Latent structure in deep generative models of language

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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:

- ...
- ...

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Notes

The plan for next week: hand in a fully outlines and bullet-pointed thesis

This is a todo list:

- Do not describe the CRF parser or inside-outside algorithm ('value recursion') in the exact framework of graphical models! These are hard to reconcile!
- $\bullet\,$ Use the general value recursion formulation and derive from there.
- Move formula derivations for the VI gradient and variance reduction to VI appendix.
- Move gradient blocking and surrogate objective to implementation appendix.
- Outline the chapter on RNNGs. Expand on sections on brains and syntax.
- Outline the chapter on syntactic evaluation.
- Describe the multitask models.

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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

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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 discriminatively 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.

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• 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. A similar strategy has recently proposed in work on semantic parsing and is called a 'syntactic scaffold' (Swayamdipta et al., 2018).

• 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

Background

In this chapter I give the background.

3.1 Syntax

- Some generic stuff on syntax, hierarchical structure in language, and constituency in natural language referencing Carnie (2010) and Everaert *et al.* (2015).
- Introduce the concept of *acceptability judgements*, with the final chapter on syntactic evaluation in mind.

3.2 Parsing

- Treebanks, in particular the Penn Treebank. Treebank preprocessing. CFGs, CNF, spans. Reference figure 3.1.
- 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.

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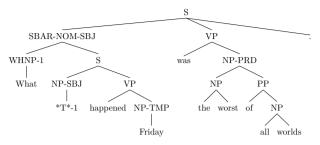
Labeled spans	Anchored rules							
(S, 0, 10)	$(S \to SBAR \varnothing, 0, 3, 10)$							
(SBAR, 0, 3)	(SBAR \rightarrow WHNP S+VP, 0, 1, 3)							
(VP, 1, 3)	$(S+VP \rightarrow \emptyset NP, 1, 2, 3)$							
÷	i:							
(NP, 7, 9)	$(NP \to \varnothing \varnothing, 7, 8, 9)$							

Table 3.1: Two conceptions of the tree in 3.1d.

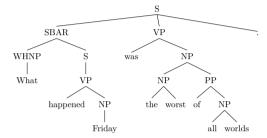
- An anchored rule is a triple (r, i, j) or four-tuple (r, i, k, j), containing a CNF rule r with span endpoints i, j, and a split-point k of the left and right child r is not a lexical rule.
- For the difference, consider the following two representations of the tree in figure 3.1d given in table 3.1.
- 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.

3.3 Language models

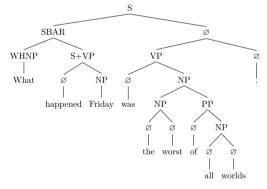
- Briefly mention some typical approaches for language modelling: count based n-gram with smoothing (Chen and Goodman, 1999; Kneser and Ney, 1995), neural n-gram (Bengio et al., 2003) and recurrent neural network (Mikolov et al., 2010). Also mention some (early) syntactic approaches: count-based (Chelba 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).



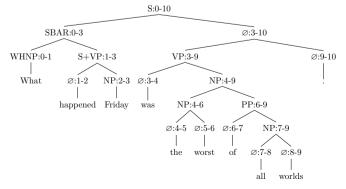
(a) Original Penn Treebank tree.



(b) Function tags and traces removed.



(c) Converted to normal form.



(d) In normal form with spans.

Figure 3.1: Converting a treebank tree (withouth part-of-speech tags).

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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).

3.4 Neural networks

Introduce all the neural networks: Ff, Rnn, Lstm, etc.

- We consider the neural networks as abstractions denoting certain parametrized functions.
- 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: $\mathbf{R}^n \to \mathbf{R}^m$.

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

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

Internally, the RNNrecursively applies an internal function f: $\mathbf{R}^n \times \mathbf{R}^m \to \mathbf{R}^m$, also called the recurrent *cell*, to the combined input of the current input and the output ouput of the previous timestep with the input at that timestep, like

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

where \mathbf{y}_0 is an initial vector that is does not depend on input.

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And RNNcan be applied to the inverse input sequence

$$reverse((\mathbf{x}_i)_{i=1}^n) \triangleq (\mathbf{x}_n, \mathbf{x}_{n-1}, \dots, \mathbf{x}_1), \tag{3.1}$$

that is, in *backward* direction:

$$Rnn^{B}((\mathbf{x}_{i})_{i=1}^{n}) = reverse(Rnn(reverse((\mathbf{x}_{i})_{i=1}^{n})))$$

$$= reverse(Rnn(\mathbf{x}_{n}, \mathbf{x}_{n-1}, \dots, \mathbf{x}_{1}))$$

$$= reverse(\mathbf{y}_{n}, \mathbf{y}_{n-1}, \dots, \mathbf{y}_{1})$$

$$= (\mathbf{y}_{1}, \mathbf{y}_{2}, \dots, \mathbf{y}_{n}).$$

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 :

$$Rnn^{B}((\mathbf{x}_{i})_{i=1}^{n}) = (\mathbf{b}_{1}, \mathbf{b}_{2}, \dots, \mathbf{b}_{n})$$
$$Rnn^{F}((\mathbf{x}_{i})_{i=1}^{n}) = (\mathbf{f}_{1}, \mathbf{f}_{2}, \dots, \mathbf{f}_{n}).$$

We can use the two functions above to construct a bidirectional RNNby combining their output

$$BIRNN((\mathbf{x}_i)_{i-1}^n) = (\mathbf{f}_1 \circ \mathbf{b}_1, \mathbf{f}_2 \circ \mathbf{b}_2, \dots, \mathbf{f}_n \circ \mathbf{b}_n), \tag{3.2}$$

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 RNNfunction, and similarly has a bidirectional equivalent BILSTM.

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

Recurrent Neural Network Grammars

4.1 Model

I describe the model.

- Specify the transition-system.
- The probabilistic model is given by

$$p(\mathbf{x}, \mathbf{y}) = \prod_{t=1}^{T} p(a_t | \mathbf{a}_{< t}) p(w_{\nu(t)} | \mathbf{a}_{< t})^{\mathbb{I}[a_t = \text{GEN}]} p(n_{\eta(t)} | \mathbf{a}_{< t})^{\mathbb{I}[a_t = \text{OPEN}]},$$

$$(4.1)$$

where ...

4.1.1 Features

The features from which the transition probabilities are predicted are computed from the entire transition history (no markov assumption) and in a syntax dependent way.

• The StackLSTM computes incremental features for the sequences on the three datastructures of the transition-system, with unbounded history.

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- A composition function computes representations of closed constituents.
- There are two options for the composition function: simple BiRNN and attention-based. The attention-based composition performed best in earlier research, so we focus on this composition.
- There is evidence that the stack- is all that is needed. We focus on the models that compute representations of all the datastructures.

4.2 Syntax and cognition

Here I describe the research into syntax and cognition using the RNNG.

Cognition RNNGs can tell us something about our brains.

- Psycholinguistic research that indicates that top-down parsing is a cognitively plausible parsing strategy (Brennan *et al.*, 2016).
- RNNGs are good statistical predictors in psycholinguistic research (Hale et al., 2018). More precisely: the sequential word-probabilities that are derived from a generative RNNG in combination with word-synchronous beam-search (Stern et al., 2017b) provide per-word complexity metrics that predict human reading difficulty well.

Syntax What do RNNGs learn about syntax?

- RNNGs learn a number of syntactic phenomena as a side product of the main objective. The attention mechanism in the composition function learns a type of 'soft' head-rules, and when trained on trees without syntactic labels the RNNG still learns representations for constituents that cluster according to their withheld gold label (Kuncoro et al., 2017).
- RNNGs are better at a long-distance verb-argument agreement task than LSTMS Linzen *et al.*, 2016; Kuncoro *et al.*, 2018.

4.3 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

$$H(Y|X) = \sum_{x \in \mathcal{X}} p_X(x)H(Y|X=x), \tag{4.2}$$

where

$$H(Y|X = x) = -\sum_{y \in \mathcal{V}} p_{Y|X}(y|x) \log p_{Y|X}(y|x).$$
 (4.3)

We estimate the quantity H(Y|X=x) with the model samples. We estimate the quantity 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 discriminative parser $p_{Y|X}$).

4.4. Related work

• 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

- Generative dependency parsing and language modelling (Buys and Blunsom, 2015a; Buys and Blunsom, 2015b; Buys and Blunsom, 2018)
- Top-down parsing and language modelling (Roark, 2001).
- Brains research with top-down parsing (Hale *et al.*, 2018; Brennan *et al.*, 2016).

Conditional Random Field parser

In this chapter I introduce an alternative parser to act as proposal model in the approximate marginalization.

- The parser is a neural Conditional Random Field (CRF) parser that combines the efficient exact inference of chart-based parsing with the rich nonlinear features of neural networks.
- The chart-based approach allows efficient exact inference, while the neural features can be relatively rich and can condition on the entire sentence.
- The neural network is used exclusively to learn good representation from which to predict local scores, while the global structured interactions are
- The parser is an adaptation of the chart-based parser introduced in Stern *et al.* (2017a), where it is trained with a margin-based objective.

5.1 Model

I describe the probabilistic model of the parser.

5.1. Model 17

1. Introduce probabilistic model, reference the appendix on CRFs C.

2. Desribe how this is an adaptation from Stern *et al.* (2017a) to probabilistic training.

Let a sentence be x_1, \ldots, x_n , where each x_i is a word. We are given a CFG (N, Σ, R, S) in Chomsky normal form. Let ψ be a function that maps any rule production $r \in R$ of the form $\langle A \to B \ C, i, k, j \rangle$ or $\langle A, i, i+1 \rangle$ to a value $\psi(r) \geq 0$. Let a tree T be a set of such rules r with the only constraint that these rules make up a tree.

Following the minimal span parser we define ψ as

$$\log \psi(A \to B \ C, i, k, j) \triangleq s_{label}(i, j, A) \tag{5.1}$$

and
$$(5.2)$$

$$\log \psi(A, i, i+1) \triangleq s_{label}(i, i+1, A), \tag{5.3}$$

and thus the potential of a tree as

$$\log \Psi(T) = \sum_{r \in T} \log \psi(r) \tag{5.4}$$

$$= \sum_{\langle A,i,j\rangle \in T} s_{label}(i,j,A), \tag{5.5}$$

(5.6)

Note that the potential function as defined in 5.1 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 5.4 corresponds exactly to the second formula in section 3 of the minimal span-based parser paper

$$s_{tree}(T) = \sum_{(\ell(i,j)) \in T} [s_{label}(i,j,\ell)]. \tag{5.7}$$

which is how I derived that 5.1 is the correct formula for the rule score. We obtain our CRF objective when we normalize this score globally

$$P(T) = \frac{\prod_{r \in T} \psi(r)}{\sum_{T' \in T} \prod_{r' \in T'} \psi(r')}$$
 (5.8)

(5.9)

or equivalently

$$\log P(T) = \sum_{r \in T} \log \psi(r) - \log \sum_{T \in T} \prod_{r \in T} \psi(r)$$
(5.10)

5.1.1 Features

I describe how the local scores are computed using neural networks.

• Give formal expression for feature function: 'LSTM minus features' with Feedforward scoring function.

5.1.2 Motivation

- Key point to make: this model regards a constituency tree as a collection of *labeled spans* over a sentence. Earlier models, both log-linear and neural, regard a constituency tree as a collection of *anchored rules* over a sentence (Finkel *et al.*, 2008; Durrett and Klein, 2015).
- A model over spanned rules puts more expressiveness in the state space of the dynamic program, because the correlations between subparts of the trees are modeled through the rich rules. The model in Stern et al. (2017a) instead puts the expressiveness in the input space by using rich neural feature representations. The state space in contrast is less structured, because the score-function is agnostic to the composition of it's children.
- Earlier approaches went even farther. These approaches enriched the grammar by lexicalizing the rules (Collins, 2003) or by breaking the grammar's independence assumptions by annotating the rule with parent and sibling labels (Klein and Manning, 2003).
- The choice to model labeled spans makes dramatically improves the speed of this model. In the section on inference we will show precisely how.

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5.2 Inference

Due to the parametrization, the model allows efficient inference. In this section we describe efficient solutions to three related problems:

- Find the best parse $\mathbf{y}^* = \arg \max_{\mathbf{y}} p(\mathbf{y}|\mathbf{x})$
- Compute the normalizer $Z(\mathbf{x}) = \sum_{\mathbf{y}} \prod_{a=1}^{A} \Psi(\mathbf{x}, \mathbf{y}_a)$, where $F = \{\Psi_a\}_{a=1}^{A}$ is the set of factors in the graph.
- Compute the entropy conditioned on \mathbf{x} , $H(\mathbf{y}|\mathbf{x})$.

All three problems can be solved with a different instance of the same two algorithm: the inside algorithm and the outside algorithm.

5.2.1 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 $0 \le i < n$

$$\alpha(A, i, i+1) = \psi(A, i, i+1)$$
 (5.12)

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

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

$$(5.13)$$

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

$$\langle A \to B \ C \rangle \in R \text{ for each } (A, B, C) \in \mathbb{N}^3,$$
 (5.14)

and recall that the labels B and C do not appear in the scoring functions in 5.1. These facts will allow us to simplify the expression in formula

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

5.13 as

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

where we've introduced a number of notational abbreviations

$$\tilde{s}_{label}(i, j, A) = \exp(s_{label}(i, j, A))$$

$$\tilde{s}_{span}(i, j) = \exp(s_{span}(i, j))$$

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

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

From equation 5.17 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:

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

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 paper²

$$s_{best}(i,j) = \max_{\ell} [s_{label}(i,j,\ell)] + \max_{k} [s_{split}(i,k,j)]. \tag{5.17}$$

²I believe there is actually an error in this equation: it should read $s_{label}(i, j, \ell) + s_{span}(i, j)$ instead of just $s_{label}(i, j, \ell)$. This is implied by the score for a single node, which is given by equation 5.1, taken directly from the paper.

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 5.17 has standard addition (+) instead.

5.2.2 Outside recursion

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

where

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

$$S'(i,j) = \sum_{A \in N} \psi(A,i,j)\beta(A,i,j)$$

5.3 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?

5.4. Related work 23

Sampler We investigate the following:

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

$$H(Y|X) = \sum_{x \in \mathcal{X}} p_X(x)H(Y|X=x), \tag{5.18}$$

where

$$H(Y|X = x) = -\sum_{y \in \mathcal{Y}} p_{Y|X}(y|x) \log p_{Y|X}(y|x).$$
 (5.19)

The quantity H(Y|X=x) can computed exactly with the CRF parser. We estimate the quantity 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.

5.4 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 encoder (Kitaev and Klein, 2018).

Semisupervised learning

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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.

6.1 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 $\nabla_{\theta} \log p_{\theta}(\mathbf{x}, \mathbf{y})$ (Baydin *et al.*, 2017).

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

$$\mathcal{L}_{U}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_{U}} \log p(\mathbf{x})$$
$$= \sum_{\mathbf{x} \in \mathcal{D}_{U}} \log \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} p_{\theta}(\mathbf{x}, \mathbf{y})$$

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.

6.2 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}

$$\log p(\mathbf{x}) = \log \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_{\lambda}(\mathbf{y} | \mathbf{x}) \frac{p_{\theta}(\mathbf{x}, \mathbf{y})}{q_{\lambda}(\mathbf{y} | \mathbf{x})}$$

$$= \log \mathbf{E}_{q} \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{y})}{q_{\lambda}(\mathbf{y} | \mathbf{x})} \right]$$

$$\geq \mathbf{E}_{q} \left[\log \frac{p_{\theta}(\mathbf{x}, \mathbf{y})}{q_{\lambda}(\mathbf{y} | \mathbf{x})} \right]$$

$$= \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right]$$

and write

$$\mathcal{E}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_{U}} \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} \mid \mathbf{x}) \right]$$

$$\leq \sum_{\mathbf{x} \in \mathcal{D}_{U}} \log p(\mathbf{x})$$

$$= \mathcal{L}_{U}(\theta, \lambda)$$
(6.1)

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 H(q)

$$\mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right] = \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) \right] - \mathbf{E}_{q} \left[\log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right]$$
$$= \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) \right] + \mathbf{H}(q),$$

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 5.

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

$$\mathcal{E}_{\text{RNNG}}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_U} \mathbf{E}_q \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} \,|\, \mathbf{x}) \right]$$
(6.2)

$$\mathcal{E}_{CRF}(\theta, \lambda) \triangleq \sum_{\mathbf{x} \in \mathcal{D}_U} \mathbf{E}_q \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) \right] + \mathbf{H}(q).$$
 (6.3)

6.3 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:

$$\nabla_{\theta} \mathcal{E}(\theta, \lambda) = \nabla_{\theta} \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} \mid \mathbf{x}) \right]$$
$$= \mathbf{E}_{q} \left[\nabla_{\theta} \log p_{\theta}(\mathbf{x}, \mathbf{y}) \right]$$
$$\approx \frac{1}{K} \sum_{i=1}^{K} \nabla_{\theta} \log p_{\theta}(\mathbf{x}, \mathbf{y}_{i})$$

where $y_i \sim q_{\lambda}(\cdot | \mathbf{x})$ for i = 1, ..., 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*

$$L(\mathbf{x}, \mathbf{y}) \triangleq \log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} \mid \mathbf{x}), \tag{6.4}$$

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

$$\nabla_{\lambda} \mathcal{E}(\theta, \lambda) = \nabla_{\lambda} \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \right]$$
$$= \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right].$$

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

$$\mathbf{E}_{q}\left[L(\mathbf{x}, \mathbf{y})\nabla_{\lambda}\log q_{\lambda}(\mathbf{y} \,|\, \mathbf{x})\right] \approx \frac{1}{K} \sum_{i=1}^{K} l(\mathbf{x}, \mathbf{y}_{i})\nabla_{\lambda}\log q_{\lambda}(\mathbf{x} \,|\, \mathbf{y}_{i})$$
(6.5)

where again $y_i \sim q_{\lambda}(\cdot | \mathbf{x})$ for i = 1, ..., 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).

6.4 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.

6.5 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.

6.6 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.

Syntactic evaluation

In this section I describe the syntactic evaluation that I perform.

7.1 Syntactic evaluation of language models

In this section we evaluate language models on a recently proposed syntactic task: to distinguish a grammatical sentence from a minimally differing ungrammatical couterpart (Marvin and Linzen, 2018).

- The task is as follows. Let (w, w^*) be a minimal pair with a grammatical sentence w and an ungrammatical sentence w^* . Then the language model p makes a correct prediction if $p(w) > p(w^*)$.
- The classification is based on the probability that the model assigns to the entire sentence. This means that the task can be applied to grammatical phenomena that are not local, e.g. that depend on a single word, or that are not sequential, like *negative* polarity items, unlike the word-prediction task in Linzen et al., 2016.
- This task can be thought of as soliciting grammatical acceptability judgements from the model, a key concept in linguistics.

7.1.1 Dataset

I describe the dataset from (Marvin and Linzen, 2018).

7.1.2 Related work

I review the literature on related syntactic evaluations and show

- Long distance subject-verb agreement with natural sentences (Linzen et al., 2016; Kuncoro et al., 2018) and nonsensical (but grammatical) sentences (Gulordava et al., 2018). Both datasets extracted automatically from a wikipedia corpus based on their predicted dependency structure. To make them nonsensical, Gulordava et al. (2018) randomly substitute words from the same grammatical category.
- Finetuning neural models to immitate grammatical acceptability judgments gathered from linguistics textbooks Warstadt *et al.* (2018).
- Training a neural machine translation model to learn question formation from their declarative counterpartMcCoy et al., 2018. Linguist argue 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. 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.
- Adversarial evaluation (Smith, 2012) (figure out what this is). One task that the paper seems to suggest is to distinguish data from the true distribution from fake data looks like the task in Marvin and Linzen (2018).

7.2 Multitask learning

One method to improve language models for the task in Linzen *et al.* (2016) is to make use of multitask learning (Enguehard *et al.*, 2017). This has also been applied in the task of

I describe the baselines based on multitask learning: language modelling with a syntactic side objective. We have two different side objectives, which gives two baseline models.

- From the language model's RNN states predict CCG supertags (Enguehard *et al.*, 2017)
- From the language model's RNN states predict labeled spans. Use features and function identical to what is used in the the scoring function of the CRF parser: 'LSTM minus' features followed by a feedforward model. This is (minor) original contribution.

We discuss these a bit.

- We hypothesize a bit about their comparative (dis)advantages.
- We compare the effect of these two multitask objectives in the syneval setting.
- We compare the two methods wrt to perplexity. Enguehard et al., 2017 showed that the CCG side objective helped the model perform much better on the syntactic task, but also helped the model reach much lower perplexity. Preliminary experiments with the labeld span side-objective showed that it also makes the model perform much better on the syntactic task, but that the perplexity is worse.

7.2.1 Background

• Give formal description of multitask learning. In our case of language modelling with syntactic side-objective, the learning objective is to maximize

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

with respect to the parameters θ , λ and ζ , where p is our model of interest, optimized for the main objective, and q is our model optimized for the side objective, which we discard after optimization.

- The key point of multitask learning is that the two models p and q share the set of parameters θ . This means that θ will be optimized to fit both objectives well.
- The parameters in λ and ζ , in turn, are optimized to the each objective separately.
- The proportion and the nature of the parameters that belong to θ is a choice of the modeller and the objective.
- Name some generic examples of multitask learning in NLP (Zhang and Weiss, 2016; Søgaard and Goldberg, 2016) and the recent work on 'syntactic scaffolds' (Swayamdipta et al., 2018).

Span labeling We describe the span label prediction.

Word labeling We describe the CCG model tagging.

7.3 Experiments

7.3.1 **Setup**

Conclusion

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

8.1 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.

8.2 Future work

We have identified possibilities for future work:

Something. Here I describe what that entails.

Acknowledgements

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.
- \bullet CRF parser lossses: our (128d + SGD) and original (250d + Adam).

A.2. Test scores 39

- 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

B.1 Data

I describe in detail the data used in the experiments:

- Data preprocessing for the PTB and unlabeled data.
- Vocabulary and UNKing for all models.

B.2 Optimization

I describe the choices made with regards to optimization.

- \bullet Optimization by automatic differentiation (Blei $\it et al.,\,2016)$
- SGD and not Adam or other adaptive methods (Stern *et al.*, 2017a) and choices of hyperparameters.
- \bullet Learning rate schedule based on development scores.
- Surrogate objective and gradient blocking Schulman et al., 2015b.

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B.3 Implementation

- We use Dynet.
- Other specifics for optimization such as how to obtain blocked gradients.

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

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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 6, 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:

$$\nabla_{\lambda} \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \right] = \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} \mid \mathbf{x}) \right]$$
(D.1)

where

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

$$\nabla_{\lambda} \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \right] = \nabla_{\lambda} \mathbf{E}_{q} \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) - \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right]$$

$$= \nabla_{\lambda} \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \left\{ q_{\lambda}(\mathbf{y} | \mathbf{x}) \log p_{\theta}(\mathbf{x}, \mathbf{y}) - q_{\lambda}(\mathbf{y} | \mathbf{x}) \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \left\{ \nabla_{\lambda} q_{\lambda}(\mathbf{y} | \mathbf{x}) \log p_{\theta}(\mathbf{x}, \mathbf{y}) - \nabla_{\lambda} q_{\lambda}(\mathbf{y} | \mathbf{x}) \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$- q_{\lambda}(\mathbf{y} | \mathbf{x}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \left\{ \nabla_{\lambda} q_{\lambda}(\mathbf{y} | \mathbf{x}) \log p_{\theta}(\mathbf{x}, \mathbf{y}) - \nabla_{\lambda} q_{\lambda}(\mathbf{y} | \mathbf{x}) \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \left\{ L(\mathbf{x}, \mathbf{y}) \nabla_{\lambda} q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \left\{ L(\mathbf{x}, \mathbf{y}) q_{\lambda}(\mathbf{y} | \mathbf{x}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right\}$$

$$= \mathbf{E}_{q} \left[L(\mathbf{x}, \mathbf{y}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} | \mathbf{x}) \right].$$

In this derivation we used the identity

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

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

$$\sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_{\lambda}(\mathbf{y} \mid \mathbf{x}) \nabla_{\lambda} \log q_{\lambda}(\mathbf{y} \mid \mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_{\lambda}(\mathbf{y} \mid \mathbf{x}) \frac{\nabla_{\lambda} q_{\lambda}(\mathbf{y} \mid \mathbf{x})}{q_{\lambda}(\mathbf{y} \mid \mathbf{x})}$$

$$= \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \nabla_{\lambda} q_{\lambda}(\mathbf{y} \mid \mathbf{x})$$

$$= \nabla_{\lambda} \sum_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} q_{\lambda}(\mathbf{y} \mid \mathbf{x})$$

$$= \nabla_{\lambda} 1$$

$$= 0.$$

D.3 Optimization

We use automatic differentiation (Baydin *et al.*, 2017) 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.*, 2015a):

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

The function BLOCKGRAD detaches 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

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

such that

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

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

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

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

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

which means that the error is of the order

$$\mu - \hat{\mu} \sim \sqrt{\frac{\mathbf{var}\left[\hat{\mu}\right]}{n}}$$

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

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

This function is also an estimator for μ , since

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \mathbf{cov}(e^X, X) &= \mathbf{E} \left[X e^X \right] - \mathbf{E} \left[X \right] \mathbf{E} \left[e^X \right] \\ &= \int_0^1 x e^x dx - \frac{e-1}{2} \\ &= 1 - \frac{e-1}{2} \approx 0.14086 \end{aligned}$$

$$\mathbf{var} \left[e^X \right] &= \mathbf{E} \left[e^{2X} \right] - (\mathbf{E} \left[e^X \right])^2$$

$$&= \int_0^1 e^{2x} dx - (1 - e^x)^2$$

$$&= \frac{e^2 - 1}{2} - (1 - e^x)^2 \approx 0.2420$$

$$\mathbf{var} \left[X \right] &= \mathbf{E} \left[X^2 \right] - (\mathbf{E} \left[X \right])^2$$

$$&= \int_0^1 x^2 dx - \frac{1}{4}$$

$$&= \frac{1}{3} - \frac{1}{4} = \frac{1}{12}.$$

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

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

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

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