Training with Adversaries to Improve Faithfulness of Attention in Neural Machine Translation

by

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Abstract

Can we trust that the attention heatmaps produced by a neural machine translation (NMT) model reflect its true internal reasoning? We isolate and examine in detail the notion of faithfulness in NMT models. We provide a measure of faithfulness for NMT based on a variety of stress tests where model parameters are perturbed and measuring faithfulness based on how often each individual output changes. We show that our proposed faithfulness measure for NMT models can be improved using a novel differentiable objective that rewards faithful behaviour by the model through probability divergence. Our experimental results on multiple language pairs show that our objective function is effective in increasing faithfulness and can lead to a useful analysis of NMT model behaviour and more trustworthy attention heatmaps. Our proposed objective improves faithfulness without reducing the translation quality and it also seems to have a useful regularization effect on the NMT model and can even improve translation quality in some cases.

**Keywords:** deep learning; neural network; neural machine translation; interpretability; attention; faithfulness
Dedication

To Mom, Dad, Poorya, and Prof. Anoop Sarkar who treated me like his own son.
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Chapter 1

Introduction

Although neural models have become the standard solutions for solving many challenging tasks including Machine Translation (MT), they are considered as black-boxes as their internal computations are not necessarily human-interpretable. In this thesis we have focused on analyzing and improving attention, as an omnipresent component in many neural models, from interpretability perspective. Thus, in Sec. 1.1 we discuss the importance of interpretability in the context of neural models. Then we focus on attention as an interpretation method and briefly mention the notion of faithfulness in Sec. 1.2. In this work we have an encoder-decoder model as our baseline and consequently we provide a brief overview of the encoder-decoder model with attention in Sec. 1.3. In Sec. 1.4 we discuss our contributions and in the end we present an overview of this thesis in Sec. 1.5.

1.1 Interpretability of Neural Models

With advances in sequence-to-sequence (Seq2Seq) models [59], Neural Machine Translation (NMT) systems augmented with attention mechanism [5] have achieved state-of-the-art in many language translation tasks. One shortcoming of NMT models, and neural models in general, is that it is usually difficult for a human interrogator to analyze or understand the true internal reasoning of the neural model for making a particular prediction [15, 18]. The underlying reason behind this difficulty is that information and concepts are represented as real-valued vectors in neural networks. Consequently it’s a challenge to interpret these vectors. Why do we want neural models to be interpretable? There can be at least two reasons for this. First of all, to debug a model during error analysis, it is crucial to know how each part of the model is contributing to the prediction and to the error. Moreover, understanding the internal workings of a model is necessary for discovering its deficiencies and improving it. This calls for interpretable neural models and also development of models and methods for understanding and explaining these models. Accordingly, this has led to a wide variety of contemporary NLP research focusing (a) different axes of interpretability including plausibility (or interchangeably human-interpretable) [19, 31] and faithfulness (agreement of an explanation with the internal reasoning of a model) [38, 20], (b) interpretation of the neural model components [7, 12, 64], (c) explaining the decisions made by neural models to humans (using expla-
nations, highlights, rationales, etc.) [51, 35, 14, 17, 6, 23], and (d) evaluating different explanation methods from different perspectives [54, 45, 49, 22, 55, 67, 34] which are all discussed in details in Chapter 2.

1.2 Attention Interpretability and Faithfulness

The advent of attention in neural models has improved the overall accuracy in many different tasks. Attention has become an omnipresent component in neural machine translation models and more generally in the architecture of neural models in NLP. The attention mechanism provides a probability distribution over the input with respect to a state variable such as decoding state in NMT. This probability distribution is used to summarize source-side information into a context-vector and is fed to the decoder as an additional signal for prediction. Along with their use in improving performance across different tasks, attention weights are widely implicitly or explicitly used to explain the predictions made by neural models [14, 16, 17]. The general idea is that attention weights can be indicators of the importance of inputs for producing a particular prediction. However, whether or not attention is a reliable source for explanation is often taken for granted. Consequently, there has been a great interest recently in the community in investigating the credibility of attention as explanation [22, 67, 55].

In this work we have focused on the faithfulness of interpretations offered by attention, that is the extent to which the model’s internal reasoning process is actually based on that interpretation. Faithfulness of these interpretations are particularly important for NLP practitioners who wish to debug their neural models and improve them. Identification of the faults of a neural model cannot be done if the neural model is not providing a faithful and trustworthy description of what it is doing. Jacovi and Goldberg [20] emphasize distinguishing faithfulness from human-interpretability in interpretability research by providing several clarifications about the terminology used by researchers. They describe the following conditions on the evaluation of how well a research project tackles the notion of faithfulness:
• Be explicit: provide a measurable evaluation of faithfulness.
• Human judgements are not relevant because we are interested in model internals.
• Do not match against gold labels (e.g. AER) because faithfulness of both correct and incorrect
decisions made by the model are equally important.
• No model is “inherently” faithful. We need to measure faithfulness not as a binary aspect of a
model (it is faithful or not) but rather as a gray-scale measure.
• A more faithful system is a necessary but not sufficient condition for model interpretation by
humans, c.f. [21].

Aligned with these criteria, we study faithfulness of NLP neural models, specifically NMT
models. We provide a faithfulness measure that is computed based on a variety of stress tests where
model parameters are perturbed and measuring how often the model output changes (Figure 1.1). Our
findings show that our objective is effective in increasing faithfulness and can lead to a useful
analysis of NMT model behaviour and more trustworthy attention heatmaps. We assert that
faithfulness is a good property to have in a model whether or not it will be useful for downstream
interpretation. A model that is faithful can be more trusted as a component in a larger end-to-end
neural model.

1.3 Encoder-Decoder Model with Attention

Given a training sentence pair \((x, y)\) where \(x = [x_1, x_2, \ldots, x_m]\) is a sentence in the source language
and \(y = [y_1, y_2, \ldots, y_n]\) is its corresponding translation in the target language, the problem of neural
machine translation is feeding \(x\) to a neural network and getting \(y\) as the output. The model we use
in this work is called "encoder-decoder" model with attention [59, 4]. The idea is that the encoder,
which is a recurrent neural network (RNN), runs over the source sentence to calculate the contextualized
representation of the source sentence. Then a second neural network which is the decoder
"decodes" this information into the target sentence. The attention mechanism is employed to calculate
the contextualized representation of the source sentence dynamically based on the decoding
step (Figure 1.2).

To be more specific, we use a bidirectional encoder, and concatenate the forward and backward
hidden hidden states to build the final representation.

\[
\begin{align*}
\tilde{h}_t &= \overset{\rightarrow}{f}_{enc}(x_t, \tilde{h}_{t-1}) \\
\overset{\leftarrow}{h}_t &= \overset{\leftarrow}{f}_{enc}(x_t, \overset{\leftarrow}{h}_{t+1}) \\
h_t &= [\tilde{h}_t, \overset{\leftarrow}{h}_t]
\end{align*}
\]  

(1.1)

Then the decoder generates output tokens using the following probability distribution:

\[p(y_t|y_{<t}, x) = \text{softmax}(g_{dec}(s_t, c_t))\]
with \( g_{dec} \) being a transformation function that produces a vocabulary-sized vector, and \( s_t \) is the hidden unit of the decoder’s RNN:

\[
s_t = f_{dec}(y_{t-1}, s_{t-1}, c_{t-1})
\]

where \( f_{dec} \) is a RNN. Here \( c_t \) is the context vector calculated by attention mechanisms:

\[
c_t = \sum_{i=1}^{m} \alpha_{t,i} h_i
\]

where \( \alpha_{t,i} \) is the normalized attention weights over the source context:

\[
\alpha_{t,i} = \frac{e^{a(s_t, h_i)}}{\sum_j e^{a(s_t, h_j)}}
\]

Here, \( a \) is a scoring function that determines the contribution of each source context vector to the final context vector. Implementation of \( a \) depends on the choice of the attention method. In this work, we use general attention [41] as the scoring function:

\[
a(s_t, h_i) = s_t^\top W_a h_i
\]
1.4 Contributions

We seek to improve faithfulness of NMT models. To this end, we make the following contributions in this work:

- We propose a measure for quantifying faithfulness in NMT.
- We introduce a novel learning objective based on probability divergence that rewards faithful behavior and which can be included in the training objective for NMT.
- We provide empirical evidence that we can improve faithfulness in an NMT model. Our approach results in a more faithful NMT model while producing better BLEU scores. Most previous work has focused on document or sentence-based classification tasks where attention models are not as directly useful as in NMT models.

We chose to study the impact of faithfulness in NMT because it is under-studied in terms of interpretability. Most previous work has focused on document or sentence-based classification tasks where attention models are not as directly useful as in NMT models. Attention is also more challenging in terms of faithfulness in the context of NMT models due to the substantial impact of the decoder component.¹

1.5 Overview

This thesis addresses the problem of faithfulness of attention in NMT. First we propose how to measure faithfulness in NMT using proposed adversarial attention as stress tests. Secondly we propose a novel method to improve faithfulness in NMT.

- in Chapter 2 we present previous works on different axes of interpretability, from interpretability methods to interpretability of attention and efforts to build inherently interpretable models.
- in Chapter 3 we demonstrate our proposal for measuring faithfulness in NMT. Our novel method for improving faithfulness in NMT is also discussed. We also mention attention sparsity as an attempt for improving faithfulness.
- in Chapter 4 we discuss our findings. We illustrate behavior of NMT in the presence of stress tests. Moreover, we show the effect of our method and attention sparsity on the faithfulness.
- We conclude our work in Chapter 5.

¹We focus on RNN based encoder-decoder models. While Transformers [63] generally produce better NMT models, in order to replace the long distance dependencies in a gated RNN, a Transformer model relies on multiple heads of attention and self-attention. Before we can tackle multi-head attention, we focus on the simpler single-head attention models and try to understand them in terms of faithfulness.
Chapter 2

Related Work

Contemporary research on interpretability of neural models cover diverse topics ranging from different interpretability methods to designing inherently interpretable neural models. In this chapter we present recent research related to our work. In Sec. 2.1 we discuss several methods for analyzing and interpreting neural models. In this work we have focused on interpretability of attention component and thus we review prior studies on understanding the semantics captured by attention in Sec. 2.2. There has been extensive research on investigating attention as an interpretation method from different axes ranging from faithfulness and plausibility to accountability and fairness. Those works are reviewed in Sec. 2.3. In this work we have also analyzed effect of sparsity for improved faithfulness. Consequently we have reviewed works regarding sparsity for better interpretability in Sec. 2.4. Our proposed method for improving faithfulness can be seen as an explanation regularizer. Several previous works have investigated regularizing explanations for better interpretability and we have reviewed them in Sec. 2.5. In the end we review prior attempts on designing inherently interpretable neural models in Sec. 2.6.

2.1 Interpretability Methods

Relevance-based interpretation is a common technique in analyzing predictions in neural models. In this method, inputs of a predictor are assigned a scalar value quantifying the importance of that particular input on the final decision. Saliency methods use the gradient of the inputs to define importance [36, 17, 13]. Layer-wise relevance propagation that assigns relevance to neurons based on their contribution to activation of higher-layer neurons is also investigated in NLP [2, 14, 3]. Another method to measure relevance is by removing the input, and tracking the difference in the network’s output [37]. While these methods focus on explaining a model’s decision, Shi et al. [56], Kádár et al. [24], Calvillo and Crocker [8] investigate how a particular concept is represented in the network.
2.2 Understanding Information Captured by Attention

Analyzing and interpreting the attention mechanism in NLP is another direction that has drawn major interest. Koehn and Knowles [28] compares alignment in NMT extracted by attention with those of fast-align and argue that attention cannot be reliably used as word alignment between source and target words, at least in the traditional sense in statistical machine translation. Ghader and Monz [16] also verify this however they show that attention is capturing useful information other than alignment. Tang and Nivre [60] investigates the role of attention in the case of word sense disambiguation (WSD) in NMT models. Counterintuitively, they show that attention pays more attention to the ambiguous noun itself and in fact encoder hidden states are handling WSD. Clark et al. [10] studies the information captured by each head in a BERT model. They conclude that some heads correspond well to linguistic notions of syntax and co-reference. Vig and Belinkov [65] focuses on structure of attention in a GPT-2 model. By visualizing attention for individual instances, they show that attention targets different part-of-speech at different layers and dependency relations are mostly captured in middle layers.

2.3 Attention and different axes of interpretability

While several studies have focused on understanding the semantic notions captured by attention [16, 64, 10], evaluating attention as an interpretability approach has garnered a lot of interest. From the faithfulness perspective, Jain and Wallace [22], Serrano and Smith [55] show that for instances in a data set there can be adversarial attention heatmaps that do not change the output of the text classifier. In other words, adversarial attention leads to no decision flip in each instance. They use this to claim that attention heatmaps are not to be trusted, or unfaithful. Wiegreffe and Pinter [67] argue against per-instance modifications at test time for two reasons: 1) in classification tasks attention may not be useful so perturbing attention is misleading. This is not true for NMT since attention is very useful in NMT. 2) they train an adversarial attention model (e.g. uniform attention) chosen to produce attention weights distant from the original attention weights while at the same time trying to minimize classification error. They show that such adversarial attention models are not as accurate as models with attention. In our work we acknowledge that attention is useful and faithful to some extent and we aim to improve faithfulness of NMT models.

While most of these works provide evidence that attention weights are not always faithful, Moradi et al. [46] confirm similar observations on the unfaithful nature of attention in the context of NMT models. Li et al. [34] is one of the few papers examining attention models in NMT. However, they are focused on the task of identifying relevant source words to explain the output translations selected by the NMT model. They look for optimal proxy models that agree with the NMT model such that the relevant source words picked as an explanation by a proxy model exhibits similar behaviour to the target model. They use the notion of fidelity over proxy models and evaluate several alternative proxy models using empirical risk minimization. Attention weights are evaluated
alongside other proxy models for this task. In contrast, our work is about improving the faithfulness of NMT models and we focus on the internal state of the NMT model rather than proxy models. They use human references, e.g. AER, for evaluating fidelity. As discussed earlier, evaluation of faithfulness cannot involved human judgements or reference data. It is possible that our faithful NMT models are also better at fidelity, but that is an open question.

While prior works have mostly failed to explicitly distinguish faithfulness from plausibility in their arguments, Jacovi and Goldberg [21, 20] focus on formalizing faithfulness and addressing evaluation of faithfulness separately from plausibility respectively.

Subramanian et al. [58] have investigated the concept of faithfulness in neural modular networks (NMN) which are employed for modeling compositionality. They question the faithfulness of the structure of the network modules describing the true abstract reasoning of the model. Similar to us, they attempt to quantify faithfulness and improve upon it. However their contributions like training with an auxiliary atomic-task supervision for improved faithfulness are specific to the context of NMNs.

Pruthi et al. [50] demonstrate that it is possible to train a model that produces a deceptive attention mask, questioning the use of attention weights as explanation from the fairness and accountability perspective.

Alvarez-Melis and Jaakkola [1] investigate the interpretability methods from the robustness perspective. They attempt to quantify robustness and show that current interpretability methods cannot be considered as robust.

2.4 Sparsity for Improved Interpretability

This line of work suggests making attention sparser so that the most contributing input word is more distinguishable over other input words. Martins and Astudillo [43] propose sparsemax as an alternative to the traditional softmax activation function, but able to output sparse probabilities and at the same time being differentiable. Malaviya et al. [42] improves sparsemax by proposing a constrained sparsemax for attention that can model fertilises to the source words and at the same time being sparse and differentiable. Zhang et al. [68] propose sparsity regularization terms such as entropy regularization to promote sparsity in the attention.

2.5 Regularizing Explanations

Recent work on explanations for black-box models has produced tools (e.g. LIME [51]) to show the implicit rules behind predictions, which can help us identify when models are right for the wrong reasons. However, these methods do not scale to explaining entire datasets and cannot correct the problems they reveal. Ross et al. [53] introduce a method for efficiently explaining and regularizing differentiable models by examining and selectively penalizing their input gradients. Rieger et al. [52] follow a similar spirit but they use ‘contextual decomposition’ [47] to extract explanations offered
by the model. Aligning attention (as explanation) with prior knowledge has also been extensively studied. Mi et al. [44], Liu et al. [40] propose to supervise attention with traditional alignment models so that attention weights match better with alignment. Zhong et al. [69] show that in the task of textual sentiment classification, attention is often misaligned with the words that contribute to attention. They propose to supervise attention with human rationale during training and they observe improved model performance. Cohn et al. [11] demonstrate that by including structural biases from traditional alignment models like positional bias and fertility in attention, it’s possible to improve the existing NMT baselines.

2.6 Self-explanatory Neural Models

Contrary to efforts for propose post-hoc explanation methods for neural models, a series of works have attempted to make neural models inherently interpretable or self-explanatory. Stahlberg et al. [57] show that the NMT model can be made self-explanatory by training it to produce the discrete decisions made by the model (from which the translations can be extracted later). Lei et al. [33] propose a model in which first a rationale is selected from the input and then is further used for prediction. Their proposed model consists of a generator and an encoder, which are trained to operate together. The generator specifies a distribution over the input to be used as candidate rationales and these are passed to the encoder for prediction. Previous work proposed to assign binary latent masks to input positions and to promote short selections via sparsity-inducing penalties such as L0 regularisation. Instead Bastings et al. [6] propose a latent model that mixes discrete and continuous behaviour allowing at the same time for binary selections and gradient-based training without RE-INFORCE. Instead of selecting part of the input as the rationale, Liu et al. [39] propose a generative explanation framework.
Chapter 3

Faithfulness in NMT

In this thesis we have two major contributions: a) quantifying faithfulness in NMT b) improving faithfulness using a novel objective. In Sec. 3.1 we explain our approach for quantifying faithfulness in NMT by putting the model under various stress tests and capturing its behavior. Then in Sec. 3.2 we present our proposed method for improving faithfulness based on a novel objective that rewards faithful behavior. We also talk about our motivation for investigating effect of sparsity on faithfulness.

3.1 Measuring Faithfulness

Intuitively, a faithful explanation should reflect the true internal reasoning of the model. Although there is no formal definition for faithfulness, a common approach in the community is to design stress tests to perturb the most relevant parts of the input, suggested by the explanation, in expectation that the model’s decision should change [20]. A common stress test is the erasure test in which the most-relevant part of the input is removed [3]. In the context of NMT, at decoding time step $t$ the attention component assigns attention weights $\alpha_t$, attending to the source word at position $m_t = \arg\max_i \alpha_{t,i}$ (or the $k$-best attended-to words in the source). These weights are often implicitly or explicitly regarded as an interpretation for the model’s prediction at the time step $t$ [61, 44, 40, 66, 32, 14, 17]. It is worth noting that erasure is only one of the possible stress tests for evaluating faithfulness. Passing more stress tests implies a more faithful model as it is resilient to more attacks or stress tests of its faithfulness. In this paper we consider three intuitive stress test cases:

- **ZeroOutMax** [3]: Here we remove attention from the most important token according to the attention weights by setting $\alpha_{t,m_t} = 0$.
- **Uniform** [46]: In this stress test all attention weights are set to be equal, $\alpha_t = \frac{1}{m} \mathbf{1}$, where $m$ is the length of the source sentence. This is to confuse the model about which part of the input is the most important one.
- **RandomPermute** [22]: In this stress test we randomly permute attention weights several times until a change in the model output is observed. We ensure that $m_t$, the most important
token according to attention, is always changed. We set \( \alpha'_t = \text{random\_permute}(\alpha_t) \) such that \( \arg\max_i \alpha'_{t,i} \neq m_t \).

Many prior studies of attention [22, 67] have used a binary measure: either attention is faithful or it is not. These studies typically are about whether attention has the potential to be useful in terms of accuracy and faithful in terms of model behaviour. In many cases, especially in the case of NMT models, attention is clearly useful and by and large it must be faithful. The question is can we measure the faithfulness and improve faithfulness. It is more natural to have a gray-scale notion of faithfulness for evaluation [20]. Following this reasoning, we define \( F(M) \) as faithfulness of attention heatmaps in model \( M \) as:

\[
F(M) = \frac{\text{# of tokens passing stress tests}}{\text{# of tokens}}
\]

\( F(M) \) is a number between 0 to 1 measuring the percentage of output tokens during inference which passed the stress tests, i.e., they changed in the presence of adversarial attention. This metric can also be regarded as a measure of trust we can assign to the attention heatmap to fully reflect the internal reasoning of the NMT model.

### 3.2 Improving Faithfulness

The conventional objective function in a sequence-to-sequence task is a cross-entropy loss \( F_{\text{acc}} \) which should be minimized:

\[
F_{\text{acc}}(\theta) = -\frac{1}{|S|} \sum_{(X,Y) \in S} \log p(Y|X; \theta)
\]

where \( S \) is the training data and \( X \) and \( Y \) are source sentence and the correct translation respectively (We use capital letters for sentences and small letters for single tokens). This training objective does not explicitly model the interpretability aspects (e.g. faithfulness) of the network and it remains unoptimized during training.

**Faithfulness Objective** In an effort to develop a model that is right for the right reason, Ross et al. [53] change the loss function of their classifier to model both right answers and right reasons instead of only the former. They achieve this by introducing a regularizing term that tends to shrink irrelevant gradients. In a similar spirit, we change our objective to account for the NMT model’s faithfulness as well as the cross-entropy score against the reference translations:

\[
F = F_{\text{acc}} + \lambda_{\text{faith}} F_{\text{faith}}
\]

\( F_{\text{faith}} \) is an additional component that rewards the model for having more faithful attention. The parameter \( \lambda_{\text{faith}} \) regulates the trade-off between between faithfulness and accuracy objectives.
Figure 3.1: We generate adversaries to the attention weights using various stress tests Uniform, ZeroOutMax, and RandomPermute. When adversarial attention weights are used, in a faithful model we expect the probability of the original output (\(\hat{y}\)) to drop significantly. We use this criteria to define a faithfulness objective function.

3.2.1 Divergence-based Faithfulness Objective

Consider a predictive model \(g_{\theta}\) in which an intermediate calculation is later employed to justify predictions:

\[
\hat{y} = \arg \max_y p(y|x) = \arg \max_y g_{\theta}(x, IC(x), y)
\]  

(3.4)

where \(IC(x)\) is the intermediate calculation on the input. A concrete example for \(IC(x)\) would be the context vector calculated by the attention mechanism.

**Hypothesis**  If there exists an intermediate calculation \(IC'(x)\), as a stress test, that conveys a contradictory post-hoc attention compared to \(IC(x)\), then \(IC(x)\) cannot be regarded as faithful for predicting \(\hat{y}\). If \(IC(x)\) is faithful, we expect the model to diverge from predicting \(\hat{y}\) when \(IC'(x)\) is employed instead.

Based on our hypothesis, we propose a divergence-based objective which mimics behavior of a faithful explanation under stress test:

\[
F_{faith} = \log p(\hat{y}|x, IC'(x))
\]

(3.5)

This objective is a negative loss that should be minimized. The minimum of this objective is achieved when the probability of the original prediction approaches zero under the stress test which
is the ideal. Thus, it promotes reduction in output probability under an adversarial intermediate calculation (Figure 3.1). It is worth noting that this objective can be potentially employed in models where outputs are modeled as soft probabilities and thus is not limited to NMT. To put a model under various stress tests we manipulate the context vector during training time by changing the attention weights and feeding it to the decoder to calculate the probability. More precisely:

$$F_{faith} = \lambda_{zom} \log p(\hat{y}|x, IC'_{zom}(x))$$
$$+ \lambda_{uni} \log p(\hat{y}|x, IC'_{uni}(x))$$
$$+ \lambda_{perm} \log p(\hat{y}|x, IC'_{perm}(x))$$

(3.6)

where $IC'_{zom}$, $IC'_{uni}$ and $IC'_{perm}$ are ZeroOutMax, Uniform and RandomPermute methods (see Sec. 3) to manipulate attention weights, respectively. \(\lambda_{\{\text{method}\}}\) parameters regulate the contribution of each objective. We use the term $F_{all}$ when all \(\lambda_{\{\text{method}\}}\) s in Eq. (3.6) are non-zero. Moreover, we use the term $F_{\{\text{method}\}}$ when \(\lambda_{\{\text{method}\}}\) is set to 1 and other regularization weights are zero.

3.2.2 On attention sparsity

Do the models trained with the faithfulness objective have sparser attention weights? Sharper attention in a model $M$ might correlate with an intensified contribution of the most-attended source hidden state on the prediction resulting in higher faithfulness.

To measure sparseness of the attention, we take an average over the normalized entropy of attention distribution for each output token during inference on test data. We use normalized entropy which is in range [0,1] to account for the fact that the range of the entropy for each output token depends on the length of the corresponding source sentence.

$$AvgEnt = \frac{1}{\sum_{i=1}^{|S|} |\hat{Y}_i|} \sum_{i=1}^{|S|} \sum_{j=1}^{|\hat{Y}_i|} \text{NormEnt}(\alpha_{i,j})$$

(3.7)

$$\text{NormEnt}(P) = - \sum_i \frac{P_i \log P_i}{\log N}$$

(3.8)

Here $\alpha_{ij}$ is the attention distribution for the output token $j$ in the generated translation of source sentence $i$, and $P$ is a discrete probability distribution. In Eq. (3.8) low entropy indicates a sharper distribution.

**Attention Entropy Regularization** Alongside investigating sparsity of the models trained by the faithfulness objective, we also train a model in which sparsity in attention is directly optimized. We used attention entropy regularization [68]:

$$F_{ent} = F_{acc} + \lambda_{ent} \sum_{i=1}^{|S|} \sum_{j=1}^{|\hat{Y}_i|} \text{Ent}(\alpha_{i,j})$$

(3.9)
where entropy of attention weights is added to the cross-entropy loss (3.2) as a regularization term.

3.2.3 Summary

In this chapter we have presented our approach for quantifying faithfulness and also improving it. We put NMT under different stress tests and define faithfulness based on the percentage of output tokens that have been preserved under those tests. We argue that faithfulness is not optimized in usual NMT objectives and we propose a novel loss based on probability divergence that rewards faithfulness behavior. Moreover we mention our motivation for experimenting with entropy regularization which is investigating if attention sparsity is related to faithfulness. In Chapter 4 we discuss our experimental setup, experiments, and findings.
Chapter 4

Experiments

In this chapter we provide results of our experiments and findings. We first explain our experimental setup including the NMT model employed, datasets used, hyperparameters and training tricks in Sec. 4.1. We also study the faithfulness of our baseline NMT model and its sensitivity to different stress tests in Sec. 4.2. In Sec. 4.3 we analyze our proposed method and its effect on faithfulness and sparsity. We provide a brief summary of this chapter in Sec. 4.4.

4.1 Experimental Setup

Data  We use the Czech-English (Cs-En) dataset from IWSLT2016\(^1\) and the German-English (De-En) dataset from IWSLT2014\(^2\). For the Czech-English dataset we use dev2010, tst2010, tst2011, tst2012, and tst2013 as the test data. For the German-English dataset we use dev2010, tst2010, tst2011, dev2012, and tst2012 as the test data. Table 4.1 shows the number of instances in different sets from the datasets used. We used Moses [29] to tokenize the dataset.

|        | Cs-En | De-En |
|--------|-------|-------|
| Train  | 101225| 160239|
| Valid  | 4601  | 7283  |
| Test   | 5716  | 6750  |

Table 4.1: Number of sentences in training, validation, and test sets across Cs-En and De-En datasets.

Architecture and Hyperparameters  We use OpenNMT [26] as our translation framework. We employ a 2 layer LSTM-based encoder-decoder [59, 9] model with global attention [41]. Dimension of the hidden states and the word embeddings for both source and target languages are set to 500. Vocabulary size for both the source and target language is set to 50000. We remove sentences with more than 50 tokens from the training data. We use Adam [25] for training our models and we

\(^1\)https://sites.google.com/site/iwsltevaluation2016/
\(^2\)https://sites.google.com/site/iwsltevaluation2014/
Table 4.2: Percentage of function and content words in the generated translation for test set.

|                | Cs-En | De-En |
|----------------|-------|-------|
| Number of tokens (+EOS) | 115993 | 139465 |
| % of function words      | 68%   | 68%   |
| % of content words       | 32%   | 32%   |

set the learning rate to 0.001. Models are trained until convergence. Our models have around 82M parameters and it took us twelve hours to train each model on two GTX 1080ti GPUs. We optimize the hyperparameters of our models using the validation set. The baseline model is trained using Eqn. (3.2) and we call it $F_{\text{baseline}}$. $\lambda_{\text{ent}}$ in Eq. (3.9) is set to 0.04. We refer to the objective as $F_{\text{all}}$ when $\lambda_{\text{zom}}, \lambda_{\text{uni}},$ and $\lambda_{\text{perm}}$ are set to 0.5, 0.375, and 0.125 respectively. $\lambda_{\text{faith}}$ is set to 1.

**Training Difficulties** Our first attempts at using the modified objective function in Eq. (3.3) trained poorly. We observed that it was difficult for the model to learn the faithfulness constraint without having already learned to assign a reasonable probability to correct translations. To address this problem we first train the NMT model using the standard unmodified objective function and then fine-tune this trained model by switching the objective function to Eq. (3.3).

### 4.2 Analyzing the baseline model

#### 4.2.1 Power of each test

We investigate behavior of the model under stress test for generation of function\(^3\) and content words. Function words (e.g., a, the, is) have little lexical meaning in contrast to content words and thus we are curious whether response of the model to stress tests differs for generation of these two groups of words. Table 4.2 shows the percentage of function and content words generated by the baseline model. As expected, the majority of the generated tokens are function words.

Table 4.3 and 4.4 show the faithfulness of the model for generation of function and content words under different stress tests. ZeroOutMax test has been the most effective method for capturing unfaithful behavior as it has resulted in the lowest faithfulness. We also determine that RandomPermute is not as effective as the Uniform and ZeroOutMax methods. Our justification is that in the RandomPermute method, it is highly probable that the context vector is biased toward a random source hidden state. Such bias can lead to significant misleading noise in the context vector which can change the prediction of the model. However, there isn’t such a bias in the Uniform or ZeroOutMax methods.

As evident from Table 4.3 and 4.4, the most strict test is when all stress tests are applied for capturing unfaithful behavior (All column).

---

\(^3\)The reference for function words (we added new function words including the EOS token to this) can be found at: [semanticsimilarity.files.wordpress.com/2013/08/jim-oshea-fwlist-277.pdf](http://semanticsimilarity.files.wordpress.com/2013/08/jim-oshea-fwlist-277.pdf)
4.2.2 Function words are more easily generated compared to content words

An important observation in Table 4.3 and 4.4 is that function words exhibit unfaithful behavior much more than content words. Faithfulness of the model for generation of content words is 78% and 76% for Czech-English and German-English respectively. However it is 33% and 32% for function words. The reason is that the production of function words rely more on the target context, in contrast to content words which rely more on the source context [62]. Accordingly, perturbation in the original attention weights likely has significantly more impact on diminishing content words compared to function words. This ties well with the main idea behind context gates in which the influence of source context and target context is controlled dynamically [62].

4.2.3 Highlighting top preserved tokens

To better understand the behavior of the model in the presence of stress test, we listed the top preserved tokens in the De-En dataset. Table 4.5 contains the top 20 content words sorted by the number of times they were preserved. It is interesting to note that for many of these frequent tokens, more than half of their total occurrences are preserved without focusing on their corresponding translation in the source sentence (e.g., “going”, “know”, “thing”, etc). In Table 4.6, we sort such tokens based

| Objective | Content Words | Function Words |
|-----------|---------------|----------------|
|           | ZOM | Uniform | RandPerm | All | ZOM | Uniform | RandPerm | All |
| $F_{baseline}$ | 83% | 90% | 94% | 78% | 46% | 48% | 64% | 33% |
| $F_{zom}$ | 91% | 93% | 98% | 86% | 84% | 87% | 95% | 74% |
| $F_{uni}$ | 84% | 98% | 97% | 83% | 56% | 98% | 91% | 54% |
| $F_{perm}$ | 86% | 95% | 96% | 83% | 74% | 97% | 98% | 71% |
| $F_{all}$ | 91% | 99% | 98% | 89% | 83% | 98% | 98% | 82% |
| $F_{ent}$ | 78% | 90% | 94% | 73% | 46% | 48% | 64% | 33% |

Table 4.3: Faithfulness metric for the generated content and function words through different objectives in the Czech-English dataset. The columns are different tests included in the Eq.(3.1).

| Objective | Content Words | Function Words |
|-----------|---------------|----------------|
|           | ZOM | Uniform | RandPerm | All | ZOM | Uniform | RandPerm | All |
| $F_{baseline}$ | 81% | 90% | 93% | 76% | 45% | 48% | 64% | 32% |
| $F_{zom}$ | 91% | 95% | 98% | 87% | 87% | 95% | 97% | 82% |
| $F_{uni}$ | 81% | 98% | 91% | 80% | 60% | 100% | 95% | 58% |
| $F_{perm}$ | 85% | 95% | 97% | 82% | 74% | 97% | 98% | 72% |
| $F_{all}$ | 91% | 98% | 98% | 89% | 87% | 100% | 99% | 86% |
| $F_{ent}$ | 81% | 90% | 93% | 76% | 47% | 47% | 64% | 33% |

Table 4.4: Faithfulness metric for the generated content and function words through different objectives in the German-English dataset. The columns are different tests included in the Eq.(3.1).
| Token   | # preserved | Coverage |
|---------|-------------|---------|
| going   | 310         | 70%     |
| people  | 237         | 46%     |
| know    | 219         | 62%     |
| world   | 215         | 67%     |
| like    | 189         | 47%     |
| think   | 176         | 50%     |
| way     | 162         | 68%     |
| get     | 160         | 53%     |
| thing   | 147         | 79%     |
| things  | 142         | 56%     |
| time    | 139         | 54%     |
| see     | 137         | 51%     |
| years   | 136         | 64%     |
| make    | 126         | 49%     |
| little  | 113         | 55%     |
| just    | 109         | 29%     |
| really  | 93          | 37%     |
| bit     | 92          | 88%     |
| said    | 89          | 59%     |
| got     | 86          | 59%     |

Table 4.5: Top 20 content words preserved by the aggregate method sorted by the number of times they were preserved.

| Token  | Coverage | Total |
|--------|----------|-------|
| bit    | 88%      | 105   |
| course | 87%      | 91    |
| thank  | 83%      | 89    |
| thing  | 79%      | 186   |
| fact   | 78%      | 74    |
| half   | 78%      | 27    |
| own    | 75%      | 75    |
| ones   | 73%      | 30    |
| states | 73%      | 30    |
| difference | 71% | 21  |
| going  | 70%      | 444   |
| turns  | 69%      | 26    |
| way    | 68%      | 237   |
| able   | 67%      | 85    |
| world  | 67%      | 323   |
| doing  | 66%      | 103   |
| planet | 65%      | 37    |
| years  | 64%      | 212   |
| know   | 62%      | 353   |
| united | 62%      | 21    |

Table 4.6: Top 20 content words preserved by the aggregate method sorted by percentage of their total occurrences that are preserved (coverage).
Table 4.7: Top 30 function words preserved by the aggregate method sorted by the number of times they were preserved.

| Token | # preserved | Coverage |
|-------|-------------|----------|
| .     | 7329        | 85%      |
| EOS   | 6364        | 94%      |
| the   | 5210        | 82%      |
| .     | 3947        | 60%      |
| of    | 3003        | 87%      |
| to    | 2923        | 86%      |
| and   | 2639        | 67%      |
| a     | 2187        | 65%      |
| that  | 1936        | 69%      |
| i     | 1737        | 76%      |
| 's    | 1732        | 95%      |
| you   | 1501        | 72%      |
| it    | 1497        | 72%      |
| is    | 1496        | 88%      |
| in    | 1364        | 64%      |
| we    | 1246        | 64%      |
| they  | 624         | 69%      |
| '    | 620         | 81%      |
| have  | 613         | 70%      |
| be    | 582         | 91%      |
| 't    | 580         | 96%      |
| 're   | 542         | 86%      |
| this  | 541         | 42%      |
| so    | 531         | 57%      |
| are   | 526         | 77%      |
| was   | 514         | 66%      |
| do    | 433         | 77%      |
| about | 417         | 65%      |
| what  | 415         | 61%      |
| can   | 400         | 54%      |

Table 4.8: Top 30 function words preserved by the aggregate method sorted by coverage.

| Token | Coverage | Total |
|-------|----------|-------|
| 't    | 96%      | 602   |
| 's    | 95%      | 1819  |
| EOS   | 94%      | 6748  |
| be    | 91%      | 641   |
| is    | 88%      | 1707  |
| of    | 87%      | 3450  |
| to    | 86%      | 3383  |
| 're   | 86%      | 631   |
| ,     | 85%      | 8582  |
| 'm    | 84%      | 311   |
| been | 82%      | 233   |
| lot   | 82%      | 148   |
| the   | 82%      | 6386  |
| "    | 81%      | 770   |
| are   | 77%      | 679   |
| do    | 77%      | 565   |
| i    | 76%      | 2290  |
| who   | 73%      | 300   |
| it    | 72%      | 2089  |
| you   | 72%      | 2099  |
| have | 70%      | 876   |
| up    | 70%      | 235   |
| they | 69%      | 904   |
| that | 69%      | 2812  |
| well | 67%      | 153   |
| and   | 67%      | 3922  |
| was   | 66%      | 774   |
| were  | 65%      | 240   |
| same  | 65%      | 154   |
| a    | 65%      | 3369  |

on their coverage, which is the percentage of their total occurrences that are not affected when a counterfactual attention is applied\(^4\).

We repeat the same process for function words (Table 4.7 and Table 4.8). As evident from Table 4.7, we have successfully yielded the same token in 94% of the occurrences of the EOS token but with a counterfactual attention. This can be explained by the previous findings suggesting special hidden units keep track of translation length [56]. As a result, the EOS token is generated upon

\(^4\)We consider only the tokens that have appeared more than 20 times. The reason is that there are many preserved words that have appeared only once (coverage=1) and it is not clear if the coverage remains the same when frequency increases.
receiving signal from these units rather than using attention. This indicates that attention weights are highly unreliable for explaining the generation of EOS tokens. This is worth noting because early generation of the EOS token is often a major reason of the under-translation problem in NMT [30]. Thus, attention weights should not be used to debug early generation of EOS, and that some other underlying influence in the network [14] might be responsible for the model’s decision in this case.

4.3 Analyzing the proposed methods

4.3.1 Impact on faithfulness

To measure the effectiveness of the proposed objectives, we choose the best model in terms of provided faithfulness but within the 0.5 BLEU score of the maximum achieved BLEU score in the validation set. The reason is that we prefer a model that is both accurate and with faithful attention-based explanations. Table 4.3 and 4.4 show the performance of the different faithfulness objective functions when generating content words and function words across different attention manipulation methods in the Czech-English (Cs-En) and German-English (De-En) datasets respectively. Results indicate that the proposed divergence-based objective has been effective in increasing the faithfulness metric. \( F_{\text{all}} \) is the most effective objective for increasing faithfulness when all stress tests are included in Eq. (3.1). When using \( F_{\text{all}} \), faithfulness of attention-based explanations for content words is increased 78% to 89%, while that of the function words is from 33% to 82% (see \( All \) column in Table 4.3). There are similar increases from 76% to 89% for content words and from 32% to 86% for function words in the De-En dataset. These results establish the effectiveness of our proposed objectives to increase the faithfulness metric. It is worth noting that increase in faithfulness of attention-based explanations for function words is much more than that of content words. This can be attributed to the fact the function words are mostly generated using the target-side information in the decoder [62, 46] and manipulating attention does not have much effect on generating them. However, our proposed faithfulness objective (\( F_{\text{faith}} \)) seems to tighten the dependence of the decoder on the attention component. This results in much more increase in faithfulness for function words compared to such content words.\(^5\) We also plot faithfulness over different checkpoints in Figure 4.1. It indicates that progress in faithfulness is much faster for function words compared to content words.

4.3.2 Effect of training with single adversary on passing other stress tests

An interesting observation in Table 4.3 and 4.4 is that training with an adversary has positive effects on the model for passing stress tests from other types of adversaries. As an example, in Table 4.3 the

\(^5\)If this dependence is not desired, it is possible not to penalize function words in the faithfulness objective. However, relying on attention for generating function words can be helpful, not necessarily for interpretability but for dealing with long-range dependencies [63] and, as a result, better translations.
Figure 4.1: Progress in faithfulness over different checkpoints. It increases much faster in function words compared to content words.

|        | De-En | Cs-En |
|--------|-------|-------|
|        | Baseline | Ours |
|        | Baseline | Ours |
| PUNC   | 0.19   | 0.70  |
| PRON   | 0.42   | 0.78  |
| VERB   | 0.47   | 0.80  |
| ADP    | 0.30   | 0.75  |
| DET    | 0.35   | 0.74  |
| PRT    | 0.13   | 0.63  |
| ADV    | 0.66   | 0.80  |
| NOUN   | 0.63   | 0.87  |
| ADJ    | 0.68   | 0.87  |
| NUM    | 0.84   | 0.86  |
| X      | 0.67   | 0.78  |

Table 4.9: Faithfulness metric within different part-of-speech (POS) tags.

column *Uniform* is the faithfulness metric when only Uniform test is employed in Eq. (3.1). When using this metric, we can observe that training a model with $F_{perm}$ increased faithfulness from 90% to 95% for content words and from 48% to 97% for function words. We can see such effect in Table 4.4 as well. This observation indicates that training with each adversary can be beneficial for making model tolerant against other types of stress tests. It seems that training with each adversary strengthens the dependence of the decoder on the attention component which can be beneficial for passing other stress tests.

### 4.3.3 POS-tag analysis

In addition to categorizing tokens into function and content words, we also analyze the effect of our proposed objective within different universal part-of-speech (POS) tags [48] in Table 4.9. Our proposed objective has increased faithfulness in each POS tag and in our both datasets. Tokens with less lexical meaning are the ones affected the most as explained in Sec. 4.3.1. As expected, punctuations (PUNC) and particles (PRT) tags have benefited the most from increase in the faithfulness. Interestingly numbers (NUM tag) have the lowest increase in faithfulness. One reason might be that they already had a high initial faithfulness and this has made further increase less likely.
4.3.4 Regularization Effect

The model checkpoints used in Tables 4.3 and 4.4 were selected based on maximum increase in faithfulness without sacrificing accuracy. To investigate if the proposed objective can have a general positive side effect in terms of accuracy, we train three independent models using the $F_{baseline}$ and $F_{all}$ objectives. To make it fair for the baseline, we also add additional steps of training for the baseline model as well to isolate the benefit of adding the faithfulness objective.

Table 4.10 contains the average BLEU score of the trained models. It indicates that the model trained with $F_{all}$, has +0.7 and +0.4 increase in BLEU score compared to the baseline for the Czech-English and German-English language pairs respectively.

| Objective | BLEU |
|-----------|------|
| Cs-En     |      |
| $F_{baseline}$ | 19.68 |
| $F_{all}$   | 20.4 |
| De-En     |      |
| $F_{baseline}$ | 24.85 |
| $F_{all}$   | 25.21 |

Table 4.10: BLEU score of the baseline and the model trained with $F_{all}$. Pairwise bootstrap resampling [27] resulted in a p-value < 0.01 which indicates the statistical significance of the observed difference.

Improved BLEU scores for the faithful model can be due to two reasons: 1) the faithfulness objective can be seen as a regularization term which prevents the model from relying too much on the target-side context and the implicit language model in the decoder, which results in increased contribution of attention on the decoder and reducing some bias in the model. 2) penalizing the model for the lack of connection between justification and prediction forces the model to learn better translations by forcing it to justify each output in a right answer for the right reason paradigm. Figure 4.2 shows some examples of how our proposed model can produce better translations.

4.3.5 Do the new models have sparser attention?

Table 4.11 shows the average entropy and average normalized entropy for the baseline, the proposed model ($F_{all}$), and the model trained with attention entropy regularization respectively. Evidently, the proposed model has not increased sparsity. On the other hand attention entropy regularization has been very effective in making attention weights sparser. But Table 4.3 and 4.4 indicates that attention entropy regularization has not been effective in increasing faithfulness. This suggests that sharper attention weights only affect the context vector and do not contribute to increased dependence of the decoder on attention. The proposed model does not end up with sparse attention, and entropy regularization has been ineffective at increasing faithfulness although it does learn a sparse attention model.
Figure 4.2: These examples show some cases where the more faithful model trained using our faithfulness objective produces better translations compared to the baseline model. In each of these cases, perturbing the attention weights has no effect on the baseline model output. The faithful model is able to focus on the source side when needed in order to produce a more accurate translation.

| Model          | AvgEnt | AvgNormEnt |
|----------------|--------|------------|
| Cs-En          |        |            |
| $F_{baseline}$ | 0.69   | 0.23       |
| $F_{alt}$      | 0.84   | 0.27       |
| $F_{ent}$      | **0.35** | **0.11**  |
| De-En          |        |            |
| $F_{baseline}$ | 0.89   | 0.29       |
| $F_{alt}$      | 1.0    | 0.32       |
| $F_{ent}$      | **0.43** | **0.14**  |

Table 4.11: Average entropy and average normalized entropy of the baseline, the proposed model ($F_{alt}$), and the model trained with attention entropy regularization.

### 4.4 Summary

In this chapter we have demonstrated our findings regarding the faithfulness of a baseline NMT model and effect of our proposed method on it and also its relation to sparsity. Our findings show that attention is much less faithful for rationalizing prediction of function words compared to content words. Moreover we show that our proposed method can successfully improve faithfulness in NMT without sacrificing accuracy and in some cases even with improved accuracy. Moreover we find that neither our proposed model has more sparse attention, nor the model trained with attention entropy regularization for increased sparsity has less unfaithful attention.
Chapter 5

Conclusion

Using attention weights to justify a model’s prediction is tempting and seems intuitive at the first glance. It is, however, not clear whether attention can be trusted for such purposes. To what extent is it trustworthy or faithful and reflect the true internal reasoning of the model? In this work we have proposed a method for quantifying faithfulness of NMT models. We have also investigated behavior of NMT under presence of different stress tests. To optimize faithfulness we have defined a novel objective function that rewards faithful behavior through probability divergence. We also show that the additional constraint in the training objective for NMT does not harm translation quality and in some cases we see some better translations presumably due to the regularization effect of our faithfulness objective. In future we intend to expand this work to language pairs where target language is not English. While this work is focused on NMT, our approach is more generally applicable to other neural models that exploit attention and where researchers are implicitly trusting attention heatmaps as a means of explanation of the model behaviour. Our faithfulness objective can be used for other NLP tasks such as text classification. We aim to investigate and improve faithfulness of attention-based explanations in more sophisticated attention models such as Transformers [63]. We can generalize our approach by designing explanatory modules in NMT through functionality separation (alignment, reordering, etc.) instead of relying only on attention. We also plan to investigate if faithful models can also be more useful for copy models and other applications of attention heatmaps in NMT.
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