LEARNING STRUCTURED PROBABILISTIC MODELS FOR SEMANTIC ROLE LABELING

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I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

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Abstract

Teaching a computer to read is one of the most interesting and important artificial intelligence tasks. Due to the complexity of this task, many sub-problems have been defined, mostly in the area of natural language processing (NLP). In this thesis, we focus on semantic role labeling (SRL), one important processing step on the road from raw text to a full semantic representation. Given an input sentence and a target verb in that sentence, the SRL task is to label the semantic arguments, or roles, of that verb. For example, in the sentence "Tom eats an apple," the verb "eat" has two roles, Eater = "Tom" and Thing Eaten = "apple".

Most SRL systems, including the ones presented in this thesis, take as input a syntactic analysis built by an automatic syntactic parser. SRL systems rely heavily on path features constructed from the syntactic parse, which capture the syntactic relationship between the target verb and the phrase being classified. However, there are several issues with these path features. First, the path feature does not always contain all relevant information for the SRL task. Second, the space of possible path features is very large, resulting in very sparse features that are hard to learn.

In this thesis, we consider two ways of addressing these issues. First, we experiment with a number of variants of the standard syntactic features for SRL. We include a large number of syntactic features suggested by previous work, many of which are designed to reduce sparsity of the path feature. We also suggest several new features, most of which are designed to capture additional information about the sentence not included in the standard path feature. We add each feature individually to a baseline SRL model, finding that the sparsity-reducing features are not very helpful, while

the information-adding features improve performance significantly. We then build an SRL model using the best of these new and old features. This model is competitive with state-of-the-art SRL models; in particular, when compared on features alone, it achieves a significant improvement over previous models.

The second method we consider is a new methodology for SRL based on labeling *canonical forms*. A canonical form is a representation of a verb and its arguments that is abstracted away from the syntax of the input sentence. For example, "A car hit Bob" and "Bob was hit by a car" have the same canonical form, {Verb = "hit", Deep Subject = "a car", Deep Object = "a car"}. Labeling canonical forms makes it much easier to generalize between sentences with different syntax. To label canonical forms, we first need to automatically extract them given an input parse. We develop a system based on a combination of hand-coded rules and machine learning. This allows us to include a large amount of linguistic knowledge and also have the robustness of a machine learning system. Since we do not have access to labeled examples of canonical forms, we train this system directly on SRL data, treating the correct canonical form as a hidden variable. Our system improves significantly over a strong baseline, demonstrating the viability of this new approach to SRL.

This latter method involves learning a large, complex probabilistic model. In the model we present, exact learning is tractable, but there are several natural extensions to the model for which exact learning is not possible. This is quite a general issue; in many different application domains, we would like to use probabilistic models that cannot be learned exactly. We propose a new method for learning these kinds of models based on *contrastive objectives*. The main idea is to learn by comparing only a few possible values of the model, instead of all possible values. This method generalizes a standard learning method, pseudo-likelihood, and is closely related to another, contrastive divergence. Previous work has mostly focused on comparing nearby sets of values; we focus on *non-local* contrastive objectives, which compare arbitrary sets of values.

We prove several theoretical results about our model, showing that contrastive objectives attempt to enforce probability ratio constraints between the compared values.

Based on this insight, we suggest several methods for constructing contrastive objectives, including contrastive constraint generation (CCG), a cutting-plane style algorithm that iteratively builds a good contrastive objective based on finding high-scoring values. We evaluate CCG on a machine vision task, showing that it significantly outperforms pseudo-likelihood, contrastive divergence, as well as a state-of-the-art max-margin cutting-plane algorithm.

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First I would like thank my advisor, Daphne Koller, for her help and guidance throughout my Ph.D. I began working in Daphne's lab as an undergraduate, so her contribution to my academic career extends back even farther. Daphne has taught me a huge amount about the research process, especially about presentation of work. This ranges from rigorously exploring and testing all aspects of a model to effectively communicating the work in papers and talks. She is also an inspiring classroom teacher; one of the main reasons I chose to study machine learning was the classes I took from her as an undergraduate.

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Chapter 1

Introduction

Teaching a computer to read is one of the most interesting and challenging problems in computer science. The field of natural language processing (NLP) developed as a response to the difficulty of this problem. One of the important developments in NLP has been the introduction and study of a number of sub-problems that break the task down into a number of more manageable sub-tasks. In this thesis, we focus on one of these tasks, semantic role labeling (SRL), an important processing step on the road from raw text to a full semantic representation.

Given an input sentence and a target verb in that sentence, the SRL task is to label the semantic arguments, or roles, of that verb. For example, in the sentence "Tom eats an apple," the verb "eat" has two roles, Eater = "Tom" and Thing Eaten = "apple". This task lies somewhere in the middle between syntax and semantics: it is more semantic than tasks such as part of speech tagging or syntactic parsing, but less semantic than tasks such as information extraction or question answering. Previous work, e.g., (Shen & Lapata, 2007; Christensen et al., 2010), have shown that using the output of an SRL system improves performance for a variety of these higher-level tasks.

Most semantic role labeling systems, including the ones presented in this thesis, take as input a syntactic analysis built by an automatic syntactic parser. SRL systems rely heavily on features extracted from the syntactic parse, particularly the *path feature*

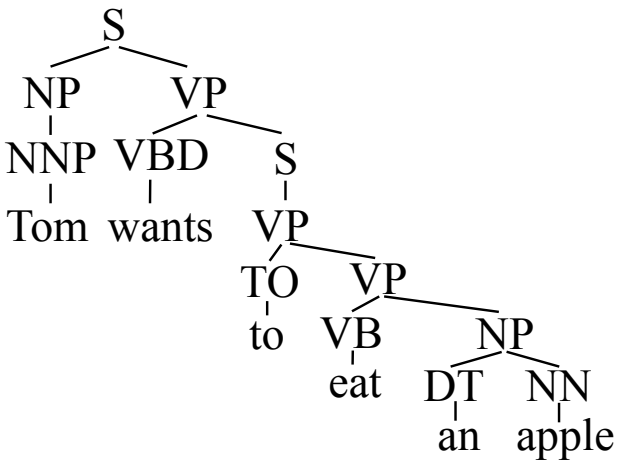


Figure 1.1: Parse of "Tom wants to eat an apple."

Tom: NP↑S↓VP↓S↓VP↓VP↓T

an apple: NP↑VP↓T

Figure 1.2: Path features for verb "eat" in Figure 1.1

(Gildea & Jurafsky, 2002), which captures the syntactic relationship between the target verb and the phrase being classified. Figures 1.1 and 1.2 show the parse and path features for several phrases in a sample sentence. The parse and the path feature are explained in more detail in Chapter 2.

Unfortunately, there are several issues with path features. First, the path feature may not contain all relevant information for the SRL task. Second, the space of possible path features is very large, resulting in very sparse features that are hard to learn.

In this thesis, we consider two ways of addressing these issues. First, we experiment with a number of variants of the standard syntactic features for SRL. We include a large number of syntactic features suggested by previous work, many of which are designed to reduce the sparsity of the path feature. We also suggest several new

features, most of which are designed to capture additional information about the sentence not included in the standard path feature.

The second method we consider is a new methodology for SRL based on labeling *canonical forms*. A canonical form is a representation of a verb and its arguments that is abstracted away from the syntax of the input sentence. For example, "A car hit Bob," and "Bob was hit by a car," have the same canonical form, {Verb = "hit", Deep Subject = "a car", Deep Object = "a car"}. Labeling canonical forms makes it much easier to generalize between sentences with different syntax. To label canonical forms, we first need to automatically extract them given an input parse. We develop a system based on a combination of hand-coded rules and machine learning. This allows us to include a large amount of linguistic knowledge and also have the robustness of a machine learning system.

This latter method involves learning a large, complex probabilistic model. Our model is structured in such a way that exact learning is tractable. However, there are several natural extensions to the model for which exact learning is not possible. This issue is not restricted to our problem; in many different application domains, we would like to use probabilistic models that cannot be learned exactly.

We propose a new method for learning these kinds of models based on *contrastive objectives*. The main idea is to learn by comparing only a few possible values of the model, instead of all possible values. This method generalizes a standard learning method, pseudo-likelihood, and is closely related to another, contrastive divergence. Previous work has mostly focused on comparing nearby sets of values; we focus on *non-local* contrastive objectives, which compare arbitrary sets of values. As we will see, using non-local contrastive terms results in significant performance gains.

1.1 Contributions and Publications

There are three main contributions of this thesis:

1. **Building an improved set of syntactic features for semantic role labeling.** While there has been some previous work, e.g., (Pradhan et al., 2005), on evaluating individual features for SRL, this thesis presents the most comprehensive study of syntactic features. Additionally, we suggest several features that incorporate additional information into the SRL system, leading to significant gains in performance.

2. **Developing a new method for semantic role labeling using canonical forms.** This system performs a much more detailed analysis of the input parse than standard SRL systems. Normalizing sentences to a common form allows significantly improved generalization between different sentences. Efficient implementation of this system involved development and use of sophisticated algorithms and data structures, as well as encoding of a large amount of linguistic knowledge. This system improves significantly over a standard (but high-performing) SRL system. This work has appeared in (Vickrey & Koller, 2008b) and a follow-up paper, (Vickrey & Koller, 2008a).

3. **Proposing non-local contrastive objectives as a means to learn complex probabilistic models.** Contrastive objectives have been described in various forms in previous work, e.g., (LeCun & Huang, 2005; Smith & Eisner, 2005), but this work focuses on local terms. Non-local methods have been suggested in the context of max-margin methods (Tsochantaridis et al., 2005), but our method is the first application of this idea to log-linear models, which, unlike margin-based models, are able to model probability distributions. We prove several theoretical results that justify the use of non-local contrastive objectives. One implication of these results is that contrastive objectives attempt to enforce probabilistic ratio constraints between compared values. Based on this insight, we propose contrastive constraint generation (CCG), which uses MAP inference to find values to include in our contrastive objective. Experimental results on a real-world machine vision task show that CCG improves significantly over local contrastive learning methods such as pseudo-likelihood and contrastive divergence, as well as the margin-based method of Tsochantaridis et al. (2005). This work has been

accepted for publication as (Vickrey et al., 2010).

1.2 Thesis Outline

Chapter 2: Background. This chapter introduces the necessary background for semantic role labeling and for learning complex probabilistic models. This chapter also includes an overview of previous work in semantic role labeling and a few basic citations in the area of probabilistic learning. More specific related work is included in each of the subsequent chapters.

Chapter 3: Evaluating Syntactic Features for Semantic Role Labeling. In this chapter, we first describe the details of our implementation of a standard SRL system. Next, we describe a number of additional syntactic features, both new and old. We then do a detailed experimental evaluation on these features and build a final model using the best features. Finally, we compare our model to several state-of-the-art SRL models on the standard CoNLL test set.

Chapter 4: Canonicalization for Semantic Role Labeling. In this chapter, we first present the idea of a canonical form. We then describe how we build an SRL system based on labeling canonical forms. We describe the linguistic knowledge that went into building the system, as well as the data structures and algorithms that allowed us to learn and perform inference in our model. Finally, we evaluate our model on the CoNLL test set and compare it to our standard SRL system.

Chapter 5: Non-Local Contrastive Objectives. In this chapter, we begin by defining contrastive objectives and discussing their relationship to several well-known learning methods. Next, we present several theoretical results, including consistency of contrastive objectives with maximum likelihood. We then propose several methods for constructing contrastive objectives, including contrastive constraint generation (CCG). Finally, we evaluate CCG on a machine vision task, comparing it to several well-known learning methods.

Chapter 2

Background

We first describe background material for semantic role labeling, followed by a discussion of learning complex probabilistic models.

2.1 Semantic Role Labeling

The first three chapters of this thesis focus on the task of *semantic role labeling* (SRL). A single instance of this problem is a sentence and a *target verb* within that sentence. The goal is to label the semantic arguments, or roles, of that verb. For example, in the sentence "Tom eats an apple," the verb "eat" has two roles, Eater="Tom" and Thing Eaten="apple". Roles are not the same as syntactic arguments (e.g., subject, direct object), although certain semantic arguments often coincide with syntactic arguments. For example, the subject of "eat" is usually the Eater, but in many sentences the Eater is not the syntactic subject of "eat" (e.g., in "Tom wanted to eat an apple", "Tom" is the subject of "want", not "eat"). For other verbs, the syntactic subject may take several possible roles. In "Tom sold the house," the syntactic subject "Tom" is the Seller, but in "The house sold," the syntactic subject "house" is the Thing Sold.

In this thesis, we focus on the PropBank (Kingsbury et al., 2002) data set and its associated role set. Other notable data sets for SRL (not discussed in this thesis) are

FrameNet (Baker & Sato, 2003)[1] and VerbNet (Schuler, 2006)[2]. These data sets are similar to PropBank but have some important differences.

PropBank contains a single set of roles which are used across all annotated verbs. These roles are divided into two types. The first type, *core arguments*, consists of verb-specific roles, labeled ARG0 through ARG5. ARG0 is generally the agent, ARG1 is generally the theme, while ARG2-ARG5 have different usages for verbs. For example, for "eat", ARG0 corresponds to the Eater, and ARG1 is the Thing Eaten. For "give", ARG0 is the Giver, ARG1 is the Gift, and ARG2 is the Recipient. The second type, *adjunct arguments*, corresponds to arguments that are not specific to particular verbs. Examples include time phrases (labeled ARGM-TMP) and location phrases (labeled ARGM-LOC). There are twelve different types of adjunct arguments.

Throughout the thesis, we use the ARGX labels for specific roles, but we often include in parentheses the verb-specific interpretation of that argument. For example, if we are talking about the ARG0 of "eat", we write ARG0(Eater).

2.1.1 SRL as an NLP Task

Semantic role labeling has a long history in linguistics and natural language processing (NLP). We will not discuss the earlier work in this thesis; Pradhan (2006), for example, gives a good overview. Semantic role labeling was reintroduced in a modern machine learning setting by Gildea & Jurafsky (2002). The standard approach to this problem is to build a classifier based on a large number of features extracted from a syntactic analysis of the sentence. In this section we will describe the basic setup of the problem and standard features used for this task.

Automatic syntactic parsers, such as the Charniak parser[3], play an essential role in most SRL systems. Until recently, most work was based on *constituency* parsers, such as the Charniak parser; in the last few years there has been a significant amount of work using *dependency parsers* for SRL. Johansson & Nugues (2008) built an early

[1] `http://framenet.icsi.berkeley.edu`
[2] `http://verbs.colorado.edu/~mpalmer/projects/verbnet.html`
[3] Available at `ftp://ftp.cs.brown.edu/pub/nlparser/`

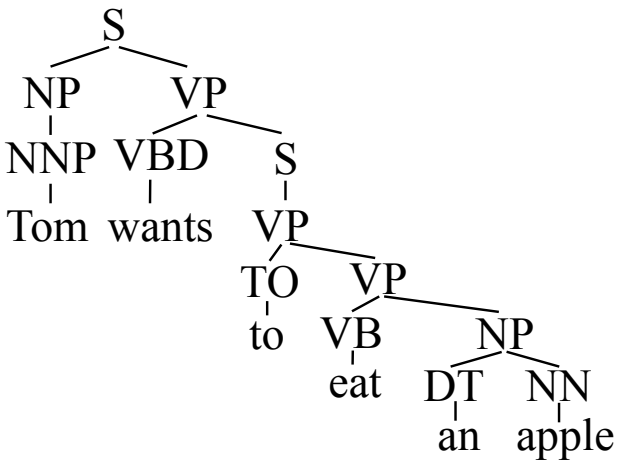


Figure 2.1: Parse of "Tom wants to eat an apple."

dependency-based SRL system, while the CoNLL 2008 shared task[4] focused on joint dependency parsing/SRL. Both types of parsers work well for SRL; the best systems using each type of parser achieve roughly comparable results. Since the different types of parse require different feature extractors, it is generally easier to choose one type and concentrate on it, particularly for more complicated methods such as the one presented in Chapter 4. In this thesis, we exclusively use constituency parses.

Figure 2.1 shows an example constituency parse. A constituency parse is a rooted tree where each node is labeled with a *category*. For example, the root of the tree in Figure 2.1 is labeled with category S, indicating that it is a sentence or sentence clause. The first child of this node is labeled with category NP, indicating a noun phrase. The leaves of the tree are labeled with the words of the sentence; the immediate parent of each leaf is labeled with that word's *part of speech tag*. A *constituent* refers to a complete subtree of the parse. Example constituents in Figure 2.1 include "Tom," "an apple," and "wants to eat an apple." The *type* of a constituent is the category of the root of the constituent subtree.

[4]Available at `http://barcelona.research.yahoo.net/conll2008/`

Problem Definition

Given a syntactic parse, standard SRL systems solve the following problem. For every sentence s, for every verb v in s, for every constituent c in the parse of s, the system must decide whether c is an argument of v, and if so, which of the possible roles it should be labeled with. Let R be the set of all possible roles (both core and adjuncts), plus one additional value "none." Each triple s, v, c is considered to be a separate training example and is labeled with a role $r \in R$: if c is an argument of v, r is the correct role of c; otherwise $r =$ "none." The data set D contains m examples; example d^i corresponds to the triple (s^i, v^i, c^i), with label $r^i \in R$. Note that none of s^i, v^i, c^i is unique to d^i; each may occur in multiple different examples.

Given this setup, we now have a straightforward (multi-class) classification problem and can use any of a variety of standard classifiers, such as logistic regression or SVM. A large amount of effort has been made in previous work to determine useful features for this task. Later in this section, we will discuss several "basic" features that are used by most high-performing systems; in Chapter 3 we will describe a number of other features that have been proposed for SRL.

Parse-related Complications

The use of automatically-generated parses introduces a complication: the correct argument phrases may not line up with a single constituent in the automatic parse. In principle, the system can recover, since any group of words from the original sentence can be covered by some set of constituents. However, this is quite difficult for the SRL classifier, so typically the system will end up with an incorrect role labeling if this happens (incorrect with respect to the most commonly used scoring metrics).

Another issue is how to deal with overlapping predictions by the role classifier. For example, suppose the role classifier decides to label a particular constituent as ARG0, but decides to label one of its children as ARG1. One simple solution to this problem is to use greedy top-down decoding, where the role assigned to a constituent is propagated (and overwrites) any labelings of its descendants. More complicated

Feature	Example	Citation
Frame	eat	(Gildea & Jurafsky, 2002)
Head Word	apple	(Gildea & Jurafsky, 2002)
Category	NP	(Gildea & Jurafsky, 2002)
Head POS	NN	(Surdeanu et al., 2003)
First Word	an	(Pradhan et al., 2005)
Last Word	apple	(Pradhan et al., 2005)

Table 2.1: Phrase features for "an apple" in Figure 2.1

Tom: NP↑S↓VP↓S↓VP↓VP↓T

an apple: NP↑VP↓T

Figure 2.2: Path features for verb "eat" in Figure 2.1. T represents the target verb.

methods have been proposed, see for example (Toutanova et al., 2005). The choice of method used to solve this problem can also influence the method used to train the system; we return to this issue in the next chapter.

Basic Features

There are two basic categories of SRL features. The first is features of the constituent, which we refer to as phrase features. Table 2.1 lists the most commonly-used (and successful) phrase features for SRL. Head words are typically computed using a heuristic head-word system, as in the head rules of Collins (1999). These features allow us to capture syntactic and lexical patters. For example, we can learn that "apple" is likely to be the ARG1 (Thing Eaten), but not the ARG0 (Eater).

The most important syntactic feature in most SRL systems is the path of category nodes from the constituent to be classified c to the target verb v (Gildea & Jurafsky, 2002). Examples of this feature are shown in Figure 2.2.[5] Path features allow systems

[5]There are several decisions to make when constructing the path feature, such as whether to use a directed or undirected path. Shown is the version of this feature we use in our models, described in more detail in Chapter 3.

to capture both general patterns, e.g., that the ARG0 of a sentence tends to be the subject of the sentence, and specific usage, e.g., that the ARG2 (Recipient) of "give" is often a post-verbal prepositional phrase headed by "to". Another commonly-used syntactic feature is the length (number of edges) in the path feature (Pradhan et al., 2005).

The final basic syntactic feature we discuss is the sub-categorization of the target verb (Gildea & Jurafsky, 2002). This feature is simply the CFG expansion of the parent of the target verb. In Figure 2.1, the sub-categorization for "eat" is $VP \rightarrow T\ NP$.

As described above, many of the roles (ARG0, ARG1, and the adjuncts) behave similarly across different verbs. To take advantage of this, we can include both a general and a frame-specific version of each feature. Consider the Head Word feature (described below). In Figure 2.1, for verb "eat" and constituent "an apple", we can extract both the general feature "head-word=apple" and the frame-specific feature "frame=eat,head-word=apple." Frame-specific versions of the head word, path, and category features are often used, as suggested by Xue & Palmer (2004), but frame-specific versions of the other feature types are less common.

Identification Classifier

There is one practical problem with the system described so far. The PropBank training set is fairly large (one million words), and in the setup described, for every verb v in every sentence s, we label every constituent c in the parse of s. This leads to a very large training set, which is made worse by the fact that training time typically scales linearly with the number of classes (in this case, the number of roles $|R| \approx 30$).

To address this issue, many systems introduce an additional preprocessing step in order to filter out constituents that are "clearly" not arguments. This is usually just a binary classifier that uses similar features to those used by the role classifier, which is supposed to answer 1 if the constituent is an argument, and -1 otherwise. This *identification* classifier is trained on the same training set as the classifier, and is then

used (at both training and test time) to reduce the set of constituents that are processed by the role classifier.[6] Often, the classification threshold for the identification classifier is set to increase recall at the cost of precision. Since constituents that are not actually arguments can make it through the filtering stage, the role classifier still needs the option to classify a constituent as "none."

2.1.2 Applications of SRL

SRL is a natural pre-processing step for tasks such as information extraction and information retrieval. For example, a typical information extraction task is to find all events of a certain type (e.g., one company buying another), along with who bought whom, when, for what price, etc. Since many such events appear in text as verbs with their associated semantic roles, it is clearly useful to be able to identify these roles automatically. More generally, SRL is an important step for any system that aims to achieve "natural language understanding."

Following is a list of applications of SRL to higher-level tasks:

Christensen et al. (2010) build a system based on SRL for open-domain information extraction (Open IE) — the task of extracting factual relationships from a text corpus without using a prespecified list of relations. Their SRL-based system obtains higher-quality extractions as compared to a state-of-the-art Open IE system.

Ponzetto & Strube (2006) use SRL as part of system that performs coreference resolution — determining when two or more phrases refer to the same real-world object. They directly use the output of a SRL system as features for their model, and show that adding these features significantly improves performance over a baseline model.

Shen & Lapata (2007) build a question-answering system which incorporates SRL data from the FrameNet data set. The resulting system performs significantly better than a system which uses only syntactic information.

[6] Ideally, we train the identification classifier in several folds of the training data, so that we do not end up with an overly confident filter on the training set.

Kim & Hovy (2006) build an opinion mining system which uses an SRL system to identify the opinion holder and opinion text.

Barnickel et al. (2009) build a large-scale automatic relation extraction system for biomedical texts whose most important component is an SRL system.

Taking a step back from individual applications, the overall pattern is that SRL systems improve performance because they perform a more-detailed analysis of the syntax and word-level semantics of the input sentence. In principle (and sometimes in practice), higher level tasks can directly incorporate these kinds of features, bypassing the need for a separate SRL system.

With this in mind, the study of SRL as a separate task is important for several reasons. First, SRL systems are a useful off-the-shelf tool which free users from reinventing these kind of detailed features and models. Second, studying SRL as a stand-alone task gives more insight into new features which may improve performance, of both SRL and higher-level systems. In this respect, SRL systems are similar to POS taggers, named entity recognizers, or syntactic parsers; much of the business of NLP is commoditizing these sub-tasks for use by higher-level systems.

2.1.3 State-of-the-art SRL Systems

There are at least four different ways in which prior work has extended the basic model. The first is to use additional features; in the following chapter we will go into detail about a wide variety of features that have been proposed for SRL. In this section, we describe three other approaches, each utilized by a different state-of-the-art SRL system.

Punyakanok et al. (2005) built the system that placed first in the CoNLL-2005 evaluation. They start with a basic SRL system as described in this chapter. They improve their system by running their classifier on not just on the top-scoring Charniak parse, but also on the next four highest-scoring Charniak parses and the highest scoring parse generated by the Collins parser (Collins, 1999). Their system then votes on the final role predictions by combining the predictions of the classifier run

on each of these six parses. This results in a very large boost in performance, which explains their system's top finish. The next three systems at CoNLL-2005 also used information from more than one parse.

Toutanova et al. (2008) looked at using joint inference for SRL. The idea is to model the interaction between different arguments of a verb in order to improve performance. Most obviously, most arguments can only appear once for a particular verb (there cannot be two Agents, for example). Other more complicated patterns can occur; for example, if there is a Recipient in the sentence, there is probably also a Gift. Toutanova et al. (2008) incorporate this information by using a reranking system, which first generates plausible labelings of all phrases in the sentence using a local classifier, and then picks among those by using more global features.

Surdeanu et al. (2007) describe the system that currently has the best reported results for SRL on the CoNLL-2005 data set. They start by building three different syntactic SRL systems. The first two models (M1 & M2) operate quite differently from the approach described in this chapter: they label the roles using sequence tagging techniques similar to those commonly used for named entity extraction and other similar tasks. Their B-I-O (beginning-inside-outside) system first uses a syntactic processor (a shallow parser for M1 and the Charniak parser for M2) to build syntactic features of each phrase. It then does linear decoding to find the optimal role assignment. The M3 system has the same setup as the basic system we describe in this chapter, classifying the constituents generated by the Charniak parser. The key idea of their work is to combine these three systems to get the final role predictions; see Surdeanu et al. (2007) for details of the combination scheme.

In this thesis, we pursue yet another direction. Our goal is to build a more sophisticated, "deeper" model of sentence syntax. We design features which capture additional information about various syntactic constructs (Chapter 3), and we design a system (Chapter 4) which not only captures this kind of information but also models the recursive structure of natural language.

2.2 Learning Complex Probabilistic Models

2.2.1 Definitions

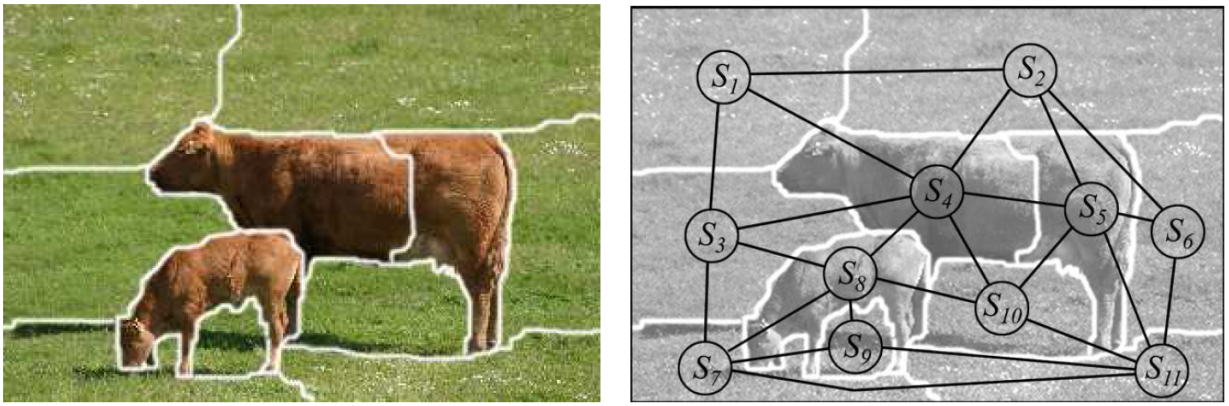
A *log-linear model* specifies a conditional probability distribution over a set of n label variables $\mathbf{Y} = \{Y_1, \ldots, Y_n\}$ given a (possibly empty) set of observed variables $\mathbf{X}$. The *model space* P_Θ is determined by a set of R feature functions $f_1(\mathbf{X}, \mathbf{Y}), \ldots, f_R(\mathbf{X}, \mathbf{Y})$; let $\mathbf{f}(\mathbf{X}, \mathbf{Y})$ be a vector containing all feature functions. A particular model $P_{\boldsymbol{\theta}}$ is defined by a vector of weights $\boldsymbol{\theta} \in \Theta$ of length R. The probability distribution associated with $P_{\boldsymbol{\theta}}$ is

$$P_{\boldsymbol{\theta}}(\mathbf{Y} = \mathbf{y} | \mathbf{X} = \mathbf{x}) = \frac{e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}, \mathbf{y})}}{Z(\mathbf{x})},$$

where $Z(\mathbf{X} = \mathbf{x}) = \sum_{\mathbf{y}} e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}, \mathbf{y})}$ is a normalization factor that ensures that the distribution sums to 1 for each $\mathbf{x}$.

One of the simplest examples of a log-linear model is logistic regression, where $\mathbf{Y}$ is a single variable to be predicted based on the input features $\mathbf{X}$. In this thesis, we focus on more complex models where $\mathbf{Y}$ consists of multiple variables. These types of models are commonly referred to as *undirected graphical models*, particularly when the connections between the label variables Y_l (as specified by the feature functions) only involve a few variables at a time. In this case, it is natural to think of the feature functions as corresponding to *edges* in a graph. This is particularly natural for *pairwise undirected graphical models*, where each feature function depends on at most two variables. Thus, each feature function depends either on only one variable (a singleton feature) or on two variables Y_{l_1}, Y_{l_2}, in which case we say there is an edge between Y_{l_1} and Y_{l_2}. Undirected graphical models are often referred to as *Markov random fields* (MRFs) when $\mathbf{x}$ is empty, and as *conditional random fields* (CRFs) (Lafferty et al., 2001) when $\mathbf{x}$ is nonempty.

Undirected graphical models allow complicated probabilistic models to be specified using relatively few parameters. This is advantageous not only computationally, but also because it enables the model to generalize better to unseen data. Undirected graphical models are used in a wide-range of applications, including natural language



(a) Over-segmentation (b) CRF Construction

Figure 2.3: CRF for classifying regions in an image (with label variables S_l)

processing, machine vision, and biological modeling. Figure 2.3 shows an example pairwise conditional random field for the task of image-region classification. Each node Y_l corresponds to a (pre-defined) region of the image; the task is to decide to which of several possible region types (e.g., "cow", "grass", "sky") the region corresponds. Neighboring regions in the graph are connected through feature functions involving those two variables. These features allow the model to capture, for example, the fact that neighboring regions are more likely to have the same type.

2.2.2 Using Log-linear Models

One of the main uses of log-linear models is in *classification problems* in which we try to predict the label variables $\mathbf{Y}$ given $\mathbf{X}$. We are given a data set D of m examples. The i^{th} example $d^i = (\mathbf{x}^i, \mathbf{y}^i)$ consists of observed features $\mathbf{x}^i$ and a correct label $\mathbf{y}^i$. We use $\hat{P}(\mathbf{Y}|\mathbf{X}) = \frac{|d^i:(\mathbf{x}^i,\mathbf{y}^i)=(\mathbf{X},\mathbf{Y})|}{\hat{Z}(\mathbf{X})}$ to refer to the empirical distribution observed in our data set D, where $\hat{Z}(\mathbf{X}) = |d^i : \mathbf{x}^i = \mathbf{X}|$. The goal is to predict $\mathbf{Y}$ as well as possible on an unseen set of test examples D_{test}.

Learning

The first task we need to solve is the *learning problem*: how to choose a good model $P_{\boldsymbol{\theta}}$ from our model space P_Θ. A common approach is to define an *objective function* over $\boldsymbol{\theta}$, and then optimize this objective to find a good choice of $\boldsymbol{\theta}$. The canonical example of this approach for a log-linear model is the log-likelihood objective,

$$LL(\boldsymbol{\theta}; D) = \sum_{(\mathbf{x}^i, \mathbf{y}^i)} \log P_{\boldsymbol{\theta}}(\mathbf{y}^i | \mathbf{x}^i).$$

This objective simply measures the average (log) probability assigned by the model $P_{\boldsymbol{\theta}}$ to the data examples d^i. This objective is concave in $\boldsymbol{\theta}$, and so as long as computing $P_{\boldsymbol{\theta}}(\mathbf{y}^i|\mathbf{x}^i)$ is feasible, it is straightforward to optimize this objective using standard convex-optimization methods such as conjugate gradient or L-BFGS (Liu & Nocedal, 1989).

Unfortunately, for many log-linear models over complex label spaces, the computation of the normalization factor $Z(\mathbf{X})$ — referred to as the *partition function* in the context of undirected graphical models — is not feasible. For example, in an undirected graphical model, the size of the label space $\mathbf{Y}$ is exponential in the number of variables Y_l. In certain cases, dynamic programming can be used to compute this sum over exponentially many values, but often exact computation of $Z(\mathbf{X})$ is not possible.

There are many approaches to this problem. One common method is to use *approximate marginal inference algorithms* to compute the statistics necessary for learning. We will not describe this approach in detail, but we briefly discuss approximate inference algorithms below. Examples of this approach include sampling methods (e.g., Markov chain Monte Carlo sampling) and message passing algorithms (e.g., belief propagation). Another common method, which we adopt in Chapter 5, is to design an alternate objective function that is easier to optimize but still prefers "good" models $P_{\boldsymbol{\theta}}$.

One well-known example of this latter approach is pseudo-likelihood (PL). Let $dom(Y_l)$ denote the set of possible values of Y_l. Let $\mathbf{y}_{-l}$ be the value of all nodes *except* node l, and $(\mathbf{y}_{-l}, y_l)$ be a combined instantiation to $\mathbf{y}$ which matches y_l for

node l and $\mathbf{y}_{-l}$ for all other nodes. The *pseudo-likelihood objective* is defined as

$$PL(\boldsymbol{\theta}; D) = \sum_{(\mathbf{x}^i, \mathbf{y}^i)} \sum_{l} \left(\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \log \sum_{a \in dom(Y_l)} e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, (\mathbf{y}^i_{-l}, a))} \right).$$

We will explain the motivation for this objective in more detail in following sections. For now, there are two important properties of this objective. First, under certain conditions, it is *consistent* with log-likelihood — that is, given an infinite amount of training data, it will learn the same parameter $\boldsymbol{\theta}$ as log-likelihood. Second, the time required to compute $PL(\boldsymbol{\theta}; D)$ is linear in the size of the training data; unlike log-likelihood, it does not scale exponentially with the number of network variables. This means that optimizing this objective is guaranteed to be computationally efficient.

Another type of alternate objective is *max-margin objectives*, including single-variable models, such as support vector machines (Cortes & Vapnik, 1995; Vapnik, 1998), and complex structured models (Taskar et al., 2003; Tsochantaridis et al., 2005). Rather than fit a probability distribution to the observed data, these methods try to enforce constraints on the (unnormalized) score function $\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i)$. As a result, computation of the partition function is not required; the model can be learned using only MAP inference (described below). However, exact optimization of these objectives is still intractable when MAP inference is intractable.

Inference

Once we have selected (learned) a model $P_{\boldsymbol{\theta}}$, we still need to actually use the model to make predictions. This typically means that given a set of features $\mathbf{x}$, we need to find the value of $\mathbf{Y}$ which maximizes $P_{\boldsymbol{\theta}}(\mathbf{Y}|\mathbf{x})$. This is known as the *maximum a-posteriori (MAP) inference problem.* This problem does *not* require computation of the partition function $Z(\mathbf{x})$ because it only requires comparison of the unnormalized scores $\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}, \mathbf{y})$.

There are some models for which computing $Z(\mathbf{x})$ is not feasible, but computing $\arg\max_{\mathbf{Y}} P_{\boldsymbol{\theta}}(\mathbf{Y}|\mathbf{x})$ is. MAP inference based on graph cuts is one important example of this (see, for example, (Kolmogorov & Zabih, 2004)). For example, suppose

we want to assign each pixel in an image to either "foreground" or "background". We allow arbitrary single-node potentials, but our model is restricted to be *associative* — the weights on the pairwise features must encourage neighboring pixels to match. Under these conditions, we can find the optimal assignment of pixels to foreground/background by constructing a special graph and then running a max-flow algorithm to find the minimum cut.

Unfortunately, in many cases where computing $Z(\mathbf{x})$ is not feasible, computing $\arg\max_{\mathbf{Y}} P_{\boldsymbol{\theta}}(\mathbf{Y}|\mathbf{x})$ is also not feasible. The solution to this problem is to use an approximate MAP inference algorithm. These methods try to find a value of $\mathbf{Y}$ with a high score but are not guaranteed to find the best possible value. One example of an approximate MAP inference algorithm is iterated conditional modes (ICM), proposed by Besag (1986). ICM is a simple greedy ascent algorithm. At each round, a variable is chosen at random; the label of this variable is then changed to the value that gives the highest score (if the current value is the best, the label is not changed). This is repeated until a local maximum is reached (i.e., no single-variable moves improve the score). Another commonly-used approximate MAP inference algorithm is max-product belief propagation (MP) (Pearl, 1988). The details of this method are not important for exposition of our work, but intuitively this method iteratively updates a set of "beliefs," one per variable, about what the best value of that variable is.

A significant advantage of MAP inference vs. marginal inference is that the MAP inference problem is just a standard combinatorial optimization problem, which has been well studied in a variety of computer-science fields. This is one of the primary motivations for the methods presented in Chapter 5: they enable us to learn a log-linear model using a MAP inference method rather than a marginal inference method.

Chapter 3

Evaluating Syntactic Features for Semantic Role Labeling

3.1 Introduction

In this chapter, we first describe our implementation of a high-performing standard SRL system. Second, we survey previous work in order to collect a long list of syntactic features proposed for SRL. Third, we propose several new features, many of which are based on incorporating additional information about specific grammatical constructs. Fourth, we systematically evaluate the relative usefulness of both the old and new features. Fifth, based on these experiments, we add the best-performing features (a mix of old and new features) to our standard SRL system, improving performance significantly. Finally, we compare to current state-of-the-art methods for SRL. While a few systems out-perform the system we describe in this chapter, our system has the best reported results among systems that classify each argument independently (non-jointly) and that use information from only a single automatic parse.

3.2 Experimental Setup

Throughout this chapter, we will present results for various SRL systems on the PropBank data set. To facilitate comparison with other work, we use the experimental setup of the CoNLL 2005 SRL task[1]. Following standard procedure, we use sections 2-21 as the training set, section 24 as the development set, and section 23 as the test set. The training set contains approximately 1 million words of text annotated with semantic role labels. All results we report are computed using the srl-eval script distributed by the CoNLL 2005 shared task.

As discussed in the previous chapter, an important element of most SRL systems is an automatic syntactic parser. In this work, we use the Charniak parser Charniak (2000), a state-of-the-art constituency parser. As noted by Toutanova et al. (2008), the Charniak parses distributed with CoNLL 2005 did not handle forward quotes correctly; for all the systems discussed in this thesis, we reparsed the training and test sets using the 2005 version of the Charniak parser.[2]

Throughout the rest of this chapter, we report results of various versions of our system on the training set (using 3-fold cross validation) and on the development set. To avoid implicitly overfitting the test set, we only report test results for a few specific feature sets, chosen based on development and training performance, *not* on test performance. We did not directly compute statistical significance intervals for our results, but we note that on the CoNLL 2005 test set, using bootstrap resampling, all submitted systems were assigned a significance interval of ± 0.8 or less F1 points. We would expect a much smaller confidence interval on the much larger training set.

3.3 Our Standard SRL System

In this section we describe the details of our implementation of the standard SRL system discussed in the previous chapter.

[1] `http://www.lsi.upc.es/~srlconll/home.html`

[2] Available at `ftp://ftp.cs.brown.edu/pub/nlparser/`

Phrase Features	Syntactic Features
Frame	Path
Head Word	Path Length
Category	Verb Subcategorization
Head POS	
First Word	
Last Word	

Table 3.1: Features used in our standard SRL system

Our system is based on multi-class logistic regression. From each data example d^i, we extract a feature vector $\mathbf{f}^i$ of length K. For each possible role $r \in R$, our model has a parameter vector $\boldsymbol{\theta}_r$ of length K. The model assigns probabilities $P(r|s,v,c) = \frac{e^{\boldsymbol{\theta}_r^T \mathbf{f}^i}}{\sum_{r'} e^{\boldsymbol{\theta}_{r'}^T \mathbf{f}^i}}$. We train the system by maximizing the L2-regularized log-likelihood,

$$\left(\sum_{d^i} \log P(r^i|s^i,v^i,c^i) \right) - \sum_r \frac{\boldsymbol{\theta}_r^T \boldsymbol{\theta}_r}{2\sigma^2}.$$

L2-regularization penalizes large weights, helping to prevent overfitting. For all results in this chapter, we use $\sigma = 1.0$; this value gave good performance on the development set for a wide variety of feature sets. It is possible that better performance might be achieved by fitting σ (on the development set) separately for each feature set. We maximize the objective using L-BFGS (Liu & Nocedal, 1989).

We use the same basic features described in Chapter 2. We prune any features that occur fewer than 3 times in the training set. Table 3.1 is a complete list of the features used by our basic system (refer to Chapter 2 for a description of these features). We now describe some specific details of our implementation of these features.

To generate the Head Word and Head POS features, we use the head-word rules of Collins (1999). As suggested by Surdeanu et al. (2003), rather than using the preposition as the head word of prepositional phrases (PPs), we instead use the head word of the object of the phrase. Also, we augment the category of all PPs with the preposition. Thus, in the sentence "I gave the ball to him," the head word of the phrase "to him" is "him," while the category of this phrase is "PP(to)."

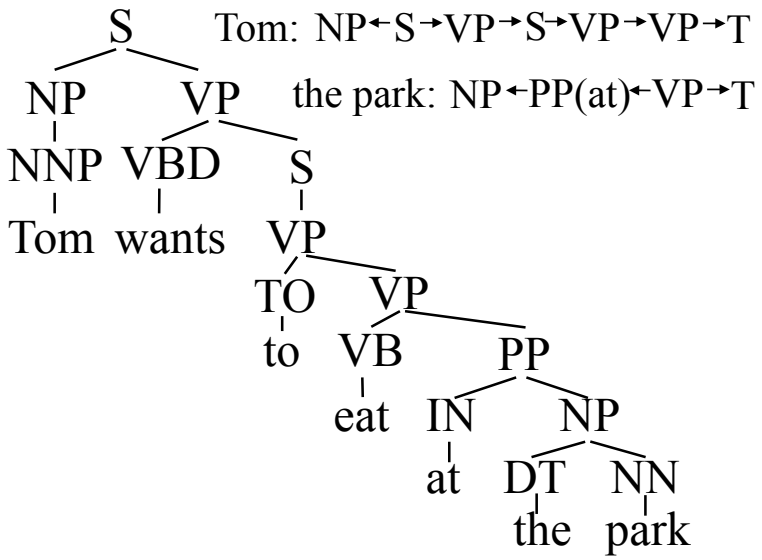


Figure 3.1: Parse with example path features for verb "eat"

There are several choices to be made regarding the path feature. In this thesis, we use directed paths (as opposed to undirected paths); we replace the category of the target verb v with "T" to make the paths tense-independent; and as above, we augment prepositional phrase categories with the head preposition. Examples of our version of the path feature are shown in Figure 3.1.

For the basic version of the subcategorization feature, we do *not* expand the categories of "PP" phrases — we consider this variant in the subsequent section. Note that in some cases, the v is not actually the head of a VP phrase; in our system, we calculate the subcategorization feature even in these cases.

In the previous chapter, we mentioned that it is important to include both frame-specific and general versions of each feature. Most systems include general versions of all features, but only include frame-specific versions of a few features (e.g. Head Word, Path, and Category). We found that using frame-specific versions of other features worked well, and so for all experiments, we include both general and frame-specific versions of all feature types.

Evaluation set	Prec.	Recall
Training (3-fold cv)	69.6	92.9
Devel	67.7	84.6
Test WSJ	68.8	83.6
Test Brown	65.6	74.6

Table 3.2: Identification classifier results

.	Train			Devel		
Features	P	R	F1	P	R	F1
Phrase	72.0	66.5	69.2	67.0	61.4	64.0
+ Path	82.4	77.3	79.8	75.5	69.3	72.3
+ Path Len	82.5	77.4	79.9	75.5	69.7	72.5
+ SubCat	**84.4**	**80.0**	**82.1**	**77.2**	**71.9**	**74.5**

Table 3.3: Results sequentially adding basic features

We used greedy top-down coding to handle overlapping predictions by the role classifier. Thus, we are primarily interested in training our classifier to identify the root of a role constituent. To this end, at training time, we throw away any constituents c whose parent is part of the same argument.

As discussed in the previous chapter, we filtered out a large number of constituents using a binary "identification" classifier trained to distinguish between role constituents and non-role constituents. Due to the lengthy training time for this model, we did not experiment with different feature sets for the identification classifier. All reported results use an identification classifier with features similar to those of the Baseline+PassPos role classifier, described in Section 3.5. We chose a filter threshold to obtain high recall without sacrificing too much precision. The evaluation metric for (only) these results is per-constituent precision/recall, which is harsher than the metric used by the CoNLL shared task, per-argument precision/recall. This difference is particularly important for arguments that span multiple constituents. Table 3.2 shows results of our identification classifier on the training, development, and test sets.

Table 3.3 shows the results for our role classifier (using the identification classifier described in the previous paragraph), starting with just the phrase features and sequentially adding the syntactic feature types. The path and subcategorization features are clearly very important, while the path length feature provides a smaller benefit. Note that the results on the training set are much higher than the development set, mostly because the Charniak parser was trained on this data. We refer to the model that uses all basic features as our "baseline" model.

3.4 Extended Syntactic Features

In this section, we consider a number of additional syntactic features. Each feature is followed either by a citation or by New if it has not been proposed in previous work. There are a several high-level ideas in these features. First, most of the features either (1) reduce the sparsity of the syntactic features or (2) add additional information not captured by the original syntactic features. The most of the features below are modifications of the path feature, but there is also a group of features which modify the subcategorization feature.

3.4.1 Sub-paths

Because of syntactic variability, the number of possible values of the path feature is very large. Combined with the fact that many verbs have few examples in our training set, this means that the path feature is very sparse. The features in this group attempt to reduce the sparsity of the path feature by extracting subsequences of the path.

Let a be the lowest common ancestor of c and v. Thus, the category of a is at the "top" of the path from c to v. Consider the path $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}S{\rightarrow}VP{\rightarrow}VP{\rightarrow}T$ (the path from "Tom" to "eat" in Figure 3.1). In this case, a is the second node in the path. We will use this path as a running example; unless otherwise indicated, for each feature type we will include the value of that feature when classifying "Tom" for

verb "eat."

Up Path: The path from c to a (inclusive). Let $u[i]$ denote the i^{th} category in this path and $|u|$ the length of this path. Example value: $NP{\leftarrow}S$. (Pradhan et al., 2005).

Down Path: The path from a to v (inclusive). Define $d[i]$ and $|d|$ as for Up Path. Example value: $S{\rightarrow}VP{\rightarrow}S{\rightarrow}VP{\rightarrow}VP{\rightarrow}T$. New.

Gen Up Path: If $|u| \geq 3$ and $|d| \geq 2$, for each $1 < i < |u|$, we construct the generalized path $u[0]{\leftarrow}u[i]{\leftarrow}u[|u|]{\rightarrow}d[|d|]$. Example value: not applicable because $|u| = 2$. (Surdeanu et al., 2007).

Gen Down Path: Analogous to Gen Up Path; requires $|u| \geq 2$, $|d| \geq 3$. Example value: $\{NP{\leftarrow}S{\rightarrow}VP{\rightarrow}T$,$NP{\leftarrow}S{\rightarrow}S{\rightarrow}T$, $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}T$, $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}T\}$. (Surdeanu et al., 2007).

3.4.2 Path Statistics

These features also try to reduce the sparsity of the path features, but instead of subsequences of the path feature, these features extract simple statistics about the path.

 # Path Clauses: Number of S* nodes in the path. Includes counts for full path, up path, and down path. Example value: Full=2, Up=1, Down=2. (Surdeanu et al., 2007).

 # Path VPs: Same as previous, but for VP*. Example value: Full=3, Up=0, Down=3. (Surdeanu et al., 2007).

Subsumption: Depth in tree of v minus depth in tree of c. Example value: 6 (depth of "eat") - 2 (depth of "Tom") = 4. (Surdeanu et al., 2007).

3.4.3 Verb Sub-categorization

As we saw in the previous section, the sub-categorization of the verb is an important syntactic feature. These features are all variants of the basic sub-categorization feature. All but **NP Subcat** add additional information to the sub-categorization,

while **NP Subcat** is designed to reduce the sparsity of the sub-categorization feature. For these features, our running example is the feature value extracted for the verb phrase "give the ball to him" when classifying the constituent "the ball" (the basic subcategorization feature in this case is $VP{\rightarrow}T\ NP\ PP$).

Lex-PP Subcat: Same as basic sub-categorization but with expanded PP categories. Example value: $VP{\rightarrow}T\ NP\ PP(to)$. New.

NP Subcat: Same as sub-categorization, but only includes NP siblings of v. Thus, this feature counts the number of NP siblings of v, plus it captures the category of parent of v. Example value: $VP{\rightarrow}T\ NP$. New.

Target Sibling: If c is a descendant of the verb phrase headed by v, the category (with PP augmentation) of the sibling of v from which c is descended. Otherwise, this feature is empty. Additionally, this category is numbered with the number of previous siblings with the same category. E.g., if c is descended from the second NP sibling of v, this feature is "NP2." Example value: $NP1$. New.

Subcat + Target Sibling: Lex-PP Subcat concatenated with Target Sibling. Example value: $VP{\rightarrow}T$ **NP** $PP(to)$. (Xue & Palmer, 2004).

3.4.4 Path Modification

Many of the new features we propose fall in this category. Each of these features modifies the original path feature, usually in order to add additional information about a specific grammatical construct. For example, the **SBAR-Mod-NP** feature gives more information about relative clauses. For these features, we include both the basic path feature and the modified version of the path feature in order to avoid excessively increasing the sparsity of the path features.

Sentence Category: If constituent c has category S, then we add NP to the category of c if c has a child with category NP; otherwise we add the first non-VP category among children of c. If there are no such children, nothing is added. Toutanova et al. (2008) proposed a binary Missing Subject feature which captures some of the same information as this feature. This feature is useful for (at least) infinitival clauses and

relative clauses. Example value: $NP{\leftarrow}S(NP){\rightarrow}VP{\rightarrow}S(){\rightarrow}VP{\rightarrow}VP{\rightarrow}T$. New.

Passive Info: If c has category VP and is passive (main verb is VBN or VBD, final helper verb is "be" or "get"), then add "-Pass" to category. In the sentence "The apple was eaten," the path from "the apple" to "eat" changes from $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}VP{\rightarrow}T$ to $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}VP\text{-}Pass{\rightarrow}T$. New.

VP-Mod-NP: If c has category VP and modifies an NP (e.g., "the boy kicking the can," "the can kicked by the boy"), add the tense of the head verb of c (either present (VBG) or past (VBN/VBD)) to the category of c. In "the boy kicking the can," the path from "the boy" to "kicking" changes from $NP{\leftarrow}NP{\rightarrow}VP{\rightarrow}T$ to $NP{\leftarrow}NP{\rightarrow}VP(Present){\rightarrow}T$. New.

SBAR-Mod-NP: If c has category SBAR and modifies an NP (e.g., "the boy whose can I kicked"), add the category of the WH-phrase at the beginning of c, plus the head word if the category is WHPP or if the head word is "whose". For example, in "the boy whose can I kicked," the path from "the boy" to "kicked" changes from $NP{\leftarrow}NP{\rightarrow}SBAR{\rightarrow}S{\rightarrow}VP{\rightarrow}T$ to $NP{\leftarrow}NP{\rightarrow}SBAR(WHNP\text{-}whose){\rightarrow}S{\rightarrow}VP{\rightarrow}T$. New.

S-TO: If c has category S and has main verb phrase with infinitival TO, add "-to". Example value: $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}S\text{-}to{\rightarrow}VP{\rightarrow}VP{\rightarrow}T$. New.

Squish VPs: If several VP categories appear consecutively in the path, replace them with a single VP. The category of a is never considered as part of such a path. Thus, we do not compress NP←VP→VP→T. This modification reduces data sparsity by combining paths that differ based on coordinations and number of helper verbs. Example value: $NP{\leftarrow}S{\rightarrow}VP{\rightarrow}S{\rightarrow}VP{\rightarrow}T$. Related to feature proposed by Pradhan et al. (2005).

3.4.5 Miscellaneous

Head Word + Path: Concatenation of head word and path. Generally, we expect the head word and path features to be independent. This feature will be helpful only if it turns out that they are not. Example value: $NP(Tom){\leftarrow}S{\rightarrow}VP{\rightarrow}S{\rightarrow}VP{\rightarrow}VP{\rightarrow}T$.

New.

Governing Category: If c has category NP, the category of the lowest ancestor of c that has category either S or VP. This feature tries to capture whether an NP is either a subject or an object of a verb. Example value: S. (Gildea & Jurafsky, 2002).

Surface Distance: For each of tokens, verbs, commas, and coordinations, counts the number of matches between c and v in the original (unparsed) sentence s. These features are very different in nature from all the other syntactic features, because they operate on the base sentence rather than the parse. Example value: Tokens=2, Verbs=1, Commas=0, Coordinations=0. (Surdeanu et al., 2007).

Starts With Particle: Based on the gold TreeBank parses, we compute for each frame the set of particles that occur with tag RP* immediately following the verb in the training set (e.g., "take off", "take up", etc.) This feature is on if c begins with a word that occurred in this way with the target verb v (whether or not that word was parsed as an RP*). (Surdeanu et al., 2007).

Position: Two Boolean features, BeforePredicate and AfterPredicate. BeforePredicate is on if c occurs before v in s. Example value: BeforePredicate=true, AfterPredicate=false. (Gildea & Jurafsky, 2002).

Passive: On if v is passive. Example value: false. (Gildea & Jurafsky, 2002).

Passive Position : Two boolean features, BeforePassivePredicate and AfterPassivePredicate. BeforePassivePredicate is on if both BeforePredicate and Passive are on. Example value: BeforePassivePredicate=false, AfterPassivePredicate=false. (Xue & Palmer, 2004).

3.5 Results and Discussion

Table 3.4 shows results for adding each feature separately to the baseline system. For almost all feature types, the results for training and development are consistent. The path modification features are by far the most successful, particularly Passive Info and Sentence Category. Of the eight features which improve over baseline on the

Feature Set	Train F1	Devel F1	Combo #
Baseline	82.1	74.5	
Up Path	+0.2	+0.1	2
Down Path	+0.2	+0.0	2
Gen Up Path	+0.1	+0.0	3
Gen Down Path	+0.1	+0.1	3
# Path Clauses	+0.0	−0.1	3
# Path VPs	+0.0	+0.1	3
Subsumption	+0.1	+0.0	3
Lex-PP Subcat	+0.2	+0.0	2
NP Subcat	+0.1	+0.3	3
Target Sibling	+0.2	−0.2	2
Subcat + Target Sibling	+0.5	+0.5	1
Sentence Category	+0.8	+0.3	1
Passive Info	+0.9	+1.0	1
VP-Mod-NP	+0.3	+0.1	1
SBAR-Mod-NP	+0.5	+0.1	1
S-TO	+0.2	+0.0	2
Squish VPs	+0.4	+0.2	1
Head Word + Path	+0.2	+0.2	2
Governing Category	+0.0	+0.0	3
Surface Distance	+0.3	+0.4	1
Particle	+0.0	−0.1	3
Position	+0.1	+0.0	2
Passive	+0.5	+0.6	–
Passive Position	+0.8	+0.9	2
Combo 1	+2.4	+2.0	
Combo 2	+2.7	+2.2	
Combo 3	+2.7	+2.2	

Table 3.4: Results (F1-only) on train and devel. All feature sets consist of baseline plus one additional feature type, except for the Combos. Results are shown as improvements over baseline; each row is independent (Combo 2 is 0.3 better than Combo 1, not 2.7 better). Each feature lists the lowest number Combo model in which it is included; all features in Combo 1 are included in Combo 2, and all features in Combo 2 are included in Combo 3.

Feature Set	Train F1	Devel F1
Combo 1	84.5	76.5
- (Subcat + Target Sibling)	84.2	76.3
- Sentence Category	84.2	76.3
- Passive Info	83.9	75.9
- VP-Mod-NP	84.3	76.3
- SBAR-Mod-NP	84.5	76.4
- Squish VPs	84.3	76.5
- Surface Distance	84.4	76.3

Table 3.5: Results of removing features one at a time from Combo 1

training set by at least 0.3, five are in this group. Of these five, four are new; and two of these (SBAR-Mod-NP and VP-Mod-NP) capture information that has not been used by any previous system. The other three features which improve by at least this much were Subcat + Target Sibling, Surface Distance, and Passive Position. The sub-path and path statistic features do not perform well; none improve over baseline by more than 0.2.

Based on these results, we consider three combination models. **Combo 1** includes the baseline features plus all features that improve over baseline on the training set by at least 0.3: Subcat + Target Sibling, Sentence Category, Passive Info, VP-Mod-NP, SBAR-Mod-NP, Squish VPs, and Surface Distance.[3] **Combo 2** includes all features from Combo 1, plus Position and Passive Position, plus all features that improve over baseline by at least 0.2: Up Path, Down Path, Lex-PP Subcat, Target Sibling, S-TO, and HeadWord + Path. **Combo 3** contains all features from Combo 2, plus all remaining (non-redundant) features: Gen Up Path, Gen Down Path, # Path Clauses, # Path VPs, Subsumption, NP Subcat, Governing Category, and Particle. Results for these models are also shown in Table 3.4. Combo 1 improves substantially over the baseline model and over the best single addition (Baseline + Passive Info). Combo 2 improves a bit over Combo 1 on both the training and development set, suggesting that the added features do contribute something extra. Finally, Combo 3 does not

[3]We found that Passive Info and Passive Position are essentially redundant; we chose the better of the two.

System	WSJ	Brown	Comb
Baseline	76.9	64.7	75.3
Baseline + PassPos	77.7	65.3	76.1
Combo 1	78.9	66.9	77.3
Combo 2	79.2	66.2	77.5
Punyakanok	79.4	67.8	77.9
Toutanova Local	78.0	65.6	∼76.3
Toutanova Joint	79.7	67.8	∼78.1
Toutanova Joint Top 5	80.3	68.8	∼78.8
Surdeanu M2	77.2	67.7	76.0
Surdeanu M3	76.5	65.4	75.0
Surdeanu Combined	80.6	70.1	79.2

Table 3.6: F1 test scores. Combined F1 for Toutanova et al. (2008) not available; we estimate using a weighted average.

improve over Combo 2, which is not surprising considering that these features made small or no difference even when added individually.

To check whether all seven of the additional features used in Combo 1 contributed to the performance of the final system, we removed each of these features independently from Combo 1. Results are shown in Table 3.5. For most of the features removing the feature leads to a noticeable drop in performance. The main exception is SBAR-Mod-NP: removing it barely affects performance, even though it gives a significant increase when added to the basic feature set and does not obviously intersect with any of the other features. It could be that Sentence Category, which (among other things) indicates whether a relative clause has a subject, is providing some of the same information that the SBAR-Mod-NP provides.

3.6 Comparison to State-of-the-art SRL Systems

Table 3.6 shows test results for four different feature sets: Baseline, Baseline + Passive Position, Combo 1, and Combo 2. We include Baseline+PassPos because the Passive Position feature is used by most high-performance SRL systems. The performance of Baseline+PassPos is already quite good; in the CoNLL 2005 evaluation, it would

System	WSJ	Brown	Comb
Combo 2	79.2	66.2	77.5
Combo 2 (reranked parses)	80.3	68.0	78.7
Punyakanok	79.4	67.8	77.9
Toutanova joint top 5	80.3	68.8	∼78.8
Surdeanu Combined	80.6	70.1	79.2

Table 3.7: Results using reranked parses

have placed at about the 75^{th} percentile among evaluated systems. We also compare to the three systems (Punyakanok et al., 2005; Toutanova et al., 2008; Surdeanu et al., 2007) discussed in the previous section. For Toutanova et al. (2008), we report results for three different models: Local, Joint, and Joint Top 5. Local is their local classification model: it classifies each constituent independently and uses only the top Charniak parse. Joint adds their reranking model, and Joint Top 5 combines information from the five best Charniak parses. For Surdeanu et al. (2007), we show results for M2, M3, and the final combined model.

To our knowledge, Combo 2 achieves the best reported results among systems that (1) use only a single Charniak parse, and (2) classify each constituent independently. The local model of Toutanova et al. (2008) is the best previous system subject to these restrictions. This is presumably due to our detailed feature selection and our new features. Among systems which use only a single Charniak parse, only the joint model of Toutanova et al. (2008) outperforms Combo 2.

As a straightforward way of incorporating additional parse information, we also ran our system using the 2006 version of the Charniak reranking parser (Charniak & Johnson, 2005).[4] This parser builds a list of the 50-best parses and reranks these parses based on additional features of each parse. Thus, it is similar to the method used by Toutanova et al. (2008) for using multiple parses (although the features are obviously different). We simply used the top parse returned after reranking as input to our system. Table 3.7 shows the results of Combo 2 applied to these parses, compared to the best results for each of the three other systems. The use of the reranked parses

[4]Available at `ftp://ftp.cs.brown.edu/pub/nlparser/reranking-parserAug06.tar.gz`

significantly improves our system, surpassing Punyakanok et al. (2005) and (almost) matching Toutanova et al. (2008). Further improvements could likely be achieved by using the self-trained parser described in McClosky et al. (2006).

Most likely, we could further improve our system by incorporating the ideas used in these three systems (voting method of Punyakanok et al. (2005) for combining multiple parses, joint modeling, and system combination). What the experimental evaluation presented here shows is that our system (which includes both previously suggested and new features) obtains the best performance when comparing purely on local features. When using reranked parses, our system achieves performance comparable to the best reported results on this task, while being comparatively easy to implement (off-the-shelf parser and straight-forward learning/inference).

Chapter 4

Canonicalization for Semantic Role Labeling

4.1 Introduction

A major problem with the standard approach to SRL is that the path feature can be quite complicated. In the sentence "He expected to receive a prize for winning," the path from "win" to its ARG0, "he", involves the verbs "expect" and "receive" and the preposition "for". The corresponding path through the parse tree likely occurs a relatively small number of times (or not at all) in the training corpus. If the test set contained exactly the same sentence but with "expected" replaced by "did not expect", we would extract a different parse path feature; therefore, as far as the classifier is concerned, the syntax of the two sentences is totally unrelated. Many verbs occur a small number of times in the training set, making the sparsity problem even worse.

In Chapter 3, we experimented with several modifications to the path features designed to help reduce sparsity. These included sub-path and path statistic features, as well as the Squish VPs path modification feature. Of these, only the Squish VPs feature gave a significant boost in performance, and this feature only handled one specific source of sparsity related to inserting helper verbs.

Verb	Deep Subject	Deep Objects
wants	Tom	to eat an apple
eat	Tom	an apple

Figure 4.1: Canonical forms for all verbs in "Tom wants to eat an apple."

In this chapter, we propose a new approach based on *canonical forms*. The canonical form for a sentence s and target verb v consists of two parts, either of which may or may not be present: a deep subject, and a (possibly empty) ordered list of deep objects. In cases where v has a syntactic subject, the deep subject is identical to the syntactic subject. However, the deep subject is also defined in many cases when the syntactic subject is missing. For example, in "Tom wants to eat an apple," "eat" is missing a syntactic subject but has deep subject "Tom." Deep objects have a similar relationship to syntactic objects. Figure 4.1 shows the canonical forms for all verbs in "Tom wants to eat an apple."

Suppose we are given a *canonicalization system*, a system that can extract the canonical form for a given sentence s and target verb v. Our main idea is to perform SRL on the canonical form, rather than on the original input sentence. The advantage of this is that (by design) canonical forms remove (most of) the syntactic variability of the original sentence.[1] Thus, it is much easier to generalize between different examples. For example, if we have only seen a particular verb in active form in the training set, we may have difficulty when we see it in passive form in the test set. However, the canonical form represents passive and active sentences in the same way, so we will be more likely to be able to correctly label the passive sentence in the test set.

In this chapter, we first define canonical form more precisely and discuss its relationship to previous work, mainly in linguistics. Second, we describe how we build a

[1] An example of variability which is not removed by our system is "He gave him the ball" vs. "He gave the ball to him".

canonicalization system. Our system makes use both of hand-coded linguistic knowledge and machine learning. It is also able to correctly model the recursive structure of natural language. Third, we describe our canonical form SRL system. Fourth, we describe how to train both the canonicalization and canonical-form SRL systems. Since we do not have labeled data for the canonicalization system, we treat the correct canonical form as a hidden variable, which allows us to train both systems using only labeled SRL data. Finally, we evaluate our system on the CoNLL 2005 shared task, showing that it performs competitively with standard SRL systems. As expected, our system performs particularly well for verbs with a small amount of training data.

4.2 Canonical Forms

In the previous section, we informally defined a canonical form as containing a deep subject and an ordered list of deep objects (either of which could be missing). We have also implied that given a sentence s and a target verb v, there is a unique correct canonical form. In this section, we will formalize the definition of correct canonical form and give further examples of canonical forms.

Given s and v, the correct canonical form is the canonical form such that the deep subject and all the deep objects are direct arguments of v. This is a simple notion intuitively, but there are several issues which make it complicated in practice.

The basic idea of our approach is to define the correct canonical form based on the semantic roles labeled in our data for the target verb v. Thus, the deep subject and deep objects should all be labeled as arguments of v.

This still leaves open the question of which argument should be the deep subject. We will *not* provide an exact criterion for determining the correct deep subject; instead, we give an intuitive definition that covers nearly every case. The deep subject is the argument of v which would be placed before the verb if we were to write a sentence in which v was the main verb of the sentence. Typically, the deep subject appears before v in the s, while the deep objects appear after v. Passive sentences are an obvious but easily handled exception. As we will see, the lack of precise definition

of the correct canonical form is not actually an issue for our system. However, if we were to attempt to label gold-standard canonical forms, there would probably be some rare cases that would need to be addressed.

There is one common situation where we wish to include a non-role constituent (at least according to PropBank) in our canonical form. This is in the case of "it" as in "It rained," and the existential "there" in "There was rain." In some sense these words have no semantic content, so it is a somewhat arbitrary decision to label or not label them. Our goal was to make the canonical form as "readable" as possible, so we chose to include these two special cases in the canonical form.

4.2.1 Related Formalisms

One area of current research which has similarities with this work is Lexical-Functional Grammars (LFGs) (Kaplan & Bresnan, 1982) (e.g., the XLE system[2]). LFGs and our approach both attempt to abstract away from the surface level syntax of the sentence. The relationship between the c-structure (syntactic structure, i.e., syntactic parse) and the f-structure (grammatical function) in an LFG is similar to the relationship between a sentence (or phrase) and the canonical form of that sentence, in that both attempt to abstract away the particular syntactic instantiation present in the sentence. The most obvious difference in our approach is that we use SRL data to train our system, avoiding the need to have labeled data specific to our method.

Combinatory Categorial Grammars (CCGs) also build a representation abstracted from the syntax of the sentence. In this method, a strong type system is introduced which maps syntactic elements into typed functions. The semantic representation of the sentence is built by recursively applying the functional representations of each node in the parse. Similar to our method, a CCG parser analyzes a sentence recursively, piece by piece. Following our work, Boxwell et al. (2009) implemented an SRL system using features generated from a CCG parser. Our system significantly outperforms their system on the CoNLL 2005 shared task (they report overall

[2] `http://www2.parc.com/isl/groups/nltt/xle/`

F1 measure of 73.5% when using automatic parses). This could be partly because we rely more heavily on the high-quality parses generated by the Charniak parser, while their transformation-based features are extracted from a separated CCG parser. Additionally, our "parsing" system, based on tree transformations, clearly differs in many aspects from the approach taken by CCG.

Lexicalized Tree-Adjoining Grammars (LTAGs) also implicitly maintain a kind of underlying representation. LTAGs have two types of syntactic operations: substitution (which is essentially the same as the substitution rule in a context-free grammar) and adjunction. Adjunction allows a tree to be inserted in the middle of another tree. For example, the sentence "I go," by using the adjunction rule with the phrase "want to," can generate the sentence "I want to go." The LTAG parse of this sentence will include the "simplified" sentence "I go," which can be used as an abstracted representation of the arguments of "go." Recently, Liu et al. (2010) built a system based on an LTAG parser which has several similarities with our work. Their system treats the correct LTAG derivation as a hidden variable and then learns a model based on maximizing performance on SRL data. As in our system, they take the top Charniak parse as given and learn a model based on this parse. They report very impressive results on the CoNLL 2005 task, achieving an overall F1 of 89.59, 9 F1 points higher than the next best system.

In terms of the specific algorithms in our system, some work has been done on packed representations. Maxwell III & Kaplan (1995) propose a packed representation similar to the data structure presented in Section 4.7, while Geman & Johnson (2002) present an inference algorithm which operates on this type of data structure. However, to our knowledge, the algorithm we present for constructing our packed representation (described in Section 4.7) has not been explored in previous work.

Another group of related work outside of SRL focuses on summarizing sentences through a series of deletions (Jing, 2000; Dorr et al., 2003; Galley & McKeown, 2007). In particular, the latter two works iteratively simplify the sentence by deleting a phrase at a time. Our approach differs from these works in several important ways. First, our transformation language is not context-free; it can reorder constituents and

then apply transformation rules to the reordered sentence. Second, we are focusing on a somewhat different task; these works are interested in obtaining a single summary of each sentence which maintains all "essential" information, while we produce a canonical form that may lose semantic content but aims to contain all arguments of a verb. Finally, training our model on SRL data allows us to avoid the relative scarcity of parallel simplification corpora and the issue of determining what is "essential" in a sentence.

Another related area of work within the SRL literature is that on tree kernels (Moschitti, 2004; Zhang et al., 2007). Like our method, tree kernels decompose the parse path into smaller pieces for classification. Our model can generalize better across verbs because it first generates canonical forms, then classifies the resulting canonical forms. Also, through iterative simplifications we can discover structure that is not immediately apparent in the original parse.

Johnson (2002) and Levy & Manning (2004) present algorithms for finding non-local dependencies given a parse tree. These methods are similar to our system in that a significant portion of the work our system does is resolving these kinds of long-range dependencies in order to generate canonical forms. The most significant difference in our work is that we incorporate this idea into a semantic role labeling system, where we are able to gain from increased generalization due to resolving these dependencies. Additionally, in order to normalize syntax as much as possible, our system handles syntactic structures not covered by these systems. For example, rewriting passive sentences as active sentences is not an example of resolving non-local dependencies, but it is an important step in generating a canonical form. An interesting area for future work is incorporating the detailed analyses in these works into a transformation-based SRL system.

4.3 Canonicalization System

In this section we describe the system we built to automatically extract canonical forms from sentences.

4.3.1 System Overview

The basic building blocks of our system are *transformation rules*. Roughly speaking, each transformation rule handles one specific kind of syntactic construct. The transformation rule can only be applied to sentences containing that construct. When applied, the rule rewrites the sentence so that it no longer uses that construct. For example, one of our rules converts a passive sentence into an active sentence. This rule, when applied to the passive sentence "I was given a chance," outputs the transformed sentence "*Someone* gave me a chance." (*Someone* is a placeholder that indicates that the subject of the active sentence is missing).

For our system to work well, we need a set of rules which covers as many common syntactic patterns as possible. One approach would be to try to automatically extract these rules from text. However, as already mentioned, we do not have data labeled with canonical forms, much less data labeled with a step-by-step series of transformations. We could try to automatically infer rules from labeled SRL data, but this approach is very difficult, requiring a search over a vast space of possible rules.

Instead, we chose to hand-construct a rule set that encodes a large amount of human-level linguistic knowledge. The rule set was built through iterative development on (training) data. Rules were added one-by-one or in groups until the rule set was capable of generating, for most ($> 95\%$) of the sentences in the training set, a canonical form containing all labeled arguments of each target verb.[3]

While hand-coding rules is an effective way to inject knowledge into the system, we also need a strategy for choosing which rules to use. A simple deterministic approach is unlikely to work well, because for many sentences, there are many possible rules which can be applied. For example, in the sentence "I wanted the chicken to eat," one rule puts "I" as the subject of "eat," while another puts "chicken" as the subject as "eat." For this reason, we took a machine learning approach to deciding how to apply the rules, which determines which rule to use based on features of the sentence

[3]Note that such a canonical form is not necessarily the correct canonical form, because it might contain non-argument constituents. However, we considered these canonical forms "good enough" as far as the SRL system was concerned.

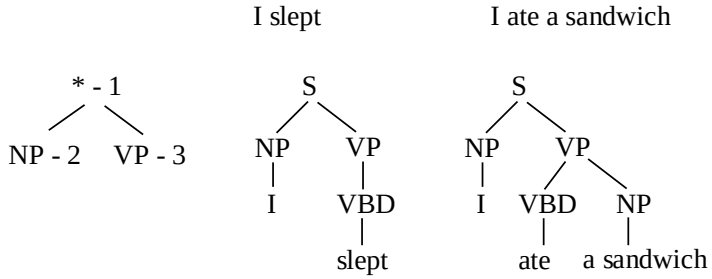


Figure 4.2: Example tree pattern and matching constituents

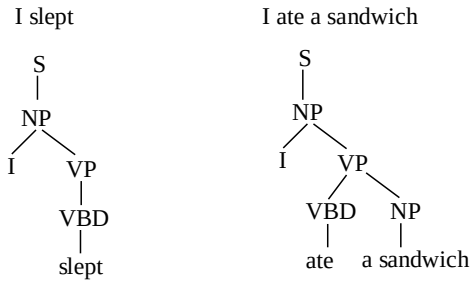


Figure 4.3: Result of applying add-child-end(3,2) in Figure 4.2. Note that the tree pattern in Figure 4.2 specifies that in each sentence, the label 3 refers to the matched VP, while the label 2 refers to the matched NP. Thus, add-child-end(3,2) moves the matched VP to be the final child of the matched NP.

and target verb.

4.3.2 Transformation Rules

A transformation rule consists of two parts: a *tree pattern* and a series of *transformation operations*. It takes as input a parse tree, and outputs a new, transformed parse tree. The tree pattern determines whether the rule can be applied to a particular parse and also identifies what part of the parse should be transformed. The transformation operations actually modify the parse. Each operation specifies a simple modification of the parse tree.

A tree pattern is a tree fragment with constraints on each node. For example,

Figure 4.2 is a tree pattern that matches any constituent in the parse tree which has an NP and a VP as children. Alongside is pictured two constituents which match this pattern. The tree pattern also assigns numerical labels to each of the matched nodes, which are used by the transformation operations as described below.

Formally, a tree pattern node X *matches* a parse-tree node A if: (1) All constraints of node X (e.g., constituent category, head word, etc.) are satisfied by node A. (2) For each child node Y of X, there is a child B of A that matches Y; two children of X cannot be matched to the same child B. (3) All constraints between children are satisfied — for example, the pattern could require that child B comes before child C in the parse. There are no other requirements. A can have other children besides those matched, and leaves of the rule pattern can match to internal nodes of the parse (corresponding to entire phrases in the original sentence). For example, the same rule can be used to transform both "Tom wanted to eat" and "Tom wanted to eat a sandwich" (into "Tom ate" and "Tom ate a sandwich"). The insertion of the phrase "a sandwich" does not prevent the rule from being applied.

A transformation operation is a simple step that is applied to the nodes matched by the tree pattern. For example, the "add-child-end" transformation operation applied to the pair of nodes (X,Y) removes X from its current parent and adds it as the final child of Y. Figure 4.3 shows an example of applying this operation to the parses in Figure 4.2.

Figure 4.4 shows a complete transformation rule that depassivizes a sentence, as well as the result of applying it to the sentence "I was given a chance." The transformation steps are applied sequentially from top to bottom. Any nodes not matched are unaffected by the transformation; they remain where they are relative to their parents. For example, "chance" is not matched by the rule and thus remains as a child of the VP headed by "give."

Note that a single transformation operation may not correspond to a linguistically sensible transformation of the parse tree. However, the transformation rules were designed so that the entire sequence of transformation operations for a particular rule should correspond to a sensible transformation of the input parse. Thus, the

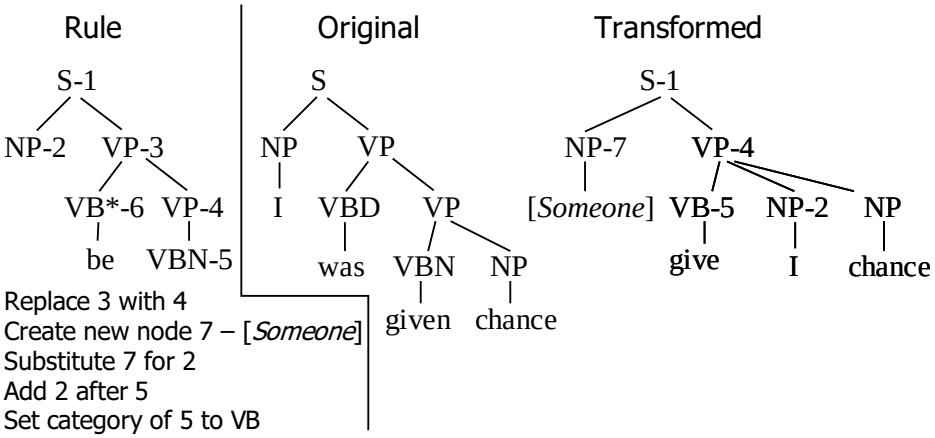


Figure 4.4: Rule for depassivizing a sentence

intermediate steps during the application of the transformation operations may not be syntactically well-formed, but the final output parse should be (assuming the transformation rule is well-designed).

4.3.3 Rule Set

Altogether, we currently have 154 (mostly unlexicalized) rules. Our general approach was to write very conservative rules, i.e., avoid making rules with low precision. We did this mainly because low-precision rules can quickly lead to a large blow-up in the number of ways to generate a canonical form from a given input sentence/target verb pair. Table 4.1 shows a summary of our rule-set, grouped by type. Note that each row lists only one possible sentence and simplification rule from that category; many of the categories handle a variety of syntax patterns. The two examples without target verbs are helper transformations; in more complex sentences, they can enable further simplifications. Another thing to note is that we use the terms Raising/Control (RC) very loosely to mean situations where the subject of the target verb is displaced, appearing as the subject of another verb.

There are two significant pieces of "machinery" in our current rule set. The first is the idea of a *floating node*, used for locating an argument within a subordinate clause.

Rule Category	#	Original	Simplified
Sentence normalization	24	Thursday, I slept.	I slept Thursday.
Sentence extraction	4	I said he slept.	He slept.
Passive	5	I was hit by a car.	A car hit me.
Misc Collapsing/Rewriting	20	John, a lawyer, …	John is a lawyer.
Conjunctions	8	I ate and slept.	I ate.
Verb Collapsing/Rewriting	14	I must eat.	I eat.
Verb Raising/Control (basic)	17	I want to eat.	I eat.
Verb RC (ADJP/ADVP)	6	I am likely to eat.	I eat.
Verb RC (Noun)	7	I have a chance to eat.	I eat.
Modified nouns	8	The food I ate …	Float(The food) I ate.
Floating nodes	5	Float(The food) I ate.	I ate the food.
Inverted sentences	7	Nor will I eat.	I will eat.
Questions	7	Will I eat?	I will eat.
Possessive	7	John's chance to eat…	John has a chance to eat.
Verb acting as PP/NP	7	Including tax, the total…	The total includes tax.
"Make" rewrites	8	Salt makes food tasty.	Food is tasty.

Table 4.1: Rule categories with sample simplifications. Target verbs are underlined.

For example, in the phrases "The cat that ate the mouse", "The seed that the mouse ate", and "The person we gave the gift to", the modified nouns ("cat", "seed", and "person", respectively) all should be placed in different positions in the subordinate clauses (subject, direct object, and object of "to") to produce the phrases "The cat ate the mouse", "The mouse ate the seed", and "We gave the gift to the person". We handle these phrases by placing a floating node in the subordinate clause which points to the argument; other rules try to place the floating node into each possible position in the sentence.

The second construct is a system for keeping track of whether a sentence has a subject, and if so, what it is. A subset of our rule set normalizes the input sentence by moving modifiers after the verb, leaving either a single phrase (the subject) or nothing before the verb. For example, "Before leaving, I ate a sandwich" is rewritten as "I ate a sandwich before leaving". In many cases, keeping track of the presence or absence of a subject greatly reduces the set of applicable transformation rules.

For example, when placing floating nodes as described above, if a subject has been identified in the subordinate clause (e.g., in "the mouse the cat ate", the subordinate clause "the cat ate" has a subject, "the cat"), the floating node cannot be placed in the subject position. Note that in some cases, the presence and identity of a subject is ambiguous; our canonicalization system will generate each candidate normalization of the sentence and will (hopefully) learn to choose the correct normalization.

As mentioned above, our rule set was developed by analyzing performance and coverage on the PropBank WSJ training set. Neither the development set nor (of course) the test set were used during rule creation.

4.3.4 Sequences of Rules

A single transformation rule handles a single syntactic construct. In many sentences, there are many different syntactic structures, often nested in a recursive fashion. To handle this, we can simply apply a sequence of rule transformations, one at a time. Assuming our rule set is written well, the output of each transformation rule should

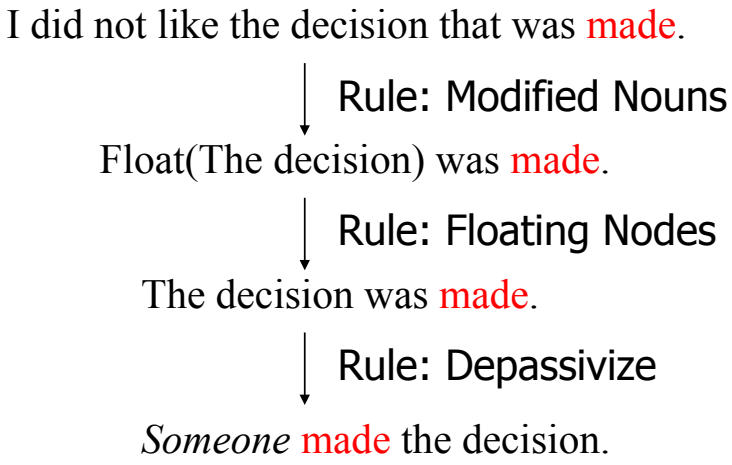


Figure 4.5: Iterative transformation rule application

be a syntactically valid parse, and so other transformation rules should in turn be applicable to the resulting parse. Figure 4.5 shows a series of rules applied to the sentence "I did not like the decision that was made," with target verb "made."

We followed an important design principle related to sequences of rules when designing our rule set: we tried to maximize reuse of each transformation rule as much as possible. For example, one of our rules transforms "Bob has a chance to eat," into "Bob eats." Consider the sentence "Bob's chance to eat has passed." One option would be to write a separate, similar rule that applies to the "X's Y to Z" construction instead of the "X has a Y to Z" construction. Instead, we wrote a new rule which rewrites *any* possessive sentence using the verb "have." This rule transforms "Bob's chance to eat has passed," into "Bob has a chance to eat." We can now apply the earlier rule to this new transformed sentence. By breaking complex transformations down into smaller building blocks, we increase the number of training examples for each transformation rule, allowing us to better learn when to use them.

Another issue worth mentioning at this point is that many of the steps do lose some semantic information. Clearly, having a chance to eat is not the same as eating. However, since our goal is to label the arguments of the verb (which in this case is simply the Eater, "I"), it is not important to maintain this information. Furthermore,

it is possible to modify the rule set to maintain this kind of information. For example, we could attach annotations to each node in the parse which keep track of information removed by previous transformation steps.

We consider a series of rules to be "finished" when it produces a parse satisfying the following constraints:

i. The root node X has category S

ii. X has a child Y with category VP

iii. X has exactly one child Z (the subject) occurring before Y. Z may be empty as described above.

iv. The main verb of the VP constituent rooted at Y is the target verb v.

We can construct a canonical from this parse in the obvious way: Z becomes the deep subject of the canonical form, and all children of Y besides v become the deep objects.

4.4 Producing Canonical Forms

For many sentence/target verb pairs (s,v), there are many possible canonical forms that can be generated using our rule set. We now describe how to efficiently generate the set of all possible candidate canonical forms for (s,v). At a high level, the algorithm is very simple. We maintain a set of derived parses S which is initialized to contain only the original, untransformed parse. One iteration of the algorithm consists of applying every possible matching transformation rule to every parse in S, and adding all resulting parses to S. With carefully designed rules, repeated iterations are guaranteed to converge; that is, we eventually arrive at a set $\hat{S}$ such that if we apply an iteration of rule application to $\hat{S}$, no new parses will be added. Note that this process does not refer to the target verb v, which means that we only need to do it once per sentence. To find canonical forms for v, we simply look through $\hat{S}$ for parses satisfying the conditions from the previous section.

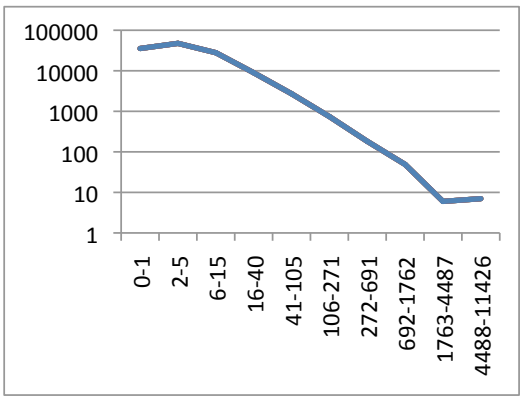


Figure 4.6: Number of (s,v) pairs (Y-axis) vs. number of canonical form/rule set pairs (buckets on X-axis)

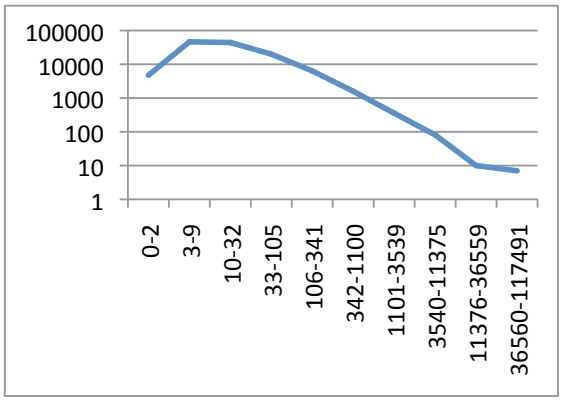


Figure 4.7: Number of (s,v) pairs (Y-axis) vs. number of canonical form/rule set/labeling triples (buckets on X-axis)

This generation procedure is conceptually simple but computationally quite expensive. Implemented naively, we would need to copy the entire parse tree at each step, and in general, this procedure could generate an exponential number of transformed parses. The first issue can be solved, and the second alleviated, using a dynamic-programming data structure similar to the one used to store parse forests (as in a chart parser). This data structure is not essential for exposition; we delay discussion until Section 4.7. Even given this compact storage, the data structure can become exponential; in practice, however, the size of the compact representation is sometimes large but manageable (statistics presented below).

Our system keeps track of the set of rules used to generate a canonical form, but not the order in which the rules were applied. If two rules affect a different part of the parse, they can be reordered arbitrarily; for this reason, in most cases, keeping track of rule application order is neither important nor feasible. Similarly, it often happens that one rule transforms a part of the parse which is discarded by a later transformation. For this reason, we maintain only minimal subsets of rules which generate a particular canonical form.

Subject to the rule set collapsing described in the previous paragraph, on the PropBank training set, the largest number of canonical form/rule set pairs generated for

a particular sentence/target verb pair was just under 5000. Figure 4.6 shows a histogram of number of canonical form/rule pairs across all sentence/target verb pairs. Note that both axes are on a log scale.

4.5 Labeling Canonical Forms

For a particular sentence/target verb pair (s, v), the output from the previous section is a set $C^{sv} = \{c_i^{sv}\}_i$ of possible canonical forms. Although labeling a canonical form is easier than labeling the original sentence, there are still many choices to be made. Additionally, the labeling task is complicated by the fact that for some sentences, there are no correct canonical forms. This happens primarily because of errors in the automatic parser, which can cause arguments to be missing from the canonical form and non-arguments to erroneously appear in the canonical form.

On the training set, we now extract a set of *role patterns* $G^v = \{g_j^v\}_j$ for each verb v. For example, the role pattern for "give" in "I gave him a sandwich" is $g_1^{give} = \{ARG0 = Subject\ NP,\ ARG1 = Object\ NP2,\ ARG2 = Object\ NP1\}$. Note that this is one atomic pattern; thus, we are keeping track not just of occurrences of particular roles in particular places in the simple sentence, but also how those roles co-occur with other roles.

For a particular simple sentence c_i^{sv}, we apply all extracted role patterns g_j^v to c_i^{sv}, obtaining a set of possible role labelings. We call a canonical form/role labeling pair a *labeled canonical form* and denote the set of candidate labeled canonical forms $L^{sv} = \{l_k^{sv}\}_k$. Note that a given pair c_i^{sv}, g_j^v may generate more than one labeled canonical form, if there is more than one way to assign the elements of g_j^v to constituents in c_i^{sv}. Also, for a sentence s there may be several labeled canonical forms that have the same assignment of roles to constituents. In particular, there may be several labeled canonical forms that assign the correct labels to all constituents; we denote this set $K^{sv} \subseteq L^{sv}$.

As mentioned earlier, we do not have access to the correct canonical forms (or the sequence of rules which generates it). Instead, we use the set K^{sv} as our notion of

correctness. This will allow us to train our model using only labeled semantic role data. Note that K^{sv} does *not* exclude canonical forms that include constituents that were not labeled as arguments.

On the PropBank training set, the number of canonical form/rule set/labeling triples generated for a particular sentence/target verb pair ranged from 1 to 120,000. The median number of triples was 13, so the majority of sentences are not expensive computationally. Figure 4.7 shows a histogram of number canonical form/rule set/labeling triples across all sentence/target verb pairs.

4.6 Probabilistic Model

We now define our probabilistic model. Given a (possibly large) set of candidate labeled canonical forms L^{sv}, we need to select a (hopefully correct) one. We assign a score to each candidate based on its features: which rules were used to obtain the canonical form, which role pattern was used, and which constituents were assigned to which roles. A log-linear model then assigns probability to each labeled canonical form equal to the normalized exponential of the score.

The first type of feature is which rules were used to obtain the canonical form. These features are indicator functions for each possible rule. Thus, we do not currently learn anything about interactions between different rules. A possible extension of this feature type includes lexicalized versions of each rule. For example, for determining control, the main verb in the sentence is important. Unfortunately, due to computational limitations, we were not able to explore this extension.

The second type of feature is an indicator function of the role pattern used to generate the labeling. This allows us to learn that "give" has a preference for the labeling $\{$*ARG0 = Subject NP, ARG1 = Postverb NP2, ARG2 = Postverb NP1*$\}$.

Our final features are analogous to those used in semantic role labeling, but greatly simplified due to our use of canonical forms: head word of the constituent; category (i.e., constituent label); and position in the canonical form. Each of these features is combined with the role assignment, so that each feature indicates a preference

Rule = Depassivize

Pattern = {ARG0 = Subj NP, ARG1 = Obj NP2, ARG2 = Obj NP1}

Role = ARG0, Head word = John
Role = ARG0, POS = NP
Role = ARG0, Position = Subj NP

Role = ARG1, Head word = sandwich
Role = ARG1, POS = NP
Role = ARG1, Position = Obj NP2

Role = ARG1, Head word = I
Role = ARG1, POS = NP
Role = ARG1, Position = Obj NP1

Figure 4.8: Features for canonical form (Subject = "John", Objects = {"me","a sandwich"}) and labeling (ARG0 = "John", ARG1 = "a sandwich", ARG2 = "I").

for a particular role assignment (i.e., for "give", head word "sandwich" tends to be ARG1). For each feature, we have a verb-specific and a verb-independent version, allowing sharing across verbs while still permitting different verbs to learn different preferences. The set of extracted features for the sentence "I was given a sandwich by John" with canonical form (Subject = "John", Objects = {"me","a sandwich"}) and labeling (ARG0 = "John",ARG1 = "a sandwich",ARG2 = "I") is shown in Figure 4.8. We omit verb-specific features to save space. Note that we "stem" all pronouns (including possessive pronouns).

For each candidate labeled canonical form l_k^{sv}, we extract a vector of features $\mathbf{f}_k^{sv}$ as described above. The probability of l_k^{sv} with respect to a weight vector $\mathbf{w}$ is defined to be $P(l_k^{sv}) = \frac{e^{\mathbf{w^T f_k^{sv}}}}{\sum_{k'} e^{\mathbf{w^T f_{k'}^{sv}}}}$.

Our goal is to maximize the total probability assigned to any $l_k^{sv} \in K^{sv}$. Therefore, for each sentence/verb pair (s, v), we want to increase $\sum_{l_k^{sv} \in K^{sv}} P(l_k^{sv})$. This expression treats the canonical form and the sequence of rules used to extract it as a hidden variable that is summed out. Taking the log, summing across all sentence/verb pairs,

and adding L2 regularization on the weights to prevent overfitting, we have our final objective $F(\mathbf{w})$:

$$\sum_{s,v} \left(\log \frac{\sum_{l_k^{sv} \in K^{sv}} e^{\mathbf{w^T f_k^{sv}}}}{\sum_{l_{k'}^{sv} \in L^{sv}} e^{\mathbf{w^T f_{k'}^{sv}}}} \right) - \frac{\mathbf{w^T w}}{2\sigma^2}$$

We train our model by optimizing the objective using standard methods, specifically L-BFGS (Liu & Nocedal, 1989). Due to the summation over the hidden variable representing the choice of canonical form, our objective is not convex. Thus, we are not guaranteed to find a global optimum. This means that initialization may affect the final results; in practice we obtained good results using the default initialization of setting all weights to 0. This may be because many sentences have only one canonical form that admits a correct role labeling and only one sequence of rules that generates this canonical form. Thus, we effectively have a large supervised set that helps to constrain the learned parameters and to guide the model in a good direction.

Consider the derivative of the likelihood component with respect to a single weight w_l:

$$\sum_{l_k^{sv} \in K^{sv}} \mathbf{f}_k^{sv}(l) \frac{P(l_k^{sv})}{\sum_{l_{k'}^{sv} \in K^{sv}} P(l_{k'}^{sv})} - \sum_{l_k^{sv} \in L^{sv}} \mathbf{f}_k^{sv}(l) P(l_k^{sv})$$

where $\mathbf{f}_k^{sv}(l)$ denotes the l^{th} component of $\mathbf{f}_k^{sv}$. This formula is positive when the expected value of the l^{th} feature is higher on the set of correct simple labelings K^{sv} than on the set of all simple labelings L^{sv}. Thus, the optimization procedure will tend to be self-reinforcing, increasing the score of correct simple labelings that already have a high score.

4.7 Simplification Data Structure

Recall that in order to generate all possible canonical forms for an input sentence s, we iteratively build a set S of transformed parses. At each step, we try applying every rule in our rule set to every parse in S. Implemented naively, this requires copying

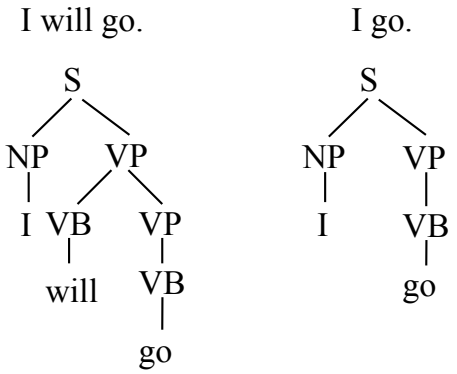


Figure 4.9: Separate parses for "I will go" and "I go"

the entire parse at each step. Furthermore, the number of possible transformed parses can be exponentially large. In this section we describe a data structure that addresses both of these computational issues.

4.7.1 Sharing Structure

Suppose we begin with "I will go" and then apply a transformation rule that removes the helper verb "will", yielding "I go". S now contains two parses, one for "I will go" and one for "I go". The simplest way to represent S is to store both parses separately, as in Figure 4.9.

However, it is clear that the two parses share a lot of structure. The root node (labeled S) and its first child subtree are the same in both parses. We can represent this shared structure through the use of a *choice node*. Figure 4.10 shows our two example sentence stored using a choice node, represented as "OR" inside a circle. We refer to a parse containing choice nodes as a *parse forest*. The set of parses represented by a particular parse forest corresponds to all possible ways of picking a choice for each choice node. Thus, in Figure 4.10, we are storing two parses, one where we choose the child constituent "will go" and one where we choose "go."

There is even more shared structure: both parses contain the constituent VP–VB–go. We can take advantage of this shared structure simply by pointing the second

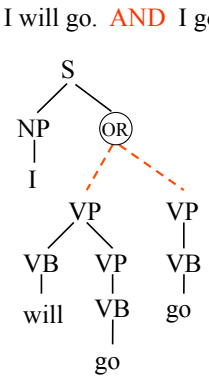


Figure 4.10: Using a choice node to share structure

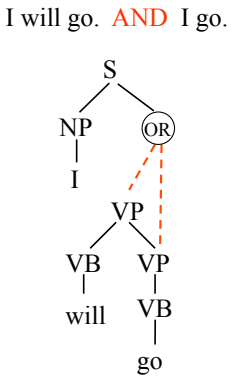


Figure 4.11: Sharing structure using a directed acyclic graph

child of the choice node at the appropriate place in the first child. The resulting data structure is shown in Figure 4.11. Note that our data structure is no longer a tree (instead, it is a directed acyclic graph), but we will continue to refer to it as a parse forest. The process for recovering the set of parses is exactly the same as before.

We say that a parse forest is valid if it has the property that given a set of choices for each choice node, the resulting structure is a tree. Put another way, every cycle in the parse forest must go through at least two children of some choice node (and thus the cycle can never be present given choices for all choice nodes).

The parse forest data structure is basically the same data structure as the chart used in chart parsing algorithms such as the CKY algorithm (Kasami, 1965; Younger, 1967). The primary difference is that a chart parse stores parses that differ only on internal labels and structure, while we store parses that represent different sentences. This makes the problem of finding a good (i.e., small) parse forest for a given set of parses much more difficult.

Recall that there were two issues we wished to address. The first was to avoid copying the entire parse every time we applied a rule. It is not hard to see that when applying a rule, we only need to create new nodes in the parse tree for every node in the transformed parse that is actually modified by the transformation rule. Typically, a transformation rule modifies only a subtree of the entire parse. We can

then simply replace the original root of this subtree with a new choice node, which points to both the untransformed version of the subtree and the newly transformed version (as in Figure 4.10). Thus, we do not need to copy anything outside of the subtree. Similarly, any descendants of nodes modified by the transformation rule do not need to be copied, because we can have both the original and transformed versions of the subtree point to the same descendants (as in Figure 4.11).

The second issue was to avoid producing an exponential number of transformed sentences. Consider the sentence "I will eat and I will drink and I will play and ..." Each subsentence can be transformed to remove the modal verb "will." This yields an exponential number of transformed sentences in the length of the parse. However, we can easily represent all such transformed sentences compactly by representing each subsentence as in Figure 4.11.

4.7.2 Rule Application

In order to maintain the advantages of the parse forest data structure, we need to be able to apply transformations without expanding the set of sentences represented by the parse forest. Fortunately, there is a straightforward way to do this.

Given a single parse tree, we apply a rule by first matching the tree pattern against a subtree of the parse and then applying the transformation operations. For concreteness, assume that we match the tree pattern top down — first we find a node that matches the constraints on the root of the tree pattern, then we match the children of the root, then their children, etc. We can do essentially the same in the parse forest. The only difference is what happens when a choice node is reached. In this case, we simply try matching against each possible child. This process could potentially be exponential in the size of the tree pattern if there were a choice node at each level. In practice, this is not an issue because our tree patterns all have under ten nodes, and most nodes in the parse forest are not choice nodes.

After this matching process, we end up with a set of expanded subtrees (note that we stop expanding the parse forest once we get to leaves of the tree pattern, since we

can share the part of the parse forest below this point). We apply the transformation operations to each of these subtrees, yielding a set of new subtrees. We then add a new choice node at the root of the transformed subtree pointing to all of these subtrees.

The result of this procedure is to apply the given transformation to *all* parses that share this particular part of the parse forest. Thus, by repeating this process for all rules and all nodes in the parse forest, we guarantee that we try all possible rules on all possible parses. Any given step of this procedure only increases the number of nodes in the parse forest by (number of nodes in the tree pattern) * (number of expanded matched subtrees).

While this procedure is reasonably efficient, it can still be improved. For example, suppose we have a parse forest representing the sentences "Bob was hit by a car" and "Bob was hit by a truck", stored as "Bob was hit by a car OR a truck". If we apply the depassivization rule to this sentence, we first expand out the entire parse (since the root of the tree pattern for the depassivize rule matches the S node at the root of the parse forest). We then apply the depassivization rule to each separately and replace the root of the parse forest with an OR node pointing to each transformed sentence as well as the original parse forest. We clearly can do much better than this: the (transformed) sentences "A car hit Bob" and "A truck hit Bob" can be represented as "A car OR a truck hit Bob". Furthermore, both "a car OR a truck" and "Bob" can be shared between the passive and active versions.

There are two useful heuristics we can apply to compactify the parse forest. The first is to merge nodes from the bottom up. Starting at the leaves of the nodes matched by the tree pattern. we check to see if the nodes were changed by the transformation operations. If not, we can remove all but one of the copies of this node. We can repeat this process, merging nodes until we get to a point where the nodes differ.

The second heuristic merges nodes top down. To guarantee we do not change the parse forest, we need two conditions to hold. First, the two merged nodes must have the same *parent* — otherwise, when we merge them, we will effectively create extra edges in the parse forest. Second, the merged nodes must differ on at most one child.

If these conditions hold, then we can merge the nodes, replacing the differing child with a choice node that points to each variant of that child.

Suppose we want to compress the sentences "Alice ate" and "Alice ran". Since these sentences differ in only one place (the verb), we can compress them as "Alice ate OR ran". However, consider the sentences "Alice ate" and "Bob ran". If we were to compress as "Alice OR Bob ate OR ran", we would have erroneously added the sentences "Alice ran" and "Bob ate" to our set.

These two heuristics are enough to fix the problems discussed above when depassivizing a sentence; in practice, they greatly reduce the final size of the parse forest. The advantage of all the compression methods mentioned so far is that they only look at the part of the parse forest currently being transformed. We also implemented a very simple global reduction step that looks for nodes that are identical (identical labels, words, and children). While further compression of the parse forest is often possible through further examination of the entire parse forest, we found that these steps (the two local heuristics plus the simple global step) were enough to keep the parse forest reasonably small.

The top-down merge actually handles another issue not yet mentioned. To produce the set of all canonical forms for a given input parse, we repeatedly apply rules to nodes in the parse forest as described above. In doing this, we may produce a given parse multiple times. In most cases, the top-down merge will automatically remove the copies by merging them back into the forest.

There are various ways in which our compression heuristics could be improved. One example would be to match entire "forests" of subtrees at once. For example, if a passive sentence has two different possible NPs for its (syntactic) subject, the current algorithm transforms each separately (hopefully recombining them in the top-down compression step). Instead, since the depassivizing rule only requires an NP, we could transform both at the same time, never needing to recombine them. Our current algorithm has difficulty when there are multiple independent choices for a particular rule; this optimization would fix this problem.

4.7.3 Adding Rule Information

There is one additional detail of our parse forest generation procedure. Recall that our probabilistic model is based on the set of rules used to generate a given canonical form. Thus, we need to keep track of the rules used to generate each parse, but we want to avoid explicitly representing every parse. It turns out that we can simply attach rule identifiers to the edges of the parse forest. The set of rules which was used to generate a given parse is simply the set of rules on the edges of that parse. The method for doing this does somewhat complicates the construction of the parse forest.

Recall that when we apply a transformation to a subtree of the parse forest, we add all transformed versions of the subtree as children of a new choice node which replaces the root of the subtree. To incorporate rule information into the parse forest, we add a label to each of the edges from the transformed subtrees to the choice node with the just-applied rule.

Furthermore, when we expand the subtree while matching the tree pattern, we also need to keep track of all rules that are labels of edges in the matched subtree. We then add all of these rules to the root of the matched subtree, adding them to the same edge where we add the newly-applied rule. This ensures that we remember that these rules were used to produce this subtree.

When applying our compression heuristics, we now must take into account the edge labels. The bottom-up merge stays the same, except that the edge labels of all children must also be the same. However, the top-down merge now becomes more complicated, because in some cases we want to push edge labels back down the graph in order to better compress the tree.

One way to explain the complication of the merge step is that when we apply a rule to produce a new subtree, it is arbitrary exactly which edges we label in the new subtree. This is because the only constraint is that each tree represented by the parse forest is labeled with the correct set of rules; it does not matter which edges are labeled. Thus, we have some flexibility in where we place the edges, so we have

to solve a small optimization problem in order to decide which assignment of rules to edges allows us to most compress the parse forest. Fortunately, this optimization is relatively straightforward to solve.

4.7.4 Inference and Learning

Again, in order for the parse forest to be useful, we must be able to do inference (probability queries about canonical forms) and learning (optimizing the parameters of our model) without expanding the set of parses represented by the parse forest. In this case, we can use a relatively straightforward extension of the inside-outside algorithm for chart parses; a similar algorithm was proposed by Geman & Johnson (2002). This allows us to compute statistics of the nodes of the parse forest in time linear in the number of edges in the parse forest. This is sufficient to make both inference and learning efficient in our model.

4.8 Experiments

We evaluated our system using the setup of the CoNLL 2005 semantic role labeling task as described in Chapter 3. As in Chapter 3, we reran the 2005 version of the Charniak parser to generate parses with the correct analysis of quotes.

Our **Baseline** SRL system for this section is the standard SRL system as described in Chapter 3, using a feature set very similar to Baseline + PassPos in Table 3.6.[4] Note that because our system uses features of the role pattern, it is doing a certain kind of joint inference, while **Baseline** classifies each constituent independently.

Our **Transforms** model takes Charniak parses as input and labels every node with Core arguments (ARG0-ARG5). Our rule set does not currently handle either referent arguments (such as "who" in "The man who ate ...") or non-core arguments (such as ARGM-TMP). For these arguments, we simply filled in using our baseline

[4]The **Baseline** system used in this section differs in a few implementation details from that of Chapter 3.

system (specifically, any non-core argument that did not overlap an argument predicted by our model was added to the labeling). Also, on some sentences, our system did not generate any predictions because no canonical forms were produced by the canonicalization system. Again, we used the baseline to fill in predictions (for all arguments) for these sentences.

Baseline and **Transforms** were regularized using a Gaussian prior; for both models, $\sigma^2 = 1.0$ gave the best results on the development set.

For generating role predictions from our model, we have two reasonable options: use the labeling given by the single highest scoring simple labeling; or compute the distribution over predictions for each node by summing over all simple labelings. The latter method worked slightly better, particularly when combined with the baseline model as described below, so all reported results use this method.

We also evaluated a hybrid model that combines the **Baseline** with our model. For a given sentence/verb pair (s, v), we find the set of constituents N^{sv} that made it past the first (identification) stage of **Baseline**. For each candidate labeled canonical form $l_k^{sv} = (c_i^{sv}, g_j^v)$ proposed by our model, we check to see which of the constituents in N^{sv} are already present in our canonical form c_i^{sv}. Any constituents that are *not* present are then assigned a probability distribution over possible roles according to **Baseline**. Thus, we rely on **Baseline** whenever the current canonical form does not contain a particular constituent. The **Combined** model is thus able to correctly label sentences when the simplification process drops some of the arguments (generally due to unusual syntax). Each of the two components was trained separately and combined only at testing time. This simple combination scheme has a significant limitation: when using **Baseline** to make a prediction, the system does not use the fact that **Transforms** had no prediction for this node.

Table 4.2 shows results of these three systems on the CoNLL 2005 task. It also shows test results for **Baseline** and **Transforms** using reranked Charniak parses (see Chapter 3), Combo 2 using reranked parses from Chapter 3, and the best reported results on this data (Surdeanu et al., 2007). Our **Transforms** model achieves

Model	Dev	Test WSJ	Test Brown	Test Both
Baseline	75.6	78.1	65.6	76.5
Transforms	**77.0**	**78.9**	67.5	**77.4**
Combined	76.8	78.8	**67.6**	77.3
Baseline (R)		79.2	67.0	77.6
Transforms (R)		80.4	69.0	78.9
Combo 2 (R)		80.3	68.0	78.7
Surdeanu		**80.6**	**70.1**	**79.2**

Table 4.2: F1 Measure using Charniak parses. (R) indicates the reranking parser was used.

Model	Test WSJ
Baseline	87.6
Transforms	88.2
Combined	**88.5**

Table 4.3: F1 Measure using gold-standard parses

a statistically significant increase over **Baseline** on all sets (according to the confidence intervals calculated for the CoNLL 2005 results), with a larger increase for the Brown test set. **Combined** and **Transforms** perform about the same; this may be partly due to the deficiencies of our combination scheme. It is worth noting that when using the uncorrected Charniak parses provided with the CoNLL distribution, **Combined** improves over **Transforms** by 0.5 F1 points on the combined test set. This is probably mostly because **Transforms** is less capable of adapting to malformed input, since it can only label arguments which end up in some canonical form. Table 4.3 shows the performance of the three models on gold standard parses; here, **Combined** does improve slightly over **Transforms**, and both improve significantly over **Baseline**.

When using reranked parses, the **Transforms** model achieves results comparable to those of Surdeanu et al. (2007). Combo 2 from Chapter 3 has very similar performance to **Transforms**; this may be partly because many of the additional features proposed in Chapter 3 were inspired by successful rules in the **Transforms** model.

We expect that by labeling canonical forms, our model will generalize well even on verbs with a small number of training examples. Figure 4.12 shows F1 measure on the WSJ test set for **Transforms** and **Baseline** as a function of training set size. As expected, **Transforms** significantly outperform the **Baseline** model when there are fewer than 20 training examples for the verb. For verbs with a very large number of

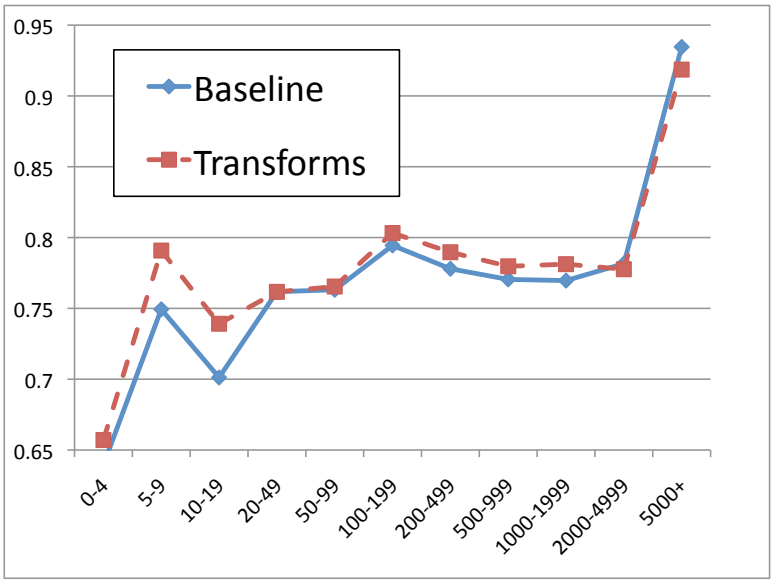


Figure 4.12: F1 Measure on the WSJ test set as a function of training set size. Each bucket on the X-axis corresponds to a group of verbs for which the number of training examples fell into the appropriate range; the value is the average performance for verbs in that bucket.

training examples, **Baseline** slightly outperforms **Transforms**; this may be because **Baseline** is better able to match the exact usage patterns of particular verbs.

We also found, as expected, that our model improved on some sentences with very long parse paths. For example, in the sentence "Big investment banks refused to step up to the plate to support the beleagured floor traders by buying blocks of stock, traders say," the parse path from "buy" to its ARG0, "Big investment banks," is quite long. The **Transforms** model correctly labels the arguments of "buy", while the **Baseline** system misses the ARG0. Unfortunately, the number of such cases was not enough to generate a significant difference in performance at an aggregate level.

To understand the importance of different types of rules, we performed an ablation analysis, shown in Table 4.4. For each major rule category in Figure 4.1, we deleted those rules from the rule set, retrained, and evaluated using the **Transforms** model. Note that deleting certain rules makes it impossible for the system to generate a

Deleted Rule Group	**Transforms**	**Combined**
None	88.24	88.47
Verb Raising/Control (all)	−1.65	−0.54
Verb Raising/Control (basic)	−1.44	−0.38
Verb Raising/Control (nonbasic)	−0.12	−0.06
Inverted Sentences/Questions	+0.10	−0.01
"Make" Rewrites	−0.44	−0.38
Modified Nouns	−1.12	−0.38
Passive	−0.31	−0.36
Possessive	−0.06	−0.02

Table 4.4: F1 Measure on WSJ test set of **Transforms** and **Combined** deleting different subsets of the rules

correct canonical form, guaranteeing failure for some arguments. To avoid parse-related issues, we trained and evaluated on gold-standard parses. Most important were rules relating to (basic) verb raising/control and modified nouns; passive and "make" rewrites were moderately important; and the removal of (nonbasic) verb raising/control, possessive, and inverted sentences/questions had little or no effect. More than anything, this indicates the relative frequency of each of these types of construction.

To get an idea of what areas our system improved over **Baseline**, we performed the same ablation analysis on **Combined**, also shown in Table 4.4. In this case, if the canonical form system does not include a constituent in the predicted canonical form, then **Baseline** is used instead. As expected, the drop in performance from removing, for example, verb raising/control (basic) is not as large. However, removing each of verb raising/control (basic), "make" rewrites, modified nouns, and passive rules leads to a noticeable drop in performance (about 0.4 F1 points in each case).

4.9 Discussion and Future Work

Besides incorporating the ideas used in the state-of-the-art SRL systems described in Chapter 3, our models could be improved in a variety of ways. One is to improve the coverage of the rule set, adding additional syntactic constructs that are not already covered. Another is to refine the currently existing rules, with the goal of incorporating additional features of the rules in order to improve canonical form selection. For example, our current system does not incorporate lexical features of the rules. Another related extension would be to add further sentence normalizations, e.g., identifying whether a direct object exists. We could also add support for non-core arguments (e.g., temporal arguments).

Another limitation of our current model is that each target verb in a sentence is labeled separately. This allows the system to produce inconsistent labelings. For example, in "I want Bob to start to eat," our system could decide that "I" is the subject of "start" and that "Bob" is the subject of "eat." Clearly, both "start" and "eat" should have the same subject.

As mentioned before, a sentence cannot be labeled entirely correctly unless the correct role pattern has been seen before; this could be fixed by better modeling of role patterns. For example, we could find clusters of verbs with similar role patterns, which would allow us to predict role patterns we have not seen yet.

Another interesting extension involves incorporating parser uncertainty into the model; in particular, our simplification system is capable of seamlessly accepting a parse forest as input. The main difficulty is pruning the parse forest in order to maintain efficiency. With this setup, the parser and simplification system could be jointly, discriminatively trained to maximize, for example, SRL performance.

The ideas in this chapter can be extended beyond the task of semantic role labeling. We could augment the system to further normalize canonical forms. For example, we could map similar verbs to a common frame and rewrite noun phrases containing nominalizations as verb phrases. Each new type of normalization (assuming it can be performed accurately) should lead to improvements in higher-level tasks. The primary

difficulty here is the lack of labeled data for further normalizations; this could perhaps be addressed in the same way as in this chapter, by treating the correct normalized form as a hidden variable.

Chapter 5

Learning with Contrastive Objectives

5.1 Introduction

At the end of Chapter 4, we suggested a number of extensions to our canonical SRL system. Several of these, particularly the suggestion to perform joint inference over all verbs in the sentence at once, greatly expand the required computation. It is unlikely that exact inference is tractable in this case, so we need to turn to approximate learning.

A syntactic parse is a fairly complex object, which makes many existing approaches to approximate learning difficult to implement. One general class of methods which is relatively easy to use even for complex objects is heuristic search, where we try to find a high-scoring configuration by taking a series of steps designed to (sooner or later) move towards higher-scoring values. Heuristic search is really just an approximate MAP procedure; unfortunately, previous work has not provided a good way to use approximate MAP solutions for learning log-linear models. In this chapter, we develop such a method. Due to additional complications in the canonical SRL model (in particular, the inclusion of hidden variables), we do not close the loop and apply these methods to semantic role labeling; instead, we evaluate our method on another

important problem, multiclass image segmentation in real-world images.

5.2 Overview

In Chapter 2, we discussed how learning log-linear models is difficult because of the complexity of computing the partition function $Z(\mathbf{x})$. Recently there has been significant interest in *contrastive methods* such as pseudo-likelihood (PL) (Besag, 1975) and contrastive divergence (CD) (Hinton, 2002). The main idea of these algorithms is to trade off the probability of the correct assignment for each labeled example with the probabilities of other, "nearby" assignments. This means that these algorithms do not need to compute the partition function $Z(\mathbf{x})$. Unfortunately, these algorithms can suffer when the distribution is highly multi-modal, with multiple distant regions of high probability.

LeCun & Huang (2005), Smith & Eisner (2005), and Liang & Jordan (2008) all consider the general case of contrastive objectives, where the contrasting set is allowed to consist of arbitrary assignments. However, previous work has not pursued the idea of *non-local* contrastive objectives. Rather than restrict the objective to considering assignments (values of $\mathbf{Y}$) that are close to the correct label, as in pseudo-likelihood and contrastive divergence, we propose methods that allow comparison to any assignment.

This chapter has two main parts. First, we prove several results that justify the use of non-local contrastive objectives. We show that a wide class of contrastive objectives are consistent with maximum likelihood, even for finite data under certain conditions. This generalizes and is a considerably stronger result than the asymptotic consistency of pseudo-likelihood. A central idea of this result is that contrastive objectives attempt to enforce probability-ratio constraints between different assignments, based on the structure of the objective. Among other consequences, this result clearly points out cases in which pseudo-likelihood (and other local methods) may fail.

Based on this insight, we propose several methods for constructing non-local contrastive objectives. We focus particularly on Contrastive Constraint Generation (CCG), a novel constraint-generation style algorithm that iteratively constructs a

contrastive objective based only on a MAP-inference procedure. While similar in flavor to the max-margin cutting plane algorithm suggested by Tsochantaridis et al. (2005), our method has the ability to obtain accurate probability estimates. We compare CCG to pseudo-likelihood, contrastive divergence, and the cutting-plane algorithm on a real-world machine vision problem; CCG achieves a 12% error reduction over the best of these, a statistically significant improvement.

5.3 Contrastive Objectives

5.3.1 Definitions

The main idea of our approach is to define small terms over subsets of $\mathbf{Y}$.

Definition 1. *Let S_j be some subset of values of $\mathbf{Y}$. The (conditional) contrastive probability distribution for S_j is $P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x}) = \frac{e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x},\mathbf{y})}}{Z_j(\mathbf{x})}$, where Z_j is the contrastive partition function $Z_j(\mathbf{x}) = \sum_{\mathbf{y} \in S_j} e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x},\mathbf{y})}$.*

We refer to this distribution as contrastive because it compares the (unnormalized) probabilities of the values of $\mathbf{Y}$ in S_j. Note that this distribution implicitly compares *normalized* probabilities: $\frac{e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x},\mathbf{y})}}{Z_j(\mathbf{x})} = \frac{P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x})}{\sum_{\mathbf{y}' \in S_j} P_{\boldsymbol{\theta}}(\mathbf{y}'|\mathbf{x})}$ due to cancellation of the global partition function.

Definition 2. *A contrastive sub-objective $C_j(\boldsymbol{\theta}; D)$ is a weighted maximum-likelihood objective with the model distribution $P_{\boldsymbol{\theta}}$ replaced by the contrastive distribution $P_{\boldsymbol{\theta},j}$ for some subset S_j:*

$$\sum_{(\mathbf{x}^i, \mathbf{y}^i): \mathbf{y}^i \in S_j} w_j(\mathbf{x}^i) \left(\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \log Z_j(\mathbf{x}^i) \right).$$

$w_j(\mathbf{x})$ is a parameter of the sub-objective that determines the overall strength of the sub-objective as well as the relative importance of each value of $\mathbf{x}$.

A *contrastive objective* $C(\boldsymbol{\theta}; D)$ is a sum of J sub-objectives C_j, each with a different subset S_j and set of weights $w_j(\mathbf{x})$. C is tractable to compute (and optimize) if

the contrastive partition functions are tractable to compute. In some cases, we can compute the contrastive partition function $Z_j(\mathbf{x})$ even if S_j contains an exponential number of values, e.g., using dynamic programming for tractable sub-structures.

We say that sub-objective C_j is *active* for example $(\mathbf{x}^i, \mathbf{y}^i)$ if $\mathbf{y}^i \in S_j$ and $w_j(\mathbf{x}^i) > 0$. The number of active sub-objectives for a particular data set D may be much smaller than the total number of sub-objectives.

For now, we assume that C is given. We will discuss how to construct contrastive objectives in Sections 5.7 and 5.8.

5.3.2 Relationship to Standard Learning Methods

The log-likelihood objective $LL(\boldsymbol{\theta}; D)$ is a contrastive objective with one sub-objective C_1, where S_1 contains all values in $\mathbf{Y}$ and $w_1(\mathbf{x}) = 1$ for all $\mathbf{x}$.

If $\mathbf{Y}$ is an MRF (or CRF), contrastive objectives are a generalization of pseudo-likelihood. To write PL as a contrastive objective, for each l, for every possible instantiation $\mathbf{y}_{-l}$, we construct one sub-objective $S_{\mathbf{y}_{-l}}$ that contains exactly the set of instantiations consistent with $\mathbf{y}_{-l}$, i.e., $(\mathbf{y}_{-l}, Y_l = a)$ for all $a \in dom(Y_l)$. All sub-objective weights $w_{\mathbf{y}_{-l}}(\mathbf{x})$ are set to 1. Since a sub-objective $C_{\mathbf{y}_{-l}}$ is only active for examples where $\mathbf{y}^i \in S_{\mathbf{y}_{-l}}$, it follows that each example participates in n sub-objectives, where n is the number of variables in the network. This yields the contrastive objective

$$\sum_{(\mathbf{x}^i, \mathbf{y}^i)} \sum_{l} \left(\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \log \sum_{a \in dom(Y_l)} e^{\boldsymbol{\theta}^T \mathbf{f}(\mathbf{x}^i, (\mathbf{y}^i_{-l}, a))} \right),$$

which is the definition of pseudo-likelihood. All of the sub-objectives in PL are *local*; they only involve instantiations that differ on a single node. Generalized pseudo-likelihood (GPL) can also easily be expressed in this framework. In GPL two or more variables are allowed to vary. This can lead to large, potentially exponential sub-objectives. In some cases, dynamic programming can render inference tractable within sub-objectives. Unlike GPL, our framework allows us to vary multiple variables

without including all possible combinations of these variables, giving us considerably more flexibility.

Another related learning method is contrastive divergence (CD), which approximates the gradient of maximum likelihood using a non-mixed Markov chain, initialized at the label of the current example. CD is generally defined by the update rule

$$\Delta\boldsymbol{\theta}_t = \sum_{(\mathbf{x}^i,\mathbf{y}^i)} f_t(\mathbf{x}^i,\mathbf{y}^i) - E_{P^k_{\boldsymbol{\theta}}}(f_t(\mathbf{x}^i,\mathbf{y}^i)),$$

where $P^k_{\boldsymbol{\theta}}$ is the distribution over $\mathbf{y}$ obtained by initializing some Markov chain Monte Carlo (MCMC) procedure at $\mathbf{x}^i$ and running for k steps.[1] CD cannot be expressed as a contrastive objective, because CD uses $P^k_{\boldsymbol{\theta}}$ to compute expectations rather than P_θ. This means that the probability-ratio matching intuitions in the next section do not hold for CD. In fact, CD does not optimize *any* objective. This means that CD requires using stochastic gradient for optimization, whereas a contrastive objective can be optimized using a variety of methods (in this paper, BFGS). Furthermore, similar to PL, standard implementations of CD are local: they compare the correct label $\mathbf{y}^i$ only to nearby values $\mathbf{y}'$.

5.3.3 Visualization of Contrastive Objectives

In this section, we present a visualization of contrastive objectives which gives insight into how they work. Figure 5.1 depicts a probability distribution and an observed data set. We assume that the probability distribution is the model distribution $P_{\boldsymbol{\theta}}$ for some parameter vector $\boldsymbol{\theta}$.

Figure 5.2 shows a representation of the gradient of the log-likelihood objective. The probability of every point is adjusted, with size proportional to how far off the current model probability is from the observed data distribution. Figure 5.3 shows the gradient of pseudo-likelihood (assuming that nearby points in the visualization corresponds to instantiations that differ on a single variable). Only neighboring points

[1] In practice, it is intractable to compute the expectation over $P^k_{\boldsymbol{\theta}}$ exactly; instead, it is estimated through sampling.

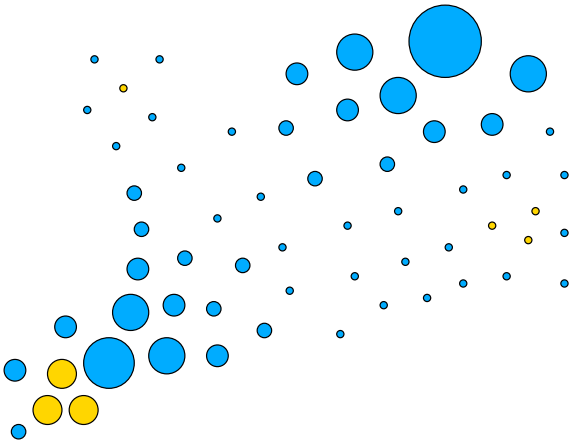


Figure 5.1: Probability distribution and observed data set. The size of each circle represents the probability assigned to that point. Yellow circles are observed data examples; each is observed once, so $|D| = 7$.

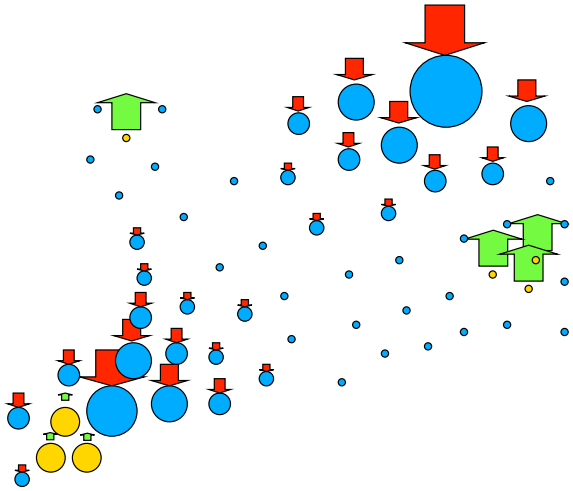


Figure 5.2: Representation of log-likelihood gradient. A green upward arrow above a point indicates positive gradient; a red downward arrow indicates negative gradient. Size of arrow indicates gradient magnitude. Very small arrows have been omitted.

are compared.

Figure 5.4 shows a single local pairwise sub-objective, which is similar to a reduced PL sub-objective. Figure 5.5 shows an example of a non-local pairwise sub-objective. This sub-objective allows us to "fix" the large blue dot at the top of the visualization. Finally, Figure 5.6 shows a sub-objective that compares points that are already "ok" (i.e., the labeled point has much higher probability than the unlabeled); the resulting gradient is small.

5.3.4 Other Related Methods

LeCun & Huang (2005) provide a general framework for learning energy functions of which contrastive objectives are an example, but do not suggest the particular log-linear form used in our work. Smith & Eisner (2005) define an objective with the same functional form as one of our sub-objectives; however, they primarily look at unsupervised learning tasks, whereas this work is mostly aimed at supervised learning.

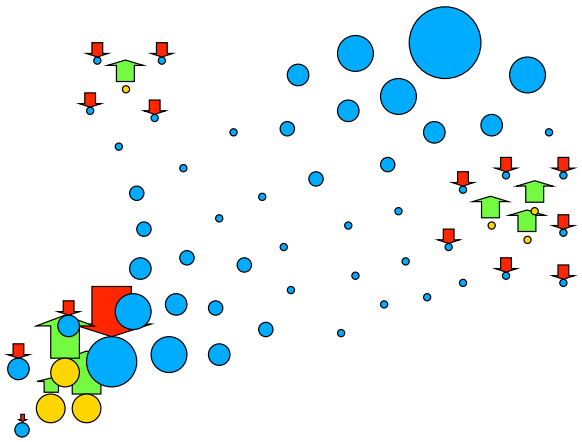


Figure 5.3: Pseudo-likelihood

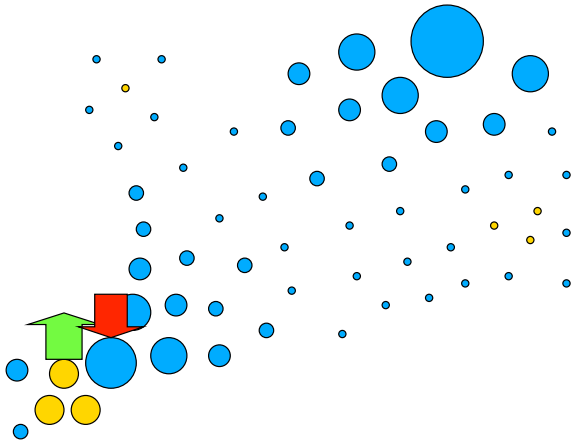


Figure 5.4: Local sub-objective

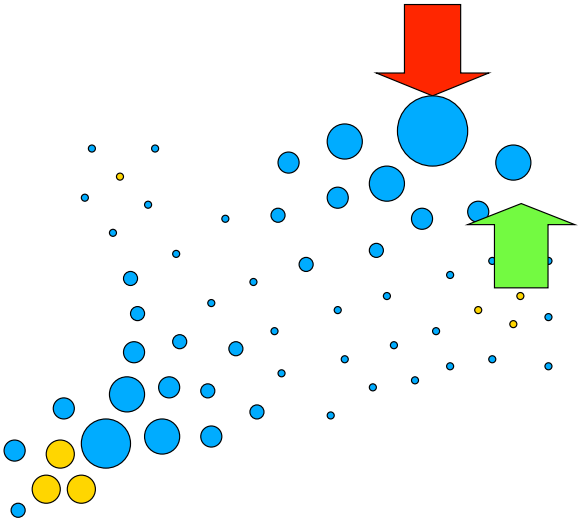


Figure 5.5: Non-local sub-objective

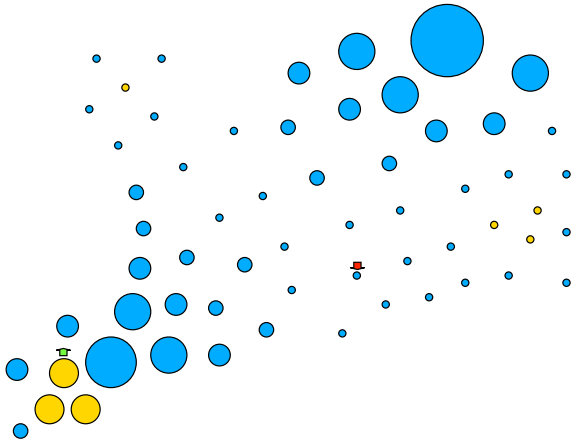


Figure 5.6: "Satisfied" sub-objective

More importantly, both of these works focus on the use of local contrastive objectives, whereas we are particularly interested in the use of non-local contrastive terms.

Liang & Jordan (2008) provide an asymptotic analysis of contrastive objectives. They show that under certain conditions, the more different assignments are covered by the objective, the more efficient the objective is as an estimator. They apply this result to compare the efficiency of pseudo-likelihood to that of maximum-likelihood. Their results suggest that increasing the number of assignments covered by the contrastive objective leads to improved learning efficiency.

Hyvärinen (2007) proposes an objective for learning binary Markov networks by trying to match ratios of probabilities between the model and the observed data. This objective minimizes squared-loss instead of log-loss; the advantage of log-loss is that contrastive objectives are a direct generalization of both log-likelihood and PL. Additionally, Hyvärinen (2007) only proposes matching local probability ratios.

Recently, Gutmann & Hyvärinen (2010) proposed a method based on learning probability ratios between the data distribution and some hand-constructed noise distribution. Similar to our method, it does not require computation of the global partition function. Unlike our method, it looks at probability ratios between different *distributions*, while our method looks at probability ratios between different *instantiations*.

Hinton et al. (2004) and Tieleman (2008) both improve CD by adding non-local contrastive terms. However, like standard CD, these methods do not correspond to any objective function. The following analysis gives a theoretical grounding to non-local contrastive learning and supplies a well-defined objective.

Max-margin-based methods, such as those proposed by Taskar et al. (2003) and Tsochantaridis et al. (2005), also are designed to avoid needing to compute the global partition function. The cutting-plane algorithm proposed by Tsochantaridis et al. (2005) is similar in spirit to our contrastive constraint-generation (CCG) approach, described in Section 5.8. Like max-margin methods, CCG can learn using only MAP inference. The primary advantage of contrastive objectives over margin-based methods is that they can calibrate probabilities between instantiations.

5.4 Theoretical Results

The main results of this section show the finite and asymptotic consistency of contrastive objectives, under suitable conditions on the model distribution $P_{\boldsymbol{\theta}}$ and sub-objectives C_j. The proofs of these theoretical results also illustrate a key feature of contrastive objectives: if two label values $\mathbf{y}, \mathbf{y}'$ are connected through a series of sub-objectives, then the objective will encourage $\frac{P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x})}{P_{\boldsymbol{\theta}}(\mathbf{y}'|\mathbf{x})}$ to match $\frac{\hat{P}(\mathbf{y}|\mathbf{x})}{\hat{P}(\mathbf{y}'|\mathbf{x})}$. This will be the main motivation for the methods we propose in Sections 5.7 and 5.8 for choosing non-local sub-objectives.

5.4.1 Consistency of Pseudo-likelihood

Before presenting the results, we review asymptotic consistency for pseudo-likelihood. We begin by establishing some notation.

Let Θ be the set of all possible parameter vectors $\boldsymbol{\theta}$, and let P_Θ denote the set of all possible models $P_{\boldsymbol{\theta}}$ obtainable using $\boldsymbol{\theta} \in \Theta$. We say that P_Θ can *represent* probability distribution $P'(\mathbf{Y}|\mathbf{X})$ if there exist parameters $\boldsymbol{\theta}' \in \Theta$ such that $P_{\boldsymbol{\theta}'}(\mathbf{Y}|\mathbf{x}) = P'(\mathbf{Y}|\mathbf{x})$ for all $\mathbf{x}$. Let $\Theta[P']$ denote the set of such $\boldsymbol{\theta}'$.

Let $P^*(\mathbf{Y}, \mathbf{X})$ be the distribution from which the data set D is drawn. Let $\{d^1, d^2, \dots\}$ be an infinite sequence of examples drawn i.i.d from $P^*(\mathbf{X}, \mathbf{Y})$; we refer to the data set composed of the first n of these as D^n, and its empirical distribution as $\hat{P}(\mathbf{y}|\mathbf{x}; D^n)$. By the strong law of large numbers, $P(\lim_{n\to\infty} \hat{P}(\mathbf{y}|\mathbf{x}; D^n) = P^*(\mathbf{X}, \mathbf{Y})) = 1$, or in short-hand $\hat{P}$ converges to P^* almost surely $\hat{P}(\mathbf{y}|\mathbf{x}; D^n) \overset{a.s.}{\to} P^*(\mathbf{y}|\mathbf{x})$ as $n \to \infty$.

Gidas (1988) proved consistency of log-likelihood and pseudo-likelihood. The statement of consistency for pseudo-likelihood is the following:

Theorem 1. *Suppose P_Θ can represent $P^*(\mathbf{Y}|\mathbf{X})$. Also, suppose that for all $\mathbf{x}$ such that $P^*(\mathbf{x}) > 0$, $P^*(\mathbf{Y}|\mathbf{x})$ is* positive*, i.e., for all $\mathbf{y}$, $P^*(\mathbf{y}|\mathbf{x}) > 0$. Let $\boldsymbol{\theta}^{(n)}$ be a sequence of weight vectors $\{\boldsymbol{\theta}^1, \boldsymbol{\theta}^2, \dots\}$ such that for all n, $\boldsymbol{\theta}^n$ optimizes $PL(\boldsymbol{\theta}; D^n)$. Then for all $\mathbf{x}$ s.t. $P^*(\mathbf{x}) > 0$, $P_{\boldsymbol{\theta}^n}(\mathbf{Y}|\mathbf{x}) \overset{a.s.}{\to} P^*(\mathbf{Y}|\mathbf{x})$ as $n \to \infty$*

This means that, provided the data is drawn from within our model class (and that

the data distribution is positive), we will converge to the correct parameters as the amount of data grows. This theorem follows from Theorem 3, proved in Section 5.4.3. Before proving asymptotic consistency for (a certain class) of contrastive objectives, we will first consider finite consistency for contrastive objectives.

5.4.2 Finite Consistency

While asymptotic representability (i.e., P_Θ being able to represent $P^*(\mathbf{Y}|\mathbf{X})$) is a standard concept in analysis of learning algorithms, finite representability (P_Θ being able to represent $\hat{P}(\mathbf{Y}|\mathbf{x})$) is less common. Suppose P_Θ can represent $\hat{P}(\mathbf{Y}|\mathbf{x})$. In many cases, we only see each $\mathbf{X} = \mathbf{x}$ one time in our data set D, which means that $\hat{P}(\mathbf{Y}|\mathbf{X})$ will have a point estimate on the correct label $\mathbf{y}^i$ for each $\mathbf{x}^i$. Thus, it can be a fairly strong condition on our model class P_Θ. However, as we will now show, it is actually a weaker condition than another commonly seen condition in analysis of learning algorithms: separability.

Typically it is assumed that Θ is exactly equal to $\mathbb{R}^R$ (i.e., any possible R-length vector of real numbers). For the purposes of the following result, we will augment Θ to also include (a certain type of) infinite-length weight vectors. Specifically, for each unit vector $\boldsymbol{\theta}' \in \mathbb{R}^R$, we include an infinite length weight vector $\boldsymbol{\theta}'_\infty$; the corresponding model distribution is $P_{\boldsymbol{\theta}'_\infty}(\mathbf{y}|\mathbf{x}) = \lim_{\lambda\to\infty} P_{\lambda\boldsymbol{\theta}'}(\mathbf{y}|\mathbf{x})$. We refer to this expanded set as Θ^∞. This augmentation simply adds certain deterministic distributions to P_Θ.

A classifier γ is a deterministic function from $\mathbf{X}$ to $\mathbf{Y}$. We say that a data set D is *separable* with respect to a set of classifiers $\Gamma = \{\gamma_k\}$ if there exists some classifier $\gamma_k \in \Gamma$ such that $\gamma_k(\mathbf{x}^i) = \mathbf{y}^i$ for all data instances d^i in D.

Lemma 1. *Let Γ_Θ be the set of classifiers $\gamma_{\boldsymbol{\theta}}$ such that $\gamma_{\boldsymbol{\theta}}(\mathbf{x}) = \arg\max_{\mathbf{y}} P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x})$ (if the* arg max *is not unique, $\gamma_{\boldsymbol{\theta}}(\mathbf{x})$ is undefined and so cannot separate with respect to $\mathbf{x}$). If D is separable with respect to Γ_Θ, then P_{Θ^∞} can represent $\hat{P}(\mathbf{Y}|\mathbf{X})$.*

Proof. Since D is separable with respect to Γ_Θ, there exists a classifier $\gamma_{\boldsymbol{\theta}}$ such that $\arg\max_{\mathbf{y}} P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x}^i) = \mathbf{y}^i$ for all data instances d^i. Let $\boldsymbol{\theta}_\lambda = \lambda\boldsymbol{\theta}$. Then $P_{\boldsymbol{\theta}_\lambda}(\mathbf{y}^i|\mathbf{x}^i) =$

$\frac{e^{\lambda\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y}^i)}}{\sum_{\mathbf{y}} e^{\lambda\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y})}} = \frac{1}{1+e^{\lambda}\sum_{\mathbf{y}\neq\mathbf{y}^i} e^{\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y})-\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y}^i)}}$. But in this last expression, all exponents are negative since $\mathbf{y}^i = \arg\max_{\mathbf{y}} P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x}^i) = \arg\max_{\mathbf{y}} \boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y})$. Thus, as $\lambda \to \infty$, $P_{\boldsymbol{\theta}_\lambda}$ converges to a point estimate on the observed label value $\mathbf{y}^i$ given each $\mathbf{x}^i$. But since D is separable, it must be that $\hat{P}$ consists of the same point estimates, and so $\lim_{\lambda\to\infty} P_{\boldsymbol{\theta}_\lambda} = \hat{P}$. But if $\boldsymbol{\theta}_\infty$ is the infinite length weight vector in the direction of $\boldsymbol{\theta}$, this means that $P_{\boldsymbol{\theta}_\infty} = \hat{P}$. □

There are a couple of things to note about this result. First, the set of classifiers Γ_Θ is precisely the set of linear separators of the form $\boldsymbol{\theta}^T\mathbf{f}(\mathbf{X},\mathbf{Y})$, a well-studied set of classifiers (and with which the notion of separability is often used). Second, although we needed to use an infinite-length weight vector to exactly represent $\hat{P}$, if the data is separable, then we can obtain an arbitrarily close approximate to $\hat{P}$ using finite-length weight vectors. We will assume exact representability for the remainder of this section, but replacing with "near-exact" representability would only slightly weaken the results (specifically, it would add an arbitrarily small approximation factor). Finally, note that the converse does *not* hold: there are data sets D such that $\hat{P}$ is representable by $P_{\Theta\infty}$ but which are not separable (either by Γ_Θ or by any other set of classifiers). Trivially, any D such that $\mathbf{y}^i$ is not deterministic given $\mathbf{x}^i$ is not separable but may still be representable.

Let $\hat{P}_j$ be the contrastive observed data distribution restricted to S_j: $\hat{P}_j(\mathbf{y}|\mathbf{x}) = \frac{|(\mathbf{x}^i,\mathbf{y}^i)=(\mathbf{x},\mathbf{y})|}{\hat{Z}_j(\mathbf{x})} = \frac{\hat{P}(\mathbf{x},\mathbf{y})}{\sum_{\mathbf{y}\in S_j}\hat{P}(\mathbf{x},\mathbf{y})}$ where $\hat{Z}_j(\mathbf{x}) = |(\mathbf{x}^i,\mathbf{y}^i) : \mathbf{x}^i = \mathbf{x}\ and\ \mathbf{y}\in S_j|$.

It will be convenient to define a slightly modified version $C'(\boldsymbol{\theta};D)$ of our contrastive objective:

$$-\sum_j \sum_{(\mathbf{x}^i,\mathbf{y}^i):\mathbf{y}^i\in S_j} w_j(\mathbf{x}^i) * (\log\frac{e^{\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i,\mathbf{y}^i)}}{Z_j(\mathbf{x}^i)} - \log\hat{P}_j(\mathbf{y}^i|\mathbf{x}^i)).$$

By definition, $C'(\boldsymbol{\theta};D)$ differs from $C(\boldsymbol{\theta};D)$ only by flipping the sign and adding a constant; thus the maxima of $C(\boldsymbol{\theta};D)$ are the same as the minima of $C'(\boldsymbol{\theta};D)$. For

the remainder of this section, we will analyze $C'(\boldsymbol{\theta}; D)$. Rewriting $C'(\boldsymbol{\theta}; D)$, we get

$$\begin{aligned}
&\sum_{j,\mathbf{x}} \hat{P}(\mathbf{x}) w_j(\mathbf{x}) \sum_{\mathbf{y} \in S_j} \hat{P}(\mathbf{y}|\mathbf{x})(\log \hat{P}_j(\mathbf{y}|\mathbf{x}) - \log P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x})) \\
&= \sum_{j,\mathbf{x}} \hat{P}(\mathbf{x}) w_j(\mathbf{x}) \frac{\hat{Z}_j(\mathbf{x})}{\hat{Z}(\mathbf{x})} \sum_{\mathbf{y} \in S_j} \hat{P}_j(\mathbf{y}|\mathbf{x}) \log \frac{\hat{P}_j(\mathbf{y}|\mathbf{x})}{P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x})} \\
&= \sum_{j,\mathbf{x}} \hat{P}(\mathbf{x}) w_j(\mathbf{x}) (\sum_{\mathbf{y} \in S_j} \hat{P}(\mathbf{y}|\mathbf{x})) KL(\hat{P}_j(\mathbf{y}|\mathbf{x}) || P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x}))
\end{aligned}$$

Thus, $C'(\boldsymbol{\theta}; D)$ is a weighted linear combination of KL-divergences.

Lemma 2. *Suppose that P_Θ can represent $\hat{P}(\mathbf{y}|\mathbf{x})$. Then for* any *contrastive objective $C'(\boldsymbol{\theta}; D)$,*

i. For any $\hat{\boldsymbol{\theta}} \in \Theta[\hat{P}]$, $C'(\boldsymbol{\theta}; D)$ has a global optimum at $\hat{\boldsymbol{\theta}}$, with $C'(\hat{\boldsymbol{\theta}}; D) = 0$.

ii. If $\boldsymbol{\theta}'$ optimizes $C'(\boldsymbol{\theta}; D)$, then for any $j, \mathbf{x}$ such that $\hat{P}(\mathbf{x}) w_j(\mathbf{x}) (\sum_{\mathbf{y} \in S_j} \hat{P}(\mathbf{y}|\mathbf{x})) > 0$, we have $P_{\boldsymbol{\theta}',j}(\mathbf{y}|\mathbf{x}) = \hat{P}_j(\mathbf{y}|\mathbf{x})$.

Proof. To prove (i), let $\hat{\boldsymbol{\theta}} \in \Theta[\hat{P}]$. Then

$$P_{\hat{\boldsymbol{\theta}},j}(\mathbf{y}|\mathbf{x}) = \frac{P_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x})}{\sum_{\mathbf{y}' \in S_j} P_{\boldsymbol{\theta}}(\mathbf{y}'|\mathbf{x})} = \frac{\hat{P}(\mathbf{x},\mathbf{y})}{\sum_{\mathbf{y} \in S_j} \hat{P}(\mathbf{x},\mathbf{y})} = \hat{P}_j(\mathbf{y}|\mathbf{x}).$$

Thus, for all $j, \mathbf{x}$, $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}) || P_{\hat{\boldsymbol{\theta}},j}(\mathbf{y}|\mathbf{x})) = 0$, and so $C'(\hat{\boldsymbol{\theta}}; D) = 0$. Since $C'(\boldsymbol{\theta}; D)$ is a weighted linear combination of KL-divergences, it is non-positive for all $\boldsymbol{\theta}$, and so $\hat{\boldsymbol{\theta}}$ is a global optimum of $C'(\boldsymbol{\theta}; D)$.

To prove (ii), suppose $\boldsymbol{\theta}'$ optimizes $C'(\boldsymbol{\theta}; D)$. From (i), it follows that $C'(\boldsymbol{\theta}'; D) = 0$. Now, since each $C'_j(\boldsymbol{\theta}; D)$ is non-negative, if $C'(\boldsymbol{\theta}'; D) = 0$, then $C'_j(\boldsymbol{\theta}'; D) = 0$ for all j. If $w_j(\mathbf{x}) > 0$ and $\sum_{y \in S_j} \hat{P}(\mathbf{x}, \mathbf{y}) > 0$, then $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}) || P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x}))$ has a positive coefficient in $C'_j(\boldsymbol{\theta}; D)$; since KL is non-negative, it follows that $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}) || P_{\boldsymbol{\theta}',j}(\mathbf{y}|\mathbf{x})) = 0$. □

Corollary 1. *Suppose that P_Θ can represent $\hat{P}(\mathbf{y}|\mathbf{x})$ and $\boldsymbol{\theta}'$ optimizes $C'(\boldsymbol{\theta}; D)$. Also suppose $\mathbf{y}_1, \mathbf{y}_2 \in S_j$, $\hat{P}(\mathbf{x}) > 0$, $\hat{P}(\mathbf{y}_1|\mathbf{x}) > 0$, and $w_j(\mathbf{x}) > 0$. Then $\frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})} = \frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})}$.*

Proof. The stated conditions ensure that the premises of Lemma 2 part (*ii*) hold. Thus, $P_{\boldsymbol{\theta}',j}(\mathbf{y}|\mathbf{x}) = \hat{P}_j(\mathbf{y}|\mathbf{x})$. But $\frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})} = \frac{\hat{P}_j(\mathbf{y}_2|\mathbf{x})}{\hat{P}_j(\mathbf{y}_1|\mathbf{x})}$ and $\frac{P_{\boldsymbol{\theta}',j}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}',j}(\mathbf{y}_1|\mathbf{x})} = \frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})}$ due to cancellation of partition functions, and we are done. □

Thus, the probability ratios according to $P_{\boldsymbol{\theta}'}$ match those according to $\hat{P}$ within a sub-objective set.

Definition 3. *We are given a set of sub-objectives C_j with weights $w_j(\mathbf{x})$. For a fixed feature value $\mathbf{x}$, we say that there is a* path *from $\mathbf{y}_1$ to $\mathbf{y}_2$ relative to probability distribution $P(\mathbf{Y}|\mathbf{x})$ if there is a sequence $S_{j_b} : b = 1, ..., k$ such that*

i. $\mathbf{y}_1 \in S_{j_1}$ *and* $\mathbf{y}_2 \in S_{j_k}$

ii. for every consecutive pair $S_{j_b}, S_{j_{b+1}}$, there exists $\mathbf{z}_b \in dom(\mathbf{Y})$ s.t. $\mathbf{z}_b \in S_{j_b}$, $\mathbf{z}_b \in S_{j_{b+1}}$, and $P(\mathbf{z}_b|\mathbf{x}) > 0$

iii. $w_{j_b}(\mathbf{x}) > 0$ for all j_b

Intuitively, this definition means that it is possible to "walk" from $\mathbf{y}_1$ to $\mathbf{y}_2$: if you are currently at value $\mathbf{y}$, you are allowed to move to any other value $\mathbf{y}'$ if $\mathbf{y}$ and $\mathbf{y}'$ both are contained in some sub-objective set S_j with positive weight $w_j(\mathbf{x})$. If $P(\mathbf{y}'|\mathbf{x}) = 0$, the walk must stop; otherwise it can continue.

Lemma 3. *Suppose that P_Θ can represent $\hat{P}(\mathbf{y}|\mathbf{x})$ and $\boldsymbol{\theta}'$ optimizes $C'(\boldsymbol{\theta}; D)$. Also, suppose that $\hat{P}(\mathbf{x}) > 0$, $\hat{P}(\mathbf{y}_1|\mathbf{x}) > 0$, and there is a path from $\mathbf{y}_1$ to $\mathbf{y}_2$ relative to $\hat{P}(\mathbf{Y}|\mathbf{x})$. Then $\frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})} = \frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})}$.*

Proof. By definition of path, there exists a sequence S_{j_b} such that $\mathbf{y}_1 \in S_{j_1}$, $\mathbf{y}_2 \in S_{j_k}$, $w_{j_b}(\mathbf{x}) > 0$, and for every consecutive pair $S_{j_b}, S_{j_{b+1}}$, there exists a $\mathbf{z}_b$ such that $\mathbf{z}_b \in S_{j_b}$, $\mathbf{z}_b \in S_{j_{b+1}}$, and $\hat{P}(\mathbf{z}_b) > 0$. This definition guarantees that the conditions of Corollary 1 hold for each sub-objective C_{j_b} (note that for C_{j_1}, both $\hat{P}(\mathbf{y}_1|\mathbf{x}) > 0$ and $\hat{P}(\mathbf{z}_1|\mathbf{x}) > 0$). It immediately follows that

$$\begin{aligned}\frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})} &= \frac{\hat{P}(\mathbf{z}_1|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})} * \frac{\hat{P}(\mathbf{z}_2|\mathbf{x})}{\hat{P}(\mathbf{z}_1|\mathbf{x})} \cdots * \frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{z}_{k-1}|\mathbf{x})} \\ &= \frac{P_{\boldsymbol{\theta}'}(\mathbf{z}_1|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})} * \frac{P_{\boldsymbol{\theta}'}(\mathbf{z}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{z}_1|\mathbf{x})} \cdots * \frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{z}_{k-1}|\mathbf{x})} \\ &= \frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})}\end{aligned}$$

□

We now have that the probability ratios according to $P_{\boldsymbol{\theta}'}(\mathbf{y}|\mathbf{x})$ match those according to $\hat{P}(\mathbf{y}|\mathbf{x})$ for any pair of values $\mathbf{y}_1, \mathbf{y}_2$ connected by a path (relative to $\hat{P}(\mathbf{Y}|\mathbf{x})$).

Definition 4. *For fixed* $\mathbf{x}$*, a set of sub-objectives* S_j *with weights* $w_j(\mathbf{x})$ span $\mathbf{Y}$ *relative to a probability distribution* $P(\mathbf{Y}|\mathbf{x})$ *if for every pair of values* $\mathbf{y}_1, \mathbf{y}_2$ *there is a path from* $\mathbf{y}_1$ *to* $\mathbf{y}_2$ *relative to* $P(\mathbf{Y}|\mathbf{x})$*.*

Note that this condition requires the total size of our sub-objectives to be at least the cardinality of $\mathbf{Y}$.

Let Θ' be the set of $\boldsymbol{\theta}'$ that optimize $C'(\boldsymbol{\theta}; D)$.

Theorem 2. *Suppose that* P_Θ *can represent* $\hat{P}(\mathbf{y}|\mathbf{x})$*. Furthermore, suppose that for every* $\mathbf{x}^i$ *(i.e., every value of* $\mathbf{X}$ *observed in* D*), our sub-objectives* S_j *with weights* $w_j(\mathbf{x}^i)$ *span* $\mathbf{Y}$ *relative to* $\hat{P}(\mathbf{Y}|\mathbf{x}^i)$*. Then* $\Theta' = \Theta[\hat{P}]$*. That is,* $\boldsymbol{\theta}'$ *optimizes* $C'(\boldsymbol{\theta}; D)$ *if and only if* $P_{\boldsymbol{\theta}'}(\mathbf{Y}|\mathbf{x}^i) = \hat{P}(\mathbf{Y}|\mathbf{x}^i)$ *for all* $\mathbf{x}^i$*.*

Proof. From Lemma 2, $\Theta[\hat{P}] \subseteq \Theta'$. We need to show that under the given conditions on $C'(\boldsymbol{\theta}; D)$, $\Theta' \subseteq \Theta[\hat{P}]$.

Let $\mathbf{x}$ be any feature value that occurs in D. Then $\hat{P}(\mathbf{x}) > 0$. Choose some $\mathbf{y}_1$ such that $\hat{P}(\mathbf{y}_1|\mathbf{x}) > 0$. By the definition of span, for every other value $\mathbf{y}_2$, there exists a path from $\mathbf{y}_1$ to $\mathbf{y}_2$ relative to $\hat{P}(\mathbf{Y}|\mathbf{x})$. From Lemma 3, $\frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})} = \frac{\hat{P}(\mathbf{y}_2|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})}$.

Suppose $\boldsymbol{\theta}'$ optimizes $C'(\boldsymbol{\theta}; D)$. Then for all $\mathbf{y}_2$, $P_{\boldsymbol{\theta}'}(\mathbf{y}_2|\mathbf{x}) = \frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})} * \hat{P}(\mathbf{y}_2|\mathbf{x})$. But $\frac{P_{\boldsymbol{\theta}'}(\mathbf{y}_1|\mathbf{x})}{\hat{P}(\mathbf{y}_1|\mathbf{x})}$ is simply some constant, and so $P_{\boldsymbol{\theta}'}$ and $\hat{P}$ differ only by a multiplicative

factor. But this immediately implies that they are the same distribution, $P_{\boldsymbol{\theta}'}(\mathbf{y}|\mathbf{x}) = \hat{P}(\mathbf{y}|\mathbf{x})$. Thus $\boldsymbol{\theta}' \in \Theta[\hat{P}]$ and $\Theta' \subseteq \Theta[\hat{P}]$. □

The optima of the log-likelihood objective are exactly $\Theta[\hat{P}]$ (provided P_Θ can represent $\hat{P}(\mathbf{y}|\mathbf{x})$). Thus, the optima of any contrastive objective fulfilling the conditions of the previous theorem are exactly the same as those of the log-likelihood objective.

5.4.3 Asymptotic Consistency

We will now extend the previous results to the case of infinite data. With the exception of Lemma 4, the proofs of all results in this section closely mirror the corresponding results from the previous section.

As before, let $\{d^1, d^2, \dots\}$ be an infinite sequence of examples drawn i.i.d from $P^*(\mathbf{X}, \mathbf{Y})$, with D^n and $\hat{P}(\mathbf{y}|\mathbf{x}; D^n)$ defined as before. Let $\boldsymbol{\theta}^{(n)}$ be a sequence of weight vectors $\{\boldsymbol{\theta}^1, \boldsymbol{\theta}^2, \dots\}$ such that for all n, $\boldsymbol{\theta}^n$ optimizes $C'(\boldsymbol{\theta}; D^n)$.

Lemma 4. *Suppose that P_Θ can represent $P^*(\mathbf{y}|\mathbf{x})$. Then for* any *contrastive objective C',*

i. For any $\boldsymbol{\theta}^* \in \Theta[P^*]$, $C'(\boldsymbol{\theta}^*; D^n) \xrightarrow{a.s.} 0$ as $n \to \infty$.

ii. For any $\boldsymbol{\theta}^{(n)}$ defined as above, for any $j, \mathbf{x}$ such that $P^*(\mathbf{x}) w_j(\mathbf{x})(\sum_{\mathbf{y} \in S_j} P^*(\mathbf{y}|\mathbf{x})) > 0$, $P_{\boldsymbol{\theta}^n, j}(\mathbf{y}|\mathbf{x}) \xrightarrow{a.s.} P^*_j(\mathbf{y}|\mathbf{x})$ as $n \to \infty$.

Proof. As noted above, $\hat{P}(\mathbf{y}|\mathbf{x}; D^n) \xrightarrow{a.s.} P^*(\mathbf{y}|\mathbf{x})$ as $n \to \infty$. This means that for $\boldsymbol{\theta}^* \in \Theta[P^*]$, $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}; D^n) || P_{\boldsymbol{\theta}^*, j}(\mathbf{y}|\mathbf{x})) \xrightarrow{a.s.} 0$ as $n \to \infty$ for all j. Thus $C'(\boldsymbol{\theta}^*; D^n) \xrightarrow{a.s.} 0$ as $n \to \infty$.

Now we prove (ii). From part (i), $C'(\boldsymbol{\theta}^*; D^n) \xrightarrow{a.s.} 0$ as $n \to \infty$. But since $\boldsymbol{\theta}^n$ optimizes $C'(\boldsymbol{\theta}; D^n)$, $C'(\boldsymbol{\theta}^n; D^n) \leq C'(\boldsymbol{\theta}^*; D^n)$ for all n. This implies that $C'(\boldsymbol{\theta}^n; D^n) \xrightarrow{a.s.} 0$ as $n \to \infty$.

Since $\hat{P}(\mathbf{y}|\mathbf{x}; D^n) \xrightarrow{a.s.} P^*(\mathbf{y}|\mathbf{x})$ as $n \to \infty$, it follows that there is some N such that for all $n \geq N$, $\hat{P}(\mathbf{y}|\mathbf{x}; D^n) > 0$ if and only if $P^*(\mathbf{y}|\mathbf{x}) > 0$. Thus, if $w_j(\mathbf{x}) \sum_{\mathbf{y} \in S_j} P^*(\mathbf{x}, \mathbf{y}) > 0$, then it is also the case that $w_j(\mathbf{x}) \sum_{\mathbf{y} \in S_j} \hat{P}(\mathbf{x}, \mathbf{y}; D^n) > 0$ for $n \geq N$. This means

that for sufficiently large n, if $w_j(\mathbf{x}) \sum_{\mathbf{y} \in S_j} P^*(\mathbf{x}, \mathbf{y}) > 0$, then $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}; D^n)||P_{\boldsymbol{\theta},j}(\mathbf{y}|\mathbf{x}))$ has a positive coefficient in $C'_j(\boldsymbol{\theta}; D^n)$.

Putting the previous two paragraphs together, $KL(\hat{P}_j(\mathbf{y}|\mathbf{x}; D^n)||P_{\boldsymbol{\theta}^n,j}(\mathbf{y}|\mathbf{x})) \overset{a.s.}{\to} 0$ as $n \to \infty$. But this implies $P_{\boldsymbol{\theta}^n,j}(\mathbf{y}|\mathbf{x}) \overset{a.s.}{\to} P^*_j(\mathbf{y}|\mathbf{x})$ as $n \to \infty$ and we are done. □

Corollary 2. *Suppose that P_Θ can represent $P^*(\mathbf{y}|\mathbf{x})$. Also suppose $\mathbf{y}_1, \mathbf{y}_2 \in S_j$, $P^*(\mathbf{x}) > 0$, $P^*(\mathbf{y}_1|\mathbf{x}) > 0$, and $w_j(\mathbf{x}) > 0$. Then for any $\boldsymbol{\theta}^{(n)}$, $\frac{P_{\boldsymbol{\theta}^n}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}^n}(\mathbf{y}_1|\mathbf{x})} \overset{a.s.}{\to} \frac{P^*(\mathbf{y}_2|\mathbf{x})}{P^*(\mathbf{y}_1|\mathbf{x})}$ as $n \to \infty$.*

Lemma 5. *Suppose that P_Θ can represent $P^*(\mathbf{y}|\mathbf{x})$. Also, suppose that $P^*(\mathbf{x}) > 0$, $P^*(\mathbf{y}_1|\mathbf{x}) > 0$, and there is a path from $\mathbf{y}_1$ to $\mathbf{y}_2$ relative to $P^*(\mathbf{Y}|\mathbf{x})$. Then for any $\boldsymbol{\theta}^{(n)}$, $\frac{P_{\boldsymbol{\theta}^n}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}^n}(\mathbf{y}_1|\mathbf{x})} \overset{a.s.}{\to} \frac{P^*(\mathbf{y}_2|\mathbf{x})}{P^*(\mathbf{y}_1|\mathbf{x})}$ as $n \to \infty$.*

Finally, we can prove full asymptotic consistency:

Theorem 3. *Suppose that P_Θ can represent $P^*(\mathbf{y}|\mathbf{x})$. Furthermore, suppose that for every $\mathbf{x}$ such that $P^*(\mathbf{x}) > 0$, our sub-objectives S_j with weights $w_j(\mathbf{x})$ span $\mathbf{Y}$ relative to $P^*(\mathbf{Y}|\mathbf{x})$. Then for any $\boldsymbol{\theta}^{(n)}$ and any $\mathbf{x}$ such that $P^*(\mathbf{x}) > 0$, $P_{\boldsymbol{\theta}^n}(\mathbf{Y}|\mathbf{x}) \overset{a.s.}{\to} P^*(\mathbf{Y}|\mathbf{x})$ as $n \to \infty$.*

Proof. Let $\mathbf{x}$ be any feature value such that $P^*(\mathbf{x}) > 0$. Choose some $\mathbf{y}_1$ such that $P^*(\mathbf{y}_1|\mathbf{x}) > 0$. From Lemma 5, for all other $\mathbf{y}_2$, $\frac{P_{\boldsymbol{\theta}^n}(\mathbf{y}_2|\mathbf{x})}{P_{\boldsymbol{\theta}^n}(\mathbf{y}_1|\mathbf{x})} \overset{a.s.}{\to} \frac{P^*(\mathbf{y}_2|\mathbf{x})}{P^*(\mathbf{y}_1|\mathbf{x})}$ as $n \to \infty$. From here it is a technical exercise to show that $P_{\boldsymbol{\theta}^n}(\mathbf{Y}|\mathbf{x}) \overset{a.s.}{\to} P^*(\mathbf{Y}|\mathbf{x})$ as $n \to \infty$, and we are done. □

From this result we can derive consistency of pseudo-likelihood for strictly positive data distributions $P_{\boldsymbol{\theta}^*}$ (i.e., $P_{\boldsymbol{\theta}^*}(\mathbf{y}|\mathbf{x}) > 0$ for all $\mathbf{y}, \mathbf{x}$), simply by noting that in the limit of infinite data, the set of active PL sub-objectives will span $\mathbf{Y}$. It is also easy to see why PL is usually not consistent with finite data (it is unlikely to span the space), and why it may not be consistent for non-positive data distributions (again, because it may not span the space).

The most important practical implication from this section is that a contrastive objective attempts to calibrate probabilities within connected components of sub-objectives but cannot calibrate probabilities between disconnected components. This

has important implications for the performance of PL (and other local contrastive objectives), as we will see in Section 5.9.

5.5 Weight Decomposition

So far we have not examined the effect of the choice of weights $w_j(\mathbf{x})$ beyond whether $w_j(\mathbf{x}) > 0$. In order to better understand the effect of the weights on the objective, we will rewrite the weights as a product of three terms, $w_j(\mathbf{x}) = w(\mathbf{x}) * \sum_{\mathbf{y}} P(C_j|\mathbf{y}, \mathbf{x})Q(\mathbf{y}|\mathbf{x})$, each of which is chosen by the designer of the contrastive objective.

The first term $w(\mathbf{x})$ allows the designer to reweight the relative importance of terms in the objective corresponding to different values of $\mathbf{x}$. This could be useful if we believe that the empirical distribution $\hat{P}(\mathbf{x})$ observed in our data does not match the true (or desired) distribution over $\mathbf{x}$ (in general, we assume that $\hat{P}(\mathbf{y}|\mathbf{x})$ must be drawn from the true underlying distribution, but this may or may not be the case for $\hat{P}(\mathbf{x})$). These weights can also be used in standard maximum likelihood training and are related to work in the area of domain adaptation (see, for example, (Mansour et al., 2009)). We will not focus on this part of the weights in this paper, assuming that they are uniform across all $\mathbf{x}$. The second term $P(C_j|\mathbf{y}, \mathbf{x})$ allows the designer to choose the relative importance of different sub-objectives for a particular value of the label variable $\mathbf{y}$ (and also relative to a feature value $\mathbf{x}$). $P(C_j|\mathbf{y}, \mathbf{x})$ is constrained to be a probability distribution such that $P(C_j|\mathbf{y}, \mathbf{x}) > 0$ only when $\mathbf{y} \in S_j$. The third term $Q(\mathbf{y}|\mathbf{x})$ is an auxiliary probability distribution that allows the designer to choose how important each $\mathbf{y}$ is to the objective.

Putting these terms together, $w_j(\mathbf{x}) = w(\mathbf{x}) * \sum_{\mathbf{y}} P(C_j|\mathbf{y}, \mathbf{x}) * Q(\mathbf{y}|\mathbf{x})$. Since P and Q are both probability distributions, the sum of all weights $w_j(\mathbf{x})$ for a given $\mathbf{x}$ is $w(\mathbf{x})$. This means that P and Q do not affect the relative influence of different values of $\mathbf{x}$. This decomposition of the weights $w_j(\mathbf{x})$ is over-parametrized; in particular, it is not hard to show that we can write any choice of $w_j(\mathbf{x})$ in this form. Specifically, let $w(\mathbf{x}) = \sum_j w_j(\mathbf{x})$, and define $P'(C_j|\mathbf{x}) = \frac{w_j(\mathbf{x})}{\sum_j w_j(\mathbf{x})}$. We now simply need to choose

distributions $P(C_j|\mathbf{y},\mathbf{x})$, $Q(\mathbf{y}|\mathbf{x})$ such that $P'(C_j|\mathbf{x}) = \sum_{\mathbf{y}} P(C_j|\mathbf{y},\mathbf{x}) * Q(\mathbf{y}|\mathbf{x})$. One way to do this is as follows. First, order $\mathbf{Y}$. Starting with $\mathbf{y}_1$, find all C_j such that $\mathbf{y}_1 \in S_j$. Set $Q(\mathbf{y}_1|\mathbf{x}) = \sum_{j:\mathbf{y}_1 \in S_j} P'(C_j|\mathbf{x})$, and set $P(C_j|\mathbf{y},\mathbf{x}) = \frac{P'(C_j|\mathbf{x})}{Q(\mathbf{y}_1|\mathbf{x})}$. It is easy to see that for j such that $\mathbf{y}_1 \in S_j$, $P'(C_j|\mathbf{x}) = P(C_j|\mathbf{y}_1,\mathbf{x}) * Q(\mathbf{y}_1|\mathbf{x})$. We now simply do the same for all remaining $\mathbf{y}$, except that we ignore any sub-objectives C_j which contain a $\mathbf{y}'$ earlier in the ordering.

5.6 Choosing Sub-objectives: Approximating LL

Based on the weight decomposition in the previous section, we can now prove a strong relationship between a particular contrastive objective and the log-likelihood function $LL(\boldsymbol{\theta}; D)$:

Lemma 6. *Let C contain a sub-objective S_{jk} for every pair of instantiations $\mathbf{y}_j, \mathbf{y}_k$ (including singleton sub-objectives where $\mathbf{y}_j = \mathbf{y}_k$). Let $w(\mathbf{x}) = |\mathbf{Y}|$ for all $\mathbf{x}$, let $P(C_{jk}|\mathbf{y},\mathbf{x}) = \frac{1}{|\mathbf{Y}|}$ if $\mathbf{y} \in C_{jk}$, 0 otherwise (i.e., P is uniform over sub-objectives containing $\mathbf{y}$), and $Q(\mathbf{y}|\mathbf{x}) = P_{\boldsymbol{\theta}_0}(\mathbf{y}|\mathbf{x})$ for some fixed parameter vector $\boldsymbol{\theta}_0$. Then $\frac{dC}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}_0} = \frac{dLL}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}_0}$.*

Proof. We have

$$\begin{aligned} w_{jk}(\mathbf{x}) &= |\mathbf{Y}| * \sum_{\mathbf{y}} I(\mathbf{y} \in \{\mathbf{y}_j, \mathbf{y}_k\}) * \frac{1}{|\mathbf{Y}|} * P_{\boldsymbol{\theta}_0}(\mathbf{y}|\mathbf{x}) \\ &= P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}). \end{aligned}$$

Plugging into the contrastive objective formula, we have

$$\sum_{jk} \sum_{(\mathbf{x}^i,\mathbf{y}^i):\mathbf{y}^i \in S_{jk}} (P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x})) P_{\boldsymbol{\theta},jk}(\mathbf{y}^i|\mathbf{x}^i)$$

$$= \sum_{(\mathbf{x}^i,\mathbf{y}^i)} \sum_{jk:\mathbf{y}^i = \mathbf{y}_j} (P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x})) P_{\boldsymbol{\theta},jk}(\mathbf{y}^i|\mathbf{x}^i)$$

Taking the derivative with respect to some parameter θ_l, we have

$$\sum_{(\mathbf{x}^i,\mathbf{y}^i)} \sum_{jk:\mathbf{y}^i=\mathbf{y}_j} (P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}^i) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i)) * \left(f_l(\mathbf{x}^i,\mathbf{y}^i) - \frac{f_l(\mathbf{x}^i,\mathbf{y}_j)e^{\boldsymbol{\theta}^T f(\mathbf{x}^i,\mathbf{y}_j)} + f_l(\mathbf{x}^i,\mathbf{y}_k)e^{\boldsymbol{\theta}^T f(\mathbf{x}^i,\mathbf{y}_k)}}{e^{\boldsymbol{\theta}^T f(\mathbf{x}^i,\mathbf{y}_j)} + e^{\boldsymbol{\theta}^T f(\mathbf{x}^i,\mathbf{y}_k)}} \right)$$
$$= \sum_{(\mathbf{x}^i,\mathbf{y}^i)} \sum_{jk:\mathbf{y}^i=\mathbf{y}_j} (P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}^i) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i)) * \left(f_l(\mathbf{x}^i,\mathbf{y}^i) - \frac{f_l(\mathbf{x}^i,\mathbf{y}_j)P_{\boldsymbol{\theta}}(\mathbf{y}_j|\mathbf{x}^i) + f_l(\mathbf{x}^i,\mathbf{y}_k)P_{\boldsymbol{\theta}}(\mathbf{y}_k|\mathbf{x}^i)}{P_{\boldsymbol{\theta}}(\mathbf{y}_j|\mathbf{x}^i) + P_{\boldsymbol{\theta}}(\mathbf{y}_k|\mathbf{x}^i)} \right).$$

Evaluating at $\boldsymbol{\theta} = \boldsymbol{\theta}_0$ and multiplying through, we get

$$\sum_{(\mathbf{x}^i,\mathbf{y}^i)} \sum_{jk:\mathbf{y}^i=\mathbf{y}_j} (f_l(\mathbf{x}^i,\mathbf{y}^i)P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}^i) + f_l(\mathbf{x}^i,\mathbf{y}^i)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) - f_l(\mathbf{x}^i,\mathbf{y}_j)P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}^i) - f_l(\mathbf{x}^i,\mathbf{y}_k)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i))$$

But since $\mathbf{y}_j = \mathbf{y}^i$ in the summation, we can cancel to get

$$\sum_{(\mathbf{x}^i,\mathbf{y}^i)} \sum_{k} \left(f_l(\mathbf{x}^i,\mathbf{y}^i)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) - f_l(\mathbf{x}^i,\mathbf{y}_k)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) \right)$$
$$= \sum_{(\mathbf{x}^i,\mathbf{y}^i)} \left(f_l(\mathbf{x}^i,\mathbf{y}^i) \sum_k P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) - \sum_k f_l(\mathbf{x}^i,\mathbf{y}_k)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) \right)$$
$$= \sum_{(\mathbf{x}^i,\mathbf{y}^i)} \left(f_l(\mathbf{x}^i,\mathbf{y}^i) - \sum_k f_l(\mathbf{x}^i,\mathbf{y}_k)P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}^i) \right).$$

But this is exactly the derivative of LL at $\boldsymbol{\theta}_0$ (observed minus expected). □

Thus, at any point $\boldsymbol{\theta}$ in weight space, we can construct a contrastive objective tangent to log-likelihood at $\boldsymbol{\theta}$. As a result, we can optimize LL using an EM-like algorithm. We initialize with weight vector $\boldsymbol{\theta}_0$. During the i^{th} Expectation step, we update $Q(\mathbf{y}|\mathbf{x}) = P_{\boldsymbol{\theta}_{i-1}}(\mathbf{y}|\mathbf{x})$. During the i^{th} Maximization step, we fix Q and use C to compute the gradient of log-likelihood at $\boldsymbol{\theta}_{i-1}$. We then take a step in the

direction of the gradient, obtaining a new weight vector $\boldsymbol{\theta}_i$. This algorithm has some similarities to an algorithm proposed by Hoefling & Tibshirani (2009) for optimizing log-likelihood using a series of pseudo-likelihoods. Significant differences are that our algorithm is more general, using any contrastive objective; and our method uses approximations that are within the parametric family of contrastive objectives, while the method proposed by Hoefling & Tibshirani (2009) approximates using a modified PL term.

There are several limitations on the practical use of this result. First, computing the auxiliary distribution Q requires computing the global partition function $Z_{\boldsymbol{\theta}_0}(\mathbf{x})$. There is a workaround, however: in addition to setting $Q(\mathbf{y}|\mathbf{x}) = P_{\boldsymbol{\theta}_0}(\mathbf{y}|\mathbf{x})$, we also (implicitly) set $w(\mathbf{x}) = |\mathbf{Y}| * Z_{\boldsymbol{\theta}_0}(\mathbf{x})$. The resulting weight $w_{jk}(\mathbf{x}) = (|\mathbf{Y}| * Z_{\boldsymbol{\theta}_0}(\mathbf{x})) * \sum_{\mathbf{y} \in C_{jk}} \frac{1}{|\mathbf{Y}|} * P_{\boldsymbol{\theta}_0}(\mathbf{y}|\mathbf{x}) = Z_{\boldsymbol{\theta}_0} * (P_{\boldsymbol{\theta}_0}(\mathbf{y}_j|\mathbf{x}) + P_{\boldsymbol{\theta}_0}(\mathbf{y}_k|\mathbf{x}) = e^{\boldsymbol{\theta}_0^T \mathbf{f}(\mathbf{y}_j, \mathbf{x})} + e^{\boldsymbol{\theta}_0^T \mathbf{f}(\mathbf{y}_k, \mathbf{x})}$. This final expression is simply the exponentiated scores of two different examples, so it is easy to compute. The cost of this modification is that we have affected the relative importance of different values of $\mathbf{x}$ in the contrastive objective C. If $\mathbf{x}$ is empty (e.g., we are working with an unconditioned Markov network), this does not affect the objective at all (beyond a multiplicative rescaling). For the general case, this will only be a problem if $Z_{\boldsymbol{\theta}_0}(\mathbf{x})$ varies wildly for different $\mathbf{x}$; even in this case, since the effect of the partition function is less direct than in maximum likelihood, we might expect approximation schemes for $Z_{\boldsymbol{\theta}_0}(\mathbf{x})$ to work well.

A second limitation is that exact computation of the gradient still requires an exponential number of sub-objectives. However, this way of looking at computing the gradient may lead to new approximation schemes for optimizing LL.

5.7 Choosing Sub-objectives: Fixed Methods

In practice we are not going to be able to span $\mathbf{Y}$ with our sub-objectives. An obvious approximation is to drop sub-objectives. The effect of this will be to partition the domain of $\mathbf{Y}$; within each connected component the objective will attempt to calibrate probabilities, but probabilities will not be calibrated across components. In

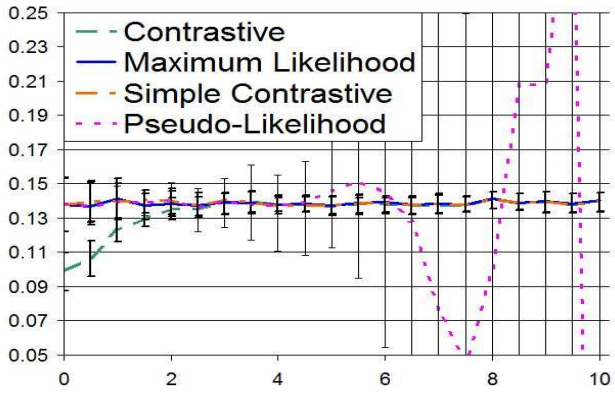


Figure 5.7: Estimate of λ_0 (y-axis) vs. λ_1 used to generate the data (x-axis). The plot shows median learned parameter value over 100 synthetic data sets, each with 1000 instances. Error bars indicate 25^{th} and 75^{th} percentile estimates. Correct $\lambda_0 = .139$. Error bars for PL extend off graph for large λ_1.

this section, we propose several techniques for constructing tractable objectives and examine some of their properties. The methods discussed in this chapter are *fixed* — a single contrastive objective is constructed and optimized. In Section 5.8, we will explore an *iterative* method, in which the contrastive objective changes as the algorithm runs.

5.7.1 Simple Fixed Methods

One obvious method for constructing sub-objectives is to use expert knowledge to determine useful values to compare. In pseudo-likelihood, for example, each sub-objective corresponds to instantiations that differ on a (particular) single variable. In generalized PL, sub-objectives contain all instantiations that differ on a particular subset of variables.

As a concrete example of a sub-objective that is not possible using (generalized) PL, we consider a binary chain MRF consisting of 10 nodes. The model is unconditional (i.e., $\mathbf{x}$ is empty), and it has only two parameters: a single bias term specifying the relative weight of 0 vs. 1; and a single affinity term that specifies how likely two

neighboring nodes are to have the same value. Thus, the log-score of an instantiation is $\lambda_0 * |y_i = 1| + \lambda_1 * |y_i = y_{i+1}|$. For large λ_1, the instantiations $\{000000000\}$ and $\{1111111111\}$ have much higher probability than any other instantiations; thus, we expect PL to have trouble fitting λ_0 in this case, since it does not directly compare the probabilities of these two instantiations. However, we can easily augment the PL objective with an additional sub-objective containing exactly these two values — we refer to this objective as Simple Contrastive. Figure 5.7 shows the error in the estimate of λ_0 as we vary the affinity parameter λ_1. Simple Contrastive is able to accurately reconstruct λ_0 for all values of λ_1, while PL is not. Contrastive objectives constructed in this way can be quite powerful but are somewhat difficult to design. We discuss this issue further in Section 5.7.3.

A different kind of approach is to use the data D to guide the selection of sub-objectives. For unconditioned Markov networks, a simple approach is to construct sub-objectives that compare different observed values of the label variables $\mathbf{y}^i$. This ensures that far-apart instantiations are compared (assuming that the data contains such instantiations). We employed this strategy for the MRF described above, augmenting PL with a single sub-objective containing all values observed in D. This objective is referred to as Contrastive. As shown in Figure 5.7, Contrastive is also effective at recovering λ_0, although for low values of λ_1, the estimate is slightly inaccurate. We discuss this further in the next section.

5.7.2 Bias

In the previous section, we made a distinction between methods that choose sub-objectives ahead of time and those that choose sub-objectives using D. We now formalize this idea and briefly discuss the differences between the two methods.

A method for choosing sub-objectives is *data-independent* if the weights $w_j(\mathbf{x})$ do not depend on D. Put another way, $w_j(\mathbf{x})$ must be the same regardless of the examples observed in D. A method is *data-dependent* if it is not data-independent. Constructing a useful data-independent contrastive objective is generally more difficult than constructing a data-dependent objective, but data-independent objectives

have a significant advantage:

Lemma 7. *Suppose that $w_j(\mathbf{x})$ does not depend on D. Then $E_{P^*}[\frac{dC(\boldsymbol{\theta};D)}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}_0}] = \frac{dC(\boldsymbol{\theta};D^*)}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}_0}$ for all $\boldsymbol{\theta}_0$, where D^* is a data set (of possibly infinite size) such that $\hat{P}(\mathbf{y}|\mathbf{x};D^*) = P^*(\mathbf{y}|\mathbf{x})$.*

Proof. Taking the derivative of $C(\boldsymbol{\theta};D)$ with respect to parameter θ_l and plugging in $\boldsymbol{\theta}_0$, we get

$$\sum_j \sum_{(\mathbf{x}^i,\mathbf{y}^i):\mathbf{y}^i \in S_j} w_j(\mathbf{x}^i) * (f_l(\mathbf{x}^i,\mathbf{y}^i) - E_{P_{\boldsymbol{\theta}_0,j}(\mathbf{y}|\mathbf{x}^i)}[f_l(\mathbf{x}^i,\mathbf{y})])$$

$$= \sum_{j,\mathbf{x}} w_j(\mathbf{x}) \sum_{\mathbf{y}\in S_j} \hat{P}(\mathbf{x},\mathbf{y})(f_l(\mathbf{x},\mathbf{y}) - E_{P_{\boldsymbol{\theta}_0,j}(\mathbf{y}|\mathbf{x})}[f_l(\mathbf{x},\mathbf{y})])$$

The only term in the expression that depends on D is $\hat{P}(\mathbf{x},\mathbf{y})$. Thus, by linearity of expectation, we have that $E_{P^*}[\frac{dC(\boldsymbol{\theta};D)}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}_0}]$ is equal to

$$\sum_{j,\mathbf{x}} w_j(\mathbf{x}) \sum_{\mathbf{y}\in S_j} E_{P^*}[\hat{P}(\mathbf{x},\mathbf{y})](f_l(\mathbf{x},\mathbf{y}) - E_{P_{\boldsymbol{\theta}_0,j}(\mathbf{y}|\mathbf{x})}[f_l(\mathbf{x},\mathbf{y})]).$$

But $E_{P^*}[\hat{P}(\mathbf{x},\mathbf{y})] = P^*(\mathbf{x},\mathbf{y})$, and we are done. If the objective data-dependent (i.e., $w_j(\mathbf{x})$ depends on D), then we can no longer push the expectation inside of the summations, and in general the equality no longer holds. □

This lemma shows that for a data-independent method, we get an unbiased estimate of the gradient at any point $\boldsymbol{\theta}_0$. Suppose that P_Θ can represent $P^*(\mathbf{y}|\mathbf{x})$. In this case, we can apply this lemma at $\boldsymbol{\theta}_0 = \boldsymbol{\theta}^*$ to get that the expectation D of the gradient at $\boldsymbol{\theta}^*$ is 0. Loosely speaking, this means that the learned parameters for different D sampled from P^* will be centered around $\boldsymbol{\theta}^*$. Data-dependent methods have no such guarantee. This bias in the gradient is precisely the reason why Contrastive in Figure 5.7 gives an inaccurate estimate for λ_0 for small values of λ_1. Since data-dependent contrastive objectives are more flexible than data-independent ones, this bias may often be acceptable in practice.

5.7.3 Data-Independent Objective Example

As we have seen, bias can be an issue for data-dependent contrastive objectives. Unfortunately, data-independent contrastive objectives are considerably harder to construct. We will now go through a detailed example of constructing a data-independent objective in order to demonstrate some of the issues that can arise.

Suppose we are trying to classify pixels of an image into a variety of different classes (e.g., person, tree, etc.); see Section 5.9 for a concrete example. In some cases, our model might correctly determine that a large part of the image belongs to the same class, but be unsure about the label (e.g., is it water or road?). Pseudo-likelihood only considers flipping a single basic unit (i.e., pixel). We will now construct a contrastive objective that flips much larger blocks of pixels.

A simple first approach would be to allow any group of adjacent pixels that are labeled with the same label in the correct labeling $\mathbf{y}^i$ to switch to a different class. This corresponds to having one sub-objective for every possible image plus every possible hole; the sub-objective contains one instantiation for each class, where all pixels in the hole are filled in with that class. Note that this contrastive objective is not a special case of Generalized PL because it does not consider all possible combinations of values for the pixels that were flipped. Unfortunately, while this contrastive objective is data-independent, it is intractable because an exponential number of sub-objectives are active for any image such that y^i has a large solid-label block — we have one active sub-objective for every possible connected sub-region of this block.

A second approach is to only allow maximal groups to be flipped. This immediately reduces the number of active sub-objectives to be linear in the number of pixels. However, it also inadvertently causes the contrastive objective to become data-dependent. Suppose that a maximal group g in $\mathbf{y}^i$ which is originally labeled "water" is flipped to be "street," creating labeling $\mathbf{y}'$. Also, suppose that adjacent to g there is another group already labeled "street." Then in $\mathbf{y}'$, g is no longer a maximal group. Thus, the sub-objective containing $\mathbf{y}^i$ and $\mathbf{y}'$ is active if $\mathbf{y}^i$ is observed in the data D, but not if $\mathbf{y}'$ is observed instead, and so this construction is data-dependent.

Fortunately, a simple tweak of this approach produces a tractable data-independent contrastive objective. We simply require that only maximal groups can be flipped; and they can only be flipped to values that are different from the values of all neighboring groups. This contrastive objective is still quite powerful and is guaranteed to produce an unbiased estimate of the gradient.

To provide one more example of a data-independent contrastive objective for this problem, we could allow *all* pixels that are labeled with a particular label a in $\mathbf{y}^i$ to flip to some other value b, but only if there are no pixels labeled b in $\mathbf{y}^i$.

Note that this discussion is similar to issues that arise when designing reversible transition distributions for Metropolis-Hastings MCMC samplers (Metropolis et al., 1953; Hastings, 1970; Chib & Greenberg, 1995). Just as here, it is important to ensure that if you can transition from y to y', then you can also transition from y' to y.

5.8 Choosing Sub-objectives: CCG

While useful for some problems, the basic approaches presented above are not particularly flexible. In this section, we propose an iterative data-dependent method for constructing contrastive objectives called Contrastive Constraint Generation (CCG).

In CCG, we begin by building an initial contrastive objective C_0 containing relatively few sub-objectives. During iteration t, we first optimize C_{t-1} to obtain a new weight vector $\boldsymbol{\theta}_t$. Next, for each example d^i, we find one or more "interesting" instantiations based on the current model $P_{\boldsymbol{\theta}_t}(\mathbf{y}|\mathbf{x})$. Finally, we construct a new contrastive objective C_t that incorporates these new instantiations into C_{t-1}. We repeat this process until convergence (or until we decide to stop). We will now describe the details of each of these steps.

Initialization. We consider two possible initializations: empty (no sub-objectives); and adding all sub-objectives from Pseudo-Likelihood.

Optimization. We optimize C_{t-1} using a method such as BFGS.

Finding Interesting Instantiations. We consider two general methods for finding new instantiations. For simplicity, we assume that only one new instantiation is generated per round per example, referred to as $\mathbf{y}_t^i$.

The first general method is to use an approximate MAP inference algorithm, such as ICM or MP (described in Section 2.2.2), to find a high probability $\mathbf{y}$ according to $P_{\boldsymbol{\theta}_t}(\mathbf{y}|\mathbf{x}^i)$. We also tried a third inference method based on dual decomposition, proposed by Komodakis et al. (2007), but this method obtained similar results to MP while being significantly slower; we do not present results for dual decomposition in this thesis.

The second general method uses a sampling algorithm such as Gibbs sampling to generate one or more instantiations. Contrastive divergence takes this second approach, with the sampling algorithm initialized at $\mathbf{y}^i$ and run for only a few steps. If we use this approximate sampling procedure, we end up with an algorithm that has many similarities with CD. The main differences are that CCG uses $P_{\boldsymbol{\theta}}$ to score the instantiations while CD uses $P_{\boldsymbol{\theta}}^k$; and CD can only use stochastic gradient methods for optimization.

Building a New Objective. We propose two simple strategies for incorporating the new instantiations. The *group* strategy: for each example d^i, build a sub-objective C_{d^i} such that, at iteration t, S_{d^i} contains the correct label $\mathbf{y}^i$ as well as $\mathbf{y}_{t'}^i$ for all $t' \leq t$ (since S_{d^i} is a set, duplicate values are ignored). This is the strategy we will take in Section 5.9. The *pairwise* strategy: for each example d^i and each $\mathbf{y}_{t'}^i$, $t' \leq t$, include a pairwise sub-objective that compares $\mathbf{y}^i$ to $\mathbf{y}_{t'}^i$. Here we can choose to ignore duplicates as in the group method, or we can weight sub-objectives based on the number of times each value has occurred. One additional choice is how to weight the additional sub-objectives against the initial sub-objectives contained in C_0.

Convergence. When duplicate instantiations are ignored, convergence is reached when, for all examples, $\mathbf{y}_t^i$ has already been seen, i.e., there exists a $t' < t$ s.t. $\mathbf{y}_t^i = \mathbf{y}_{t'}^i$. Otherwise, we could stop when the round-to-round decrease in the training error becomes small (or some other performance-based metric is satisfied).

As we will see in Section 5.9, this type of method works well in practice, particularly

Figure 5.8: Original image and correct region labeling

when our method for finding instantiations produces instantiations far away from $\mathbf{y}^i$.

5.9 Experimental Results

In this section, we explore the application of CCG to a real-world machine vision problem. We use the street scenes image data set described by Gould et al. (2009), consisting of 710 images. Every pixel in each image is labeled with one of eight classes. To reduce the computational burden and to have access to more coherent features, we take as input the regions as predicted in Gould et al. (2009). An example segmentation into regions is shown in Figure 5.8. This limits the maximum pixel-wise accuracy: the best-possible labeling of regions for this data obtains pixel-wise error of 12.0% (Lower Bound in Table 5.1).

Our model for this task is a conditional random field using intra-region (single node) and inter-region (pairwise) features, also taken from Gould et al. (2009). The single node features capture appearance features of each class: road tends to be gray, sky is blue and textureless, etc. The edge features capture relationships between neighboring regions. Unlike classification for pixels or super-pixels, it is not the case that a region of one class is extremely likely to border other regions with that class,

since regions can cover entire objects. The edge features can capture relationships like "cars" are next to "roads" or "cars" are not next to "water".

We tested the following learning algorithms:

Independent (I). Only the singleton potentials are used during training. This method is equivalent to logistic regression with individual regions as training examples.

Pseudo-Likelihood (PL). See Section 5.3.2.

Contrastive Divergence (CD). Each iteration, we generate a single sample for each data example d^i and use it to compute a stochastic approximation to the gradient. We use Gibbs sampling to generate the samples, following standard practice for CD (see, for example, Bengio (2009)). We tested three variants: CD-1, which generates samples using one round of Gibbs[2]; CD-10, which uses 10 rounds of Gibbs per sample; and CD-100, using 100 rounds. We ran each variant for a total of 10,000 seconds, which corresponded to 50k, 16.5k, and 2k iterations, respectively.

Max-margin Cutting Planes (MM). This is a constraint-generation algorithm proposed by Tsochantaridis et al. (2005). This method uses a margin-based objective, which tries to find a weight vector $\boldsymbol{\theta}$ such that for every d^i, the score $\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i, \mathbf{y}^i)$ of the correct label $\mathbf{y}^i$ is larger than $\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i, \mathbf{y}) + \Delta(\mathbf{y}, \mathbf{y}^i)$ for any other $\mathbf{y}$, where $\Delta(\mathbf{y}, \mathbf{y}^i)$ is a loss function that measures how far away $\mathbf{y}$ is from $\mathbf{y}^i$. For these experiments, we use pixel-wise error as our loss function. The cutting plane algorithm finds at each step the most violated constraint, which corresponds to, for each d^i, finding the $\mathbf{y}$ that maximizes $\boldsymbol{\theta}^T\mathbf{f}(\mathbf{x}^i, \mathbf{y}) + \Delta(\mathbf{y}, \mathbf{y}^i)$; it then adds a new constraint based on these values. To find the most violated constraint, we tried using (appropriately modified versions of) both ICM and MP, which we refer to as ICM-MV and MP-MV. For our reported results, we initialize with an empty constraint set; initializing with constraints corresponding to PL instantiations did not improve performance. This method has a hyper-parameter C which we chose to maximize performance on a small subset of the test set. This method usually converges in about 150-170 iterations.

Contrastive Constraint Generation (CCG). This is our method as described

[2]In one round of Gibbs sampling, each node is resampled once, in random order.

in Section 5.8. For initialization, we tried empty initialization and using the PL sub-objectives. We tried seven total ways of generating instantiations. First, we use the same sampling procedures as the CD variants — Gibbs-1, Gibbs-10, and Gibbs-100. This version of our algorithm is closely related to CD. Next, we ran the approximate map procedures ICM and MP on the current model to generate instantiations. Finally, we use the most-violated constraint procedures ICM-MV and MP-MV. We refer to, for example, CCG with MP instantiations and empty initialization as CCG(MP); with PL initialization, CCG(MP+PL). The number of iterations required to reach convergence varied based on the initialization and instantiation method, from about 20 iterations for CCG(ICM) to 85 with CCG(MP+PL), while for the Gibbs variants, convergence is not reached within 100 iterations (we stopped at this point).

To evaluate the learned weights, we need a maximum a-posterior (MAP) inference algorithm to produce the most likely labeling at test time. We found that ICM consistently outperformed MP as a test-time inference algorithm, so for the main results in this section we use ICM for test-time inference. Results are generated using 10-fold cross-validation on the 710 images, reporting pixel-wise error. Standard deviations are computed based on the individual results for each fold.

Table 5.1 shows all tested algorithms except for CCG with empty initialization; Figure 5.9 shows the same results in chart form. Based on the computed standard deviations, a difference in error of about .01 is statistically significant according to an unpaired t-test. There are two important things to note in this table. First, methods using non-local instantiations clearly outperform methods using the more local instantiations generated by Gibbs sampling (even when Gibbs is run for 100 rounds). The best non-local method, CCG(MP-MV+PL), decreases absolute error over the best local method, CCG(Gibbs-100+PL), by 2.7%, a 12% relative reduction in error. Second, CCG significantly outperforms the other non-local method, MM, by a similar margin; CCG(MP-MV+PL) reduces absolute error from MM(ICM-MV) by 2.7% (12% relative error reduction).

Interestingly, CCG is the only algorithm to improve substantially over Independent. In particular, PL more than doubles the pixel-wise error rate. This can be explained

Learning Method	Error	SD
Lower Bound	.120	.005
Independent	.225	.014
PL	.461	.044
CD-1	.225	.016
CD-10	.219	.015
CD-100	.225	.014
MM(ICM-MV)	.217	.009
MM(MP-MV)	.218	.007
CCG(Gibbs-1+PL)	.225	.016
CCG(Gibbs-10+PL)	.218	.015
CCG(Gibbs-100+PL)	.217	.015
CCG(ICM+PL)	.200	.013
CCG(MP+PL)	.198	.015
CCG(ICM-MV+PL)	.192	.011
CCG(MP-MV+PL)	**.190**	.013

Table 5.1: Pixel-wise ICM test error with standard deviation (SD)

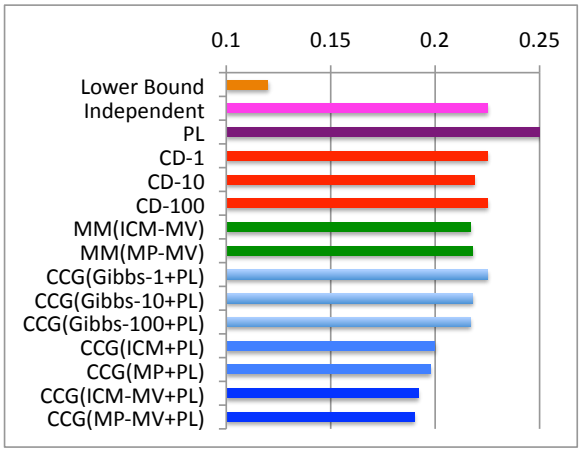


Figure 5.9: Pixel-wise ICM test error. Colors denote groups of similar algorithms. The bar for PL extends off the chart.

by the fact that labels of neighboring regions are highly correlated — PL relies heavily on this during training, but at test time, the neighbors are no longer given. The strong locality of PL is a significant disadvantage for this problem.

For all three instantiation generation methods, initializing CCG using PL resulted in small but noticeable gains when using ICM at test time (absolute difference ranging from .004 to .007). Additionally, it significantly reduced the number of iterations required to reach convergence. Interestingly, if we use MP as the test-time inference method, we get extremely bad results if we use an empty initialization (absolute difference ranging from .145 to .295).

So far, we have reported the number of iterations for each algorithm, which measures how many times the instantiation generation method was called. However, the algorithms perform differing amounts of work at each iteration, ranging from CD (least) to CCG (most). Figure 5.10 shows test accuracy vs. running time for the CD variants as well as for CCG(ICM+PL). The number of iterations pictured is 50k, 16.5k, 2k, and 6, for CD-1, CD-10, CD-100, and CCG(ICM+PL), respectively. CD-1

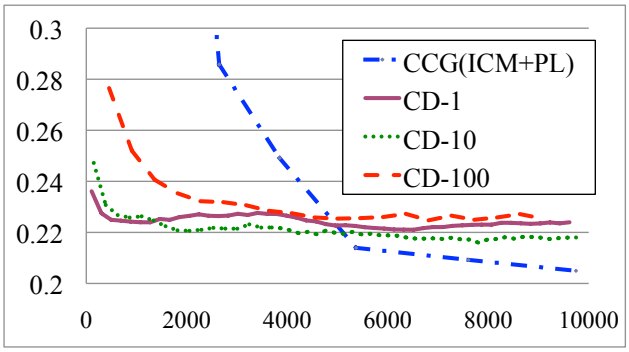


Figure 5.10: Test Error vs. Running Time (in seconds)

has converged, CD-10 probably has, while CD-100 has not. Despite the very small number of iterations for CCG, it is already significantly outperforming CD at this point. This shows that the non-local instantiations generated by ICM are much more informative than the instantiations generated by Gibbs sampling.

In fact, the difference between local and non-local methods is even greater than this graph suggests. After six iterations, CCG(Gibbs-1+PL), CCG(Gibbs-10+PL), and CCG(Gibbs-100+PL) have error rates .234, .227, and .229, respectively, vs. .205 for CCG(ICM+PL); all have similar running times. In general, CD-n is much faster than CCG(Gibbs-n+PL), with comparable results at convergence (although neither type was run to full convergence for all values of n). The main reason for this is that batch optimization is much slower than stochastic optimization, at least initially. In future work, we plan to implement a stochastic gradient descent version of CCG and compare it to CD.

MM is quite fast, requiring only 3 minutes to fully converge. There is no obvious method for choosing additional constraints to add to the objective after reaching convergence, so we do not have a way to trade off time vs. performance for MM. Most likely, MM is stuck at a sub-optimal solution due to the use of approximate MAP inference.

We also examined the effect of different test-time inference strategies on the results. We tried three algorithms: ICM, MP, and Singleton. In the Singleton method, we

Learning Method	Inference (Test)		
	Single	ICM	MP
Singleton	.225	.225	.225
PL	.235	.461	.549
CD(Gibbs-1)	.235	.225	.241
MM(ICM-MV)	.223	.217	.218
CCG(MP+PL)	.206	.198	.210
CCG(MP-MV+PL)	**.203**	**.190**	**.201**

Table 5.2: Comparison of Inference Methods

dropped all pairwise potentials and simply predicted based on the single node potentials. Table 5.2 shows the results for the one algorithm in each family for each of these strategies. As promised, ICM performs better than MP across the board. A partial explanation is that MP does not always converge. Singleton as a test-time inference algorithm (i.e., ignoring the pairwise potentials at test time) is surprisingly close to ICM. This table also shows that a substantial part of the advantage of CCG over the other methods is improved learning of the single-node potentials. This advantage over local methods is likely a more subtle version of the problems that PL has on this data: undertraining the single node potentials because it relies too much on information which is given in the training data but not the test data.

5.10 Discussion and Future Work

It is interesting to compare the natural approximation methods for LL versus contrastive objectives. The natural way to approximate a contrastive objective is to drop sub-objectives. As already mentioned, the effect of this is to drop all constraints over unconnected sub-components; however, we still maintain probability ratio constraints within sub-components. On the other hand, the standard way to approximately optimize LL is to approximate the partition function Z. This affects the probability ratios between every pair of instantiations $\mathbf{y}, \mathbf{y}'$, but to a lesser extent than if $\mathbf{y}$ and $\mathbf{y}'$ were in different sub-components in a contrastive objective. An interesting test would

be to compare the effect of approximations to Z (e.g., using variational techniques) to dropping sub-objectives.

Another interesting area for future research is how to decide between a few, large sub-objectives and many small sub-objectives. Our theoretical results show that under certain conditions, the two objectives lead to the same set of optimal parameters. However, in practical settings these conditions are not achievable. Thus, an empirical question remains about the relative merits of the two approaches. One important thing to note is that the use of multiple small sub-objectives rather than one large sub-objective gives us additional degrees of freedom through the sub-objective weights, $w_i(\mathbf{x})$. These weights allow us to emphasize constraints between particular subsets of assignments, which might be beneficial in some settings.

Another future direction is to further develop the theoretical basis of contrastive objectives. As mentioned earlier, (Liang & Jordan, 2008) provide results which suggest that increasing coverage of the contrastive objective increases learning efficiency. An interesting open question is whether it is possible to characterize which assignments contribute the most to the quality of the objective.

We introduced the chapter by discussing the connection to the complex probabilistic model described in Chapter 4. As we mentioned, this model has an additional complication because of the existence of hidden variables. We leave as future work extension of the theoretical results and algorithms to this case.

Chapter 6

Conclusion

The field of natural language processing and machine learning in general often have a tension between optimizing for a particular task and building a general purpose intelligent system. This thesis includes examples of both lines of work. Chapter 3 presents a simple, well-engineered classifier which achieves high-performance on the SRL task, while Chapter 4 presents a more ambitious system which takes a different approach to SRL than previous work.

This latter system could be extended beyond SRL in a variety of ways. For example, we could augment the system to further normalize canonical forms. Similar verbs could be mapped to the same frame, noun phrases containing nominalizations could be mapped to verb phrases, coreferent entities could be collapsed, etc. Even more, we could build higher-level normalizations, combining multiple canonical forms across sentences into structures such as events or narratives. The general principle employed by our work on canonical form SRL is to learn a system that builds normalized semantic structures through a series of linguistically-informed steps. The most obvious way forward is to expand the scope of these steps.

The biggest challenge in this direction is the lack of labeled data for these normalized forms. Perhaps this can be addressed in the same way we handled the lack of data for canonical forms: by using other, already existing labeled data as an indirect signal.

Extending backward, the system might also be improved by incorporating parsing

decisions into the model (for example, by taking a parse forest as input). Combining the forward and backward extensions leads to a system that can jointly reason about all steps in the processing pipeline.

A major challenge in all of these extensions is that as we add more and more complexity to the model, exact inference and learning will no longer be tractable. Approximate MAP inference through heuristic search is one of the most powerful and accessible methods for dealing with these types of models. The learning method presented in Chapter 5 is a powerful new tool for taking advantage of this kind of MAP inference algorithm.

Many interesting real-world models, including the canonical form model presented in this thesis, involve hidden variables. There are interesting theoretical and practical questions involved in extending our method to this case. For example, we could either attempt to sum out the hidden variable (difficult in most cases) or maximize over it (easier, but still probably requires approximation). Ultimately, which works better is an empirical question which will need to be explored for a variety of applications.

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