B.2Optimization64table.caption.64

Latent syntax in a deep generative model of language

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Contents

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ABSTRACT

In this thesis I investigate the question: *What are effective ways of incorporating syntactic structure into neural language models?*

In this thesis I:

- study a class of neural language models that merges generative transition-based parsing with recurrent neural networks in order to model sentences together with their latent syntactic structure;
- propose a new globally trained chart-based parser as an alternative proposal distribution used in the approximate marginalization;
- propose effective methods for semisupervised learning, making the syntactic structure a latent variable;
- perform targeted syntactic evaluation and compare the model's performance with that of alternative models that are based on multitask learning.

I find that:

- ...
- ...

Acknowledgements

1

Introduction

This thesis investigates the question: *What are effective ways of incorporating syntactic structure into neural language models?*

We study a class of neural language models that explicitly model the hierarchical syntactic structure in addition to the sequence of words (Dyer *et al.*, 2016; Buys and Blunsom, 2015b; Buys and Blunsom, 2018). These models merges generative transition-based parsing with recurrent neural networks in order to model sentences together with their latent syntactic structure. The syntactic structure that decorates the words can be latent, and marginalized over, or can be given explicitly, for example as the prediction of an external parser. Although these are fundamentally joint model, they can be evaluated as regular language models (modeling only words) by (approximate) marginalization of the syntactic structure. In the case of the RNNG (Dyer *et al.*, 2016), exact marginalization is intractable due to the parametrization of the statistical model, but importance sampling provides an effective approximate method. An externally trained discriminative parser is used to obtain proposal samples. Other models provide exact marginalization, but this typically comes at the cost of a less expressive parametrization, for example one in which the features cannot be structure-dependent (Buys and

Blunsom, 2018).

In this thesis I study the RNNG (Dyer *et al.*, 2016) and investigate:

The approximate marginalization I propose an alternative proposal distribution and investigate the impact.

- I propose a new discriminative chart-based neural parser that is trained with a global, Conditional Random Field (CRF), objective. The parser is an adaptation of the minimal neural parser proposed in Stern *et al.* (2017a), which is trained with a margin-based objective.
- This contrast with the choise of Dyer *et al.* (2016) for a transition-based parser as proposal, a discrminatively trained RNNG.
- We posit that a globally trained model is a better proposal distribution than a locally trained transition based model: a global model has ready access to competing analyses that can be structurally dissimilar but close in probability, whereas we hypothesize that a locally trained model is prone to produce locally corrupted structures that are nearby in transition-space.
- In a transition based parser more diverse samples can be obtained by flattening the transition distributions. This causes the model to be less confident in its predictions. A downside is that this approach causes the model to explore parts of the probability space which it has not encountered during training.
- The above is a general challenge for greedy transition based models that can be answered to by training with dynamic oracles (Goldberg and Nivre, 2013), also called 'exploration' ((Ballesteros *et al.*, 2016; Stern *et al.*, 2017a). These approaches can be considered instances of imitation learning (Vlachos, 2013; He *et al.*, 2012).
- We do not consider these directions in this thesic. Dynamic oracles can produce substantial improvements in constituency parsing performance, but they must be custom designed for each transition system (Fried and Klein, 2018).

Semi-supervised training by including unlabeled data To make joint models competitive language models they need to make use of the vast amounts of unlabeled data that exists.

- A major drawback of these syntactic language models is that they require annotated data to be trained, and preciously little of such data exists.
- We extend the training to the unsupervised domain by optimizing a variational lower bound on the marginal probabilities that jointly optimizes the parameters of proposal model ('posterior' in this framework) with the joint model.
- We obtain gradients for this objective using the score function estimator (Fu, 2006), also known as REINFORCE (Williams, 1992), which is widely used in the field of deep reinforcement learning, and we introduce an effective baseline based on argmax decoding (Rennie *et al.*, 2017), which significantly reduces the variance in this optimization procedure.
- Our CRF parser particularly excels in the role of posterior thanks the independence assumptions that allow for efficient exact computation of key quantities: the entropy term in the lower bound can be computed exactly using Inside-Outside algorithm, removing one source of variance from the gradient estimation, and the argmax decoding can be performed exactly thanks to Viterbi, making the argmax baseline even more effective.

Alternative, simpler, models There are alternatives to the methods that this thesis investigates.

- Multitask learning of a neural language model with a syntactic side objective is a competitive and robust alternative method to infuse neural language models with syntactic knowledge.
- Training the syntactic model on data that mixes gold trees with predicted 'silver' trees for unlabeled data is a competitive and robust alternative to fully principled semi-supervised learning.

- We propose a simple multitask neural language model that predicts labeled spans from the RNN hidden states, using a feature function identical identical to that used in the CRF parser.
- We consider these alternatives in order to quantify significance of the latent structure and the semisupervised training as measured by some external performance metric.

Targeted syntactic evaluation TBA

2

Background

In this chapter I give background to this thesis.

2.1 Syntax

Introduce the background on syntax relevant for the chapters on parsing, and the syntactic evaluation. My aim is to provide a succinct and compelling answer to the inevitable question: *Why do we care about constituency structure?* In particular I want to firmly establish the concept of constituents, and secondly I want to set some of the ground for the syntactic evaluation that we perform in the final chapter.

- Introduce the central question: what are sentences, strings or structures? Is a sentence a string of words in linear order, or are the words combined in a hierarchical structure? (Everaert *et al.*, 2015; Frank *et al.*, 2012)
- The notion of a constituent, and constituent tests Carnie (2010) and Huddleston and Pullum (2002).
- Hierarchical structure (of these constituents) Everaert *et al.* (2015).
- The lexical and phrasal categories of constituent analysis.

- Evidence for structured sentence processing from psycholinguistic research (Hale, 2001; Levy, 2008; Brennan *et al.*, 2016).
- Introduce the concept of *acceptability judgements*, with the final chapter on syntactic evaluation in mind.

In the following exposition we primarily follow Huddleston and Pullum (2002), with some excursions into Carnie (2010) and Everaert *et al.* (2015). The first source is a well established reference grammar of the English language that is relatively agnostic with respect to theoretical framework, whereas the the later two sources are more firmly rooted in a particular framework[1]. We take the following three pricinpiles (about English syntax!) from (Huddleston and Pullum, 2002) as guiding:

(i) Sentences consist of parts that may themselves have parts.

(ii) These parts belong to a limited range of types.

(iii) The constituents have specific roles in the larger parts they belong to.

Constituents Sentences consist of parts that may themselves have parts. The parts are groups of words that function as units, and they are called *constituents*. Consider the simple sentence *A bird hit the car*. The immediate constituents are *a bird* (the subject) and *hit the car* (the predicate). The phrase *hit the car* can be further analyzed as containing the constituent *the car*. The ultimate constituents of a sentence are the atomic words, and the entire analysis is called the constituent structure of the sentence. This structure can be indicated succinctly with the use of brackets

[A bird [hit [the car]]]

or less succinctly as a tree as in figure 2.1. Evidence for the existence of these constituents can be provided by examples such as the following, which are called constituent tests (Carnie, 2010). Consider inserting the adverb *apparently* into our example sentence, indicating the alleged

[1] Broadly subsumable under the label *generative grammar*.

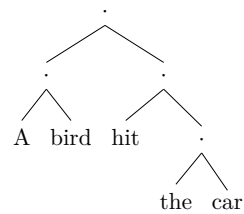


Figure 2.1: Sentence 2.1 as a tree. (TODO: draw this without labels.)

status of the event described in the sentence. In principle there are six positions available for the placement of *apparently* (including before, and after the sentence). However, only three of these placements are actually permissible[2]:

1. *Apparently* a bird hit the car.
2. *An *apparently* bird hit the car.
3. A bird *apparently* hit the car.
4. *A bird hit *apparently* the car.
5. *A bird hit the *apparently* car.
6. A bird hit the car, *apparently*.

Based on the bracketing in 2.1 we can formulate a general constraint: the adverb must not interrupt any constituent. Indeed, this explains why *actually* cannot be placed anywhere inside *hit the car* and not between *a* and *bird*. For full support, typically results from many more such test are gathered, and in general these tests can be much more controversial than in our simple example (Carnie, 2010).

Syntactic categories The constituents of a sentence belong to a limited range of types that form the set of syntactic categories (Huddleston and Pullum, 2002). Two types are distinguished: lexical categories (part of speech) and phrasal categories. The tree in figure 2.1 can be represented in more detail by adding syntactic categories, see figure 2.2.

[2]We use an asterisk '*' to indicate a sentence that is judged ungrammatical, as is customary in linguistics.

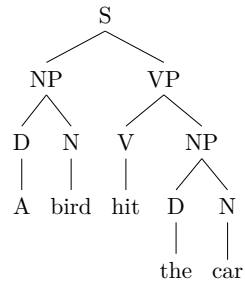
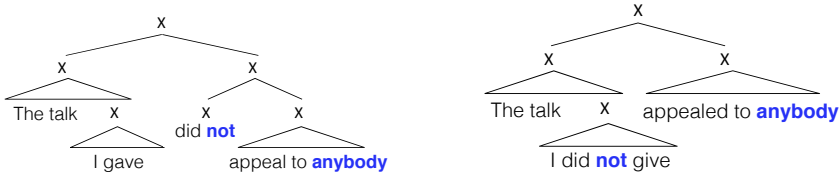


Figure 2.2: A tee specified with lexical (D, N, V) and phrasal categories (S, NP, VP).

Hierarchical structure The constituents have specific roles in the larger parts they belong to (Huddleston and Pullum, 2002). This structure provides constraints that are not explainable from the linear order of the words themselves. Consider the following example about the syntactic behaviour of *negative polarity items* (NPIs)[3] such as *anybody*:

1. The book that I bought did *not* appeal to *anybody*.
2. * The book that I bought appealed to *anybody*.

From this example we might formulate the hypothesis that the word *not* must linearly precede the word *anybody*. A counter example refutes this linear hypothesis:



(a) In licensing context. **(b)** Not in licensing context.

Figure 2.3: Negative Polarity. Figure taken from Everaert *et al.*, 2015. (TODO: draw in qtree, but how to make the nested roofs?)

[3] A negative polarity item is, to first approximation, a word or group of words that is restricted to negative context (Everaert *et al.*, 2015). More generaly they are words that need to be licensed by a specific *licencing context* (Giannakidou, 2011).

1. *The book I did *not* buy appealed to *anybody*.

Instead, the constraints that govern this particular pattern depend on hierarchical structure: the word *not* must "structurally precede" the word *anybody* (Everaert *et al.*, 2015). Figure shows the constituent structure of both sentences. The explanation goes as follows (put this in my own words): "In sentence 2.3 (a) the hierarchical structure dominating *not* also immediately dominates the hierarchical structure containing *anybody*. In sentence 2.3 (b), by contrast, *not* sequentially precedes *anybody*, but the triangle dominating *not* fails to also dominate the structure containing *anybody*."

Cognitive reality Does all this exist in the human brain? These people say *yes*: (Hale, 2001; Levy, 2008; Brennan *et al.*, 2016).

Controversy Theoretical syntax is rife with controversy, and wildly differing viewpoints exist. In fact, for each point made in our short discussion, the exact opposite point has been made as well:

- Constituents are fundamental (Huddleston and Pullum, 2002; Carnie, 2010) *versus* word-word relations are all you need (Tesnière, 1959; Nivre, 2005; Hudson, 2010).

- Hierarchical structure is a core feature of language (Everaert *et al.*, 2015) *versus* sequential sentence structure has enough explanatory power Frank *et al.*, 2012. The claim is that (2) is cognitively more fundamental than (1),

es [[can [be analysed] [as [hierarchically structured]]]]

Sentences [can be analysed] [as hierarchically structured]

  which is exactly contrary to the analyses above. This is more similar to the NLP task of *chunking*, or shallow parsing.

- Studies in cognitive neuroscience and psycholinguistics show that human sentence processing is hierachical (Hale, 2001; Levy, 2008; Brennan *et al.*, 2016) *and* they show that it is not (Conway and Pisoni, 2008; Christiansen *et al.*, 2012; Gillespie and Pearlmutter,

2011; Gillespie and Pearlmutter, 2013) (selected from the survey in Frank *et al.* (2012)).

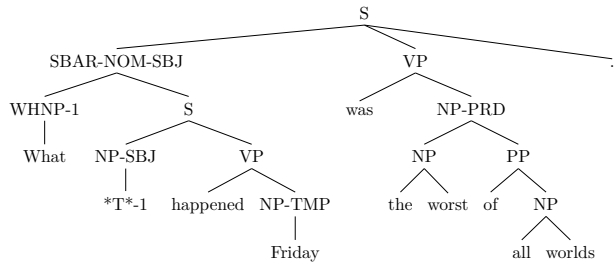
In this research I take a position of extreme pragmatism with respect to syntax: it is whatever our dataset says it is. Which means in our case, the Penn Treebank has the final word on the subject. And is language hierachical or linear? That is exactly what we inted to ivestigate from a statistical and computational viewpoint.

2.2 Parsing

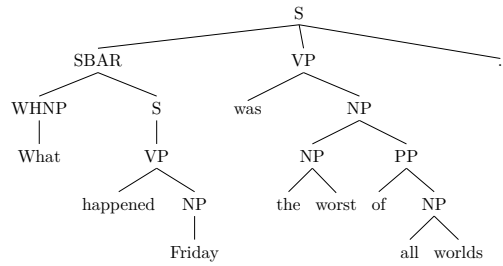
- Treebanks, in particular the Penn Treebank. Treebank preprocessing. CFGs, CNF, spans. Reference figure 2.4.
- The two conceptions of a tree: as a set of *labeled spans* or as a set of *anchored rules*.
- A labeled span is a triple (ℓ, i, j) of a syntactic label ℓ together the left and right endpoints i, j that the label spans.
- An *anchored rule* is a triple (r, i, j) or four-tuple (r, i, k, j), containing a CNF rule r with span endpoints i, j, and a split-point k of the left and right child r is not a lexical rule.
- For the difference, consider the following two representations of the tree in figure 2.4d given in table 2.1.
- Algorithms for parsing: global chart based, local transition based
- Dynamic programming inference versus search heuristics.
- Modelling types: generative, discriminative, log-linear, count-based, feature-based, neural network features.

2.3 Language models

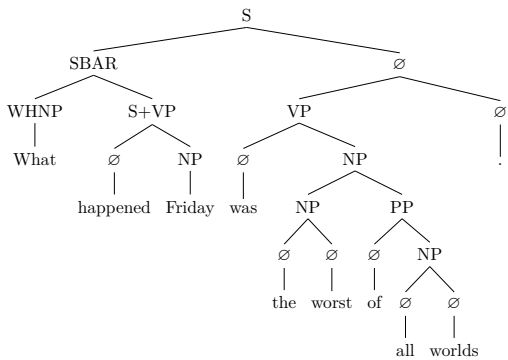
- Briefly mention some typical approaches for langugage modelling: count based n-gram with smoothing (Chen and Goodman, 1999;



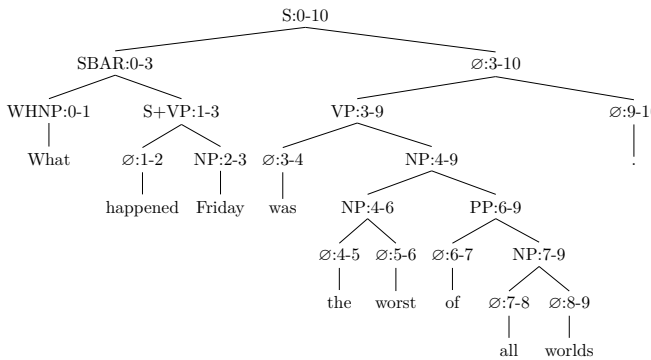
(a) Original Penn Treebank tree.



(b) Function tags and traces removed.



(c) Converted to normal form.



(d) In normal form with spans.

Figure 2.4: Converting a treebank tree (withouth part-of-speech tags).

Labeled spans	Anchored rules
(S, 0, 10)	(S → SBAR ∅, 0, 3, 10)
(SBAR, 0, 3)	(SBAR → WHNP S+VP, 0, 1, 3)
(VP, 1, 3)	(S+VP → ∅ NP, 1, 2, 3)
⋮	⋮
(NP, 7, 9)	(NP → ∅ ∅, 7, 8, 9)

Table 2.1: Two conceptions of the tree in 2.4d.

Kneser and Ney, 1995), neural n-gram (Bengio *et al.*, 2003) and recurrent neural network (Mikolov *et al.*, 2010). Also mention some (early) syntactic approaches: count-based (Chelba and Jelinek, 2000; Pauls and Klein, 2012), neural (Emami and Jelinek, 2005), and top-down parsing related (Roark, 2001).

- Explain the metric perplexity.
- Briefly mentions some typical datasets and some benchmarks (dataset, perplexity, number of parameters, training time).
- Mention some downsides of the perplexity metric: conflating different sources of succes in next-word prediction (simple collocations, semantics, syntax).
- Note that there exists some alternatives to perplexity: adversarial evaluation (Smith, 2012), subject-verb agreement (Linzen *et al.*, 2016) and grammatical acceptability judgments (Marvin and Linzen, 2018).

2.4 Neural networks

Introduce all the neural networks.

- We consider the neural networks as abstractions denoting certain parametrized functions FF, RNN, LSTM, etc.

- Let $\mathbf{x}$ and $\mathbf{y}$ be vectors in respectively $\mathbf{R}^n$ and $\mathbf{R}^m$.

  A *feedforward neural network* is a parametrized function FF from $\mathbf{R}^n$ to $\mathbf{R}^m$ such that

  $$\text{FF}(\mathbf{x}) = \mathbf{y}.$$

  A *recurrent neural network* is a parametrized function RNNthat takes a sequence of vectors $(\mathbf{x}_i)_{i=1}^n = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ in $\mathbf{R}^n$ and produces a sequence of output vectors in $(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n)$ in $\mathbf{R}^m$:

  $$\text{RNN}((\mathbf{x}_i)_{i=1}^n) = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n).$$

  Internally, the RNNrecursively applies a function $f : \mathbf{R}^n \times \mathbf{R}^m \to \mathbf{R}^m$ that is defined by the recursion

  $$\begin{aligned}\mathbf{y}_t &= f(\mathbf{x}_t, \mathbf{y}_{t-1}) \\ &= f(\mathbf{x}_t, f(\mathbf{x}_{t-1}, \mathbf{y}_{t-2})) \\ &\vdots \\ &= f(\mathbf{x}_t, f(\mathbf{x}_{t-1}, f(\ldots f(\mathbf{x}_1, \mathbf{y}_0)))),\end{aligned}$$

  which is how the vectors $\mathbf{y}_i$ are computed. That is, f takes the input $\mathbf{x}$ of the current timestep t and the output $\mathbf{y}$ of the previous timestep $t-1$ and returns a new ouput for timestep t. The initial vector $\mathbf{y}_0$ does not depend on the input, and can be fixed or part of the function's set of parameters.

  An RNNcan be applied to the input sequence in reverse, that is, in the *backward* direction:

  $$\begin{aligned}\text{RNN}_B((\mathbf{x}_i)_{i=1}^n) &= \text{reverse}(\text{RNN}(\text{reverse}((\mathbf{x}_i)_{i=1}^n))) \\ &= \text{reverse}(\text{RNN}(\mathbf{x}_n, \mathbf{x}_{n-1}, \ldots, \mathbf{x}_1) \\ &= \text{reverse}(\mathbf{y}_n, \mathbf{y}_{n-1}, \ldots, \mathbf{y}_1) \\ &= (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n),\end{aligned}$$

  where we defined a

  $$\text{reverse}((\mathbf{x}_i)_{i=1}^n) \triangleq (\mathbf{x}_n, \mathbf{x}_{n-1}, \ldots, \mathbf{x}_1), \tag{2.1}$$

For consistency we will refer to the RNNin the regular, *forward*, direction as RNN_F. To stress the difference between the different outputs obtained from the two directions, we will denote the output vectors obtained in the regular, forward, direction with $\mathbf{f}_i$ and the vectors obtained in the backward direction with $\mathbf{b}_i$:

$$\text{RNN}_F((\mathbf{x}_i)_{i=1}^n) = (\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n)$$
$$\text{RNN}_B((\mathbf{x}_i)_{i=1}^n) = (\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_n)$$

The two functions above can used to construct a *bidirectional* RNNby combining the output of each as

$$\text{BIRNN}((\mathbf{x}_i)_{i=1}^n) = (\mathbf{f}_1 \circ \mathbf{b}_1, \mathbf{f}_2 \circ \mathbf{b}_2, \ldots, \mathbf{f}_n \circ \mathbf{b}_n), \tag{2.2}$$

where we use $\circ$ to denote vector concatenation, *i.e.*$\mathbf{x} \circ \mathbf{y}$ is a vector in $\mathbf{R}^{n+m}$.

An LSTMis a particular way to construct the RNNinternal function f, and similarly has a bidirectional equivalent denoted BILSTM.

- The function FFis defined as follows:
- The function LSTMis defined as follows
- (Minibatch) SGD optimization.

3

Recurrent Neural Network Grammars

In this chapter we introduce the Recurrent Neural Network Grammar (RNNG), a probabilistic model of sentences with explicit phrase structure, introduced by Dyer *et al.* (2016).

3.1 Model

The discriminative RNNG is a discriminative transition based parser that uses regular RNNs to summarize the actions in the history and the words on the buffer into vectors, and uses a special RNN with a syntax-dependent recurrence to obtain a vector representation of items on the the stack. Depending on the perspective, the generative RNNG can be considered a generative instantiation of the RNNG, jointly modelling the words instead of merely conditioning on them. And although But it can be seen as a structured model of language that predicts words together with their structure. From the view of parsing, the generative RNNG simply dispends with the buffer of the discriminative RNNG to instead predict the words that decorate the tree. But as a model of sentences, it can be understood as kind of structured RNN: it predicts words incrementally, but compresses and labels them recursively whenever they form a complete constituents.

Transition sytem The RNNG uses a transition system crafted for top-down parsing. The discriminative transition system has three actions:

- OPEN(X) opens a new nonterminal symbol X in the partially constructed tree.
- SHIFT moves the topmost word x from the buffer onto the stack.
- REDUCE closes the open constituent by composing the symbols in it into a single item representing the content of the subtree. This allows nodes with an arbitrary number of children.

How these actions work to build a tree is best illustrated with an example derivation, given in table 3.1. The actions are constrained in order to only derive well-formed trees:

- SHIFT can only be excecuted if there is at least one open nonterminal (all words must be under some nonterminal symbol).
- OPEN(X) requires there to be words left on the buffer (all constituents must eventually hold terminals).
- REDUCE requires there to be at least one terminal following the open nonterminal, and the topmost nonterminal can only be closed when the buffer is empty (all nodes must end under a single root node).

The generative transition system is derived from this system by replacing the SHIFT action, which moves the word x from the buffer into the open constituent on the stack, with an action that *predicts* the word:

- GEN(x) predicts that x is the next word in the currently open constituent, and puts this word on the top of the stack.

The buffer is dispensed with and is replaced by a similar structure that records the sequence words predicted so far. An example derrivation parallel to the discriminative example is given in table 3.2.

	Stack	Buffer	Action
0		*The* | *hungry* | *cat* | *meows* | .	OPEN(S)
1	(S	*The* | *hungry* | *cat* | *meows* | .	OPEN(NP)
2	(S | (NP	*The* | *hungry* | *cat* | *meows* | .	SHIFT
3	(S | (NP | *The*	*hungry* | *cat* | *meows* | .	SHIFT
4	(S | (NP | *The* | *hungry*	*cat* | *meows* | .	SHIFT
5	(S | (NP | *The* | *hungry* | *cat*	*meows* | .	REDUCE
6	(S | (NP *The hungry cat*)	*meows* | .	OPEN(VP)
7	(S | (NP *The hungry cat*) | (VP	*meows* | .	SHIFT
8	(S | (NP *The hungry cat*) | (VP | *meows*	.	REDUCE
9	(S | (NP *The hungry cat*) | (VP *meows*)	.	SHIFT
10	(S | (NP *The hungry cat*) | (VP *meows*) | .		REDUCE
11	(S (NP *The hungry cat*) (VP *meows*) .)		

Table 3.1: Discriminative transition sequence that parses an input sentence. Items are separated by the midline symbol |.

Probabilistic model Fundamentally, the model is a probability distribution over transition actions $\mathbf{a} = (a_1, \ldots, a_T)$ that generates a tree $\mathbf{y}$. Conditionally, given a sequence of words $\mathbf{x}$, in the discriminative model, and jointly predicting $\mathbf{x}$ in the generative model. Put simply, the model is thus defined as

$$p(\mathbf{a}) = \prod_{t=1}^{T} p(a_t \mid a_{<t}), \tag{3.1}$$

where in the discriminative case $p(\mathbf{a}) = p(\mathbf{y} \mid \mathbf{x})$ and in the generative model $p(\mathbf{a}) = p(\mathbf{x}, \mathbf{y})$.

The exact model however is slightly more complicated, a consequence of the difference between the discrminative and the generative actions, and a consequence of practical concerns regarding the implementation. To define the model precisely we need to introduce some things. First we define the set of discriminative actions as

$$A_{\mathcal{D}} = \{\text{SHIFT}, \text{OPEN}, \text{REDUCE}\}, \tag{3.2}$$

and the set of generative actions as

$$A_{\mathcal{G}} = \{\text{GEN}, \text{OPEN}, \text{REDUCE}\}. \tag{3.3}$$

We define a finite set of nonterminal symbols, for example

$$N = \{\text{S}, \text{NP}, \ldots, \text{WHNP}\},$$

	Stack	Terminals	Action
0			OPEN(S)
1	(S		OPEN(NP)
2	(S | (NP		GEN(*The*)
3	(S | (NP | *The*	*The*	GEN(*hungry*)
4	(S | (NP | *The* | *hungry*	*The* | *hungry*	GEN(*cat*)
5	(S | (NP | *The* | *hungry* | *cat*	*The* | *hungry* | *cat*	REDUCE
6	(S | (NP *The hungry cat*)	*The* | *hungry* | *cat*	OPEN(VP)
7	(S | (NP *The hungry cat*) | (VP	*The* | *hungry* | *cat*	GEN(*meows*)
8	(S | (NP *The hungry cat*) | (VP | *meows*	*The* | *hungry* | *cat* | *meows*	REDUCE
9	(S | (NP *The hungry cat*) | (VP *meows*)	*The* | *hungry* | *cat* | *meows*	GEN(.)
10	(S | (NP *The hungry cat*) | (VP *meows*) | .	*The* | *hungry* | *cat* | *meows* | .	REDUCE
11	(S (NP *The hungry cat*) (VP *meows*) .)	*The* | *hungry* | *cat* | *meows* | .	

Table 3.2: Generative transition sequences that *generates* a sentence together with its constituency structures.

and a finite alphabet of words, for example

$$\Sigma = \{\text{all}, \text{friday}, \ldots, \text{worst}\}.$$

Then in the discriminative model $\mathbf{a}$ is an element of $A^T_{\mathcal{D}}$, and in the generative model $\mathbf{a}$ is an elemtnt of $A^T_{\mathcal{G}}$, both with the restriction that the actions form a valid tree $\mathbf{y}$. The sequence of nonterminals $\mathbf{n}$ in N^K is the sequence of nonterminal nodes obtained from $\mathbf{y}$ by pre-order traversal. An a sentence $\mathbf{x}$, finally, is an element of Σ^N.

Finally, let $\mathbf{1}_{\{a_t = \text{OPEN}\}}$ be the indicator function for the event that the action a_t is to open a new nonterminal, and similarly let $\mathbf{1}_{\{a_t = \text{GEN}\}}$ be the indicator function for the event that the action a_t is to generate a word. Then we can introduce two functions that map between sets of indices to indicate the number of times a particular action has been taken at each time step:

$$\mu : [T] \to [M] : \mu(t) = \sum_{i=0}^{t-1} \mathbf{1}_{\{a_i = \text{OPEN}\}},$$

and

$$\nu : [T] \to [N] : \nu(t) = \sum_{i=0}^{t-1} \mathbf{1}_{\{a_i = \text{GEN}\}}.$$

We are now in the position to write down the exact models. Let $\mathbf{a}$ be a sequence from $A_{\mathcal{D}}^T$. Then the model for the discrminative RNNG is

$$p(\mathbf{y} \mid \mathbf{x}) = p(\mathbf{a} \mid \mathbf{x}) \tag{3.4}$$

$$= \prod_{t=1}^{T} p(a_t \mid \mathbf{x}, a_{<t}) p(n_{\mu(t)} \mid \mathbf{x}, a_{<t})^{\mathbf{1}\{a_t = \text{OPEN}\}}. \tag{3.5}$$

Let $\mathbf{a}$ be a sequence from $A_{\mathcal{G}}^T$, which include the actions that generate words[1], then the model for the generative RNNG is

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{a}) \tag{3.6}$$

$$= \prod_{t=1}^{T} p(a_t \mid a_{<t}) p(n_{\mu(t)} \mid a_{<t})^{\mathbf{1}\{a_t = \text{OPEN}\}} p(x_{\nu(t)} \mid a_{<t})^{\mathbf{1}\{a_t = \text{GEN}\}}. \tag{3.7}$$

The probabilities over next actions at time step t are given by classifiers on a vector $\mathbf{u}_t$[2], which represents the parser configuration at that timestep:

$$p(a_t \mid a_{<t}) \propto \exp(\mathbf{h}) \qquad \text{where } \mathbf{h} = \text{FF}_\alpha(\mathbf{u}_t) \tag{3.8}$$

$$p(n_{\mu(t)} \mid a_{<t}) \propto \exp(\mathbf{h}) \qquad \text{where } \mathbf{h} = \text{FF}_\beta(\mathbf{u}_t) \tag{3.9}$$

$$p(x_{\nu(t)} \mid a_{<t}) \propto \exp(\mathbf{h}) \qquad \text{where } \mathbf{h} = \text{FF}_\gamma(\mathbf{u}_t) \tag{3.10}$$

where $\{\alpha, \beta, \gamma\}$ are separate parameters. How the vector $\mathbf{u}_t$ is constructed is outlined in the next section.

Note on actions We could have defined the actions differently as

$$A_{\mathcal{D}} = \{\text{REDUCE}, \text{SHIFT}\} \cup \{\text{OPEN}(n) \mid n \in N\},$$

and

$$A_{\mathcal{G}} = \{\text{REDUCE}\} \cup \{\text{OPEN}(n) \mid n \in N\} \cup \{\text{GEN}(x) \mid x \in \Sigma\},$$

and defined $p(\mathbf{a})$ as in 3.1. However, in the case of the generative model this is particularly inefficient from a computational perspective.

[1] Note that under this action set $p(a_t \mid a_{<t}, \mathbf{x}_{<t}) = p(a_t \mid a_{<t})$, given the fact that the words in $\mathbf{x}_{<t}$ are contained in $a_{<t}$.

[2] For brevity we omit the conditioning on $\mathbf{x}$, which was redundant already in the case of the generative model.

Note that the set Σ is generally very very large[3], and observe that the normalization in 3.8 requires a sum over all actions, while a large number of the actions do not generate words. Besides, the presentation in 3.4 and 3.6 is conceptually cleaner: first choose an action, then, if required, choose the details of that action. For these reasons combined we opt for the two-step prediction. For consistency we extend this modelling choice to the discriminative RNNG. And although it appears that Dyer *et al.* (2016) model the sequences according to 3.1, followup work takes our approach and models the actions of the generative RNNG as in equation 3.6 (Hale *et al.*, 2018).

3.1.1 Features

The transition probabilities are computed from the vector $\mathbf{u}_t$ that summarizes the parser's entire configuration history at time t. This vector is computed incrementally and in a syntax-dependent way. It is defined as the concatenation of three vectors, each summarizing one of the three datastructures separately:

$$\mathbf{u}_t = [\mathbf{s}_t, \mathbf{b}_t, \mathbf{h}_t],$$

Here, $\mathbf{s}_t$ represents the stack, $\mathbf{b}_t$ represents the buffer, and $\mathbf{h}_t$ represents the history of actions.

The vectors $\mathbf{b}_t$ and $\mathbf{h}_t$ are computed each with a regular RNN; the history vector in the forward direction, and the buffer in the backward direction, to provide a lookahead.

$$\mathbf{h}_t = \text{RNN}^f(\mathbf{a})[t],$$
$$\mathbf{b}_t = \text{RNN}^b(\mathbf{x})[t].$$

The vector $\mathbf{s}_t$ represents the partially constructed tree that is on the stack, and its computation depends on this partial structure by using a structured RNN that encodes the tree in top-down order while recursively compressing constituents whenever they are completed. The RNN incrementally computes a new hidden state based on incoming

[3] On the order of tens of thousands.

nonterminal and terminal symbols while these are respectively opened and shifted, as a regular RNN would, but rewrites this history whenever the constituent that they form is closed. Whenever a REDUCE action is predicted, the RNN rewinds its hidden state to before the constituent was opened; the items making up the constinuent are composed into a single vector by a composition function; and this composed vector is then fed into the rewound RNN as if the subtree where a single input. The closed constituent is now a single item represented by a single vector. Due to the nested nature of constituents this procedure recursively compresseses subtrees.

Consider this example following the parser states in table 3.1. At step 5, the stack contains the five items

$$(\text{S} \mid (\text{NP} \mid \textit{The} \mid \textit{hungry} \mid \textit{cat}$$

which were each first represented by a lookup embedding vector, and then encoded by a regular, sequential, forward RNN. Now a REDUCE action is predicted. The items are popped from the stack until the first open bracket has been popped, which in this example is the item (NP. This process also rewinds the RNN state to before this bracket was openend, bringing it back to its encoding of the stack at state 1. The composition now computes a vector representation for the 5 popped items, computing a representation for the single item

$$(\text{NP } \textit{The hungry cat}).$$

The RNN is updated with this single input, which results in the encoding of stack at step 6, and finalizes the reduction step.

To see how this process is recursive, consider the reduction that takes the stack from the five items

$$(\text{S} \mid (\text{NP} \mid \textit{The} \mid (\text{ADJP } \textit{very hungry}) \mid \textit{cat}$$

to the two items

$$(\text{S} \mid (\text{NP } \textit{The } (\text{ADJP } \textit{very hungry}) \textit{ cat}).$$

You can see that the (ADJP *very hungry*) has already been composed into a single item, and now it takes part in the compression at a higher level.

Composition function Two kinds of functions have been proposed to for the composition described above: the original function based on a bidirectional RNN (Dyer *et al.*, 2016), and a more elaborate one that additionally incorporates an attention mechanism (Kuncoro *et al.*, 2017). Both methods encode the invidual items that make up the constituent with a bidirectional RNN but while the simpler version merely concatenates the endpoint vectors, the attention based method computes a convex combination of all these vectors, weighted by predicted attention weights. Kuncoro *et al.* (2017) show that the attention-based composition performs best and so we only consider this function.

3.2 Training

The discriminative and generative model are trained to maximize the objective

$$\mathcal{L}(\theta) = \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} p_\theta(\mathbf{y} \mid \mathbf{x}),$$

respectively

$$\mathcal{L}(\theta) = \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} p_\theta(\mathbf{x}, \mathbf{y}),$$

by gradient-based optimization on the parameters θ.

3.3 Inference

The two formulations of the RNNG have complementary applications: both models can be used for parsing, but the generative model can additionally be used as a language model. How these problems can be solved is the topic of this section.

3.3.1 Discriminative model

Parsing a sentence $\mathbf{x}$ with the discriminative model corresponds to solving the following search problem of finding the maximum *a posteriori* (MAP) tree

$$\hat{\mathbf{y}} = \arg\max_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} p_\theta(\mathbf{y} \mid \mathbf{x}).$$

Solving this exactly is intractable due to the parametrization of the model. At each timestep, the model conditions on the entire history derivation history which excludes the use of dynamic programming to solve this efficiently. Instead we rely on an approximate search strategy. There are two common approaches for this: greedy decoding and beam search. We only focus on the first. Greedy decoding is precisely what it suggests: at each timestep we greedily select the best local decision

$$a_t^* = \arg\max_a p_\theta(a|a_{<t}^*).$$

The predicted parse is then the approximate MAP tree $\mathbf{y}^*$ constructed by the sequeunce $\mathbf{a}^* = (a_1^*, \cdots, a_m^*)$.

3.3.2 Generative model

Given a trained generative model p_θ we are interested in solving the following two problems: parsing a sentence $\mathbf{x}$

$$\hat{\mathbf{y}} = \arg\max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} p_\theta(\mathbf{x}, \mathbf{y}),$$

and computing its marginal probability

$$p(\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} p_\theta(\mathbf{x}, \mathbf{y}).$$

Either inference problem is intractable as either problem would require exhaustive enumeration of and computation over all possible action sequences. Luckily, both can be effectively approximated with the same method: importance sampling using a conditional proposal distribution $q_\lambda(\mathbf{y} \mid \mathbf{x})$ (Dyer *et al.*, 2016).

Approximate marginalization The proposal distribution allows us to rewrite the marginal probability of a sentence as an expectation under

this distribution:

$$\begin{aligned} p(\mathbf{x}) &= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} p_\theta(\mathbf{x}, \mathbf{y}) \\ &= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_\lambda(\mathbf{y}|\mathbf{x}) \frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \\ &= \mathbf{E}_q \left[\frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \right] \end{aligned}$$

This expectation can be approximated with a Monte Carlo estimate

$$\mathbf{E}_q \left[\frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \right] \approx \frac{1}{K} \sum_{i=1}^{K} \frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})}, \tag{3.11}$$

using proposal samples $\mathbf{y}_i$ sampled from the proposal model q_λ conditioning on $\mathbf{x}$.

Approximate MAP tree To approximate the MAP tree $\hat{\mathbf{y}}$ we use the same set of proposal samples as above, and choose the tree $\mathbf{y}$ from the proposal samples that has the highest probability probability under the joint model $p_\theta(\mathbf{y}, \mathbf{x})$.

Proposal distribution In order to avoid division by zero, the proposal distribution must satisfy the property that for all $\mathbf{x}$ and $\mathbf{y} \in \mathcal{Y}(\mathbf{x})$

$$p(\mathbf{x}, \mathbf{y}) > 0 \Rightarrow q(\mathbf{y}|\mathbf{x}) > 0.$$

We additionally want that samples can be obtained efficiently, and that their conditional probability can be computed. All these requirements are met by the discriminative RNNG: samples can be obtained by ancestral sampling over the transition sequences. For this reason Dyer *et al.* (2016) use this as their proposal. However, any discriminatively trained parser that meets these requirements can be used alternatively, and in chapter 4 we will propose such an alternative.

3.4 Experiments

We perform three types of experiments with the RNNG:

- We reproduce the parsing f-scores and perplexities from (Dyer *et al.*, 2016), and some more.
- We evauluate 'how good the model is' as a sampler.

Supervised model We investigate the following.

- We train with standard hyperparameter settings and optimizer, and replicate the original results. We will get a little lower with the discriminative model because we do not use tags.
- We evaluate F-score with 100 samples (as many proposal trees as possible).
- We evaluate perplexity with varying number of samples: 1 (argmax), 10, 20, 50, 100 (default). The peplexity evaluation with the argmax prediction gives an impression of the uncertaty in the model (Buys and Blunsom, 2018).

Sampler We investigate the following:

- We asses the conditional entropy of the model. This is most quantitative. Recall that conditional entropy is defined as

$$\mathrm{H}(Y \mid X) = \sum_{x \in \mathcal{X}} p_X(x) \mathrm{H}(Y \mid X = x), \tag{3.12}$$

  where

$$\mathrm{H}(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} p_{Y|X}(y \mid x) \log p_{Y|X}(y \mid x). \tag{3.13}$$

  We estimate the quantity $\mathrm{H}(Y \mid X = x)$ with the model samples. We estimate the quantity $\mathrm{H}(Y \mid X)$ by a sum over the development dataset. For the probabilities $p_X(x)$ we use the marginalized probabilities of the joint RNNG (with samples from the discrminative parser $p_{Y|X}$).
- We asses for some cherry picked sentences. This is more qualitative. These sentences should be difficult or ambiguous. Or they can

be ungramatical when taken from the syneval dataset. We can evaluate their entropy, and the diversity of samples, for example to see if there are clear modes. We can make violinplots of the probabilities of the samples. We can compute the f-scores of the samples compared with the argmax tree.

3.5 Related work

3.5.1 Generative parsing

- Generative dependency parsing and language modelling (Titov and Henderson, 2007; Buys and Blunsom, 2015a; Buys and Blunsom, 2015b; Buys and Blunsom, 2018)
- Top-down parsing and language modelling (Roark, 2001).

3.5.2 Syntax and cognition

The RNNG has been at the center of experiments into unsupervised syntactic induction

Syntax RNNGs learn about syntax beyond their supervision. The attention mechanism in the composition function learns a type of 'soft' head-rules[4], in which most of the attention weight is put on the item that linguist consider the synactic head of such constituents. Another finding shows that when trained on unlabeledd trees, the RNNG learns representations for constituents that cluster according to their withheld gold label (Kuncoro *et al.*, 2017). Additionally RNNGs are much better at a long-distance subject-verb agreement task than LSTMS (Linzen *et al.*, 2016; Kuncoro *et al.*, 2018), which advantage they owe to the composition function that by repeatedly compressing intervening structure decreases the distance between the two words at stake.

Cognition RNNGs can tell us something about our brains. Psycholinguistic research has shown that top-down parsing is a cognitively plausi-

[4] A head is the lexical item in a phrase that determines the syntactic category of that phrase.

ble parsing strategy (Brennan *et al.*, 2016), and recently, RNNGs have been shown to be particularly good statistical predictors for human sentence comprehension (Hale *et al.*, 2018). In this experiment, the sequential word-probabilities derived from a generative RNNG[5] provide a per-word complexity metric that predict human reading difficulty well. Much better at least than predictions from the word probabilities obtained from a purely sequential RNN language model.

[5]Obtained by using 'word-synchronous beam-search' (Stern *et al.*, 2017b).

4

Conditional Random Field parser

../src/bibliography

This chapter introduces a neural Conditional Random Field (CRF) parser that can be used as an alternative proposal distribution for the approximate marginalization of the RNNG. The model is a span-factored CRF that independently predicts scores for labeled spans over the sentence using neural networks. The scores then interact in a chart-based dynamic program, giving a compact description of the distribution over trees.

This approach combines the efficient exact inference of chart-based parsing, the rich nonlinear features of neural networks, and the global training of a CRF. The chart-based approach allows efficient exact inference alowing for exact decoding and global sampling while the neural features can be complex and can condition on the entire sentence. The CRF training objective [...something about receiving information about all substructures...]. The parser is an adaptation of the chart-based parser introduced in Stern *et al.* (2017a) to global CRF training. The original is trained with a margin-based objective. Our interest in in this model is as a proposal distribution, which requires probabilistical training.

In this chapter:

- I present the parser and describe how it is an adaptation of earlier (neural) crf parsing and the maximum margin trained parser of Stern *et al.* (2017a).
- I show how the several inference problems of interest can be solved exactly: prediction, entropy, sampling.
- We train the parser in a supervised fashion and show it's adequacy as a parser.
- We invesitage how samples are obtained from this parser.

4.1 Model

The model is a CRF over labeled spans that form a tree. We write $\mathbf{y}_a = (i, j, \ell)$ for a labeled span and consider a tree as a collection of these $\mathbf{y} = \{\mathbf{y}_a\}_{a=1}^{A}$. We define the score of a tree as the product of nonnegative local potentials $\Psi(\mathbf{x}, \mathbf{y}_a) \geq 0$. The function Ψ scores each span seperately, conditional one the entire sentence. The probability of a tree is the globally normalized score of the tree:

$$p(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{a=1}^{A} \Psi(\mathbf{x}, \mathbf{y}_a), \tag{4.1}$$

where

$$Z(\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \prod_{a=1}^{A} \Psi(\mathbf{x}, \mathbf{y}_a)$$

is the normalizing constant that sums over all the possible parse trees and makes sures that the probability distribution sums to 1. This normalizing constant can be computed efficiently with the inside algorithm.

By factorizing a tree over labeled spans we make an even stronger assumption than that typically made by factorizating over anchored context-free rules, see table 2. By scoring just labels for spans the potential function has no access to information about the direct substructure under the node, such as the child nodes and split point, and this puts a

greater burden on it. The function can rely less on the tree structure and must thus rely more on the structure of the input sentence. But the stronger factorization will also greatly reduce the size of the state-space of the dynamic programs, greatly speeding up training and inference, an the burden of the feature function will be carried by a rich neural network parametrization. Together, this will make the parser fast and very effective.

4.1.1 Features

The scoring function Ψ is implemented with neural networks following the design of the minimal scoring function of Stern *et al.* (2017a). The local potentials can only make minimal use of structural information, as we argued above, but they can depend on the entire sentence. This suggest the use of RNN encodings. The representation of a span (i, j) is the concatenation of the difference between forward and backward vectors computed by a bidirectional RNN

$$\mathbf{s}_{ij} = [\mathbf{f}_j - \mathbf{f}_i; \mathbf{b}_i - \mathbf{b}_j], \tag{4.2}$$

illustrated in figure 4.1. The score for a label is computed from this vector using a feedforward network:

$$\log \Psi(\mathbf{x}, \mathbf{y}_a) = \Big[\text{FF}(\mathbf{s}_{ij})\Big]_\ell. \tag{4.3}$$

This architecture is rightly called minimal, but it works surprisingly well: Stern *et al.* (2017a) experiment with more elaborate functions based on concatenation of vectors (a strict superset of the minus approach) and biaffine scoring (inspired by (Dozat and Manning, 2016)), but these function improve marginally, if they do at all.

4.1.2 Motivation

The model regards a constituency tree as a collection of *labeled spans* over a sentence. Earlier CRF models for constituency parsing, both log-linear and neural, factorize trees over *anchored rules* (Finkel *et al.*, 2008; Durrett and Klein, 2015). This puts most of the expressiveness of the model in the state space of the dynamic program, modelling

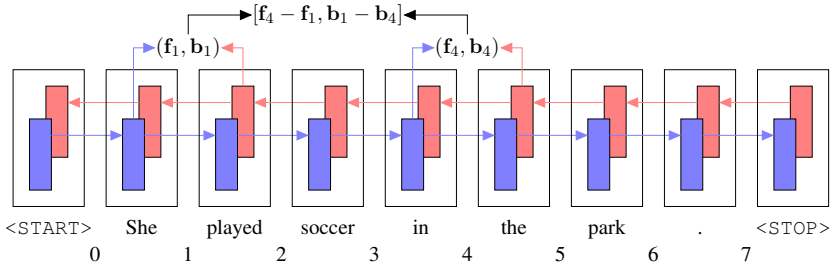


Figure 4.1: Representation for the span $(1, 4)$ computed from RNN encodings. Taken without permission from Gaddy *et al.* (2018).

interactions between subparts of the trees through their interaction in the rules, instead of at the feature level. The model in Stern *et al.* (2017a) removes part of this structure, and puts more expressiveness in the input space by using rich neural feature representations conditioning on the entire sentence. The discrete interaction between the local scores remains only at level of labeled spans. This dramatically improves the speed of this model, which will become evident in the next section.

Chart based parsing shows a move from grammar to features. The work of Hall *et al.* (2014) shows how the log-linear CRF model of Finkel *et al.*, 2008 can work with bare unnanotated grammars when relying more on surface features of the sentence, and Durrett and Klein (2015) show how these surface features can be replaced with dense neural features. The work of (Stern *et al.*, 2017a) moves one step further: the grammar is dispensed with altogether, making the model span-factored, and the scoring function is given the full power of neural networks.

Contrast this with generative parsing based on treebank grammars, where features are not available because the models are not conditional. Instead, these models rely entirely on detailed rule information. Basic treebank grammars do not parse well because the rules provide too little context, and good results can only be obtained by enriching grammars. Hence the independence assumptions in the grammar are typically weakened, not strengtehened. Such approaches lexicalize rules (Collins, 2003), annotate the rule with parent and sibling labels (Klein and Manning, 2003), or automatically learn refinements of nonterminal

categories (Petrov *et al.*, 2006).

The closest predecessor to our model is the neural CRF parser of Durrett and Klein (2015), which predicts local potential for anchored rules using a feedfoward network. This differs from our approach in two ways. Their method requires a grammar, extracted from a treebank beforehand, whereas our approach implictly assumes all rules are possible rules in the grammar. Secondly, their scoring function conditions only on the parts of the sentence directly under the rule, dictated by the use of a feedforward network, whereas our scoring function computes a score bassed on representations computed from the entire sequence.

4.2 Inference

Because the model is span-factored it allows efficient inference. In this section we describe efficient solutions to four related problems:

- Find the best parse $\hat{\mathbf{y}} = \arg\max_{\mathbf{y}} p(\mathbf{y} \mid \mathbf{x})$
- Compute the normalizer $Z(\mathbf{x}) = \sum_{\mathbf{y}} \prod_{a=1}^{A} \Psi(\mathbf{x}, \mathbf{y}_a)$.
- Obtain a sample $y \sim p(\mathbf{y} \mid \mathbf{x})$.
- Compute the entropy $H(\mathbf{y})$ conditional on $\mathbf{x}$.

These problems are solved by different instances of the same two algorithms: the inside algorithm and the outside algorithm. We first describe how these quantities will be used, and then how these are computed. For each labeled span, the inside algorithms comptutes the inside values

$$\alpha = ...$$

and the outside algorithm computes the outside values

$$\beta = ..$$

Given these quantities, we can directly solve three problems described above.

Lognoramlizer The lognormalizer is the inside value at the root node

- $Z(\mathbf{x}) = \alpha(ROOT, 1, n)$.

Entropy Derivation for entropy...

Parse Semirings... Viterbi from inside... Replacing the max with plus. sum-product, max-product, etcetera.

4.2.1 Inside recursion

In this derivation we follow Michael Collins notes on the Inside-Outside Algorithm.[1] We have the following general result for the inside value α. For all $A \in N$, for all $0 \leq i < n$

$$\alpha(A, i, i+1) = \psi(A, i, i+1) \tag{4.4}$$

and for all (i, j) such that $1 \leq i < j \leq n$:

$$\alpha(A, i, j) = \sum_{A \to BC} \sum_{k=i+1}^{j-1} \psi(A \to B\ C, i, k, j) \cdot \alpha(B, i, k) \cdot \alpha(C, k, j) \tag{4.5}$$

Note that we are considering a CFG in which the rule set is complete, i.e.

$$\langle A \to B\ C \rangle \in R \text{ for each } (A, B, C) \in N^3, \tag{4.6}$$

and recall that the labels B and C do not appear in the scoring functions in **??**. These facts will allow us to simplify the expression in formula 4.5 as

$$\begin{aligned}
\alpha(A, i, j) &= \sum_{B \in N} \sum_{C \in N} \sum_{k=i+1}^{j-1} \tilde{s}(i, j, A) \cdot \alpha(B, i, k) \cdot \alpha(C, k, j) \\
&= \tilde{s}(i, j, A) \cdot \sum_{k=i+1}^{j-1} \sum_{B \in N} \alpha(B, i, k) \cdot \sum_{C \in N} \alpha(C, k, j) \\
&= \tilde{s}(i, j, A) \cdot \sum_{k=i+1}^{j-1} S(i, k) \cdot S(k, j)
\end{aligned}$$

[1] http://www.cs.columbia.edu/~mcollins/io.pdf

where we've introduced a number of notational abbreviations

$$\tilde{s}(i,j,A) = \exp(s(i,j,A))$$
$$S(i,j) = \sum_{A \in N} \alpha(A,i,j)$$

Note that this is the exact same formula as **??**.

From equation 4.9 we can deduce that we in fact do even need to store the values $\alpha(i,j,A)$ but that it suffices to only store the marginalized values $S(i,j)$. In this case, the recursion simplifies even further:

$$\begin{aligned} S(i,j) &= \sum_{A \in N} \alpha(A,i,j) \\ &= \sum_{A \in N} \tilde{s}(i,j,A) \cdot \sum_{k=i+1}^{j-1} S(i,k) \cdot S(k,j) \\ &= \left[\sum_{A \in N} \tilde{s}(i,j,A) \cdot \right] \left[\sum_{k=i+1}^{j-1} S(i,k) \cdot S(k,j) \right] \end{aligned}$$

where we put explicit brackets to emphasize that independence of the subproblems of labeling and splitting. We can now recognize this as the 'inside' equivalent of the expression from the paper[2]

$$s_{best}(i,j) = \max_{\ell}[s(i,j,\ell)] + \max_{k}[s_{split}(i,k,j)]. \tag{4.9}$$

The recursions are the same; the semirings are different. The viterbi recursion given above is in the ViterbiSemiring, which uses the max operator as $\oplus$; the inside recursion given in 4.9 has standard addition $(+)$ instead.

[2] I believe there is actually an error in this equation: it should read $s(i,j,\ell) + s_{span}(i,j)$ instead of just $s(i,j,\ell)$. This is implied by the score for a single node, which is given by equation **??**, taken directly from the paper.

4.2.2 Outside recursion

$$
\begin{aligned}
\beta(A,i,j) &= \sum_{B\to CA\in R}\sum_{k=1}^{i-1}\psi(B\to CA,k,i-1,j)\cdot\alpha(C,k,i-1)\cdot\beta(B,k,j) \\
&\quad + \sum_{B\to AC\in R}\sum_{k=j+1}^{n}\psi(B\to A,C,i,j,k)\cdot\alpha(C,j+1,k)\cdot\beta(B,i,k) \\
&= \sum_{B\in N}\sum_{C\in N}\sum_{k=1}^{i-1}\psi(B,k,j)\cdot\alpha(C,k,i-1)\cdot\beta(B,k,j) \\
&\quad + \sum_{B\in N}\sum_{C\in N}\sum_{k=j+1}^{n}\psi(B,i,k)\cdot\alpha(C,j+1,k)\cdot\beta(B,i,k) \\
&= \sum_{k=1}^{i-1}\left[\sum_{B\in N}\psi(B,k,j)\cdot\beta(B,k,j)\right]\cdot\left[\sum_{C\in N}\alpha(C,k,i-1)\right] \\
&\quad + \sum_{k=j+1}^{n}\left[\sum_{B\in N}\psi(B,i,k)\cdot\beta(B,i,k)\right]\cdot\left[\sum_{C\in N}\alpha(C,j+1,k)\right] \\
&= \sum_{k=1}^{i-1}S'(k,j)\cdot S(k,i-1) + \sum_{k=j+1}^{n}S'(i,k)\cdot S(j+1,k)
\end{aligned}
$$

where

$$
\begin{aligned}
S(i,j) &= \sum_{A\in N}\alpha(A,i,j) \\
S'(i,j) &= \sum_{A\in N}\psi(A,i,j)\beta(A,i,j)
\end{aligned}
$$

4.3 Experiments

We perform three types of experiments with the CRF parser:

- We show that the model is a good supervised parser. We train the model supervised on the PTB and show the f-score on the PTB test set.
- We evaluate the joint RNNG with samples from the CRF parser. We compare the perplexity and fscore with RNNG case.

- We evauluate 'how good the model is' as a sampler.

Supervised model We investigate the following.

- We have some optimization and hyperparameter choices here. The original paper uses Adam with 0.001 and a LSTM of dimension 250, which gives the model around 2.5 million parameters. For the discriminative RRNG we use SGD with 0.1, and hidden sizes of 128 gives the model around 800,000 parameters.

- I suggest two experiments: (1) use the default setting from (Stern *et al.*, 2017a) and (2) use the settings for the RNNG with a hidden size to match the 800,000 parameters.

Proposal model We investigate the following:

- We evaluate validation F-score and perplexity.

- We evaluate F-score with 100 samples (as many proposal trees as possible).

- We evaluate perplexity with varying number of samples: 1 (argmax), 10, 20, 50, 100 (default). The peplexity evaluation with the argmax prediction gives an impression of the uncertaty in the model (Buys and Blunsom, 2018).

- We perform learning rate decay and model selection based on a development score computed with the samples from the discriminative RNNG. Undecided: should we train a separate joint RNNG with CRF samples?

Sampler We investigate the following:

- We asses the conditional entropy of the model. This is most quantitative. Recall that conditional entropy is defined as

$$\mathrm{H}(Y|X) = \sum_{x \in \mathcal{X}} p_X(x) \mathrm{H}(Y|X = x), \tag{4.10}$$

where

$$\mathrm{H}(Y|X=x) = -\sum_{y \in \mathcal{Y}} p_{Y|X}(y|x) \log p_{Y|X}(y|x). \tag{4.11}$$

The quantity $\mathrm{H}(Y|X=x)$ can computed exactly with the CRF parser. We estimate the quantity $\mathrm{H}(Y|X)$ by a sum over the development dataset. For the probabilities $p_X(x)$ we use the marginalized probabilities of the joint RNNG (with samples from the CRF parser $p_{Y|X}$).

- We asses for some cherry picked sentences. This is more qualitative. These sentences should be difficult or ambiguous. Or they can be ungramatical when taken from the syneval dataset. We can evaluate their entropy, and the diversity of samples, for example to see if there are clear modes. We can make violinplots of the probabilities of the samples. We can compute the f-scores of the samples compared with the argmax tree.

4.4 Related work

Here I describe related work, and in particular earlier approaches to (neural) CRF-parsing.

1. Of course (Stern *et al.*, 2017a)
2. CRFs (Sutton and McCallum, 2012)
3. CRF parsing with linear and nonlinear features (Finkel *et al.*, 2008; Durrett and Klein, 2015)
4. Attempts to simplify the grammar and thus the state-space of the dynamic program (Hall *et al.*, 2014).
5. Recent extension of Stern *et al.* (2017a), with same model but different features (Kitaev and Klein, 2018).

Earlier work on CRF parsing consider a tree as a collection of anchored rule productions productions Finkel *et al.*, 2008; Durrett and

Klein, 2015, and hence define the score of a tree as the product over clique potentials on anchored rules:

$$\log \psi(A \to B\ C, i, k, j) = \log \psi(A, i, j) \tag{4.12}$$

$$\tag{4.13}$$

discarding the rest of the span information. The function is then defined as

$$\log \psi(A, i, j) \triangleq s(i, j, A), \tag{4.14}$$

and thus the potential of a tree as

$$\log \Psi(T) = \sum_{r \in T} \log \psi(r) \tag{4.15}$$

$$= \sum_{\langle A,i,j \rangle \in T} s(i, j, A), \tag{4.16}$$

$$\tag{4.17}$$

Note that the potential function as defined in **??** disregards most of the information in a binary rule. In particular we see that B, C and k, the labels and split-point of the children, are discarded.

Now note that equation 4.15 corresponds exactly to the second formula in section 3 of the minimal span-based parser paper

$$s_{tree}(T) = \sum_{(\ell(i,j)) \in T} [s(i, j, \ell)]. \tag{4.18}$$

which is how I derived that **??** is the correct formula for the rule score.

5

Semisupervised learning

In this chapter we show how the RNNG can be trained on unlabeled data. Together with the regular, supervised, objective, this derives a way to perform semisupervised training.

- I formulate an unsupervised objective for the RNNG that we can combine with the supervised objective to perfom semisupervised training.
- I introduce an approximate posterior in the form of a discriminative parser and derive a variational lower bound on the unsupervised objective.
- I show how to obtain gradients for this lowerbound by rewrinting the gradient into a form that is called the score function estimator (Williams, 1992; Fu, 2006).

Notation In this chapter we write $\mathbf{x}$ for a sentence, $\mathbf{y}$ for a (latent) constituency tree, and $\mathcal{Y}(\mathbf{x})$ for the *yield* of $\mathbf{x}$, all trees that can be assigned to $\mathbf{x}$. Furthermore, let $\mathcal{D}_L = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ be a labeled dataset of sentences $\mathbf{x}$ with gold trees $\mathbf{y}$, and let $\mathcal{D}_U = \{\mathbf{x}_i\}_{i=1}^M$ be an unlabeled dataset consisting of just sentences $\mathbf{x}$. We denote our generative RNNG

with p_θ and when we write q_λ we will mean either the discriminative RNNG or the CRF parser.

5.1 Objective

We define the following general semi-supervised objective

$$\mathcal{L}(\theta, \lambda) \triangleq \mathcal{L}_S(\theta) + \mathcal{L}_U(\theta, \lambda).$$

The supervised objective $\mathcal{L}_S$ is optimized over $\mathcal{D}_L$ and $\mathcal{L}_U$ the unsupervised objective optimized over $\mathcal{D}_U$. We introduce $\alpha \in \mathbb{R}_{\geq 0}$ as an arbitrary scalar controlling the contribution of the unsupervised objective.

Supervised objective We define the supervised objective $\mathcal{L}_S(\theta)$ as

$$\mathcal{L}_S(\theta) \triangleq \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}_L} \log p_\theta(\mathbf{x}, \mathbf{y})$$

This objective is optimized as usual using stochastic gradient estimates:

$$\nabla_\theta \mathcal{L}_S(\theta) \approx \frac{N}{K} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{B}} \nabla_\theta \log p_\theta(\mathbf{x}, \mathbf{y}),$$

where $\mathcal{B} \subseteq \mathcal{D}_U$ is a mini-batch of size K sampled uniformly from the dataset. We rely on automatic differentiation to compute $\nabla_\theta \log p_\theta(\mathbf{x}, \mathbf{y})$ (**baydin2017automatic**).

Unsupervised objective We define the unsupervised objective $\mathcal{L}_U(\theta, \lambda)$ as

$$\begin{aligned}\mathcal{L}_U(\theta, \lambda) &\triangleq \sum_{\mathbf{x}\in\mathcal{D}_U} \log p(\mathbf{x}) \\ &= \sum_{\mathbf{x}\in\mathcal{D}_U} \log \sum_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} p_\theta(\mathbf{x}, \mathbf{y})\end{aligned}$$

This is a language modelling objective, in which we treat $\mathbf{y}$ as latent. We have noted the a consequence the lack of independence assumptions

of the RNNG is that the sum over trees $\mathbf{y}$ is not tractable. To optimize this objective we must thus fall back on approximate methods.

5.2 Variational approximation

We optimize the unsupervised objective using variational inference (Blei *et al.*, 2016). We introduce a posterior $q_\lambda(\mathbf{y}|\mathbf{x})$ parametrised by λ and use Jensen's inequality to derive a variational lower bound on the objective $\mathcal{L}_U(\theta, \lambda)$. First we bound the likelihood of one $\mathbf{x}$ in $\mathcal{D}_U$

$$\begin{aligned}
\log p(\mathbf{x}) &= \log \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_\lambda(\mathbf{y}|\mathbf{x}) \frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \\
&= \log \mathbf{E}_q \left[\frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \right] \\
&\geq \mathbf{E}_q \left[\log \frac{p_\theta(\mathbf{x}, \mathbf{y})}{q_\lambda(\mathbf{y}|\mathbf{x})} \right] \\
&= \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big]
\end{aligned}$$

and write

$$\begin{aligned}
\mathcal{E}(\theta, \lambda) &\triangleq \sum_{\mathbf{x} \in \mathcal{D}_U} \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \\
&\leq \sum_{\mathbf{x} \in \mathcal{D}_U} \log p(\mathbf{x}) \\
&= \mathcal{L}_U(\theta, \lambda) \qquad (5.1)
\end{aligned}$$

as a lower bound on our true objective $\mathcal{L}_U$. This is a particular instance of the evidence lower bound (ELBO) (Blei *et al.*, 2016). The quantity can be rewritten to reveal an entropy term $\mathrm{H}(q)$

$$\begin{aligned}
\mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] &= \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) \Big] - \mathbf{E}_q \Big[\log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \\
&= \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) \Big] + \mathrm{H}(q),
\end{aligned}$$

which gives this objective an intuitive interpretation. On the one hand, the objective aims to

Posterior The posterior q can be any kind of models, with the only condition that for all $\mathbf{x}$ and $\mathbf{y} \in \mathcal{Y}(\mathbf{x})$,

$$p(\mathbf{x}, \mathbf{y}) > 0 \Rightarrow q(\mathbf{y}|\mathbf{x}) > 0.$$

This condition is fulfilled by any discriminatively trained parser with the same support as the joint RNNG p. We have two obvious choices at hand: the discriminatively trained RNNG, and the CRF parser that we introduced in chapter 4.

An interesting advantage of the CRF parser is that we *can* compute the entropy $\mathrm{H}(q)$ exactly. This contrasts with the discriminative RNNG, where $\mathrm{H}(q)$ can only be approximated. To make this explicit we introduct separate ELBO objectives:

$$\mathcal{E}_{\text{RNNG}}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_U} \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \tag{5.2}$$

$$\mathcal{E}_{\text{CRF}}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_U} \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) \Big] + \mathrm{H}(q). \tag{5.3}$$

5.3 Optimization

Just like the supervised objective $\mathcal{L}_U$ we optimize the lower bound $\mathcal{E}$ by gradient optimization, which means that we need to compute the gradients $\nabla_\theta \mathcal{E}(\theta, \lambda)$ and $\nabla_\lambda \mathcal{E}(\theta, \lambda)$.

Gradients of joint parameters The first gradient is easy and permits a straightforward Monte-Carlo estimate:

$$\begin{aligned}
\nabla_\theta \mathcal{E}(\theta, \lambda) &= \nabla_\theta \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \\
&= \mathbf{E}_q \Big[\nabla_\theta \log p_\theta(\mathbf{x}, \mathbf{y}) \Big] \\
&\approx \frac{1}{K} \sum_{i=1}^{K} \nabla_\theta \log p_\theta(\mathbf{x}, \mathbf{y}_i)
\end{aligned}$$

where $y_i \sim q_\lambda(\cdot|\mathbf{x})$ for $i = 1, \ldots, K$ are samples from the approximate posterior. We can move the gradient inside the expectation because q does not depend on θ, and note that $\nabla_\theta \log q_\lambda(\mathbf{y}|\mathbf{x}) = 0$.

Gradients of posterior parameters The second gradient is not so straightforward and requires us to rewrite the objective into a form that is called the *score function estimator* (Fu, 2006). Firstly we define a *learning signal*

$$L(\mathbf{x}, \mathbf{y}) \triangleq \log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}), \tag{5.4}$$

and use the identity in equation D.1 that we derive in the appendix

$$\begin{aligned}\nabla_\lambda \mathcal{E}(\theta, \lambda) &= \nabla_\lambda \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y})\Big] \\ &= \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x})\Big].\end{aligned}$$

In this rewritten form the gradient is in the form of an expectation, and that does permit a straightforward MC estimate:

$$\mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x})\Big] \approx \frac{1}{K} \sum_{i=1}^{K} L(\mathbf{x}, \mathbf{y}_i) \nabla_\lambda \log q_\lambda(\mathbf{x}|\mathbf{y}_i) \tag{5.5}$$

where again $y_i \sim q_\lambda(\cdot|\mathbf{x})$ for $i = 1, \ldots, K$ are independently sampled from the approximate posterior. This estimator has been derived in slightly different forms in Williams (1992), Paisley *et al.* (2012), Mnih and Gregor (2014), Ranganath *et al.* (2014), and Miao and Blunsom (2016) and is also known as the REINFORCE estimator (Williams, 1992).

5.4 Variance reduction

We introduce the two baselines:

- Feedforward baseline (Miao and Blunsom, 2016).
- Argmax baseline from Rennie *et al.* (2017) which is exact in the CRF, and approximate in the RNNG.
- The CRF has no variance in estimating the entropy.

5.5 Experiments

- Experiments with the two baselines and the two posteriors.

- Compare to a simple baseline: supervised learing on mixed gold-silver trees (partially predicted).
- Analyze the variance reduction provided by the different baselines.

5.6 Related work

- Discrete latent variables in neural models (Miao and Blunsom, 2016; Yin *et al.*, 2018).
- Semisupervised training for the RNNG (Cheng *et al.*, 2017).
- Argmax baseline Rennie *et al.*, 2017.
- Training with the policy gradient of a risk-objective as a surrogate for training with a dynamic oracle (Fried and Klein, 2018).

6

Syntactic evaluation

Language models are typically evaluated by the perplexity they assign on held out data. And thus did we evaluate our language models in the previous chapters. In this chapter we look at alternatives. In particular, we look at evaluation that specifically probes the syntactic abilities of a language model. To this end we take the dataset introduced by Marvin and Linzen (2018), which presents a comprehensive set of syntactic challenges, and evaluate the models presented thus far against them. The dataset consists of constructed sentence pairs that differ in only one word, where one sentence is grammatical and the other is not, and the task is to assign higher probability to the grammatical sentence. We can think of this task as soliciting comparative *acceptability judgements*, which is a key concept in linguistics. We will refer to this dataset as SYNEVAL, for *syntactic evaluation*.

Organization The chapter is organized as follows. First, I introduce the SYNEVAL dataset and describe syntactic phenomena that it tests, and review how this dataset relates to other work on syntactic evaluation. I then describe multitask learning as an approach already suggested to improve language models for this task, and introduce a novel mul-

titask model based on span labeling. Finally I evaluate all the models introduced in this thesis on this dataset and discuss the results.

6.1 Syntactic evaluation

A shortcoming of perplexity is that the metric conflates various sources of succes (Marvin and Linzen, 2018). A language model can make use of many aspects of language to predict the probability of a sequence of words. And although we would like the probability of a sentence to depend on high-level phenomena such as syntactic well-formedness or global semantic coherence, a language model can also focus on lower hanging fruit such as collocations and other semantic relations predicted from local context. Syntax is especially difficult to evaluate given that most sentences in a corpus are grammatically simple (Marvin and Linzen, 2018). Arguably, this conflation is also the appeal: perplexity is a one size fits all metric. But for a fine-grained analysis we must resort to a fine-grained metric.

Recently, a series of papers has introduced tasks that specifically evaluate the syntactic abilities of language models (Linzen *et al.*, 2016; Gulordava *et al.*, 2018; Marvin and Linzen, 2018). And such tasks can be very revealing. The task introduced by Linzen *et al.* (2016) is to predict the correct conjugation of a verb given an earlier occuring subject—especially in the precense of distracting subjects that intervene[1]. This task has revealed that lower perplexity does not imply greater succes on this task (Tran *et al.*, 2018), and that an explicitly syntactic model like the RNNG significanlty outperforms purely sequential models, especially with increasing distance between the subject and the verb (Kuncoro *et al.*, 2018). This type of agreement is one of the phenomena evaluated in SYNEVAL.

Dataset The SYNEVAL dataset consists of contrastive sentence pairs that differ in only one word. Let $(\mathbf{x}, \mathbf{x}')$ be this minimal pair, with grammatical sentence $\mathbf{x}$ and an ungrammatical sentence $\mathbf{x}'$. Then a language model p makes a correct prediction on this pair if $p(\mathbf{x}) > p(\mathbf{x}')$.

[1] E.g. *Parts* of the river valley *have/has*.

The classification is based on the probability of the entire sequence. This makes the task applicable to grammatical phenomena that involve interaction between multiple words, or where the word of contention does not have any left context. This contrasts with the task introduced in Linzen *et al.* (2016). This approach is also more natural for a model like the RNNG, where the probability of the sentence is computed by marginalizing over all latent structures, whereas individual word probabilities can only be obtained when conditioning on a single structure—for example a predicted parse—as is done in Kuncoro *et al.*, 2018.

The sentence pairs fall into three categories that linguists consider to depend crucially on hierachical syntactic structure (Everaert *et al.*, 2015; Xiang *et al.*, 2009):

1. Subject-verb agreement (The farmer *smiles.*)
2. Reflexive anaphora (The senators embarassed *themselves.*)
3. Negative polarity items (*No* authors have *ever* been famous.)

The dataset contains constructions of increasing difficulty for each of these category. For example, the distance between two words in a syntactic dependency can be increased by separating them with a prepositional phrase: *The farmer next to the guards smiles.* In this example *the guards* additionally forms a distractor for the proper conjugation of *smiles*, making the example extra challenging.

The dataset is constructed automatically using handcrafted context-free grammars. The lexical rules are finegrained so that the resulting sentences reasonably coherent semantically. In particular there are rules for animate and innanimate objects so a sentence like *The apple laughs* cannot be constructed. The total dataset consists of around 350,000 sentence pairs.

Categories The following list is the complete set of categories that are evaulated in the SYNEVAL dataset, taken from Marvin and Linzen (2018) with slight .[2]

1. **Simple agreement**:

[2]There is a slight confusion in the

   (a) The farmer *smiles*.

   (b) *The farmer *smile*.

2. **Agreement in a sentential complement**:

   (a) The mechanics said the author *laughs*.

   (b) *The mechanics said the author *laugh*.

3. **Agreement in short VP coordination**:

   (a) The authors laugh and *swim*.

   (b) *The authors laugh and *swims*.

4. **Agreement in long VP coordination**:

   (a) The author knows many different foreign languages and *enjoys* playing tennis with colleagues.

   (b) *The author knows many different foreign languages and *enjoy* playing tennis with colleagues.

5. **Agreement across a prepositional phrase**:

   (a) The author next to the guards *smiles*.

   (b) *The author next to the guards *smile*.

6. **Agreement across a subject relative clause**:

   (a) The author that likes the security guards *laughs*.

   (b) *The author that likes the security guards *laugh*.

7. **Agreement across an object relative**:

   (a) The movies that the guard likes *are* good.

   (b) *The movies that the guard likes *is* good.

8. **Agreement across an object relative (no *that*)**:

   (a) The movies the guard likes *are* good.

   (b) *The movies the guard likes *is* good.

9. **Agreement in an object relative**:

   (a) The movies that the guard *likes* are good.

   (b) *The movies that the guard *like* are good.

10. **Agreement in an object relative (no *that*)**:
    (a) The movies the guard *likes* are good.
    (b) *The movies the guard *like* are good.
11. **Simple reflexive anaphora**:
    (a) The author injured *himself*.
    (b) *The author injured *themselves*.
12. **Reflexive in sentential complement**:
    (a) The mechanics said the author hurt *himself*.
    (b) *The mechanics said the author hurt *themselves*.
13. **Reflexive across a relative clause**:
    (a) The author that the guards like injured *himself*.
    (b) *The author that the guards like injured *themselves*.
14. **Simple NPI**:
    (a) *No* authors have ever been famous.
    (b) **Most* authors have ever been famous.
15. **Simple NPI (the)**:
    (a) *No* authors have ever been popular.
    (b) **The* authors have ever been popular.
16. **NPI across a relative clause**:
    (a) *No* authors that *the* guards like have ever been famous.
    (b) **Most* authors that *no* guards like have ever been famous.
17. **NPI across a relative clause (the)**:
    (a) *No* authors that *the* guards like have ever been famous.
    (b) **The* authors that *no* guards like have ever been famous.

For the full list of lexical items used in the constructions we refer the reader to Marvin and Linzen (2018).

Related work There has been a surge recently of work on syntactic evaluation. Linzen *et al.* (2016) introduce the task of long distance subject-verb agreement and Gulordava *et al.* (2018) make this test more challenging by turning the sentences nonsensical while keeping them grammatical. Both datasets are extracted from a wikipedia corpus based on properties of their predicted dependency parse. To make the sentences nonsensical, Gulordava *et al.* (2018) randomly substitute words from the same grammatical category.[3] Warstadt *et al.* (2018) fine-tune neural models to learn to immitate grammatical acceptability judgments gathered from linguistics textbooks. McCoy *et al.* (2018) Train a neural machine translation model to learn how to turn a declarative sentence into a question. Linguist have argued that the transformations required to generate one from the other provide strong evidence for the existence of hierarchical structure in language Everaert *et al.*, 2015.[4] Finally, targeted evaluation has been introduced previously for semantic comprehension by Zweig and Burges (2011) in a sentence completion task, and minimal contrastive sentence pairs have been used to evaluate neural machine translation by Sennrich (2017).

6.2 Multitask learning

One method that makes language models perform better in the tasks described in this chapter is to provide stronger syntactic supervision by using multitask learning (Enguehard *et al.*, 2017; Marvin and Linzen, 2018). Multitask learning is a simple yet effective way of providing additional supervision to neural models by combining multiple tasks in one single objective, and has been succcesfully applied in natural language processing Collobert and Weston, 2008; Collobert *et al.*, 2011; Zhang and Weiss, 2016; Søgaard and Goldberg, 2016. By combining

[3] An approach inspired by Chomsky's (in)famous sentence *Colorless green ideas sleep furiously* that is both grammatical and nonsensical.

[4] These pairs play a central role as empirical evidence in the argument—known as the *argument from the poverty of the stimulus*—that humans have an innate predisposition for generalizations that rely on hierarchical structure rather than linear order (Chomsky, 1980). Sequence-to-sequence neural machine translation, on the other hand, is a fully sequential model that involves no hierarchical structure or transformations.

objectives that share parameters the model is encouraged to learn representations that are useful in all the tasks.

In this section I describe two simple baselines for the syntactic evaluation task that are based on multitask learning. Both methods are based on language modelling with a syntactic side objective. The first side objective is to predict combinatory categorical grammar (CCG) supertags (Bangalore and Joshi, 1999) for each word in the sentence, and is proposed in (Enguehard *et al.*, 2017). The second side objective is to label spans of words with their category. This objective is inspired by the label scoring function in the CRF parser introduced in chapter 4.This is similar to an approach found in recent work on semantic parsing where a similar side-objective is used and where it is called a 'syntactic scaffold' (Swayamdipta *et al.*, 2018). The exact form of our side-objective is novel, as far as the author is aware of, and is parametrized in a considerably simpler way. Both objectives are challenging and should require representations that encode a fair amount of syntactic information.

Multitask objective In our case we combine a language model p with a syntactic model q, and optimize these jointly over a single labeled dataset $\mathcal{D}$[5]. In this case, we maximize the objective

$$\mathcal{L}(\theta, \lambda, \xi) = \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \log p_{\theta,\lambda}(\mathbf{x}) + \log q_{\theta,\xi}(\mathbf{y}|\mathbf{x}) \tag{6.1}$$

with respect to the parameters θ, λ and ξ. The key feature of multitask learning is that the two models p and q share the set of parameters θ and that in objective 6.1 these parameters will thus be optimized to fit *both* the models well. The parameters in λ and ξ are optimized for their respective objectives separately. The proportion and the nature of the parameters that belong to θ is a choice of the modeller and determines how both objectives influence one another. In the following paragraphs we specify this parametrization.

[5]Note that it is our choice to focus on only a single dataset, and that multitask learning is principle more flexible than that, providing the option to combine multiple disjoint datasets in a single objective.

Language model The main model p is a regular RNN language model on sentences $\mathbf{x} = (x_1, \ldots, x_n)$:

$$\log p_{\theta,\lambda} = \sum_{i=1}^{n} \log p_{\theta,\lambda}(x_i \mid \mathbf{x}_{<i}),$$

where the probabilities are computed by linear regression on a feature vector $\mathbf{f}_{i-1}$ as

$$p_{\theta,\lambda}(x \mid \mathbf{x}_{<i}) \propto \exp \left[\mathbf{W}^\top \mathbf{f}_{i-1} + \mathbf{b}\right]_{x_i}.$$

where the parameters $\xi = \{\mathbf{W}, \mathbf{b}\}$ are specific to the language model. The features $\mathbf{f}_i$ are computed using a forward RNNparametrized by θ,

$$[\mathbf{f}_1, \ldots, \mathbf{f}_n] = \text{RNN}^f_\theta(\mathbf{x}).$$

These features are also used in the side objective, and it is in this precise sense that the parameters θ are shared between p and q.

Word labeling This side objective is taken from Enguehard *et al.* (2017) and is the side objective that is used in the multitask model of Marvin and Linzen (2018). Let $\mathbf{y} = (y_1, \ldots, y_n)$ be a sequence of CCG supertags for the sentence $\mathbf{x}$, with one tag for each word. The side model is then a simple greedy tagging model:

$$\log q_{\theta,\xi}(\mathbf{y} \mid \mathbf{x}) = \sum_{i=1}^{n} \log q_{\theta,\xi}(y_i \mid \mathbf{x}).$$

The probability over tags for position i are computed from $\mathbf{f}_i$ using a feedforward network parametrized by ξ

$$q_{\theta,\xi}(y_i \mid \mathbf{x}) \propto \exp \left[\text{FF}_\xi(\mathbf{f}_i)\right]_{y_i}.$$

Span labeling This side objective is inspired by the label scoring function of the CRF parser, and is novel as a multitask objective, as far as I know. Let $\mathbf{y}$ be a sequence of labeled spans $\mathbf{y}_k = (\ell_k, i_k, j_k)$

that are obtained from a gold parse tree for $\mathbf{x}$. Then the side model q predicts a label ℓ for a sentence $\mathbf{x}$ given span endpoints i and j:

$$\begin{aligned}\log q_{\theta,\xi}(\mathbf{y} \mid \mathbf{x}) &= \sum_{k=1}^{K} \log q_{\theta,\xi}(\mathbf{y}_k \mid \mathbf{x}) \\ &= \sum_{k=1}^{K} \log q_{\theta,\xi}(\ell_k \mid \mathbf{x}, i_k, j_k).\end{aligned}$$

We define a span feature as in the CRF parser

$$\mathbf{s}_{ij} = \mathbf{f}_j - \mathbf{f}_i$$

and compute a distribution over labels using a feedforward network parametrized by ξ

$$q_{\theta,\xi}(\ell \mid \mathbf{x}, i, j) \propto \exp\left[\text{FF}_{\xi}(\mathbf{s}_{ij})\right]_{\ell}.$$

This model differs from the supertagging model in the interaction between features that follows from the definition of $vecs_{ij}$. This simple definition puts significant strain on the features, which is precisely what we want.

6.3 Experiments

In this section we report the results on the dataset.

- Marvin and Linzen (2018) provide results with a number of
- To provide baselines we also train

evaluate a number of models on the examples and also provide results of human judgements gathered.

Human evaluation via amazon mechanical turk.

N-gram language model with kneser ney smoothing.

RNN language model (LSTM).

RNN language model with multitask learning.

6.3.1 Setup

- Following the example of Marvin and Linzen (2018) we train a regular LSTM language model, and a multitask LSTM language model with CCG supertagging. We additionally train
- For the language train 10 independent runs of each model and report means and standard deviations of their accuracy on the SYNEVAL dataset.

Details about training can be found in appendix B

6.3.2 Results

7

Conclusion

Here is a narrative summary of what I have shown in this thesis.

7.1 Main contributions

The main n contributions of thesis are:

Global training of a chart based neural parser. Here I describe what that entails.

Semisupervised training of RNNGs. Here I describe what that entails.

Effective baselines for the score function estimator. Here I describe what that entails.

7.2 Future work

We have identified possibilities for future work:

Something. Here I describe what that entails.

Appendices

A

Figures

In this appendix I will put figures, for cases where there are just too many. For example:

- The barplots of the syntactic evaluation
- The training losses for the various models
- The valuation perplexity and f-score during training.

A.1 Training plots

We show training plots that are means with standard deviation bands over 10 runs. We have two types of plots: losses and development scores.

Development scores Plots with development scores.

- DiscRNNG + GenRNNG-disc + GenRNNG-crf + CRF (small) development fscores.
- CRF parser lossses: our (128d + SGD) and original (250d + Adam).

- GenRNNG-disc + GenRNNG-crf development perplexity
- Language models: lstm + lstm-ccg + lstm-span development perplexity
- GenRNNG + LSTM development perplexity.

Training losses Plots with training losses.

A.2 Test scores

Here we show violin plots that show the distribution of the test scores.

A.3 Samples

Here we put figures to illustrate the samples.

A.4 Syntactic evaluation

Here we put more bar-charts for the syntactic evaluation.

B

Implementation

This appendix reports all details about the implementation of the models, including the datasets and their pre-processing, optimization, and hyperparameters. We have made some deliberate choices which we will motivate. As a general rule, we choose simplicity over maximal performance: we use a minimal scheme for dealing with unknown words, we use only word embeddings, which we learn from scratch, and use regular SGD optimization. The reason: to compare the models in a minimal setting so as to maximally focus on the essential modelling differences between the models. All code is available at github.com/daandouwe/thesis.

B.1 Data

B.1.1 Datasets

Penn Treebank We use a publicly available version of the Penn Treebank (PTB) that was preprocessed and published by Cross and Huang (2016), and that has since been used in the experiments of Stern *et al.* (2017a) and Kitaev and Klein (2018). The data is divided along the standard splits of sections 2-21 for training, section 22 for de-

velopment, and section 23 for testing. The dataset comes with predicted tags, which is for training neural parsers, but note, however, that none of our models use these tags. The dataset is availllable at https://github.com/jhcross/span-parser/data.[1]

One Billion Word Benchmark In the experiments on semisupervised learning we use the One Billion Word Benchmark (OBW) dataset (Chelba *et al.*, 2013) to obtain unlabeled data. This is a common dataset for large-scale language modelling (Jozefowicz *et al.*, 2016), and has the advantage that it has sentences seperated by a newline; a requirement for the RNNG language model, which should only be applied to entire sentences and not to longer or shorter segments.[2] The dataset in its entirety is far too large for our purposes, so instead we select sentences from the first section of the training data[3] by selecting the first 100,000 sentences that have at most 40 words. Because the OBW uses slightly different tokenization and standardization of characters than the Penn Treebank we perform a number of processing steps to smooth out these difference. First, we escape all brackets following the Penn Treebank convention (*e.g.* replacing `(` with `-LRB-`) and do the same for the quotation marks (*e.g.* replacing `"` with `"`). Finally, tokenization of negation is handled differently in the OBW, and we change this to the PTB convention (*e.g.* replacing `don 't` with `do n't`). These simple changes together avoid a lot of incoherences when combining this dataset with the PTB. The dataset is publicly availllable at http://www.statmt.org/lm-benchmark/, and scripts for preprocessing are availllable at github.com/daandouwe/thesis/scripts.

CCG supertags For the multitask language model with CCG supertagging we use the CCGBank (Hockenmaier and Steedman, 2007) processed by Enguehard *et al.* (2017) into a word-tag format. This is the dataset

[1] Although I do not know how it is possible to make the PTB public, given the licensing restrictions of the LDC, I am very thankful that it was done. Now, all the data used in this thesis is publicly availllable.

[2] For this reason we cannot use the otherwise appealing Wikitext dataset (Merity *et al.*, 2016): this dataset has sentences grouped into paragraphs.

[3] Section `news.en-00001-of-00100`.

also used by Marvin and Linzen (2018). It follows the same splits of the Penn Treebank as described above, and restricts the size of the tagset from the original 1363 different supertags to 452 supertags that occurred at least ten times, replacing the rest of the tags with a dummy token. The dataset is publicly availlable at https://github.com/BeckyMarvin/LM_syneval/tree/master/data/ccg_data.

B.1.2 Vocabularies

We use two types of vocabularies corresponding to the two types of models that we study this thesis: a vocabulary for the discriminative models and a vocabulary for the generative models. The vocabulary used in the discrminative models contains all words in the training data, whereas the vocabulary used in the generative models only includes words that occur at least 2 times in the training data[4]. Finally, in the semisupervised models we construct the vocabulary from the labeled and unlabeled datasets combined. To keep the vocabulary size manageable in this larger dataset we restrict the vocabulary of the generative model to words that occur at leest 3 times.

Unknown words We use a single token for unknown words, and during training replace each word w by this token with probability $1/(1 + \text{freq}(w))$, where $\text{freq}(w)$ is the frequency of w in the training data. In this we follow Stern *et al.* (2017a), and this is a different approach from Dyer *et al.* (2016) who use a set of almost 50 tokens each with detailed lexical information about the unknown word in question.[5] This elaborate approach is common in parsing but certainly not in language modelling (Dyer *et al.*, 2016), for which reason we opt for the simpler scheme of a single token.

Embeddings All word embeddings are learned from scratch: the embeddings are considered part of the model's parameters and are opti-

[4]This makes training of the generative model faster, because the softmax normalization involves less terms in the sum, and additionaly avoids the statistical difficulty related to predicting words that occur just once. The discrminative model has neither of these problems, since the words are only conditioned on

[5]This approach is taken from the Berkeley parser (Petrov *et al.*, 2006).

Table B.1: Vocabularies

mized jointly with the rest of them, starting from random initialization (Glorot and Bengio, 2010). While we surmise that more elaborate embeddings should improve performance of the models[6], such investigation is othogonal to our work. We furthermore do not experiment with any kind of subword information in the embeddings and, as noted before, make no use of tags in any of the models. The influence of such embeddings on the discriminate parser of Stern *et al.* (2017a) is analysed extensively by Gaddy *et al.* (2018), who investigate all combinations of word, tag, and character-LSTM embeddings, and find that the best model[7] improves on the worst model[8] by only 0.8 F1, which is a relative improvement of just 1%. We believe this justifies our basic approach.

B.2 Implementation

All our models are implemented in python using the Dynet neural network library (Neubig *et al.*, 2017b), and use automatic batching (Neubig *et al.*, 2017a). Automabatching enables efficient training of ours model, for which manual batching is not possible.

Optimization All our models are optimized with stochastic gradient-based methods, in which we use mini-batches to compute stochastic approximations of the model's gradient on the entire dataset. We use mini-batches subsampled from the dataset and let Dynet compute the gradients using automatic differentiation (Neubig *et al.*, 2017b; Baydin *et al.*, 2018). For all our supervised models we use regular stochastic gradient descent (SGD), with an initial learning rate of 0.1, and anneal this based on performance on a development set. This follows the recomendations of Wilson *et al.* (2017), who show that on models and

[6]See for example the impact of ELMo embeddings (Peters *et al.*, 2018) on the performance of the parser in Kitaev and Klein (2018) (an adaptation of the chart parser in Stern *et al.* (2017a)).

[7]A tie between the model that uses all embeddings concatenated and the model that uses just the character-LSTM, both with an F1 of 92.24.

[8]Using only word embeddings, at an F1 of 91.44.

Table B.2: Optimization

Table B.3: Model parameters

datasets similar to ours this method finds good solutions and is more robust against overfitting than methods with adaptive learning rates. This also follows Dyer *et al.* (2016), who obtain their best RNNG models using this optimizer and learning rate. For our semisupervised model we do rely on adaptive gradient methods, and use Adam (Kingma and Ba, 2014) with the default learning rate[9] of 0.001. Adaptive learning are considered more suitable for dealing with the dramatic variability in magnitude of the surrogate obective (Ranganath *et al.*, 2014; Fried and Klein, 2018). We use minibatches

We normalize the learning signal: "This variability makes training an inference network using a fixed learning rate difficult. We address this issue by dividing the centered learning signal by a running estimate of its standard deviation. This normalization ensures that the signal is approximately unit variance, and can be seen as a simple and efficient way of adapting the learning rate." (Mnih and Gregor, 2014).

Surrogate objective and gradient blocking Schulman *et al.*, 2015.

Hyperparameters For the RNNG we follow exactly the hyperparameters from the published papers. For the CRF parser

- Dropout of ...

[9] To be precise, this is the value α in Kingma and Ba (2014).

C

Conditional Random Fields

In this appendix I describe CRF's for factor graphs, together with the message passing algorithms from which forward-backward and inside-outside are derived.

D

Variational Inference

In this appendix we give an account of variational inference in general of amortized variational inference in particular. We focus on amortized inference with discrete latent variables, and in particular when the variables are structured. We then derive the score function gradient, as used in chapter 5, and we describe techniques to reduce the variance of this estimator.

D.1 Variational Inference

We will write some generic things about variational inference.

- Variational inference for exponential families, with conjugate priors (Jordan *et al.*, 1999; Wainwright and Jordan, 2008; Blei *et al.*, 2016).
- With amortized inference, using neural networks, for non-conjugate models (Kingma and Welling, 2014; Rezende *et al.*, 2014) and in particular the reparametrization trick that makes these models efficiently trainable.
- Reparametrization for discrete latent variables (Maddison *et al.*,

2017; Jang *et al.*, 2017).

- The generalization of this reparametrization trick in automatic differentiation variational inference (Kucukelbir *et al.*, 2017).
- Black box variational inference, which uses the same combination of score function gradient with variance reduction that we resort to (Ranganath *et al.*, 2014).

D.2 Score function estimator

In this section we provide a detailed derivation of the score function estimator:

$$\nabla_\lambda \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \Big] = \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \tag{D.1}$$

where

$$L(\mathbf{x}, \mathbf{y}) \triangleq \log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x})$$

$$\begin{aligned}
\nabla_\lambda \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \Big] &= \nabla_\lambda \mathbf{E}_q \Big[\log p_\theta(\mathbf{x}, \mathbf{y}) - \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big] \\
&= \nabla_\lambda \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \Big\{ q_\lambda(\mathbf{y}|\mathbf{x}) \log p_\theta(\mathbf{x}, \mathbf{y}) - q_\lambda(\mathbf{y}|\mathbf{x}) \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big\} \\
&= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \Big\{ \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \log p_\theta(\mathbf{x}, \mathbf{y}) - \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \log q_\lambda(\mathbf{y}|\mathbf{x}) \\
&\qquad - q_\lambda(\mathbf{y}|\mathbf{x}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big\} \\
&= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \Big\{ \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \log p_\theta(\mathbf{x}, \mathbf{y}) - \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big\} \\
&= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \Big\{ L(\mathbf{x}, \mathbf{y}) \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \Big\} \\
&= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \Big\{ L(\mathbf{x}, \mathbf{y}) q_\lambda(\mathbf{y}|\mathbf{x}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big\} \\
&= \mathbf{E}_q \Big[L(\mathbf{x}, \mathbf{y}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) \Big].
\end{aligned}$$

In this derivation we used the identity

$$\nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) = q_\lambda(\mathbf{y}|\mathbf{x}) \nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}),$$

which follows from the derivative

$$\nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) = \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) q_\lambda(\mathbf{y}|\mathbf{x})^{-1}.$$

We

$$\begin{aligned}
\sum_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} q_\lambda(\mathbf{y}|\mathbf{x})\nabla_\lambda \log q_\lambda(\mathbf{y}|\mathbf{x}) &= \sum_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} q_\lambda(\mathbf{y}|\mathbf{x}) \frac{\nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x})}{q_\lambda(\mathbf{y}|\mathbf{x})} \\
&= \sum_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} \nabla_\lambda q_\lambda(\mathbf{y}|\mathbf{x}) \\
&= \nabla_\lambda \sum_{\mathbf{y}\in\mathcal{Y}(\mathbf{x})} q_\lambda(\mathbf{y}|\mathbf{x}) \\
&= \nabla_\lambda 1 \\
&= 0.
\end{aligned}$$

D.3 Optimization

We use automatic differentiation (**baydin2017automatic**) to obtain all our gradients. In order to obtain the gradients in formula D.1 using this method we rewrite it in the form of a *surrogate objective* (Schulman *et al.*, 2015):

$$\mathcal{L}_{\text{SURR}}(\theta, \lambda) = \frac{1}{K}\sum_{i=1}^{K} \log q_\lambda(\mathbf{x}|\mathbf{y}_i)\textsc{BlockGrad}(L(\mathbf{x}, \mathbf{y}_i)). \tag{D.2}$$

The function BLOCKGRADdetaches a node from its upstream computation graph. This turns it effectively into a scalar. More precisely, let f be function (computed by a node in the computation graph) with parameters θ and input $\mathbf{x}$, then

$$\textsc{BlockGrad}(f_\theta(\mathbf{x})) \triangleq f(\mathbf{x}),$$

such that

$$\nabla_\theta \textsc{BlockGrad}(f_\theta(\mathbf{x})) = \nabla_\theta f(\mathbf{x}) = 0.$$

Automatic differentiation of equation D.2 with respect to λ will give us the exact expression we are looking for

$$\nabla_\lambda \mathcal{L}_{\text{SURR}}(\theta, \lambda) = \frac{1}{K} \sum_{i=1}^{K} L(\mathbf{x}, \mathbf{y}) \nabla_\lambda \log q_\lambda(\mathbf{x}|\mathbf{y}_i),$$

hence the adjective *surrogate*.

D.4 Variance reduction

We have derived an estimator for the gradient of the posterior parameters in the unsupervised objective. This estimator is unbiased, but is known to have high variance, often too much to be useful (Paisley *et al.*, 2012). Two effective methods to counter this are control variates and baselines (Ross, 2006).

Variance of estimator First, let's analyze the variance of our estimator. Note that our expectation is of the general form

$$\mu \triangleq \mathbf{E}\left[f(X)\right]$$

and that we estimate this quantity by generating n independent samples $X_1, \ldots, X_n \sim P(X)$ and computing

$$\hat{\mu} \triangleq \frac{1}{n} \sum_{i=1}^{n} f(X_i).$$

This is an unbiased estimator for μ with error

$$\left[(\mu - \hat{\mu})^2\right] = \mathbf{var}\left[\hat{\mu}\right] = \frac{\mathbf{var}\left[\hat{\mu}\right]}{n},$$

which means that the error

$$\mu - \hat{\mu} = O\left(\sqrt{\frac{\mathbf{var}\left[\hat{\mu}\right]}{n}}\right)$$

and reducing it linearly requires a quadratic number of samples.

In our particular case, the function f is

$$f_{X=x}(Y) \triangleq L(X, Y) \nabla_\lambda \log q_\lambda(Y|X = x)$$

where we have made explicit that y is the random variable, and x is given.

Control variates Consider a function $g(X)$ with known expectation

$$\mu_g \triangleq \mathbf{E}\left[g(X)\right]$$

Then we can define a new function $\hat{f}$ such that

$$\hat{f}(X) \triangleq f(X) - g(X) + \mu_g.$$

This function is also an estimator for μ, since

$$\begin{aligned}\mathbf{E}\left[\hat{f}(X)\right] &= \mathbf{E}\left[f(X)\right] - \mu_g + \mu_g \\ &= \mathbf{E}\left[f(X)\right],\end{aligned}$$

and a computation shows that the variance of the new function is

$$\begin{aligned}\mathbf{var}\left[\hat{f}(X)\right] &= \mathbf{E}\left[(f(X) - g(X) + \mu_g) - \mu)^2\right] \\ &= \mathbf{E}\left[(f(X) - g(X) + \mu_g)^2\right] - 2\,\mathbf{E}\left[(f(X) - g(X) + \mu_g)\mu\right] + \mathbf{E}\left[\mu^2\right] \\ &= \mathbf{E}\left[(f(X) - g(X) + \mu_g)^2\right] - 2\,\mathbf{E}\left[(f(X) - g(X) + \mu_g)\right]\mu + \mu^2 \\ &= \mathbf{E}\left[(f(X) - g(X) + \mu_g)^2\right] - 2\mu^2 + \mu^2 \\ &= \mathbf{E}\left[f(X)^2 + g(X)^2 + \mu_g^2 - 2f(X)g(X) + 2f(X)\mu_g - 2g(X)\mu_g\right] - \mu^2 \\ &= \mathbf{E}\left[f(X)^2\right] - \mathbf{E}\left[f(X)\right]^2 \\ &\qquad - 2(\mathbf{E}\left[f(X)g(X)\right] - \mathbf{E}\left[f(X)\right]\mathbf{E}\left[g(X)\right]) \\ &\qquad + \mathbf{E}\left[g(X)^2\right] - \mathbf{E}\left[g(X)\right]^2 \\ &= \mathbf{var}\left[f(X)\right] - 2\,\mathbf{cov}\left[f(X), g(X)\right] + \mathbf{var}\left[g(X)\right]\end{aligned}$$

This means we can get a reduction in variance whenever

$$\mathbf{cov}\left[f(X), g(X)\right] > \frac{1}{2}\,\mathbf{var}\left[g(X)\right].$$

The function g is called a *control variate*—it allows us to control the variance of f.

From the equality above we can see that this will be the case whenever $f(X)$ and $g(X)$ are strongly correlated. Our choice of control

variate will be made with the that in mind. Furthermore, $\mathbf{E}\left[g(X)\right]$ must be known. What is an optimal control variate? Typically a control variate of the form ag is chosen with fixed, and a is optimized to maximize the correlation. This brings us to the generic formulation of a control variate:

$$\hat{f}(X) \triangleq f(X) - a(g(X) - \mathbf{E}\left[g(X)\right])$$

with variance

$$\mathbf{var}\left[\hat{f}(X)\right] = \mathbf{var}\left[f(X)\right] - 2a\,\mathbf{cov}\left[f(X), g(X)\right] + a^2\,\mathbf{var}\left[g(X)\right]$$

We take a derivative of this with respect to a

$$\frac{d}{da}\,\mathbf{var}\left[\hat{f}(X)\right] = -2\,\mathbf{cov}[f(X), g(X)\right] + 2a\,\mathbf{var}\left[g(X)\right]$$

Setting this to zero and solving for a we obtain the optimal choice for a

$$a = \frac{\mathbf{cov}\left[f(X), g(X)\right]}{\mathbf{var}\left[g(X)\right]}. \tag{D.3}$$

Plugging in this solution into the expression for $\mathbf{var}\left[\hat{f}(X)\right]$ and dividing by $\mathbf{var}\left[f(X)\right]$ we get

$$\frac{\mathbf{var}\left[\hat{f}(X)\right]}{\mathbf{var}\left[f(X)\right]} = 1 - \frac{\mathbf{cov}[f(X), g(X)\right]}{\mathbf{var}\left[f(X)\right]\mathbf{var}\left[g(X)\right]} \tag{D.4}$$

$$= 1 - \mathbf{corr}^2\left[f(X), g(X)\right], \tag{D.5}$$

which shows that given this choice of a the reduction in variance is directly determined by the correlation between $f(X)$ and $g(X)$.

Bringing this all together, we let our new estimator be

$$\mathbf{E}\left[f(X)\right] = \mathbf{E}\left[\hat{f}(X)\right] \approx \frac{1}{n}\sum_{i=1}^{n}[f(X_i) - ag(X_i)\right] - \mu_g$$

Example (Ross, 2006) Suppose we want to use simulation to determine

$$\mathbf{E}\left[f(X)\right] = \mathbf{E}\left[e^X\right] = \int_0^1 e^x dx = e - 1$$

with $X \sim \mathcal{U}(0,1)$. A natural control variate to use in this case is the random variable X itself: $g(X) \triangleq X$. We thus define the new estimator

$$\begin{aligned}\hat{f}(X) &= f(X) - g(X) + \mathbf{E}\left[g(X)\right] \\ &= e^X - X + \frac{1}{2}.\end{aligned}$$

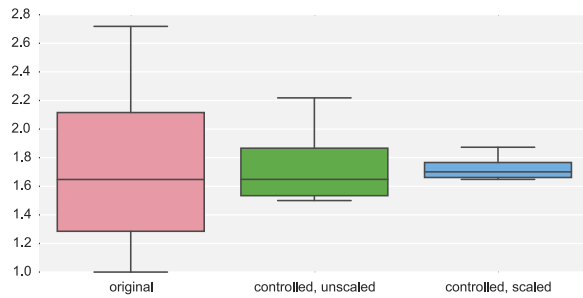
To compute the decrease in variance with this new estimator, we first note that

$$\begin{aligned}\mathbf{cov}(e^X, X) &= \mathbf{E}\left[Xe^X\right] - \mathbf{E}\left[X\right]\mathbf{E}\left[e^X\right] \\ &= \int_0^1 xe^x dx - \frac{e-1}{2} \\ &= 1 - \frac{e-1}{2} \approx 0.14086 \\ \mathbf{var}\left[e^X\right] &= \mathbf{E}\left[e^{2X}\right] - (\mathbf{E}\left[e^X\right])^2 \\ &= \int_0^1 e^{2x} dx - (1-e^x)^2 \\ &= \frac{e^2-1}{2} - (1-e^x)^2 \approx 0.2420 \\ \mathbf{var}\left[X\right] &= \mathbf{E}\left[X^2\right] - (\mathbf{E}\left[X\right])^2 \\ &= \int_0^1 x^2 dx - \frac{1}{4} \\ &= \frac{1}{3} - \frac{1}{4} = \frac{1}{12}.\end{aligned}$$

When we choose a as in formula D.3 we can use formula D.4 to compute that

$$\begin{aligned}\frac{\mathbf{var}\left[\hat{f}(X)\right]}{\mathbf{var}\left[f(X)\right]} &= 1 - \frac{(0.14086)^2}{\frac{0.2420}{12}} \\ &\approx 0.0161.\end{aligned}$$

This is a reduction of 98.4 percent! A simulation illustrates what this looks like in practice with ... samples:


2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
original
controlled, unscaled
controlled, scaled

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