Enforcing Constraints on Outputs with Unconstrained Inference

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Abstract

Increasingly, practitioners apply neural networks to complex problems in natural language processing (NLP), such as syntactic parsing, that have rich output structures. Many such applications require deterministic constraints on the output values; for example, requiring that the sequential outputs encode a valid tree. While hidden units might capture such properties, the network is not always able to learn them from the training data alone, and practitioners must then resort to post-processing. In this paper, we present an inference method for neural networks that enforces deterministic constraints on outputs without performing post-processing or expensive discrete search over the feasible space. Instead, for each input, we nudge the continuous weights until the network’s unconstrained inference procedure generates an output that satisfies the constraints. We find that our method reduces the number of violating outputs by up to 94%, while improving accuracy in constituency parsing.

1 Introduction

Suppose we have trained a sequence-to-sequence network (Cho et al., 2014; Sutskever et al., 2014; Kumar et al., 2016) to perform a structured prediction task such as constituency parsing (Vinyals et al., 2015). We would like to apply our network to novel, unseen examples, but still require that the network’s outputs obey the appropriate set of hard-constraints; for example, that the output sequence encodes a valid parse tree. Enforcing these constraints is important because down-stream tasks, such as relation extraction or coreference resolution, often assume that the constraints hold.

Unfortunately, there is no guarantee that the neural network will learn these constraints from the training data alone. Although in some cases, the outputs of state-of-the-art systems almost always obey the constraints for the test-set of the data on which they are tuned (Vinyals et al., 2015); in practice, the quality of machine learning systems are much lower when run on data in the wild (e.g., because small shifts in domain or genre change the underlying data distribution). In such cases, the problem of constraint violations may become significant.

This raises the question: how should we enforce hard constraints on the outputs of a neural network? We could perform expensive discrete search or manually construct a list of post-processing rules for the particular problem domain of interest. Though, we might do even better if we continue to train the neural network at test-time to learn how to satisfy the constraints on each input. Such a learning procedure is applicable at test-time because learning constraints requires no labeled data: rather, we only require a function that measures the extent to which a predicted output violates a constraint.

In this paper, we present an inference method for neural networks that enforces output constraints by adjusting the network’s weights at test-time. Given an appropriate function that measures the extent of a constraint violation, we can express the hard constraints as an optimization problem over the continuous weights and apply back-propagation to change them. That is, by iteratively adjusting the weights so that the neural network becomes increasingly likely to produce an output configuration that obeys
the desired constraints. Much like scoped-learning, the algorithm customizes the weights for each example at test-time (Blei et al., 2002), but does so in a way to satisfy the constraints.

1.1 Motivating Example

As a motivating example, consider a sequence-to-sequence network that inputs a sentence and outputs a sequence of “shift-reduce” commands that encode the sentence’s parse tree. Briefly, the shift-reduce commands control a parsing algorithm by indicating how and when to use its stack. Each command controls whether to shift (s) a token onto the stack, reduce (r) the top of the stack into a parent tree node, or push (1) the current reduction back onto the stack. To be successful, the network must generate commands that imply a valid tree over the entire input sentence. However, the decoder outputs just a single command at a time, producing some outputs that are not globally-consistent, valid shift-reduce programs.

In such cases, the output may not have enough shifts to include every input token in the tree or may attempt to reduce when the stack is empty. For example, the following input sentence “So it’s a very mixed bag.” comprises ten space-delimited tokens (the quotations are part of the input), but an unconstrained sequence-to-sequence network could output an invalid sequence with only nine shifts sssr!rr!ssrr!rr!ssrrrrrr!r. We must introduce another shift so the last token is pushed onto the stack and issue another reduce so it is inserted into the tree.

We could attempt to fix the output with post-processing, but where is the right place to insert these commands in the sequence? There are 406 = \binom{29}{2} candidate locations. Further complicating our post-processing dilemma is the fact that the output contains several other errors that are seemingly unrelated to the constraint. Instead, we could attempt to fix the problem with a more sophisticated decoder, but this is difficult because the decoder outputs a single character at each time-step and our constraints are global, limiting corrections to the end of the sequence when it is too late to rectify an earlier decision. A beam search is less myopic, but in practice most of the output mass is peaked on the best output token, resulting in little improvement.

Instead, we could apply the method we present in this paper: when applied to the above example, it takes only 12 back-propagation steps to remove enough probability mass from the invalid output space to allow the network’s unconstrained decoding process to produce a valid output sequence:

\[
\text{ssr!sr!ssssrr!rr!ssrrrrrr!} \quad \text{(initial output)} \\
\text{ssr!ssssrr!rr!rr!ssrrrrrr!} \quad \text{(12 steps)}
\]

Interestingly, the network generates an additional s command at the beginning of the sequence while also producing a cascade of error correction in later time steps: the new output now satisfies the constraints and is a perfectly correct parse. Of course, enforcing constraints does not always lead to an improvement in accuracy, but we find that often it does in practice, especially for a well-trained network. When applied to a parsing task, we find that our method is able to completely satisfy constraints in up to 94% of the outputs that initially had constraint violations. Further, enforcing constraints in this way consistently increases the accuracy across a wide range of models and inference techniques.

2 Background

Consider a neural network that generates a variable length output vector \( y = \{y_i\}_{i=1}^{ny} \) from a variable length input vector \( x = \{x_i\}_{i=1}^{nx} \). For example, in image classification, the input vector encodes fixed multi-dimensional tensor of pixel intensities and the output vector comprises just a single element corresponding to the discrete class label. In sequence-to-sequence, the input might be a variable length vector of French tokens, and the output would be a variable length vector of its English translation. It is sometimes convenient to think of the network as a function from input to output

\[
f(x; W) \rightarrow y \tag{1}
\]

However, for the purpose of exposition, we separate the neural network into a real-valued model (negative energy function) that scores the compatibility of the outputs (given the weights and input) and an inference procedure that searches for high scoring outputs.

For the model, let \( y_i \) be a discrete output from an output unit and let \( \psi(y_i; x, W) \) be its corresponding real-valued log-space activation score (e.g., the log of the softmax for locally normalized models or simply a linear activation value for globally normalized models). Define the negative energy \( \Psi \) over a collection of output values \( y \) as an exponentiated sum of...
Then, inference is the problem of finding the values of the outputs $y$ that maximize the negative energy given fixed inputs $x$ and weights $W$. Thus, we can rewrite the neural network as the function:

$$f(x; W) \mapsto \arg\max_y \Psi(y; x, W)$$  \hspace{1cm} (3)

The purpose of separating the model from the inference procedure is so we can later formalize our optimization problem. We emphasize that this formulation is consistent with existing neural networks. Indeed, inference in feed-forward networks is a single feed-forward pass from inputs to outputs. When the outputs only depend on each other through hidden states that only depend on earlier layers of the network, feed-forward inference is exact in the sense that it finds the optimum of Equation 3. For recurrent neural networks (RNNs), each output depends on hidden states that are functions of previous output values. However, we can still think of the usual procedure that produces the highest scoring output at each time step as a local greedy approximation to global inference; of course, the procedure can optionally be improved with a beam.

3  Constrained inference for neural networks

A major advantage of many neural networks is that once trained, inference is extremely efficient. However, constraints can render inference intractable due to discrete search. Our goal is to take advantage of the fact that unconstrained inference is inexpensive and design a constrained inference algorithm that exploits such a procedure as a black box. Our method iteratively adjusts the weights for each test-time input, concentrating the probability mass on the feasible region so that unconstrained inference becomes increasingly likely to generate an output that satisfies the constraints.

In this work, we focus on constraints that require the outputs to belong to an input-dependent context-free language $L^x$ (CFL). The idea is to treat the output space of the neural network as the terminal symbols, and devise the appropriate production rules and non-terminals to express constraints on them. An advantage of employing CFLs over other formalisms such as first order logic (FOL) is that CFLs are intuitive for expressing constraints on the outputs, especially for language models and sequence-to-sequence networks. For example, when modeling Python or Java code, it is easy to express many of the desired programming language’s constraints using a CFL, but cumbersome in FOL. Indeed, CFLs are an expressive class of languages.

3.1 Motivation

To motivate our algorithm, we begin with the ideal optimization problem and argue that unlike for linear models with local constraints, the resulting Lagrangian is not well suited for globally constrained inference in neural networks. We ultimately settle upon an alternative objective function that reasonably models our constrained inference problem. Although our algorithm lacks the theoretical guarantees enjoyed by classic relaxation algorithms we nevertheless find it works well in practice.

Consider the following constrained inference problem for neural networks

$$\max_y \Psi(x, y, W)$$

s.t. $y \in L^x$ \hspace{1cm} (4)

Naively enforcing the constraint requires combinatorial discrete search, which is intractable in general. Instead, we prefer a smooth optimization problem with meaningful gradients to guide the search.

With this in mind, let $g(y, L) \mapsto r$ for $r \in \mathbb{R}_+$ be a function that measures a loss between a sentence $y$ and a grammar $L$ such that $g(y, L) = 0$ if and only if there are no grammatical errors in $y$. That is, $g(y, L) = 0$ for the feasible region and is strictly positive everywhere else. For a large class of CFLs, $g$ could be the least errors count function \cite{lyons1974estimation} or a weighted version thereof. We could then express CFL membership as an equality constraint and minimize the Lagrangian

$$\min_{\lambda} \max_y \Psi(x, y, W) + \lambda g(y, L)$$  \hspace{1cm} (5)

However, this dual leads to difficult optimization algorithms because there is just a single dual variable.

Instead, observe that the network’s weights control the negative energy of the output configurations. By properly adjusting the weights, we can affect the outcome of inference by removing mass from invalid outputs. The weights are likely to generalize much better than the single dual variable because in most neural networks, the weights are tied across space
(e.g., CNNs) or time (e.g., RNNs). As a result, lowering the negative energy for a single invalid output has the effect of lowering the negative energy for an entire family of related, invalid outputs; enabling faster search. With this in mind, it is tempting to replace the single dual-variable with a “dual neural-network” that is parameterized by a set of “dual weights.” This is powerful because we have effectively introduced an exponential number of “dual variables” (via the energy, which scores each output) that we can easily control via the weights; although similar, the new optimization is no longer equivalent to the original:

$$\min_{W_\lambda} \max_y \Psi(x, y, W) + \Psi(x, y, W_\lambda)g(y, \mathcal{L})$$  \hspace{1cm} (6)

While a step in the right direction, the objective still requires combinatorial search because (1) the maximization involves two non-linear neural networks and (2) a greedy decoding algorithm is unable to cope with the global loss $g(\cdot)$ because the constraints do not factorize over the individual outputs. In contrast, the functions involved in classic Lagrangian relaxation methods for NLP have multipliers for each output variable that can be combined with linear models to form a single unified decoding problem for which efficient inference exists (Koo et al., 2010; Rush et al., 2014; Rush & Collins, 2012).

### 3.2 Algorithm

Since our non-linear functions and global constraints do not afford us the same ability, we must modify the optimization problem for a final time so that we can employ the network’s efficient inference procedure as a black-box. Therefore, we (1) remove the negative-energy term that involves the original weights $W$ and compensate with a regularizer that attempts to keep the dual weights $W_\lambda$ as close (closeness governed by $\alpha$) to these weights as possible and (2) maximize exclusively over the network parameterized by $W_\lambda$ while ignoring the constraint term during the maximization. This results in the following optimization problem:

$$\min_{W_\lambda} \Psi(x, \hat{y}, W_\lambda)g(\hat{y}, \mathcal{L}) + \alpha\|W - W_\lambda\|_2$$  \hspace{1cm} (7)

While this appears to be a brutal modification, it is reasonable because by definition of the constraint loss $g(\cdot)$, the global minima must correspond to outputs that satisfy all constraints. Further, we expect to find high-probability optima if we initialize $W_\lambda = W$. Moreover, the objective is intuitive: if there is a constraint violation in $\hat{y}$ then $g(\cdot) > 0$ and we lower the negative energy of $\hat{y}$ to make it less likely. Otherwise, $g(\cdot) = 0$ and we leave the negative energy of $\hat{y}$ unchanged.

To optimize the objective, our algorithm alternates maximization to find $\hat{y}$ and minimization w.r.t. $W_\lambda$. In particular, we first approximate the maximization step by employing the neural network’s inference procedure (e.g., greedy decoding or beam-search) to find $\hat{y}$. Then, given a fixed $\hat{y}$, we minimize the objective with respect to the $W_\lambda$ by performing stochastic gradient descent (SGD). Since $\hat{y}$ is fixed, the constraint loss term becomes a constant in the gradient; thus, making it easier to employ external black-box constraint losses (such as those based on compilers) that may not be differentiable.

As a remark, note the similarity to REINFORCE (Williams, 1992): output sentences are states, the decoder outputs are actions and the constraint-loss is a negative reward. Indeed the gradient of the objective (Equation 7) w.r.t. $W_\lambda$ is a REINFORCE gradient. However, unlike REINFORCE, our algorithm terminates early: upon discovery of an output that satisfies all constraints.

AlGORITHM 1 Constrained Inference for Neural Networks

| Inputs: test instance $x$, input specific CFL $\mathcal{L}_x$, pretrained weights $W$ |
|---|
| $W_\lambda \leftarrow W$ #reset instance-specific weights |
| while not converged do |
| $y \leftarrow f(x; W_\lambda)$ #perform inference using weights $W_\lambda$ |
| $\nabla \leftarrow g(y, \mathcal{L}_x)\frac{\partial}{\partial W_\lambda}\Psi(x, y, W_\lambda) + \alpha\|W - W_\lambda\|_2$ #compute constraint loss |
| $W_\lambda \leftarrow W_\lambda - \eta \nabla$ #update instance-specific weights with SGD or a variant thereof |
| end while |

### 4 Application to Parsing

Consider the structured prediction problem of syntactic parsing in which the goal is to input a sentence comprising a sequence of tokens and output a tree describing the grammatical parse of the sentence. One way to model the problem with neural networks is to linearize the representation of the parse tree and then employ the familiar sequence-to-sequence model (Vinyals et al., 2015).

Let us suppose we linearize the tree using a sequence of shift ($s$) and reduce ($r, r!$) commands that con-

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1 In some networks (e.g., feed-forward networks), it may be possible to perform the argmax exactly.
control an implicit shift-reduce parser. Intuitively, these commands describe the exact instructions for converting the input sentence into a complete parse tree: the interpretation of the symbol $s$ is that we shift an input token onto the stack and the interpretation of the symbol $r$ is that we start (or continue) reducing (popping) the top elements of the stack, the interpretation of a third symbol $!$ is that we stop reducing and push the reduced result back onto the stack. Thus, given an input sentence and an output sequence of shift-reduce commands, we can deterministically recover the tree by simulating a shift-reduce parser. For example, the sequence `ssrr!ssr!rr!rr!` encodes a type-free version of the parse tree `(S (NP the ball) (VP is (NP red)))` for the input sentence “the ball is red.” It is easy to recover the tree structure from the input sentence and the output commands by simulating a shift-reduce parser, performing one command at a time as prescribed by the classic algorithm.

Note that for output sequences to form a valid tree over the input, the sequence must satisfy a number of constraints. First, the number of shifts must equal the number of input tokens $n_x$, otherwise either the tree would not cover the entire input sentence or the tree would contain spurious terminal symbols. Second, the parser cannot issue a reduce command if there are no items left on the stack. Third, the number of reduces must be sufficient to leave just a single item, the root node, on the stack.

We can express most of these constraints with a CFL

$$\mathcal{L} = \{ G \rightarrow sRr! \\ R \rightarrow sRr \\ R \rightarrow Rr! \\ R \rightarrow RR \\ R \rightarrow \epsilon \}$$

(8)

Intuitively, Rule 1 states that a valid shift-reduce command set must begin with a shift (since stack is initially empty, there is nothing to reduce) and end with a reduce that places the final result on the stack. Rule 2 states that if we do a shift, then we need to reduce the shifted token at some point in the future. Rule 3 states that if we do not shift then we are allowed to reduce only if we also push the result on the stack. Rule 4 allows for multiple subtrees. Rule 5 is the base case.

Note, however, that this grammar is for a general purpose shift-reduce language, but we need to constrain the number of shifts to equal the number of input tokens $n_x$. Since the constraint is a bit verbose to express with production rules, we can instead write the regular language $(s(r!))^m (r!)^*$. Where $m$ is the number of elements in $x$ and intersect it with our CFL.

$$\mathcal{L} = \mathcal{L} \cap (s(r!))^m (r!)^*$$

(9)

Rather than relying on a general purpose algorithm to compute $g(y, \mathcal{L})$ that measures the number of grammatical errors, we instead implement it specifically for our language. Let $ct_{i=0}^{n} (b(i))$ be the function that counts the number of times proposition $b(i)$ is true. Now, define the following loss

$$g(y, \mathcal{L}) = \sum_{i \in \{s, !\}} \max (0, ct_{i=0}^{n} (y_i = s)) + \sum_{j} \max (0, ct_{j=0}^{n} (y_j = r) - ct_{j=0}^{n} (y_j \in \{s, !\})) + (ct_{i=0}^{n} (y_i = r) - ct_{i=0}^{n} (y_i \in \{s, !\}))$$

The first term provides loss when the number or shifts equals the number of input tokens, the second term provides loss when attempting to reduce an empty stack and the third term provides loss when the number of reduces is not sufficient to attach every lexical item to the tree.

5 Related work

There has been recent work in applying neural networks to structured prediction problems. For example, the recent structured prediction energy networks (SPENS) combines graphical models and neural networks via an energy function defined over the output variables (Belanger & McCallum, 2016). SPENS focuses on soft constraints (via the energy function) and performs inference by relaxing the binary output variables to be continuous and then backpropagating into them. In contrast, our method focuses on hard constraints and we backpropagate into the weights rather than into the outputs directly. We could combine our method with SPENS to handle soft constraints; for example, by back-propagating the output energy into the weights instead of the relaxed outputs themselves.

There has been recent work on applying neural networks to parsing problems that require the ability to handle hard constraints. For example, by employing a sequence-to-sequence network (Vinyals et al., 2015) or a custom network designed for shift reduce parsing (Dyer et al., 2016). The former requires the output to form a valid parse tree and hence they employ post-processing to ensure this property. The latter satisfies constraints as part of the decoding
process by sampling over a combinatorial space. Our approach avoids post processing and discrete search.

Another intriguing approach is to distill the hard constraints into the weights at training time using a teacher network (Hu et al., 2016). The method is appealing because it does not require constrained inference or combinatorial search. However, the method must achieve a difficult balance between the loss due to the training data and the loss due to the constraint violations. Further, it would crucially rely on network’s ability to generalize the constraints learned on the training data to the testing data.

Finally, our method highly resembles dual decomposition and more generally Lagrangian relaxation for structured prediction (Koo et al., 2010; Rush et al., 2010; Rush & Collins, 2012). In such techniques, it is assumed that a computationally efficient inference algorithm can maximize over a superset of the feasible region (indeed this assumption parallels our exploitation of the fact that unconstrained inference in the neural network is efficient). Then, the method employs gradient descent to gradually concentrate this superset onto the feasible region until the constraints are satisfied. However, for computational reasons, these techniques assume that the constraints factorize over the output and that the functions are linear so that they can be combined into a single model. In contrast, we have a single dual variable so we instead minimize with respect to the weights, which generalize better over the output. Further, we are unable to combine the dual into a single model over which we can do inference because the network is highly non-linear.

6 Experiments

In this section we empirically evaluate our constrained inference procedure on two sequence-to-sequence tasks. The first is a transduction task between two simple languages, which we describe next. The second is the sequence-to-sequence shift-reduce parsing task described in Section 4. Both tasks impose hard constraints on the output of the sequence-to-sequence network. In the transduction task, the output must belong to the target language and obey domain-specific constraints, and in the parsing task, the output sequence of shift-reduce commands must encode a valid parse tree.

We are interested in answering the following questions (Q1) how well does the sequence-to-sequence network learn the constraints from data (Q2) for cases in which the network is unable to learn the constraints, is our method able to actually enforce the constraints and (Q3) does the method enforce constraints without compromising the quality of the network’s output. Q3 is particularly important because we adjust the weights of the network at test-time and this may lead to unexpected behavior.

6.1 Experimental procedure

In each experiment, we learn a sequence-to-sequence network on a training set and then evaluate the network directly on the test set using a traditional inference algorithm to perform the decoding (either greedy decoding or beam-search). Then, to address (Q1) we measure the failure-rate (i.e., the ratio of test sentences for which the network infers an output that fails to fully satisfy the constraints). In order to address (Q2) we evaluate our method on the failure-set (i.e., the set of output sentences for which
the original network produces invalid constraint-violating outputs) and measure our method’s conversion rate; that is, the percentage of failures for which our method is able to completely satisfy the constraints (or “convert”). Finally, to address (Q3), we evaluate the quality (e.g., accuracy or F1) of the output predictions on the network’s failure-set both before and after applying our method.

For parsing, in which the F1 measure is only defined on valid parse trees, we perform a domain-specific post-processing heuristics to satisfy the constraints. In particular, we simulate a shift-reduce parser on the output, but enforce constraints locally: a reduce on an empty stack is ignored, a shift on an empty input queue is ignored, and additional shifts and reduces are added at the end to ensure the final tree spans the entire input sentence.

6.2 Simple Transduction Experiment

A transducer \( T : \mathcal{L}_S \rightarrow \mathcal{L}_T \) is a function from a source language to a target language. In our experiment, we employ a known \( T \) to generate input/output training examples and train a sequence-to-sequence network to learn \( T \) on that data. Crucially, there are hard constraints on the output (for example, the output must belong to \( \mathcal{L}_T \), and other problem-specific constraints that may in general depend on the input sentence). If the network is unable to learn all the constraints from data, then our method is applicable and we can evaluate its performance.

For our task, we choose a simple transducer, similar to those studied in recent work (Grefenstette et al., 2013). The source language \( \mathcal{L}_S \) is \((az|bz)^*\) and the target language \( \mathcal{L}_T \) is \((aaa|zb)^*\). The transducer is defined to map occurrences of \( az \) in the source string to \( aaa \) in the target string, and occurrences of \( bz \) in the source string to \( zb \) in the target string. For example, \( T(bzazbz) \rightarrow zbbaazb \) The training set comprises 1934 sequences of length 2–20 and the test set contains sentences of lengths 21–24. We employ shorter sentences for training to require generalization to longer sentences at test time.

For this experiment, we employ a thirty-two hidden unit single-layered, attention-less, sequence-to-sequence long short-term memory (LSTM) in which the decoder LSTM inputs the final encoder state at each decoder time-step. We train the network for 1000 epochs using RMSProp to maximize the likelihood of the output (decoder) sequences in the training set. The network achieves perfect train accuracy while learning the rules of the target grammar \( \mathcal{L}_T \) perfectly, even on the test-set.

However, despite learning the train-set perfectly, the network fails to learn the input-specific constraint that the number of a’s in the output should be three times the number of a’s in the input. It is not surprising that the network fails to learn this constraint because doing so would require counting and memorizing the number of input a’s over long sequences of characters. In contrast, learning the constraint that the output must belong to \( \mathcal{L}_T \) is relatively easy because only local rules govern the regular language. Since the network fails to learn the triple-a constraint, it gives us an opportunity to study the performance of our constrained inference method. We implement the following loss for this constraint: 

\[
g(y, L_T) = (n + m)^{-1} \left( (3 \sum x_i I(x_i = a)) - (\sum y_i I(y_i = a)) \right)^2
\]

where \( n + m \) the combined input/output length, normalizes between 0 and 1. For constrained inference we run Algorithm 1 by initializing \( W_\lambda = W \) and employing vanilla stochastic gradient descent with a learning rate of 0.05 and no weight decay. We cap the number of iterations at a maximum of 100.

On the “azbz task,” our method achieves a conversion rate of 65.2% after 100 iterations, while also improving the accuracy on the failure-set from 75.2% to 82.4%. This improvement is encouraging because it demonstrates that modifying the weights at test-time may not lead to undesirable behavior after all. Also, we investigate which set of weights the algorithm should modify at test-time in order to best satisfy the constraints: modifying all the weights (65.2% conversion rate) works better than modifying just the encoder, decoder, or output units in isolation, which achieve conversion rates of (resp. 58.2, 57.4, 20.9). Two important practical lessons we learn from working with this task are (1) the regularizer is actually unnecessary because the network does not drift far enough from the initialization \( W_\lambda = W \) to cause undesirable behavior and (2) normalizing the constraint loss \( g(\cdot) \) (e.g., between 0 and 1) is important because it provides optimization stability by preventing the the loss from growing unbounded with the length of the predicted output sequence.

We also provide data-cases that highlight both success and failure (Tables 12). The title of these tables is the input and the desired ground truth output. The rows show the network’s output at each iteration (as indicated). The loss column is Equation 7.
Table 3: Parsing Networks (BS9 means beam size 9)

| name   | F1    | greedy | hidden | layers | dropout |
|--------|-------|--------|--------|--------|---------|
| Net0   | 71.54 | 67.80  | 128    | 3      | no      |
| Net1   | 71.64 | 66.88  | 128    | 2      | no      |
| Net2   | 72.97 | 68.89  | 256    | 3      | no      |
| Net3   | 78.14 | 74.53  | 128    | 3      | no      |
| Net4   | 81.26 | 78.32  | 172    | 3      | yes     |

and the final column is the token-wise accuracy between the output and the ground truth.

Note that the example in which our method improves accuracy is interesting because it demonstrates that our algorithm is able to harness the global constraints to correct errors at earlier time-steps. Note that this is not possible for a local method that enforces constraints at each time-step during the decoding process. The reason is that such an approach is not able to revisit the mistakes at early time-steps that lead to constraint violations at later time-steps.

### 6.3 Syntactic Parsing Experiment

We investigate the behavior of the constraint satisfaction algorithm on the shift-reduce parsing task described in Section 4. For the parsing task, we transform the Wall Street Journal (WSJ) portion of the Penn Tree Bank (PTB) into shift-reduce commands in which each reduce command has a phrase-type (e.g., noun-phrase or verb-phrase). We employ the traditional split of the data with section 22 for dev, section 23 for test, and remaining sections 01-21 for training. We evaluate on the test set with evalb F1.

While state-of-the-art networks almost always produce sequences that define valid trees (Vinyals et al., 2015); in practice, the parsing quality of even the best systems degrade in the wild (e.g., due to domain, genre, tokenization, out-of-vocabulary words and data-distribution changes in general). Thus, it is important to understand the behavior of sequence-to-sequence networks in a wider range of more realistic accuracy regimes in which the constraint violations are likely to be more prolific.

To this end, we train many sequence-to-sequence networks with different hyper-parameters in order to produce a variety of networks that differ in parsing quality. We limit ourselves to the WSJ subset of the PTB (roughly 40k training sentences). We select five networks that vary in quality with F1 scores ranging from the low-seventies to the low-eighties (Table 3). The model name indicates the relative quality with Net0 being the worst and Net4 being the best. Note that these networks employ attention, following previous work (Vinyals et al., 2015).

We study the behavior of the constraint-satisfaction method on the five networks using various inference procedures for decoding: greedy decoding and beam-search with a beam-size of two, five, and nine (resp. beam2, beam5, beam9). Beam-search is less myopic than greedy-decoding and would likely perform better both in terms of F1 and in terms of the number of outputs that define valid trees.

We report the results in Table 5. The left-most column indicates the inference procedure employed in the experiment. The indicated inference procedure is employed both for the initial network prediction and in the inner loop of our algorithm. The failure-rate is given as a fraction of violated outputs over the total number of test examples. This statistic indicates the extent to which constraint-violations are a problem for each initial network prior to applying constrained inference. Note that we first run greedy decoding and then run beam-search on greedy’s failure-set to produce an even smaller failure-set for the beam-search conditions. Thus, examples in the beam-search failure-sets are particularly challenging for the network because they elude both beam-search and greedy decoding.

In order to address question Q2—the ability of our approach to satisfy constraints—we measure conversion rates. As before, the conversion rates are the percentage of the examples in the failure-sets for which the constraint-satisfaction method is able to satisfy all the constraints. Across all the experimental conditions, the conversion rates are high, often above 80 and sometimes above 90. The conversion rates appear to correlate with the quality of the underlying parsing system: across the different inference algorithms, conversion rates tend to be higher for Net3 and Net4 than for Net0 and Net1.

Next, in order to address question Q3—the ability of our approach to satisfy constraints without negatively affecting output quality—we measure the F1 scores on the failure-sets both before and after applying the constraint satisfaction algorithm. Since this F1 measure is only defined on valid trees, we employ heuristic post-processing, as described earlier, to ensure all outputs are valid. We find that

http://nlp.cs.nyu.edu/evalb/
<“So it’s a very mixed bag.”> → sssr!ssssrr!srr!rr!ssrrrrrr!

| iteration | output | loss      | accuracy |
|-----------|--------|-----------|----------|
| 0         | sssr!srrrrrrr! | 0.0857   | 33.3%    |
| 11        | sssr!srrrrrr! | 0.0855   | 33.3%    |
| 12        | sssr!srrrrrrr! | 0.0000   | 100.0%   |

Table 4: A shift-reduce example for which the method successfully enforces constraints. The initial output has only nine shifts, but there are ten tokens in the input. Enforcing the constraint not only corrects the number of shifts to ten, but changes the implied tree structure to the correct tree.

| Inference | Network | Failure rate (n/2415) | Conversion rate (%) | F1 (before) | F1 (after) |
|-----------|---------|-----------------------|---------------------|-------------|------------|
| Greedy    | Net0    | 886                   | 69.86               | 58.47       | 60.41      |
|           | Net1    | 971                   | 73.12               | 59.03       | 59.82      |
|           | Net2    | 474                   | 88.40               | 58.77       | 61.18      |
|           | Net3    | 611                   | 88.05               | 62.17       | 64.49      |
|           | Net4    | 317                   | 79.81               | 65.62       | 68.79      |
| Beam 2    | Net0    | 602                   | 82.89               | 60.45       | 61.35      |
|           | Net1    | 707                   | 86.14               | 61.30       | 61.26      |
|           | Net2    | 269                   | 82.53               | 61.31       | 61.37      |
|           | Net3    | 419                   | 94.27               | 65.40       | 66.65      |
|           | Net4    | 206                   | 87.38               | 66.61       | 71.15      |
| Beam 5    | Net0    | 546                   | 81.50               | 61.43       | 63.25      |
|           | Net1    | 615                   | 84.72               | 61.99       | 62.86      |
|           | Net2    | 220                   | 80.91               | 61.63       | 63.34      |
|           | Net3    | 368                   | 92.66               | 67.18       | 69.4       |
|           | Net4    | 160                   | 87.50               | 67.5        | 71.38      |
| Beam 9    | Net0    | 552                   | 80.62               | 61.64       | 62.98      |
|           | Net1    | 613                   | 83.69               | 62.83       | 63.95      |
|           | Net2    | 225                   | 80.00               | 61.04       | 62.52      |
|           | Net3    | 360                   | 93.89               | 67.83       | 70.64      |
|           | Net4    | 153                   | 91.50               | 68.66       | 71.69      |

Table 5: Evaluation of the proposed constrained-inference procedure. Failure rate is the size of the failure-set over the size of the test set (2.4k). Conversion rate is the percentage of sentences in the failure-set that the method completely satisfies. The F1 (before) column evaluates the performance of the base inference algorithm on the failure-set. The F1(after) column evaluates the performance of the constrained-inference algorithm on the same failure-set.
in every case, except one, our approach satisfies constraints in a way that improves the quality of the parses (as compared to employing post-processing). While the improvement is somewhat modest, it is consistent across nearly every model and inference algorithm. Again, we observe the largest improvements with the more accurate networks (Net3 and Net4).

Table 4 contains a successful example that we had previously highlighted in Section 1. The algorithm satisfies the constraints, and also corrects the output errors yielding a perfectly correct parse. Note that in order to reduce visual clutter, we omit type information in this version of the experiment.

Finally, on outputs that our algorithm converts, we report the number of iterations that it takes. Across all conditions, it takes 5–7 steps to convert 25% of the outputs, 15–20 steps to convert 50%, 39–57 steps to convert 80%, 58–73 steps to convert 90% and 77–84 steps to convert 95%. We observe that higher quality networks (Net3, Net4) require more iterations. This might be because (a) the failure-set of these nets contain sentences that are inherently more difficult or (b) their weights are larger requiring more steps to induce behavioral changes.

7 Conclusion

We presented an algorithm for satisfying constraints in neural networks that avoids combinatorial search, but employs the network’s efficient unconstrained procedure as a black box. We evaluated the algorithm on two sequence-to-sequence tasks, a synthetic transducer problem and a real-world shift-reduce parsing problem. We found that lower accuracy networks tend to produce outputs with more constraint violations, that our method is able to rectify these violations (on up to 94.3% of sentences), and that enforcing the constraints in this way improves the accuracy (dispelling some initial concerns that adjusting the weights at test-time would result in erratic behavior).

An exciting area of future work is to generalize our method and explore the idea of neural Lagrangian relaxation, in which a neural network replaces the dual variable in the Lagrangian optimization problem. In much the same way that neural networks have successfully modeled the latent variables in variational learning, we hope that the networks could learn the Lagrange variables and provide extremely fast amortized inference for constrained optimization.

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