-of-the-art research. This architecture is not appropriate for sequence labeling tasks however because of neural network components that are unique to the relation classification task as explained below. As a consequence, we use a related but slighter different architecture based on Collobert et al. (2011) for the sequence labeling tasks and share neural network weights of the early layers between the two architectures.

In the architecture described in Nguyen and Grishman (2015) each word s_i of an input sentence s is first mapped to a word-vector $\mathbf{v}_i \in \mathbb{R}^d$ through a word-embedding matrix to form a sentence matrix $\mathbf{S}$. In our experiment, we initialize the word-embedding matrix with $d = 300$ dimensional GloVe vectors trained on the Common Crawl corpus (commoncrawl.org). To ensure that the dimensionality of $\mathbf{S}$ is consistent across sentences, we compute the longest sentence length K of the sentences in the SemEval and ACE corpora and pad shorter sentences with a padding token as a preprocessing step, such that $\mathbf{S} = [\mathbf{v}_1, \ldots, \mathbf{v}_K]^T$.

To indicate which words in the input sentence are the relation arguments, we compute the distance between each word index i and the index of the first relation argument words $e1$ and $e2$ as $i - e1$ and $i - e2$ for the first and second argument respectively. These distances are mapped into real valued position vectors $\mathbf{p}_{1i}$ for the distance $i - e1$ for each word, and $\mathbf{P}_{2i}$ for the distance $i - e2$ for each word, both in $\mathbb{R}^{d'}$. From these we construct the position matrices $\mathbf{P}_1 = [\mathbf{p}_{11}, \ldots, \mathbf{p}_{1K}]^T$ and $\mathbf{P}_2 = [\mathbf{p}_{21}, \ldots, \mathbf{p}_{2K}]^T$. We use the three matrices $\mathbf{S}$, $\mathbf{P}_1$ and $\mathbf{P}_2$ to form the augmented sentence matrix $\mathbf{S}' = [\mathbf{S} \mid \mathbf{P}_1 \mid \mathbf{P}_2] \in \mathbb{R}^{K \times (d+2d')}$.

The $K \times (d + 2d')$ dimensional augmented sentence matrix is used as input for a convolutional neural network layer. The convolution filters are applied over the full height of augmented sentence matrix in windows of n tokens over the K dimensional axis. In other words, each convolution filter is a weight matrix $\mathbf{W} \in \mathbb{R}^{n \times (d+2d')}$. The output of the convolutional neural at position i is:

$$\sigma\left(w_0 + \sum_{j=i}^{i+n} \mathbf{S}'_i \mathbf{W}_i^T\right)$$

Where σ is the rectified linear activation function, $\mathbf{W}_i$ and $\mathbf{S}'_i$ is the i'th row of the convolutional filter matrix and augmented sentence matrix respectively, and w_0 is a bias term. In our experiment we use 150 filters of each window size, and window sizes n of 2, 3, 4 and 5 for a total of 600 convolutional filters.

We apply max-pooling to the output of each convolutional filter yielding a 600 dimensional feature vector, which is used as input for a soft-max output layer. See figure 5.5 for a diagram.

For the sequence classification tasks we use a convolutional neural network architecture based on Collobert et al. (2011). This architecture is virtually identical to the architecture used for the relation classification task, with the exception of the position features. To predict the tag for word s_i in the sentence s, a window of K tokens around s_i is transformed into a sentence matrix $\mathbf{S} = [\mathbf{v}_{i-\frac{K}{2}}, \ldots, \mathbf{v}_i, \ldots, \mathbf{v}_{i+\frac{K}{2}}]^T \in \mathbb{R}^{K \times d}$ where $\mathbf{v}_i \in \mathbb{R}^d$ is taken from a word-embedding matrix. For words where $i \pm K/2$ exceeds the sentence border a padding token is used. The sentence matrix $\mathbf{S}$ is used directly as input to the convolutional layer. In other words, the convolutional filter weights $\mathbf{W}$ for sequence classification tasks have dimensionality $n \times d$, where n is the convolution filter window size.

The subtle differences between the network architecture used for sequence and relation classification leads to some practical difficulties: Since most symbolic differentiation software used for neural network training such as TensorFlow or Theano use

matrix-vector formulations of the convolution operation, neural network weights must be expressed as matrices in these frameworks (Abadi et al., 2016; Theano Development Team, 2016). This means that the convolutional filter weights $\mathbf{W}$ cannot easily be shared between the sequence classification tasks and the relation classification tasks, since the filters have dimensionality $n \times d$ in one and $n \times d + 2d'$ in the other.

For this reason, we test three different strategies for for sharing neural network weights between the target and auxiliary tasks. Firstly, we test the enticingly simple strategy of Collobert and Weston (2008) and share only the word-embedding, and, when possible, the position-embedding matrix between the target and auxiliary tasks.

Secondly, extend the architecture of Nguyen and Grishman (2015) to a **multi channel convolutional network** as introduced in Kim (2014). The idea of a channel in this context is similar to a color channel in a digital image: An image is often represented as a stack of three matrices where each matrix component denotes color intensity in a color channel.

We can use the idea of multi-channel convolutional neural networks to modify the architecture proposed by Nguyen and Grishman (2015) to accommodate sharing convolutional filter weights between the networks for the target and auxiliary task. Specifically, we can produce two identical sentences matrices from an input sentence. One is used to produce the augmented sentence matrix, one is kept as is. We can feed the augmented sentence matrix into a task-specific convolutional layer, and the un-augmented sentence matrix into a convolutional layer that can be shared with auxiliary tasks.

Thirdly, because the ACE 2005 relation classification task and SemEval 2010 Task 8 require exactly the same architecture, we can readily share both the embeddings and the convolutional filters over the augmented sentence matrix. We therefore test this weight sharing strategy as well, but only when using ACE 2005 as an auxiliary task. A diagram of neural network weights are shared between tasks can be seen in figure 5.6

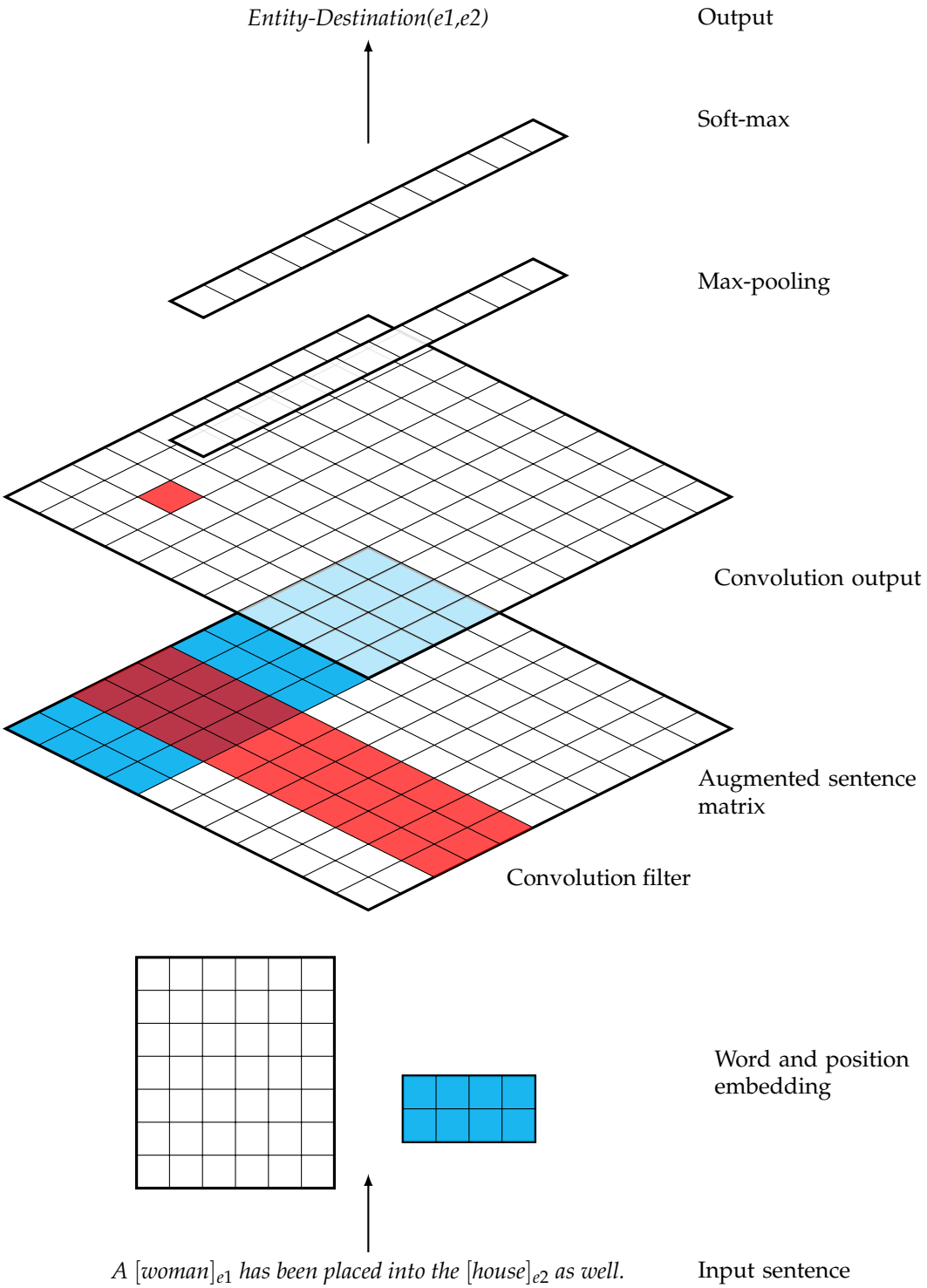


Figure 5.5
Diagram of the convolutional neural network for relation classification. The input sentence is mapped to a sentence matrix by concatenating the word-vector for each word in the word embedding matrix and the position-vector for each word-position in the position embedding matrix for both entities. The position embedding components of the architecture is shown in blue. This forms a $K \times d + 2d'$ matrix. Convolution filters are applied along the K-axis of the sentence matrix to produce the convolution output. Each element in the convolution output matrix corresponds to one convolution filter applied at one position of the sentence matrix. An example convolutional filter and its corresponding output unit is shown in red. Max-pooling is applied to the convolution output to obtain a feature-vector. This vector is used as input to a soft-max output layer.

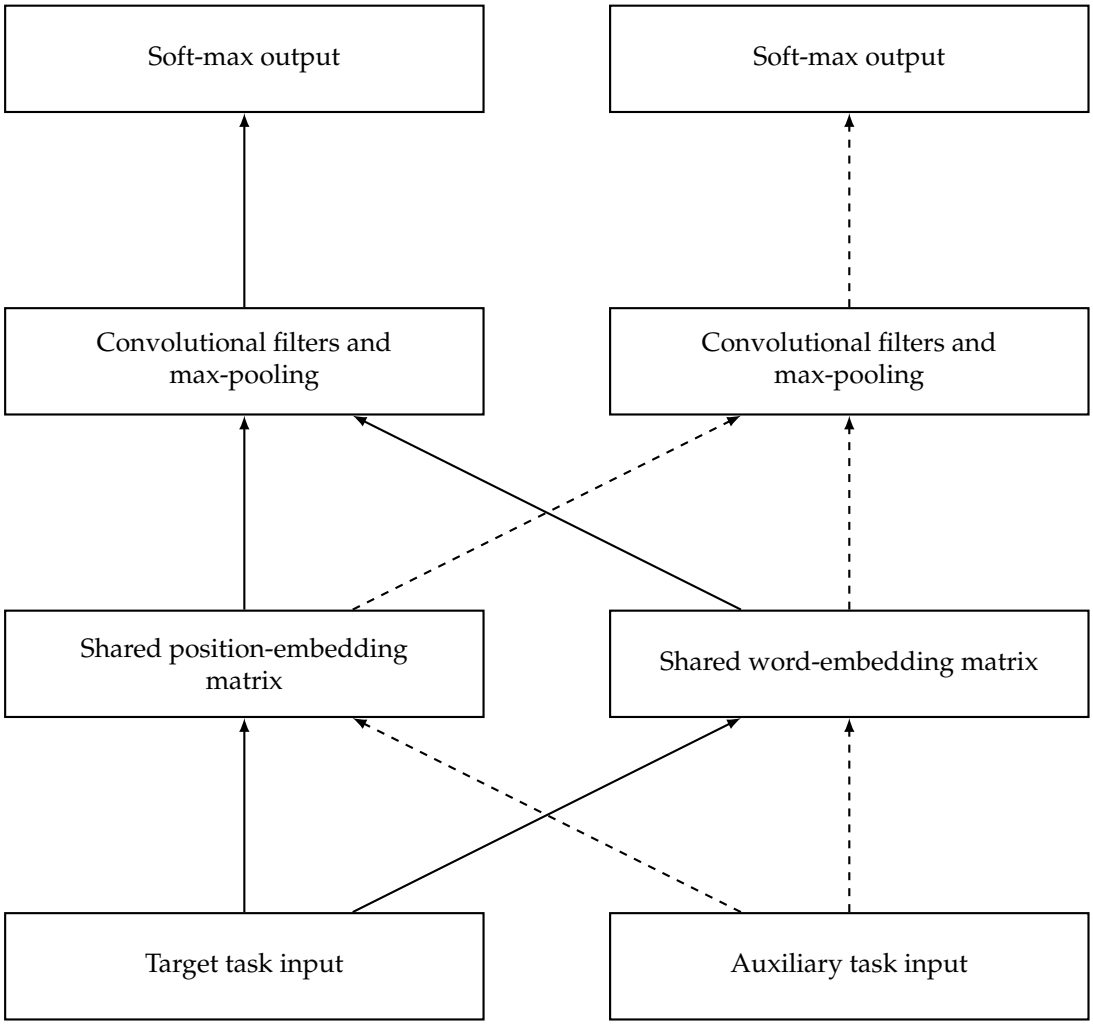


Figure 5.6
Diagram of the weight sharing strategy in which only the embedding matrices are shared between the auxiliary and target task. The solid lines show how network activations flow from the target task to the target output. Dashed lines show how the activations flow through the auxiliary network.

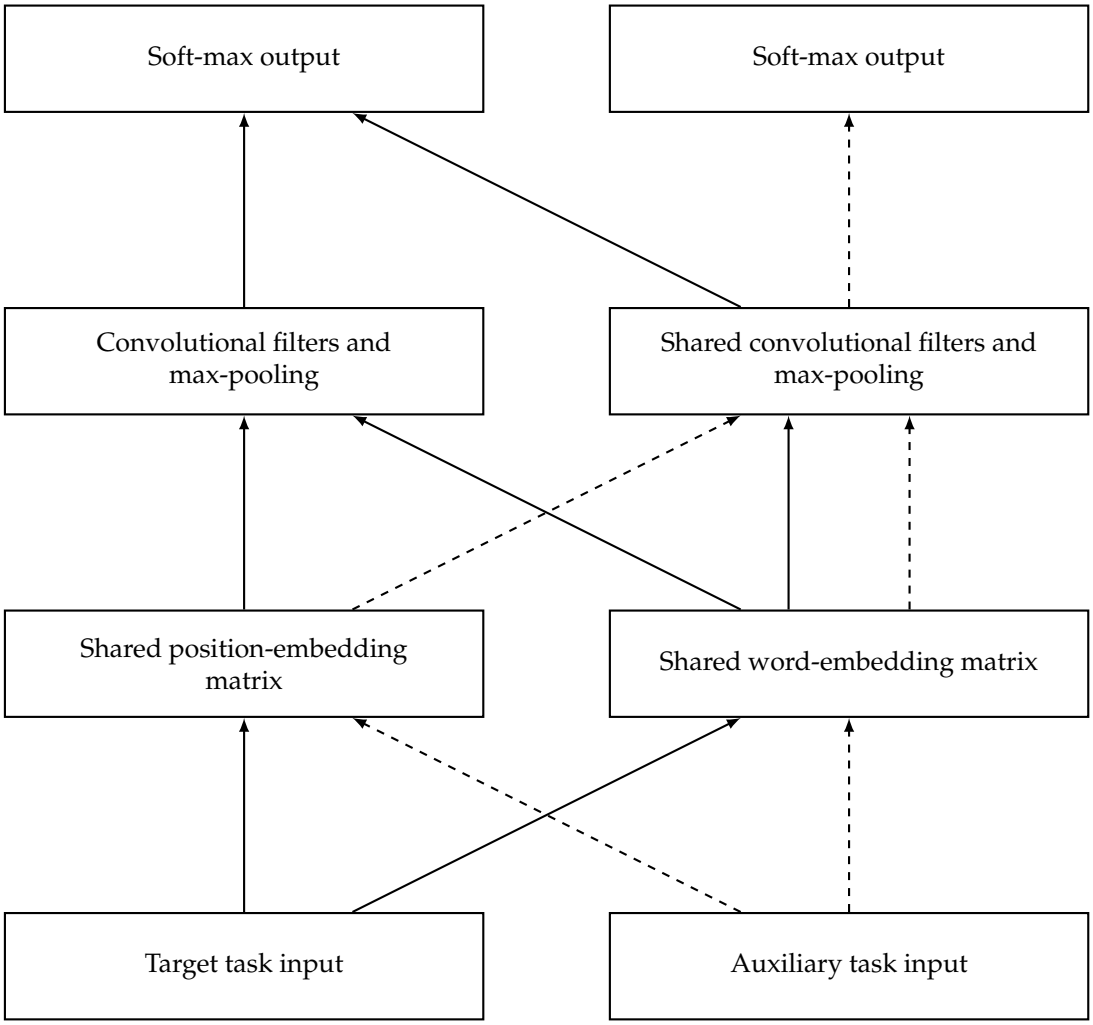


Figure 5.7
Diagram of how neural network weights are shared when using a multi channel convolutional network to enable sharing convolutional filters. The solid lines show how network activations flow from the target task to the target output. Dashed lines show how the activations flow through the auxiliary network.

5.5 Algorithm

Our main goal is to investigate the sample complexity dynamics of learning a relation classification task in a multi-task learning setting when the data available for the target task is limited. To this end, we compare the generalization error of a deep learning model trained only on SemEval 2010 Task 8, the target task, with the generalization error of a deep learning model trained jointly on the SemEval data and one of the auxiliary tasks described in 5.3.

We proceed as follows: We vary the amount of data from the target task by a set of fractions. For every fraction f we perform 5-fold cross validation on the target data to yield 5 macro F1 scores. We use the training data from the 4 training folds of target data and the auxiliary data to train the architectures described in 5.4. We use an algorithm similar to Mou et al. (2016) and Bingel and Søgaard (2017): We uniformly select one of the two tasks, sample a mini-batch from the training data of that task, and perform one gradient descent update with respect to cross-entropy error using the Adam algorithm described in section 3.2.2.

This process is iterated until an early stopping criterion on a target task validation set is met. Specifically, $1/10$ of target training data is set aside for early stopping validation. Training is halted when the cross-entropy error on the early stopping dataset has not improved for 200 iterations of mini-batch gradient descent. Finally, the model weights are reset to their best recorded value.

When the patience is exceeded we record the cross-validation macro-F1 on the target task test fold using the best recorded weights. Since neural network training is a random search procedure with respect to weight initialization and mini-batch sampling we run this experiment for each fraction f 5 times, yielding a total of 25 random cross-validation splits. We have provided the algorithm used in our experiments as pseudocode in algorithm 1. The code can be downloaded at `github.com/suned/thesis`.

5.6 Summary

In this section we have summarized the state of related work for deep multi-task learning for relation classification. We found that no previous investigation of the usefulness of deep multi-task learning for relation classification exists.

We have described the SemEval 2010 Task 8 dataset which we use as a benchmark in our experiments. In this context, we discussed the need for a benchmark dataset that gives us confidence about the generality of an experiment that uses it. We have called into question whether the SemEval dataset has this quality. Nevertheless, we have decided to use it as a benchmark in our experiments because of its status as the de facto standard dataset for relation classification experiments.

Moreover, we have described each auxiliary task for which we test the impact of hard neural network weight sharing on the target task. Finally, we have described the neural network architectures used, and how we adapt them to enable weight sharing, as well as the algorithm used to train this architecture.

We continue by presenting the results obtained from our experiments.

Algorithm 1 *Pseudocode for our deep multi-task learning experiment.*

Require: Target dataset $\mathcal{D}_{target}$
Require: Auxiliary dataset $\mathcal{D}_{aux}$
Require: mini-batch size b
  function CROSSVALIDATION($\mathcal{D}$)
    return *K train and test cross validation folds.*
  end function
  function SAMPLE(set S of size N, f)
    return *$N \times f$ samples from S sampled uniformly*
  end function
  function INITIALIZEWEIGHTS( )
    return initialized neural network weight vector $\mathbf{w}$
  end function
  function GRADIENTDESCENT($\mathcal{D}$, $\mathbf{w}$)
    return *the weight vector* $\mathbf{u}$ *resulting from a single gradient descent step on* $\mathcal{D}$ *with the weights* $\mathbf{w}$ *using the Adam algorithm*
  end function
  function MACROF1($\mathbf{w}$,$\mathcal{D}$)
    return *Macro F1 of the neural network parameterized by* $\mathbf{w}$ *on* $\mathcal{D}$
  end function
  function REPORT(s, f)
    report score s and fraction f to user
  end function
  for all *5 iterations* **do**
    for $f \in \{\frac{0}{5}, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1\}$ **do**
      for $\mathcal{D}_{trainFold}, \mathcal{D}_{val} \in$ CROSSVALIDATION($\mathcal{D}_{target}$) **do**
        $\mathcal{D}_{earlyStopping} \leftarrow$ SAMPLE($\mathcal{D}_{trainFold}$, $\frac{1}{10}$)
        $\mathcal{D}_{train} \leftarrow \mathcal{D}_{trainFold} \setminus \mathcal{D}_{earlyStopping}$
        $\mathcal{D}_f \leftarrow$ SAMPLE($\mathcal{D}_{train}$, f)
        $\mathbf{w}_0 \leftarrow$ INITIALIZEWEIGHTS( )
        $\mathbf{w}_{best} \leftarrow \mathbf{w}_0$
        $i \leftarrow 1$
        while *patience not exceeded* **do**
          $\mathcal{T} \leftarrow$ SAMPLE($\{\mathcal{D}_f, \mathcal{D}_{aux}\}$, $\frac{1}{2}$)
          $\mathcal{B} \leftarrow$ SAMPLE($\mathcal{T}$, $\frac{|\mathcal{T}|}{b}$)
          $\mathbf{w}_i \leftarrow$ GRADIENTDESCENT($\mathcal{B}$, $\mathbf{w}_{i-1}$)
          $i \leftarrow i + 1$
          if $\hat{E}(\mathbf{w}_i, \mathcal{D}_{earlyStopping})$ *was the best recorded* **then**
            $\mathbf{w}_{best} \leftarrow \mathbf{w}_i$
          end if
        end while
        $s \leftarrow$ MACROF1($\mathbf{w}_{best}$, $\mathcal{D}_{val}$)
        REPORT(s,f)
      end for
    end for
  end for

Part 6

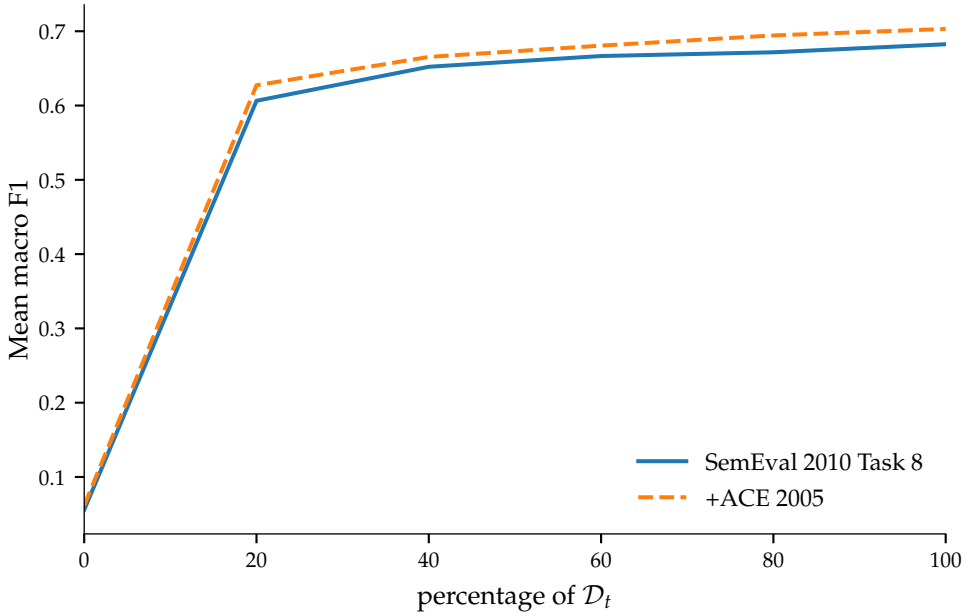
Results

In this section we present the results obtained in the experiment detailed in the previous sections. We visualize the effect of multi-task learning on generalization error estimated by cross-validation for each of the proposed weight sharing strategies. Specifically, we plot the mean macro F1 for each cross-validation experiment as a function of the fraction of target data available for training. This produces a so called **learning curve** that indicates how generalization error improves as the amount of training data is increased in both the single-task and multi-task setting.

Moreover, we perform statistical tests of significance using one sided t-testing on the cross-validation data collected for each fraction f of target data in order to determine if the observed differences between single-task and multi-task learning can be explained by variation due to random weight initialization and and stochastic gradient descent.

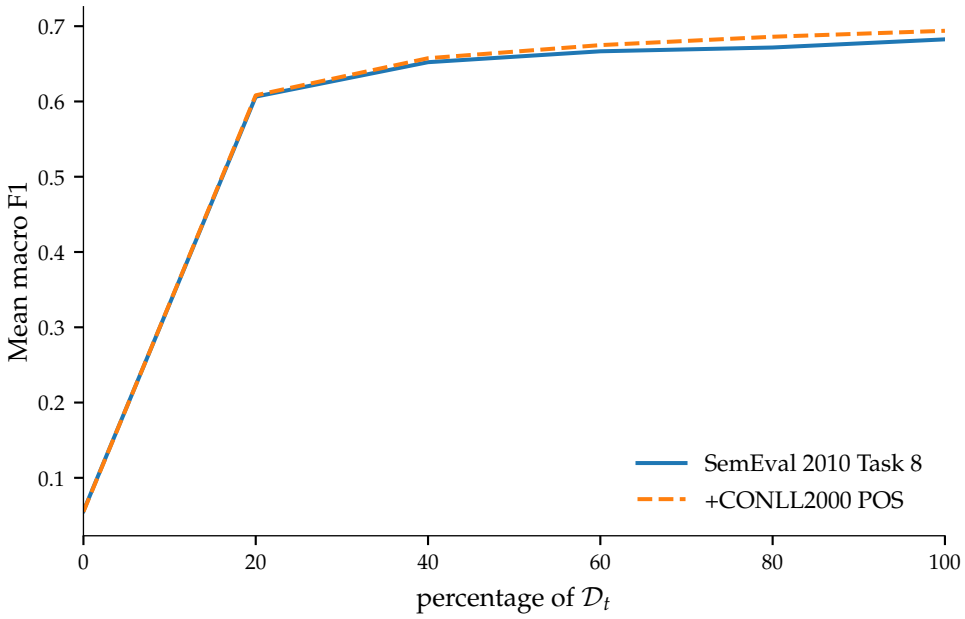
6.1 Shared Embeddings

In this section we present the results obtained for SemEval 2010 Task 8 in a single-task and multi-task setting using the simple weight sharing strategy discussed in section 5.4 in which only the word and position embedding matrices are shared between tasks. Each plot contains two curves: one learning curve for SemEval 2010 Task 8 when learnt as a single task, and one when learnt simultaneously with an auxiliary task. In addition we present tables containing the p-value of one-sided t-tests between the macro $F1$ scores of multi-task and single-task experiments grouped by the fraction of target data f.



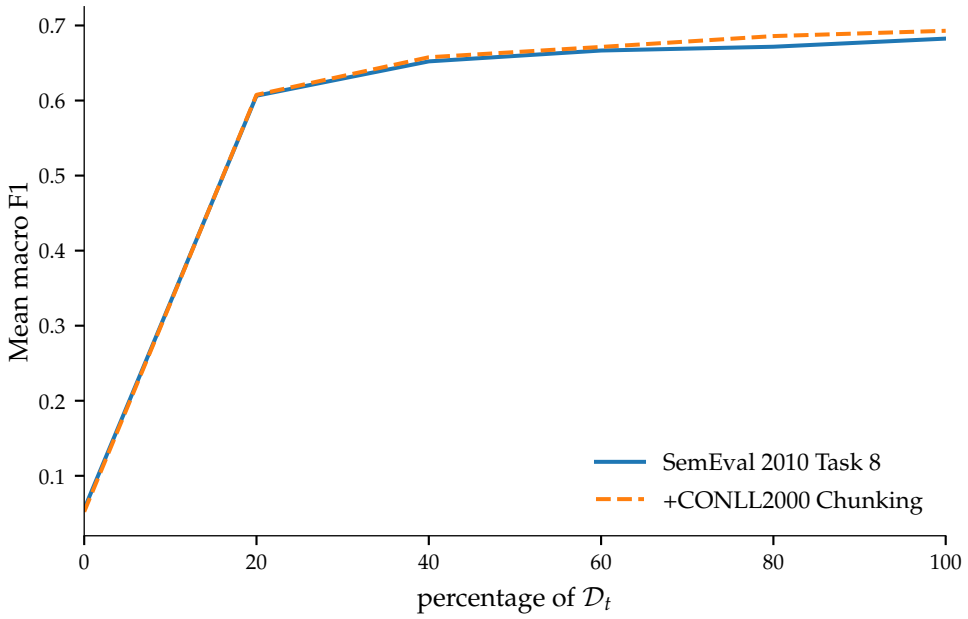
Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.058	**.622**	.664	.681	.682	.693
***p*-value**	.359	**.033**	.088	.054	.192	.106

Figure 6.1
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with ACE 2005 with shared position and word embedding matrices. The learning curves indicate a slight improvement of multi-task learning over single-task learning when the target data is reduced by 80%. In all other cases the observed differences are due to variation due to weight initialization and other stochastic properties of the training procedure with high probability.



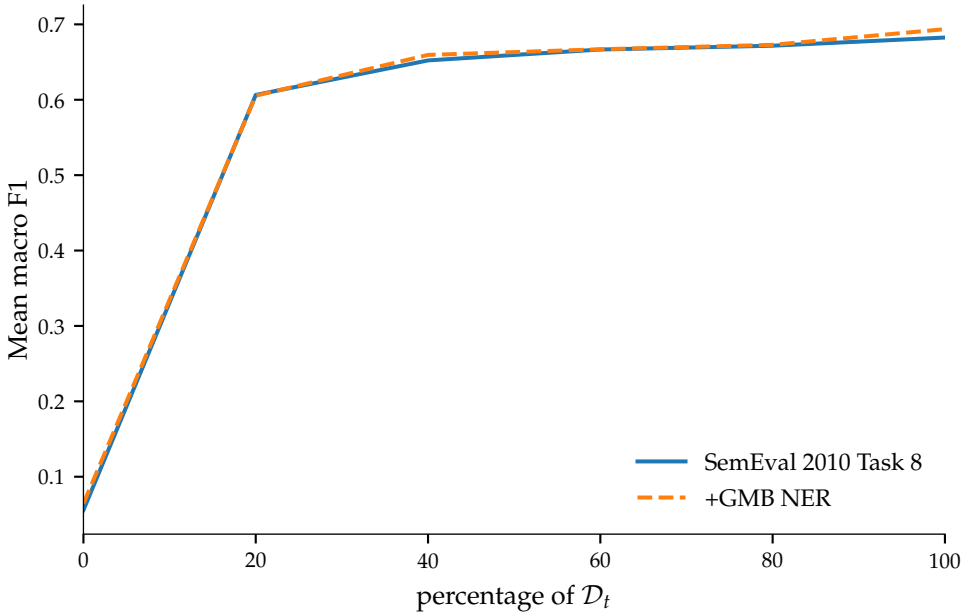
Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.052	.610	.654	.675	.686	.694
***p*-value**	.329	.316	.422	.187	.055	.092

Figure 6.2
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with the CONLL2000 part-of-speech tagging task. The observed differences can with high probability be explained by the stochastic nature of the experiment.



Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.050	.608	.655	.674	.686	.686
p**-value**	.236	.414	.371	.223	.058	.389

Figure 6.3
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with the CONLL2000 chunking task. Here we also see no statistically significant gains in generalization performance for the multi-task learning setting.

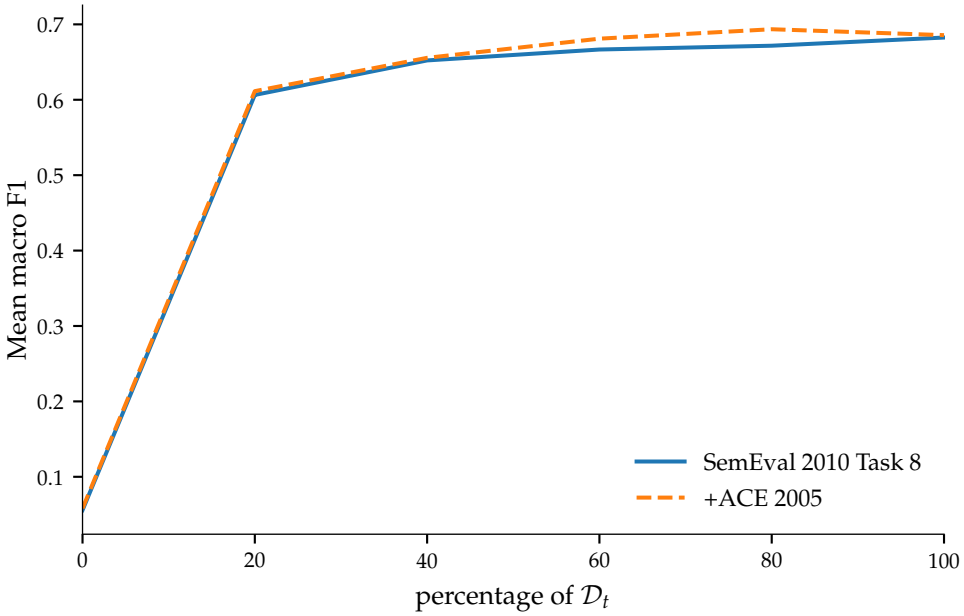


Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.064	.605	.659	.667	.673	.694
p-value	.237	.455	.242	.487	.452	.113

Figure 6.4
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with GMB named entity recognition. The differences in generalization performance between the two approaches are most likely due to the stochastic nature of the experiment.

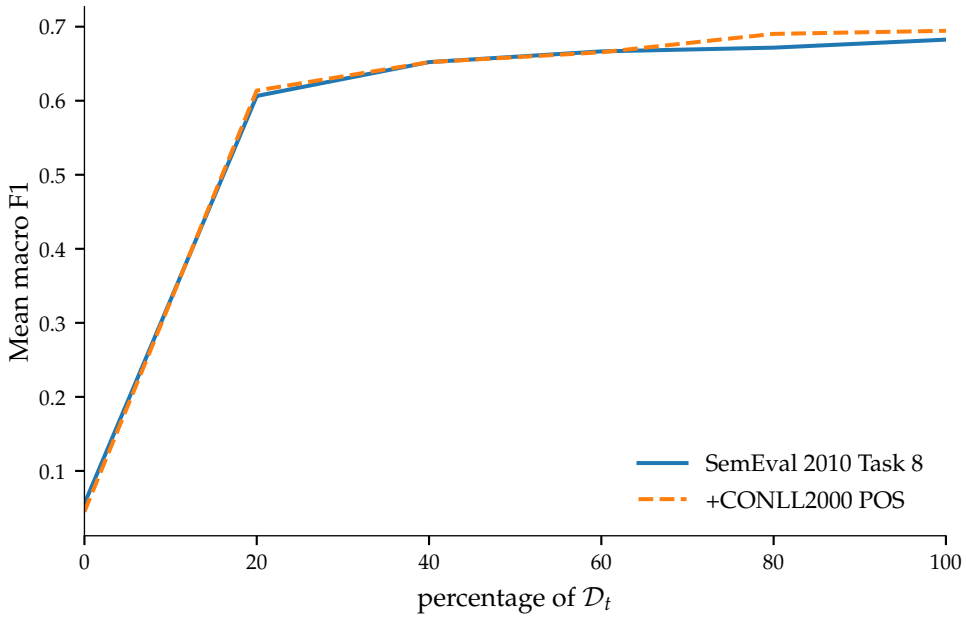
6.2 Shared Side Channel Convolutional Filters

In this section we present the results obtained for SemEval 2010 Task 8 in a single-task and multi-task setting using the multi-channel weight sharing strategy discussed in section 5.4. The presentation format is the same as in the last section.



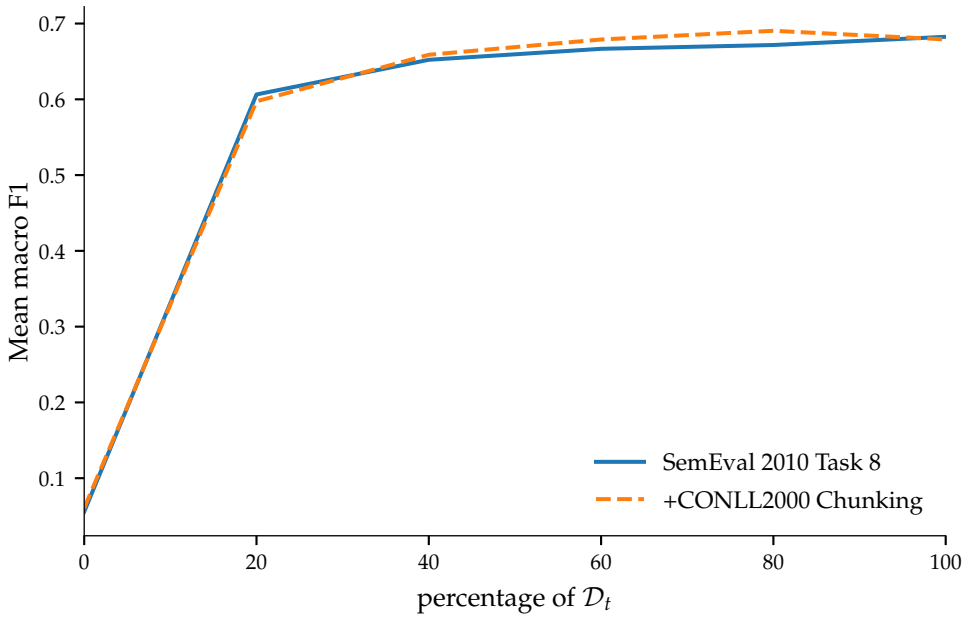
Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.058	.611	.656	.681	**.694**	.686
p-value	.419	.346	.382	.099	**.034**	.405

Figure 6.5
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with ACE 2005. The learning curves indicate that there is a significant difference between single-task and multi-task learning when the target data is reduced by 20%.



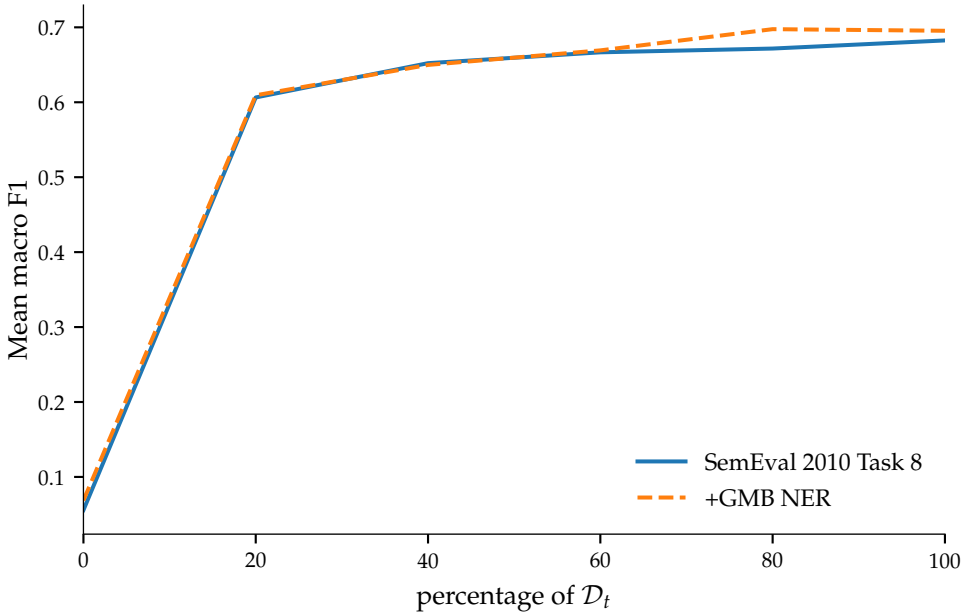
Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.045	.614	.652	.665	.690	.694
***p*-value**	.155	.251	.497	.464	.054	.158

Figure 6.6
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with CONLL2000 part-of-speech. There are no significant differences between the two curves.



Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.061	.597	.659	.679	.690	.679
p**-value**	.338	.238	.292	.161	.060	.379

Figure 6.7
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with the CONLL2000 Chunking task. Once again there are no significant differences between the single-task and multi-task learning setting.

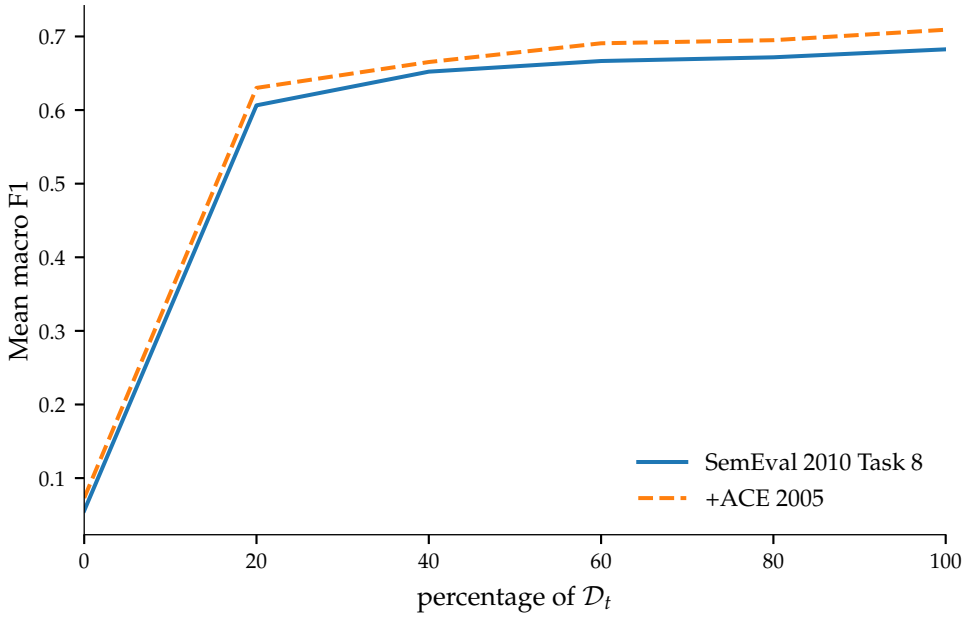


Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.069	.609	.650	.669	**.698**	.695
***p*-value**	.159	.398	.424	.417	**.015**	.128

Figure 6.8
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with GMB named entity recognition. The learning curves indicate a significant difference in generalization performance between single-task and multi-task learning with the target data is reduced by 20%.

6.3 Shared Convolutional Filters

Here we present the results for the final weight sharing strategy: sharing the convolutional filters for the augmented sentence matrix. As discussed, this strategy is only practically feasible



Percentage of $\mathcal{D}_t$	0	20	40	60	80	100
Mean single-task macro $F1$	.056	.606	.652	.667	.672	.683
Mean multi-task macro $F1$	.073	**.630**	.665	**.691**	**.695**	**.709**
p-value	.121	**.022**	.139	**.015**	**.023**	**.011**

Figure 6.9
Learning curves and hypothesis tests for SemEval 2010 Task 8 trained as a single task and in a multi-task setting with ACE 2005. There are significant differences in the generalization performance between the multi-task and single task at most points along the learning curves.

6.4 Summary

The results presented in this section are mixed: The weight sharing strategies in which just the position and word embedding matrices are shared do not in general lead to tangible improvements in generalization performance for multi-task learning. The only proposed weight sharing strategy that lead to significant improvements in generalization performance is the convolutional filter sharing approach in which the convolutional filters over the augmented sentence matrix are shared. This approach is unfortunately only practically feasible when sharing the weights with an auxiliary relation classification task. In the next section we provide an analysis of these results.

Part 7

Discussion

In the previous section we saw that all but one weight sharing strategy tested in our deep multi-task learning experiments did not lead to significant improvements in generalization error for relation classification. In this section, we reflect on this result in order to outline the conclusions we can draw.

7.1 Impact of Limited Weight Sharing

As discussed, the neural network architecture adopted from Nguyen and Grishman (2015) puts certain limitations on how neural network weights can be shared between tasks in practice. The solution to this problem of sharing only the position and word embedding matrices was motivated by Collobert and Weston (2008). They show that sharing the word vector weights of convolutional neural network architectures between auxiliary syntactic labeling tasks such as part-of-speech tagging and a target semantic role labeling task leads to significant improvements in generalization error for the target task.

However, all the tasks that are learnt simultaneously in Collobert and Weston (2008) are derived from annotations of the same sections of the PropBank corpus (Kingsbury and Palmer, 2002). When annotations for auxiliary tasks are taken from different corpora, the potential benefits made possible by sharing only the word embedding is limited by the degree of overlap of words occurring in both corpora. The set of words that occur in a corpora is commonly referred to as it's **vocabulary**. The only way an auxiliary task can benefit the target task is if the weights that are updated while learning from an auxiliary task are also used by the target task. When sharing only the word embedding, this happens only when a word is in both the auxiliary vocabulary and in the target vocabulary.

In Collobert and Weston (2008) the vocabulary overlap is maximal since all annotations for all tasks pertain to the same text. This is not the case for the corpora used in our experiments as seen in figure 7.1. We speculate that the reason we observe better results when sharing convolutional filter weights as compared to sharing just the embedding matrices is in large part due to the fact that the convolutional filters are guaranteed to be used by both tasks. Intuitively, one task may then benefit the other if the features detected by a filter learnt by one task is useful for the other.

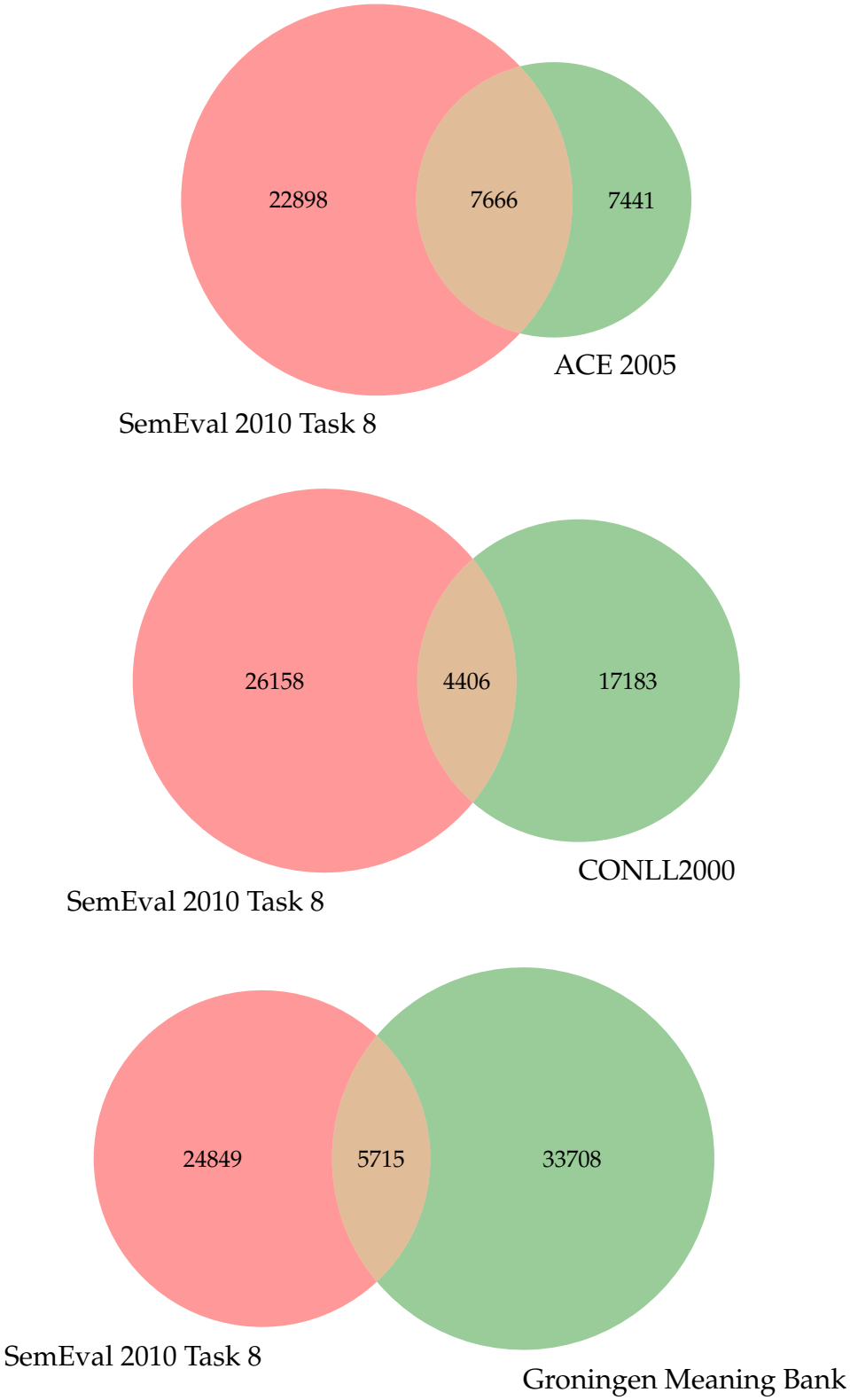


Figure 7.1
Vocabulary overlap between the corpora used in our experiments. The Venn diagrams show the number of tokens occurring in both the SemEval 2010 Task 8 vocabulary and each of the vocabularies of the auxiliary tasks.

7.2 Semantic Relations are Inconsistently Defined

The reasoning in the previous section does not explain why the multi-channel weight sharing strategy and sharing convolutional filters over the augmented sentence matrix when learning the ACE 2005 relation classification as an auxiliary task leads to different results. The differences in generalization performance between these two approaches indicate that there are few convolutional features of the un-augmented sentence matrix that are learnable from the ACE 2005 dataset that are useful for the target task.

This result suggests that there must be general differences in patterns of semantic and syntactic information encoded in word vectors alone that are good predictors of relation types in the two datasets. This is surprising given that, superficially, there is a clear semantic overlap between some of the relations in the two tasks as argued in section 5.2. However, as pointed out in Handschuh et al. (2016), the objective of relation classification is ill-defined in the sense that the restrictions on what constitutes a valid relation varies from dataset to dataset. This leads to some important general differences between the relations found in the ACE 2005 relation classification task and SemEval 2010 Task 8.

We have already discussed the definition of a valid relation enforced during the annotation process of the SemEval dataset in section 5.2. To reiterate, they were:

- Relation arguments cannot depend on discourse knowledge (e.g they can't be pronouns).
- Relation arguments cannot appear in separate sentential clauses.

No such restrictions are present in the ACE 2005 annotation guidelines

These differences between annotation guidelines lead to significant differences between the types of relations that appear in the two datasets. The sentence:

> *The fifty essays collected in this volume testify to most of the prominent themes from Professor Quispel's scholarly career*

is a canonical example of *Member-Collection(essays, volume)* taken from the SemEval dataset. As typical for the SemEval dataset, the arguments belong to different noun phrases: *the fifty essays* and *this volume*. The two noun phrases are separated by words that are informative of the *Member-Collection* relation, namely *collected in*.

Contrast this with the following canonical example of the *Personal-Social(his, father-in-law)* relation from the ACE 2005 dataset:

> *The fact that this guy was such an idiot to go back and let his father-in-law kill him shows he wasn't the most stable of people*.

Here, the arguments belong to the same noun phrase *his father-in-law*. We speculate that the kind of convolutional feature detectors that are useful for classifying relations where both relation arguments appear in the same noun phrase are not very useful for classifying relations where the arguments appear in separate noun phrase.

This indicates that there are examples in the ACE 2005 dataset that requires the network to learn semantic and syntactic feature detectors that are unlikely to be useful for detecting canonical SemEval relations.

If this syntactic and semantic pattern mismatch between the relations in the two datasets occur frequently enough, we speculate that it explains why learning ACE 2005 as an auxiliary task only leads to improvements in generalization performance when the convolutional filters over the augmented sentence matrix that also contains position information is shared between the target and auxiliary tasks. In this weight sharing scheme, the training examples in ACE 2005 that are more similar to the examples in SemEval can benefit the target network with more powerful feature detectors that incorporate position information.

We can estimate the frequency of this syntactic pattern as follows: Construct a syntactic parse tree for the sentence in which $relation(arg1, arg2)$ occurs. Traverse the tree bottom-up from the leaves corresponding to $arg1$ and $arg2$ in turn. Record the first noun phrase node encountered between the leaves and the root. Denote this node as the nearest-ancestor noun phrase of the argument. Let the predicate $sameNP(arg1, arg2)$ be a logical predicate on the arguments of the relation that is true when they share a nearest-ancestor noun phrase node. Count the examples in each dataset for which $sameNP(arg1, arg2)$ is true.

We have counted the number of samples for which $sameNP(arg1, arg2)$ is true for both the SemEval dataset and the ACE 2005 dataset using the Stanford PCFG parser (Klein and Manning, 2003). In addition, we have counted the number of relations in which one of the arguments is a pronoun denoted by the predicate $pronoun(arg1, arg2)$. The results can be seen in figure 7.2. Specifically we see that more than half of the samples in the ACE 2005 dataset are made up of sentences in which the relation arguments share a nearest-ancestor noun phrase node. In the SemEval dataset, there are hardly any samples of this sort.

This leads to the following conclusion: the inconsistent requirements for what constitutes a valid relation in the two datasets as expressed by the annotation guidelines lead to samples in which the syntactic and semantic indicators of the presence of a semantic relation are very different. This inconsistency is not conductive for multi-task learning, since it makes it unlikely that the features that are useful for one task is also useful for the other. We have identified only two major differences in the general syntactic patterns of the relations between the two datasets. We speculate that a more thorough analysis would lead to more. This indicates that if we want to re-use annotated data for relation classification, it calls for the development of a general, unambiguous definition of relation classification as a task as is argued in Handschuh et al. (2016).

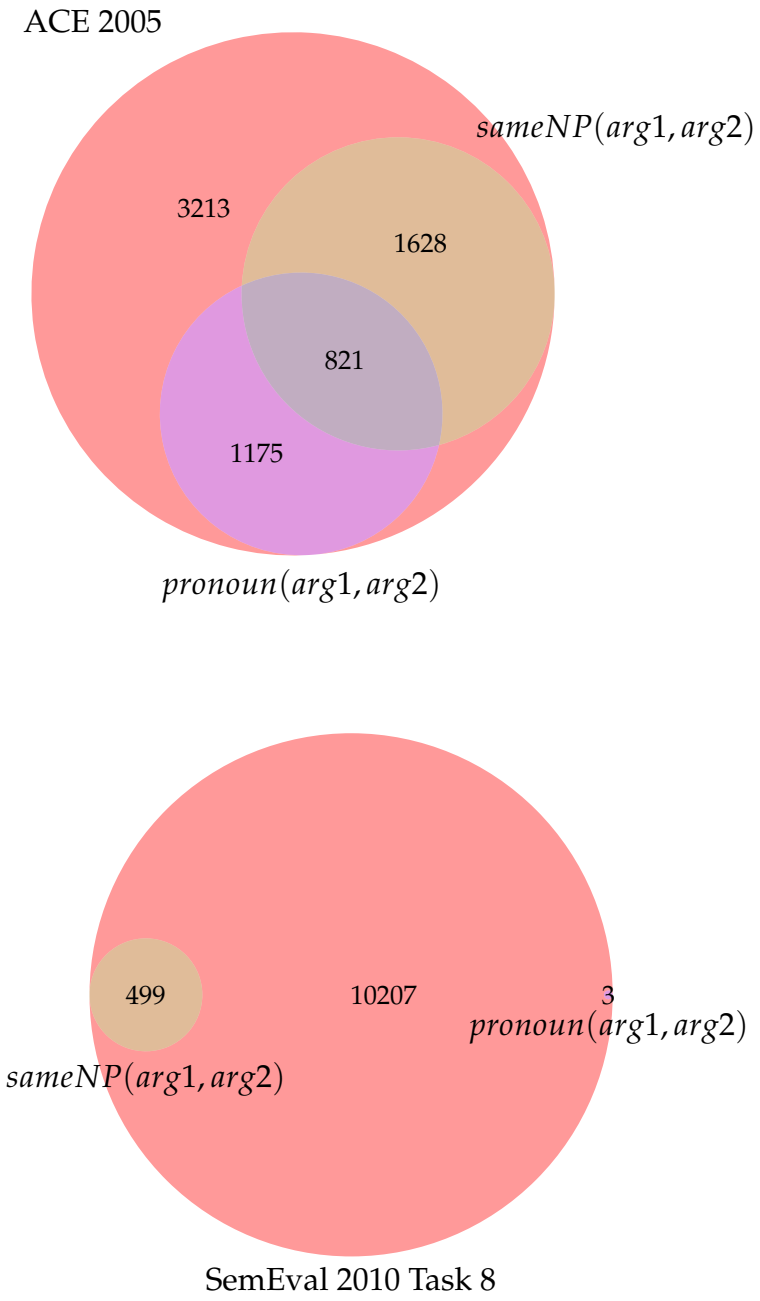


Figure 7.2
Venn diagram of relations where the relation arguments are part the same noun phrase or one relation is a pronoun for the ACE 2005 dataset and the SemEval 2010 Task 8 dataset.

The argument we have presented in this section is speculative in nature because it's difficult to inspect exactly what kinds of feature detectors a convolutional neural network for natural language processing tasks learn. In contrast, convolutional neural

networks for image recognition tasks learn feature detectors that can very intuitively be seen as general edge or line detectors in the early layers, and more specialized object detectors in the the layers close to the output (Goodfellow et al., 2016). This makes it easy to reason about whether the early layers of networks tasked with learning two different things are learning similar feature detectors, which in turn makes it easier to predict whether sharing the weights of early layers between them can lead to generalization improvements.

If a similar language for describing what is detected by convolutional filters in a neural network for a language processing task could be developed, this this would be a significant step towards answering the questions: *which tasks are useful as auxiliary tasks?* and *how should weights of the networks for two tasks be shared?*

7.3 The Need for A Unifying Theory of Multi-Task Learning

As discussed in section 4.4, empirical experiments as those in this thesis are the most reliable way to investigate which auxiliary tasks to use and how neural network weights be shared in order for multi-task learning to improve generalization for a specific application. The lack of theoretical understanding presents us with a problem: When a deep multi-task learning experiment leads to a negative result it may be due to unfit auxiliary tasks, an unfit neural network architecture or both.

The sequence classification tasks we have tested do not lead to generalization gains for any of the architectures that we have tested. Whether or not changing the neural network architecture can yield generalization gains by multi-task learning remains to be seen. The major question is: how much energy should we spend on experimenting with this and that architecture before we conclude that two tasks are unrelated? Or, if we do see generalization improvements on the target task, how can we know that our network architecture really takes advantage of all the useful information in the auxiliary tasks, and that further gains are not possible still?

We believe a unified theory of multi-task learning that can provide answers to these types of questions is an important goal for future research. In particular, such a theory should provide us with statistical tests that can be applied to two tasks and indicate whether generalization gains should be possible by learning them simultaneously. This is an ambitious goal since it involves making predictions about the neural network features induced by a particular dataset. Nonetheless, we believe the potential for efficient development of multi-task learning systems with high performance that such a theory would make possible would be extremely valuable in both business and research.

7.4 Summary

In this section we have reflected on the results of our deep multi-task learning experiments. We have argued that when combining text data from disparate corpora, sharing only the word embedding is effective only to the extent that the vocabulary of those corpora overlap.

Moreover, we have argued that the differences in annotation guidelines for SemEval 2010 Task 8 and the ACE 2005 relation classification task lead to important

differences in the resulting learning problems which may make multi-task learning less effective. This suggests a need for a more general consensus on the goal of relation classification as a task if we want to re-use annotated data. We have suggested that reasoning about performance differences between models is difficult because we lack a language for describing what is learnt by convolutional neural networks for natural language processing tasks. Developing such a language would be a helpful tool for pursuing multi-task learning with convolutional neural networks for natural language processing tasks.

Finally we have discussed the need for a unifying theory of multi-task learning that predicts if an auxiliary task should lead to gains in generalization performance. With the current state of the theoretical background, there is no way of knowing if a useless auxiliary task could not be made useful by for example changing the network architecture.

Part 8

Perspectives

In this section we reflect on the points highlighted in the previous section. We focus on suggesting multi-task learning strategies for relation classification that we believe still needs to be explored in order to determine if even better generalization gains is possible. We begin by exploring alternative neural network architectures that remove the weight sharing limitations of the architecture proposed by Nguyen and Grishman (2015). We then turn to suggestions for other possible auxiliary tasks. We end the section with a discussion of the the pros and cons of multi-task learning vs. feature engineering.

8.1 Alternative Neural Network Architectures

As discussed, the architecture suggested by Nguyen and Grishman (2015) puts limitations on how neural network weights can be shared in practice. This section provides basic outlines for how to construct a neural network architecture that removes these limitations.

8.1.1 Convolutional Neural Network with Argument Markers

It is generally accepted that a successful relation classification system needs as input some representation of which words of the input sentence constitute the relation arguments (Nguyen and Grishman, 2015; Zhang and Wang, 2015; Jiang, 2009). The solution proposed by Nguyen and Grishman (2015) is to augment the sentence matrix formed from the concatenated word vectors pertaining to the input with position vectors that encode distances to the relation arguments.

This has the unfortunate effect of hindering weight sharing of the convolutional filter weights between the relation classification network and sequence classification networks in practice, since it induces a mismatch of the dimensionality of the respective convolutional filter matrices.

Other researchers have found that it's possible to remove the position features completely if each sentence is pruned such that the first and last word constitute the first and last relation argument words (Santos et al., 2015). This suggests that the specific representation of relation argument positions is unimportant.

One strategy for equalizing the sentence matrix dimensionality is therefore to adapt a relation argument position representation that does away with the position embedding. The pruning strategy of (Santos et al., 2015) is one path forward. We speculate that simply marking the relation arguments with special beginning and end tokens would also work. By equalizing the dimensionality of the sentence matrix for the relation classification network and the sequence prediction networks sharing the convolutional filter weights is made possible, which may lead to better results than we have reported here.

8.1.2 Recurrent Neural Network

Zhang and Wang (2015) describes a recurrent neural network architecture for relation classification that can also be used for a multi-task learning. In this architecture, the word vector for each word is fed into a bi-directional recurrent network layer. This produces a sequence of feature vectors that are the concatenation of the output of each application of the recurrent layer in both directions. Zhang and Wang (2015) apply max-pooling on the components of these feature vectors, and feed the resulting vector into a logistic regression layer. The relation arguments are marked simply by adding special tokens before and after each argument.

It's possible to share the weights of the recurrent layer with a sequence classification model by adding an output layer to each feature vector produced by the bidirectional recurrent layer as is done in for example Bingel and Søgaard (2017). Since the dimensionality of the weight matrices depend only on the dimensionality of the word embedding matrix and the output dimensionality of the recurrent layer, this does away the limitation induced by the position features in the architecture proposed by Nguyen and Grishman (2015).

8.2 Alternative Auxiliary Tasks

In this section we investigate other auxiliary natural language processing tasks that have the potential for improving relation classification generalization which were not tested in our experiment. We discuss the goal of each task and investigate neural network architectures that permit hard parameter sharing with a relation classification network.

8.2.1 Semantic Role Labeling

The goal of relation classification is ultimately to produce a compact representation of the semantic roles of words in text when those roles constitute an instance of a relation in the inventory of interest. **Semantic role labeling** can be seen as a generalization of this problem. The goal in semantic role labeling is to label the arguments for so called predicates in a sentence. The term *predicate* stems from logic and roughly means a function that performs a logical test on its arguments, i.e maps it to a truth value.

In natural language processing, the term predicate is often used to refer to words, often verbs, that expect certain arguments so to speak. A particular example of this is the idea of transitive and intransitive verbs. A transitive verb has a direct and

possibly an indirect object, for example *brought* in *he brought her a glass of water* where *her* is the indirect object and *a glass of water* is the direct object. Intransitive verbs takes no objects, such as *laughs* in *she laughs*. We can express the transitivity of these verbs by representing them as predicates that take a fixed number of arguments, for example *brought(her, a glass of water* and *laughs(she)*.

The goal of semantic role labeling is to predict the predicate arguments given a sentence and a predicate in that sentence (Jurafsky and Martin, 2009). PropBank and FrameNet are two datasets frequently used for this task (Kingsbury and Palmer, 2002; Baker et al., 1998). See figure 8.1 for an example.

[The San Fransisco Examiner]	issued	[a special edition]	yesterday
ARG1	PREDICATE	ARG2	

Figure 8.1
Example predicate labeling derived from PropBank.

Semantic role labeling tasks can be solved with neural networks. Collobert et al. (2011) describe a convolutional architecture very similar to the architecture of Nguyen and Grishman (2015). Specifically, they approach semantic role labeling as a sequence labeling task where the goal is to assign BIO labels indicating whether a token is a the beginning, inside or outside of a predicate argument. To indicate which word is the predicate, they augment the window matrix formed by the word vectors of the window with position features that encode the distance to the predicate. It's possible to share the convolutional filters of this architecture by using the multi-channel or argument marker strategy described in 8.1.1.

As discussed, semantic role labelling and relation classification are highly related tasks. We speculate that a representation that is useful for predicting the roles of words with respect to predicates in the sentence will also be good for predicting semantic relations.

8.2.2 Typed Dependency Parsing

The objective in typed dependency parsing is to predict and label binary grammatical relations that hold among words in a sentence such as the subject or object of the verb (Jurafsky and Martin, 2009). This can be expressed using a tree structure where the words of the sentence are the nodes and the grammatical relations among them are the edges. See figure 8.2 for an example.

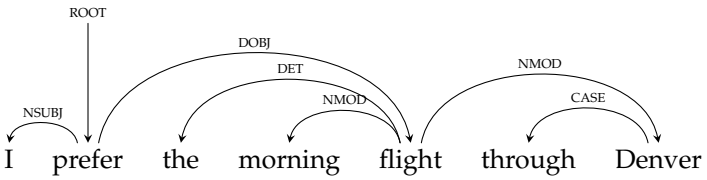


Figure 8.2
A typed dependency parse tree using the Universal Dependency Set (De Marneffe et al., 2014).

A directed edge is added from a so called head word to another token if the morphology of the token is directly dependent on the head word. For example, the verb-subject relationship between the verb *prefer* and *I* determines that the form of the nominal subject should be *I* and not *me* for example.

The advantage of typed dependency parses is that they give approximations to the semantic relationships between predicates and their arguments, such as transitive verbs and their subject and objects. This makes dependency parse trees highly useful features for information extraction systems (Jurafsky and Martin, 2009).

Typed dependency parsers can be implemented as neural networks. Recently, Kiperwasser and Goldberg (2016) demonstrated that word vectors and bidirectional recurrent neural network features could be trained jointly with a structured prediction objective that predicts the dependency graph. The word embedding and bidirectional recurrent neural network weights could be shared with the model proposed by Zhang and Wang (2015) to empirically investigate the usefulness of typed dependency parsing as an auxiliary task.

8.3 Pipelining Vs. Multi-Task Learning

In this thesis we have investigated the possibility of re-using labeled data by using it to automatically learn a representation that improves generalization for a target task when data for this task is limited. In truth, labeled natural language data for auxiliary tasks can be re-used for this purpose in a different manner: by training a system that predicts labels for target task data. These predictions can be used as input features to the system for the target task. For example, we could use the CONLL2000 data to train a system that predicts chunk and part-of-speech tags for the SemEval data. We might then then use these tags as input to the relation classification network.

This approach is in fact the standard mode of operation for natural language processing practitioners. Using all of the linguistic knowledge available to us to manually produce a good representation may let us use a smaller hypothesis space for the target task without penalizing the training error. Vapnik-Chervonkis analysis gives us confidence that learning with a smaller hypothesis space reduces the need for training data. Therefore, using the auxiliary data not as output information used to automatically find a good representation, but as input information, by manually creating a **pipeline** of natural language processing systems that produces a good representation for the target task, we may be able to use the auxiliary data to learn with a small hypothesis space and thereby reduce the need for labeled training data for the target task.

The main issue with such a pipeline method is **error propagation**, where classification errors early in the pipeline lead to classification errors on the target task (Collobert et al., 2011). Whether multi-task learning is preferable to pipelining in the context of relation classification is a question that, with our current understanding, may only be investigated empirically. Such a comparative study would be a significant undertaking, and we therefore suggest it as a possible future experiment that may

improve our understanding of, not only when pipelining is preferable to multi-task learning, but also what makes an auxiliary task beneficial.

8.4 Summary

In this section we have suggested two alternative neural network architectures that may lead to better results with deep multi-task learning than we have presented here: one convolutional architecture that does away with the position features, and one recurrent architecture.

In addition, we have suggested two auxiliary tasks which we believe may lead to improved generalization performance for relation classification: semantic role labeling and typed dependency parsing. Finally, we have suggested a comparative study be conducted that investigates how pipelining versus multi-task learning natural language tasks affects sample complexity dynamics of the target task.

Part 9

Conclusion

This thesis represents a first step towards understanding whether multi-task learning is a useful technique for improving generalization performance of a deep learning model for relation classification. We began our investigation by exploring relation classification as a natural language processing task. We found that relation classification is a difficult problem because of the high degree of variance and ambiguity of natural language. Because of these challenges, hand-crafted rules that depend on syntactic parses of the input text do not scale well to large inventories of target relations and large scale corpora.

We then proceeded to explain how supervised machine learning techniques can be used to solve the relation classification problem as an alternative. We saw how Vapnik-Chervonenkis analysis tells us that the number of training examples N and the complexity of the hypothesis space $m(N, \mathcal{H})$ are the two main conditions governing the success of supervised machine learning techniques.

In continuation, we have introduced convolutional neural networks as a concrete way to implement a hypothesis space that is well suited for multi-task learning. We have discussed how to search this hypothesis space using iterative gradient based methods, and the challenges that comes with this approach.

We have explored extensions of Vapnik-Chervonenkis analysis to the multi-task learning setting. These theoretical results in general tells us that learning multiple tasks simultaneously can strengthen the statistical guarantees on the distance between training error $\hat{E}$ and generalization error E. However, these theoretical contributions do not show how multi-task learning can lead to increased generalization performance in an absolute sense, by decreasing the training error and the complexity of the hypothesis space simultaneously.

We have designed and carried out an experiment that tests the effectiveness of deep multi-task learning on a benchmark relation classification task. Specifically we have searched the research literature and found a convolutional neural network architecture that achieves good results for the relation classification problem. We found however that this architecture made multi-task learning by hard weight sharing impractical. For this reason we adapted this network architecture by proposing three weight sharing strategies:

- Shared word and position embeddings in which only the embedding matrices of the target and auxiliary model is shared.
- Shared side channel convolutional filters in which we extend the original architecture to a multi-channel convolutional network that allows sharing convolutional filters over a sentence matrix without appended relation argument position information.
- Shared convolutional filters in which we share convolutional filters across the augmented sentence matrix that contains information about the relation argument positions. This approach is only practically feasibly when the auxiliary task is another relation classification task.

We have empirically compared the sample complexity dynamics of single-task learning and multi-task learning of the target task. Our results are mixed: The shared word and position embedding architecture does not in general lead to statistically significant improvements in target task generalization. The shared side channel architecture leads to occasional improvements of target task generalization. The weight sharing strategy that shares convolutional filters over the augmented sentence matrix reliably produces improvements in generalization error.

We have analyzed these results. We have explained that sharing only embedding matrices leads to a low degree of weight sharing when the learning tasks are defined over different corpora. Moreover, we have suggested that the disparate results when using an auxiliary relation classification task may be caused by inconsistent definitions of what constitutes a valid semantic relation. This suggests a need for a consensus on the goal of relation classification as a task if we want to re-use annotated data. Finally, we have discussed the need for a unifying theory of multi-task learning that can provide statistical tests on datasets that can reveal whether implementing a learning system that uses these sets as auxiliary data is wasted effort.

We have proposed a number of experiments that might be carried out as future work. Specifically, we have proposed alternative neural network architectures and auxiliary tasks that may lead to better results than we have presented here. We have also suggested a study that compares the sample complexity dynamics of pipelining vs. multi-task learning in order to determine which approach is best suited to reduce the data annotation burden.

Our initial results show that deep multi-task learning of relation classification is a feasible strategy for reducing the data annotation burden, provided the designer of the learning system is able to identify the right auxiliary tasks and the right network architecture. As discussed however, in the absence of a theory of multi-task learning that reveals precisely what that entails, this process mostly consists of trial and error. Therefore, there is much work still to be done to better our understanding of how learning several tasks simultaneously can help machines learn how to classify semantic relations.

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