A Closer Look at Transformer Attention for Multilingual Translation

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Abstract

Transformers are the predominant model for machine translation. Recent studies also showed that a single Transformer model can be trained to learn translation for multiple different language pairs, achieving promising results. In this work, we investigate how multilingual Transformer models pay attention when translating different language pairs. To achieve this, we first conduct automatic pruning to eliminate a large number of noisy heads and then assess the functions and behaviors of the remaining heads in both self-attention and crossattention. We find that different language pairs, in spite of having different syntax and word orders, tend to share the same heads for the same functions, such as syntax heads and reordering heads. However, the different characteristics of different language pairs can clearly cause interference in function heads and affect head accuracies. Additionally, we reveal an interesting behavior of the Transformer cross-attention: the deep-layer cross-attention heads work in a cooperative way to learn different options for word reordering, which may be caused by the nature of translation tasks having multiple different gold translations in the target language for the same source sentence.¹

1 Introduction

For traditional statistical machine translation, such as phrase-based translation (Koehn et al., 2003), the translation process is very clear: source phrases are translated into target phrases according to translation rules and then target phrases are reordered to ensure the fluency of the target sentence. However, in state-of-the-art neural translation models (Bahdanau et al., 2014; Vaswani et al., 2017; Chen et al., 2018), how the model learns to translate is substantially less obvious. The behavior of the Transformer model (Vaswani et al., 2017) remains particularly hazy, as it contains many different selfand cross-attention heads in different layers.

A number of existing studies conducted analyses of functions and behaviors of attention heads in Transformer translation models. Voita et al. (2019b) found that the Transformer attention is noisy, as most of the Transformer heads can be pruned away without significant loss in translation quality. They also identified three important functions of self-attention in the Transformer encoder, such as heads focusing on syntax. Ferrando and Costa-jussà (2021) demonstrated that the crossattention of the Transformer model frequently attends to uninformative source words to balance the contribution of source and target context for predicting the next word. Chen et al. (2020) showed that some cross-attention heads learn alignment for the current target word, achieving higher accuracies than cross-attention heads that learn alignment for the next target word. However, these methods only analyzed attention in bilingual models, not for multilingual Transformer models.

Multilingual translation, i.e., training a single Transformer to learn translation for multiple different language pairs, has received much attention in recent years and obtained promising results (Wang et al., 2020; Kim et al., 2021; Pires et al., 2023). A number of studies investigated how a multilingual Transformer learns to translate different language pairs. Several of these (Lin et al., 2021; Wang et al., 2020; Xie et al., 2021) learned language-dependent weight masks to identify language-dependent subnetworks. Pires et al. (2023) trained the multilingual Transformer to learn language-specific layers and improved translation quality. Chiang et al. (2022) and Kim et al. (2021) assessed how different language pairs share important heads in multilingual Transformer models.

However, prior work has not yet studied the specific functions and behaviors of different attention heads in multilingual Transformer models. In this

¹Code and scripts for reproducing our results can be found https://github.com/jingyiz/ multilingual-translation-attention-head-analysis.

paper, we investigate functions and behaviors² of both self-attention and cross-attention for multilingual translation. We find that different language pairs with different syntax and different word orders tend to share the same heads for the same functions (such as syntax heads and reordering heads), but the different characteristics of different language pairs can clearly cause interference in function heads and affect head accuracies compared to bilingual models. We further obtain an interesting finding about how the Transformer learns word reordering: different cross-attention heads in deep layers work in a cooperative way to learn different options for reordering. This may result from the fact that there are multiple different gold translations (reorderings) in the target language for the same source sentence³.

2 Related Work

There are a number of studies on analyzing layer representations of different Transformer layers. Voita et al. (2019a) used canonical correlation analysis and mutual information estimators to study how information flows across Transformer layers for different learning objectives. Kudugunta et al. (2019) used Singular Value Canonical Correlation Analysis (SVCCA) to analyze how representations evolve in a multilingual translation model. Xu et al. (2021b) analyzed how word translation evolves in Transformer layers and showed that translation already happens progressively in encoder layers and even in the input embeddings, by measuring word translation accuracy of different Transformer layers. These methods did not analyze the specific functions of attention heads.

Other prior work analyzed Transformer attention to better understand a particular aspect of the translation process. Tang et al. (2021) analyzed Transformer attention for negation translation and showed that negation is often rephrased during training, which can make it more difficult for the model to learn a reliable link between source and target negation. Tang et al. (2018) analyzed Transformer cross-attention for learning word sense disambiguation (WSD) and showed that cross-attention is likely to distribute more attention to the ambiguous noun itself rather than context tokens, in comparison to other nouns, which suggests that the Transformer learns to encode contextual information necessary for WSD in the encoder hidden states. Additionally, Tang et al. (2018) also noticed that, from shallow layers to deep layers, the cross-attention accuracy for aligning the next target word first increases and then decreases. However, we our study is the first to reveal the cooperative behavior of cross-attention heads.

There is also prior work that studied representation sharing in multilingual translation. Firat et al. (2016) proposed a multiway, multilingual model with language-specific encoders and decoders and showed result quality improvements over models trained on only one language pair. Several authors (Zhang et al., 2021; Bapna and Firat, 2019; Zhu et al., 2021) considered language-dependent gating and adaptation for layer representations. Xu et al. (2021a) proposed parallel encoder and decoder layers with language-dependent weighted layer aggregation. Wang et al. (2019) presented a universal representer to replace both encoder and decoder models to enable parameter sharing between encoder and decoder and they made the representer sensitive for specific languages using language-sensitive embedding, attention, and discriminator. Zhu et al. (2020) incorporated a language-aware interlingua into the encoder-decoder architecture, which enables the model to learn a language-independent representation from the semantic spaces of different languages, while still allowing for languagespecific specialization of a particular language pair. Additionally, Shaham et al. (2023) showed that controlling the proportion of each language pair in the training data can balance the amount of interference between languages in multilingual models. Yuan et al. (2023) developed a detachable model by assigning each language (or group of languages) to an individual branch that supports plug-and-play training and inference with a novel efficient training recipe. Xu et al. (2023) investigated how to utilize intra-distillation to learn more language-specific parameters and then showed the importance of these language-specific parameters. However, these methods did not investigate the head functions in multilingual models.

²Following Voita et al. (2019b)'s work, we use a weightbased method for analyzing attention head behaviors. It is also possible to use a norm-based method (Kobayashi et al., 2020), which may provide a more detailed interpretation of the inner workings of Transformers compared to weight-based methods in some cases.

³In the training data of translation models, it is rather rare that the same source sentence has multiple different translated target sentences, but it is very common that the same source phrase has multiple different translated target phrases. Therefore, translation models are able to learn to translate a source sentence into different target sentences.

| | DeEn | FrEn | RoEn | EnDe | EnFr | EnRo | Average |
|----------------------------|-------|-------|-------|-------|-------|-------|---------|
| R-bi | 25.90 | 29.47 | 31.46 | 21.94 | 31.08 | 25.74 | 27.59 |
| R-multi | 25.88 | 29.85 | 34.07 | 21.70 | 31.00 | 26.17 | 28.11 |
| R-finetune | 26.48 | 29.91 | 34.96 | 22.61 | 31.79 | 27.21 | 28.82 |
| R-prune ($\lambda = 25$) | 26.31 | 29.76 | 34.87 | 22.31 | 31.46 | 27.12 | 28.63 |
| R-prune ($\lambda = 35$) | 26.23 | 29.56 | 34.82 | 22.05 | 31.40 | 27.21 | 28.54 |

Table 1: Translation results (BLEU) on the test sets.

| Train | | |
|-------|-------|---|
| DeEn | 2.5M | Europarl v7, TED2020, News-Commentary v11 |
| FrEn | 2.5M | Europarl v7, TED2020, News-Commentary v11 |
| RoEn | 0.9M | Europarl v8, TED2020, SETIMES2 |
| Valid | | |
| DeEn | 5,014 | newstest2009, newstest2010 |
| FrEn | 5,014 | newstest2009, newstest2010 |
| RoEn | 1,999 | newsdev2016 |
| Test | | |
| DeEn | 9,006 | newstest2011, newstest2012, newsdev2013 |
| FrEn | 9,006 | newstest2011, newstest2012, newsdev2013 |
| RoEn | 1,999 | newstest2016 |
| | | |

Table 2: Datasets and their number of sentence pairs.

3 How Do Transformers Pay Attention for Multilingual Translation?

3.1 Methodology and Experimental Setup

Bilingual Baseline. We used the original Transformer model in its base setting (Vaswani et al., 2017) (i.e., the same model parameters, training parameters and inference parameters) as our bilingual baseline model and conducted translation experiments for six translation directions⁴: German \leftrightarrow English (De \leftrightarrow En), French \leftrightarrow English $(Fr \leftrightarrow En)$, and Romanian \leftrightarrow English (Ro \leftrightarrow En). For each translation direction (such as $De \rightarrow En$), we trained a Transformer model using the training data and validation data for this translation direction as shown in Table 2.⁵ Following Vaswani et al. (2017), we trained each model for 100k training steps. However, because our training data size for a single translation direction is smaller than in their work, 100k training steps caused overfitting in our models. Therefore we computed the validation loss after each training epoch and then chose the best validation checkpoint for evaluation. Translation results on the test sets are given in Table 1 as R-bi.

| | $\lambda = 25$ | $\lambda = 35$ |
|--------|----------------|----------------|
| DeEn | 74 | 54 |
| FrEn | 58 | 49 |
| RoEn | 74 | 52 |
| EnDe | 85 | 64 |
| EnFr | 65 | 53 |
| EnRo | 81 | 56 |
| Shared | 55 | 45 |
| Total | 14 | 14 |

Table 3: Number of remaining heads after automatic pruning for different translation directions. "Shared" means the number of heads that remain for all six translation directions. "Total" refers to the original number of all heads before automatic pruning.

Multilingual Translation. For multilingual translation, we trained a single Transformer to learn translation for all six translation directions. We combined all training data in Table 2 together and added a special token at the beginning of each source sentence to indicate which target language we desire the model to generate, following Johnson et al. (2017). We used the same base setting of the original Transformer with 100k training steps for our multilingual model. During training of the multilingual model, we computed the validation loss for the combined validation data after each training epoch and found that the validation loss continuously decreased, so we used the final checkpoint of the multilingual model for evaluation. The evaluation results of the multilingual model are given in Table 1 as R-multi. In the results, we can observe that the multilingual model obtained comparable or higher translation quality compared to our bilingual baseline for different language pairs.

Finetuning. We then finetuned⁶ the multilingual model for each translation direction using direction-

⁴We chose these language pairs because parallel sentences with gold-standard word alignments are available (Zhang and van Genabith, 2021) for these language pairs, which can be used to analyze target-to-source attention (alignment).

⁵For subword segmentation, we applied byte pair encoding (Sennrich et al., 2016) and learned a joint vocabulary of size 32k for all languages in our experiments.

⁶Finetuning a multilingual model for a given translation direction (i.e., multilingual pretraining) is very popular for low-resource language pairs and can significantly improve translation quality. We find that finetuning generally did not change the functions of different heads (see Figure 1) but did improve the accuracies of function heads for the given translation direction (see Table 12).



Figure 1: Functional heads (red: rare word head (R); yellow: positional head (-1 and +1); purple: syntactical head (S); green: C-alignment head (C); blue: N-alignment head (N)) contained in (a) the multilingual model (R-multi); (b) finetuned models (R-finetune); (c) pruned models with $\lambda = 25$; (d) pruned models with $\lambda = 35$. From left to right, the three columns of figures represent S2S, T2T, and T2S attention. Each figure shows attention heads from the first layer to the last layer (top-down) and each layer contains 8 heads. Black denotes heads that are pruned away.

specific training and validation data.⁷ During finetuning, we set the maximum number of finetuning steps to 50k and computed the validation loss after each training epoch, and finally used the best validation checkpoint for evaluation. We found that models for all six directions converged during finetuning (the best validation checkpoint is not the last checkpoint). The results of the finetuned models are given in Table 1 as R-finetune. As shown in Table 1, finetuning a pre-trained multilingual translation model for a specific translation direction can improve the translation quality for the given translation direction (i.e., R-finetune > R-multi). Table 1 also shows that the finetuned models can achieve higher translation quality compared to the bilingual models (R-bi) for all translation directions in our experiments.

Head Pruning. As shown by Voita et al. (2019b), Transformer attention is noisy, i.e., many attention heads carry no important function and can be pruned away without significant loss in translation quality. Following them, we conduct automatic pruning to identify important heads and analyze their functions. For each translation direction, we continue to finetune the already converged model (R-finetune) with a regularization loss (Louizos et al., 2017) along with the original translation loss to prune away useless heads. With the regularization loss, the model learns a 0/1 gate for each head. Heads with a 0 gate are pruned away. A weight λ is assigned to the regularization loss to control the amount of heads to be pruned, i.e., a higher weight for the regularization loss will result in more heads being pruned away. Translation results after head pruning are given in Table 1 and the number of remaining heads for each translation direction is

⁷For example, when we finetuned the multilingual model for the De \rightarrow En direction, we only used training and validation data with German in the source and English in the target.

| | DeEn | FrEn | RoEn | EnDe | EnFr | EnRo |
|------|------|------|------|------|------|------|
| Accu | 0.31 | 0.36 | 0.19 | 0.33 | 0.36 | 0.26 |

Table 4: Accuracy of the rare word head.

listed in Table 3.⁸ At $\lambda = 35$, roughly 2/3 of all heads were pruned away and the average BLEU only decreased by 0.28. Table 3 also shows that different language pairs tended to share important heads, as most of the remaining heads remained for all six translation directions.

3.2 Head Function Analysis

We analyzed the behavior of the remaining heads to understand their functions.

Source-to-source Rare-word Heads. We find that one source-to-source (S2S) attention head in the first encoder layer tends to attend to the most infrequent word of the input sentence, which agrees with the bidirectional findings of Voita et al. (2019b). The maximum weight of this head is assigned to one of the least two frequent words in the input sentence roughly 30% of the time, as shown in Table 4 for most language pairs. We also find that this behavior of attending to rare words does not occur in target-to-target (T2T) and target-to-source (T2S) attention, as all T2T and T2S heads achieved less than 10% accuracy at attending to the two least frequent words. The S2S rare word head is marked in red in Figure 1.⁹

Self-attention Positional Heads. We find that some self-attention heads in both the encoder and the decoder tend to attend to neighbors (+1 or -1 position). We call a self-attention head "positional" if its maximum attention weight is assigned to neighbors at least 80% of the time. For example, if the maximum weight of a head is assigned to the -1 relative position more than 80% of the time, then this head is identified as a positional -1 head, as shown in Figure 1. Table 5 shows positional heads found in the finetuned models (R-finetune). We find that different language

| | head | directions |
|----------|------|-------------------------------|
| S2S (-1) | 1:6 | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| | 2:6 | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| | 0:1 | EnDe,EnFr |
| S2S (+1) | 1:7 | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| T2T (-1) | 0:5 | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| | 0:7 | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| | | |

Table 5: Positional heads in the finetuned models (R-finetune). "1:6" denotes the 6th head in the 1st layer.

| | German | French | Romanian | English |
|--------|--------|--------|----------|---------|
| obj | 1 | -2 | -1 | -2 |
| nsubj | 1 | 1 | 2 | 1 |
| advmod | 1 | 1 | 1 | 1 |
| amod | 1 | -1 | -1 | 1 |

Table 6: The highest-probability relative distance for different dependency relationships (forward direction).

pairs generally share the same positional heads, and positional heads only occur in shallow encoder and decoder layers. As shown in Figure 1, positional heads essentially remain unchanged during finetuning. However, during pruning, some positional heads are eliminated and some new positional heads emerge, mostly because positional attention is easy to learn and therefore this function tends to migrate from one head to another during automatic pruning.

Self-attention Syntactical Heads. We find that some self-attention heads in both the encoder and the decoder learn syntactical dependencies, i.e., the maximum attention weight is assigned to a syntactically related word of the current word. We call a self-attention head "syntactical" if it learns a dependency relationship with an accuracy at least 10% higher than the baseline accuracy of this relationship. The baseline accuracy of a dependency relationship is the accuracy of a fictional head that always attends to the most likely relative position of this relationship. For example, for the obj dependency relationship in English, the correct dependency typically is encountered at the -2 relative position (38% of cases), which is the most likely relative position for this relationship. Hence, a fictional head that always attends to the -2 relative position will achieve 38% accuracy for this relationship, and 38% can serve as the baseline accuracy for the English obj relationship. For different languages, the most likely relative position of the obj relationship is different, as shown in Table 6. We look at four important dependency relation-

⁸The base Transformer model contains 144 attention heads in total: 48 self-attention heads in the encoder, 48 selfattention heads and 48 cross-attention heads in the decoder. Cross-attention and self-attention in both the encoder and the decoder have 6 layers and each layer contains 8 heads.

⁹Figure 1 shows functional heads identified for at least one translation direction. For example, all syntactical heads identified for different translation directions as shown in Table 7 and Table 9 are marked as *S* heads in Figure 1. Black heads are heads that were pruned away for all translation directions during automatic pruning.

| \checkmark | 3:6 | amod-f | DeEn,FrEn |
|-------------------------|---|---|---|
| | | amod-b | FrEn,RoEn |
| | | advmod-f | FrEn |
| | | nsubj-f | EnDe |
| × | 3:2 | obj-b | DeEn,RoEn,EnDe,EnFr |
| | | nsubj-f | DeEn |
| \checkmark | 2:0 | obj-b | RoEn,EnDe,EnFr |
| | | nsubj-f | DeEn,EnDe |
| \checkmark | 2:2 | obj-f | RoEn,EnDe,EnFr,EnRo |
| × | 5:5 | obj-b | DeEn,RoEn,EnRo |
| | | nsubj-f | DeEn |
| \checkmark | 4:2 | obj-f | DeEn,RoEn,EnDe |
| × | 2:1 | amod-f | DeEn |
| | | amod-b | RoEn |
| | | | |
| | | obj-b | RoEn |
| × | 4:1 | obj-b nsubj-f | RoEn DeEn,EnDe,EnFr |
| × | 4:1 3:4 | • | |
| $\overline{\checkmark}$ | | nsubj-f | DeEn,EnDe,EnFr |
| × ✓ × | | nsubj-f obj-f | DeEn,EnDe,EnFr RoEn,EnDe |
| \checkmark | 3:4 | nsubj-f obj-f nsubj-b | DeEn,EnDe,EnFr RoEn,EnDe DeEn |
| \checkmark | 3:4 | nsubj-f obj-f nsubj-b obj-f | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn |
| \checkmark | 3:4 | nsubj-f obj-f nsubj-b obj-f advmod-b | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn |
| | 3:4 5:1 5:0 0:0 3:7 | nsubj-f obj-f nsubj-b obj-f advmod-b amod-b nsubj-f nsubj-b | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn FrEn,RoEn |
| | 3:4 5:1 5:0 0:0 | nsubj-f obj-f nsubj-b obj-f advmod-b amod-b nsubj-f | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn FrEn,RoEn FrEn,EnDe |
| | 3:4 5:1 5:0 0:0 3:7 | nsubj-f obj-f nsubj-b obj-f advmod-b amod-b nsubj-f nsubj-b | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn FrEn,RoEn FrEn,EnDe FrEn |
| | 3:4 5:1 5:0 0:0 3:7 2:5 | nsubj-f obj-f nsubj-b obj-f advmod-b amod-b nsubj-f nsubj-f advmod-f | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn FrEn,RoEn FrEn,EnDe FrEn FrEn |
| | 3:4 5:1 5:0 0:0 3:7 2:5 5:3 | nsubj-f obj-f nsubj-b obj-f advmod-b amod-b nsubj-f nsubj-f advmod-f obj-f | DeEn,EnDe,EnFr RoEn,EnDe DeEn RoEn RoEn FrEn,RoEn FrEn,EnDe FrEn FrEn FrEn RoEn |

Table 7: Dependency relationships learned by S2S syntactical heads in the finetuned models. \times means the head is pruned away with automatic pruning at $\lambda = 35$, while \checkmark means the head remains after pruning.

| | DeEn | | | | | |
|-----|---------------------|------|------|------|------|------|
| 2:2 | 0.06 | 0.43 | 0.44 | 0.65 | 0.51 | 0.54 |
| 4:2 | 0.06 0.46 | 0.44 | 0.48 | 0.53 | 0.45 | 0.48 |

Table 8: Accuracy of S2S heads for the obj-f relationship in the finetuned models. Among all S2S heads, head "2:2" achieved the highest obj-f accuracy for EnDe, EnFr, and EnRo; head "4:2" achieved the highest obj-f accuracy for DeEn, FrEn, and RoEn.

ships¹⁰: obj (v \rightarrow o), nsubj (v \rightarrow s), advmod (v \rightarrow a), and amod (n \rightarrow a). For each of these 4 relationships, we consider both the forward and the backward directions. Ultimately, we thus investigate whether a head learns any of the 8 relationships obj-f, obj-b, nsubj-f, nsubj-b, advmod-f, advmod-b, amod-f, and amod-b. We find a head can learn different dependency relationships, as shown in Tables 7 and 9. The most important dependency relationship learned by the Transformer is obj, as more than half of all syntactical heads mainly learn the obj relationship. Tables 7 and 9 further show that some translation directions share some syntactical heads (e.g., DeEn, RoEn, and EnDe share the

| \checkmark | 3:6 | obj-f advmod-f | DeEn,FrEn,RoEn,EnDe,EnRo DeEn,EnDe,EnFr EnDe |
|--|--|--|--|
| | | amod-f amod-b | EnRo EnRo |
| | | nsubj-f | EnDe |
| \checkmark | 2:6 | obj-f nsubj-f advmod-f | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo EnDe EnDe |
| | 3:5 | | |
| v | 5:5 | obj-f nsubj-f | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo EnDe |
| | | advmod-f | EnDe |
| \checkmark | 2:3 | nsubj-b | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| | | amod-f | EnRo |
| | 3:3 | nsubj-b | DeEn,FrEn,RoEn,EnDe,EnFr,EnRo |
| \checkmark | 2:2 | obj-f | DeEn,EnDe,EnRo |
| | | nsubj-f | EnDe |
| | 1.7 | advmod-f | EnDe |
| v | 1:5 | amod-f amod-b | EnFr,EnRo EnRo |
| | | advmod-f | EnFr |
| | | obj-f | EnRo |
| \checkmark | 1:6 | obj-f | DeEn,RoEn,EnDe,EnFr,EnRo |
| × | 1:2 | advmod-f | DeEn,EnDe,EnFr |
| | | nsubj-f | EnDe |
| | | obj-f | EnDe |
| \checkmark | 2:1 | amod-f | EnFr,EnRo |
| | | nsubj-f | EnDe |
| | | advmod-f | EnDe |
| | 2.4 | obj-f | EnDe |
| v | 3:4 | obj-f nsubj-b | DeEn,EnDe,EnRo EnRo |
| × | 5:5 | obj-f | DeEn,FrEn,RoEn,EnDe |
| × | 2:5 | obj-f | EnDe,EnRo |
| | | advmod-b | EnRo |
| | 0:2 | obj-f | EnDe,EnRo |
| ✓ | 4:5 | obj-f | EnDe,EnRo |
| | $\frac{5:0}{4:4}$ | obj-f | DeEn,FrEn |
| × | 4:4 | | EnDo |
| | | obj-f amod-f | EnRo EnRo |
| | 1.0 | amod-f | EnRo |
| \checkmark | 1:0 | amod-f obj-f | EnRo EnRo |
| ✓ | 1:0 | amod-f obj-f amod-b | EnRo |
| ✓ | | amod-f obj-f | EnRo EnRo EnRo |
| | | amod-f obj-f amod-b nsubj-b amod-b nsubj-f | EnRo EnRo DeEn EnRo EnDe |
| | 2:4 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f | EnRo EnRo DeEn EnRo EnDe EnDe |
| | 2:4 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe |
| $ \begin{array}{c} \checkmark \\ \hline \times \\ \hline \checkmark \\ \hline \end{matrix} $ | 2:4 1:3 4:0 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f nsubj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe |
| $ \begin{array}{c} \checkmark \\ \hline \times \\ \hline \checkmark \\ \hline \end{array} $ | 2:4 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe |
| $\begin{array}{c} \checkmark \\ \hline \times \\ \hline \checkmark \\ \hline \end{matrix}$ | 2:4 1:3 4:0 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f nsubj-f obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe EnDe EnDe |
| $\begin{array}{c} \checkmark \\ \hline \times \\ \hline \checkmark \\ \hline \end{matrix}$ | 2:4 1:3 4:0 3:7 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f nsubj-f obj-f amod-b | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe EnRo EnRo EnRo |
| $ \begin{array}{c} \checkmark \\ \hline \times \\ \hline \checkmark \\ \hline \times \\ \end{array} $ | 2:4 1:3 4:0 3:7 4:6 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f obj-f amod-b obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo |
| | 2:4 1:3 4:0 3:7 4:6 4:7 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f obj-f obj-f amod-b obj-f obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo EnRo EnRo |
| | 2:4 1:3 4:0 3:7 4:6 4:7 5:1 4:1 5:3 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo EnRo EnRo EnRo EnRo |
| | 2:4 1:3 4:0 3:7 4:6 4:7 5:1 4:1 5:3 5:6 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f nsubj-b | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo EnRo EnRo EnRo EnRo |
| | 2:4 1:3 4:0 3:7 4:6 4:7 5:1 4:1 5:3 5:6 3:1 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f nsubj-b obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo EnRo EnRo EnRo EnRo |
| | 2:4 1:3 4:0 3:7 4:6 4:7 5:1 4:1 5:3 5:6 3:1 0:1 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f nsubj-b obj-f obj-f | EnRoEnRoEnRoDeEnEnRoEnDeEnDeEnDeEnDeEnRoEnRoEnRoEnRoEnDeEnDeEnRoEnDe |
| | 2:4 1:3 4:0 3:7 4:6 4:7 5:1 4:1 5:3 5:6 3:1 | amod-f obj-f amod-b nsubj-b amod-b nsubj-f advmod-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f obj-f nsubj-b obj-f | EnRo EnRo DeEn EnRo EnDe EnDe EnDe EnDe EnDe EnRo EnRo EnRo EnRo EnRo EnRo EnRo EnRo |

Table 9: Dependency relationships learned by T2T syntactical heads in the finetuned models. \times means the head is pruned away with automatic pruning at $\lambda = 35$, while \checkmark means the head remains after pruning.

¹⁰We used the parsing results by the Stanford parser (Manning et al., 2014) as the ground truth label in our experiments.

| Head | DeEn | FrEn | RoEn | EnDe | EnFr | EnRo |
|---------|------------------------------|------|------|------|------|------|
| 0:7 | 0.88 | 0.81 | 0.86 | 0.85 | 0.77 | 0.72 |
| 1:5 | 0.81 | 0.76 | 0.82 | 0.77 | 0.73 | 0.77 |
| 2:5 | 0.88 | 0.84 | 0.85 | 0.81 | 0.75 | 0.68 |
| 2:7 | 0.88 0.81 0.88 0.81 | 0.73 | 0.84 | 0.77 | 0.80 | 0.87 |

Table 10: Accuracy of C-alignment heads.

S2S "4:2" head for the obj-f relationship in Table 7), but not all translation directions share all syntactical heads. For a more direct overview of how different translation directions share syntactical heads, Table 8 gives the accuracy of different S2S heads for the obj-f relationship, which clearly shows that the "2:2" head mainly learns obj-f for EnDe, EnFr, and EnRo, while the "4:2" head mainly learns obj-f for DeEn, FrEn, and RoEn. Meanwhile, the S2S "2:2" head acquires nearly 0 obj-f accuracy for the DeEn direction, although this head is the most accurate obj-f head for EnDe, EnFr, and EnRo.

Cross-attention C-alignment Heads. We find that some cross-attention heads in the shallow layers learn word alignment for the current target word, i.e., the maximum weight is assigned to the source word aligned to the current target word. If a head achieves more than 80% accuracy for aligning the current target word, we call such a head a "C-alignment" head. When we calculate the alignment accuracy¹¹, we only consider situations when the current target word is a content word¹², as function words generally do not have clear alignments between different languages. By attending to the contextualized representation of the source word aligned to the current target word, C-alignment heads can help to retrieve the full context of the current target word (both the leftside and right-side context), in contrast to targetto-target self-attention, which can only attend to the left-side context of the current target word. Table 10 gives the accuracy of C-alignment heads in the finetuned models (R-finetune), showing that Calignment heads generally learn the current word alignment for all translation directions, while the highest-accuracy C-alignment head for different directions may differ.

| Head | DeEn | FrEn | RoEn | EnDe | EnFr | EnRo |
|------|------|------|------|------|------|------|
| 2:0 | 0.70 | 0.67 | 0.66 | 0.62 | 0.72 | 0.65 |
| 3:0 | 0.72 | 0.72 | 0.69 | 0.65 | 0.68 | 0.56 |
| 3:7 | 0.73 | 0.72 | 0.72 | 0.74 | 0.77 | 0.77 |
| 4:0 | 0.78 | 0.80 | 0.75 | 0.76 | 0.76 | 0.71 |
| 4:2 | 0.78 | 0.81 | 0.78 | 0.79 | 0.77 | 0.78 |
| 4:5 | 0.66 | 0.70 | 0.66 | 0.64 | 0.62 | 0.60 |
| 4:6 | 0.67 | 0.71 | 0.68 | 0.64 | 0.70 | 0.59 |
| 4:7 | 0.82 | 0.83 | 0.81 | 0.81 | 0.75 | 0.75 |
| 5:4 | 0.69 | 0.74 | 0.70 | 0.65 | 0.72 | 0.63 |
| 5:5 | 0.63 | 0.70 | 0.67 | 0.67 | 0.66 | 0.59 |
| 5:6 | 0.66 | 0.71 | 0.66 | 0.68 | 0.61 | 0.65 |

Table 11: Accuracy of N-alignment heads.

Cross-attention N-alignment Heads. We further find that some cross-attention heads in the deep layers learn word alignment for the next target word, i.e., the maximum weight is assigned to the source word aligned to the next target word. As the next word is unknown at the current decoding step, N-alignment heads are rather learning to predict the next target word than just aligning the next target word. Therefore, the N-alignment accuracies are generally lower than the C-alignment accuracies. We identify "N-alignment" heads as heads that achieve more than 70% accuracy for aligning the next word. When we calculate the N-alignment accuracy, we again only consider situations when the next target word is a content word, as before for the C-alignment accuracy. Figure 1 shows that C-alignment heads occur in shallow layers and N-alignment heads occur in deep layers, which indicates that the Transformer decoder appears to first use C-alignment heads to obtain the context of the current target word, and then, based on the context of the current target word, predicts which word to generate next. Table 11 gives the accuracy of N-alignment heads in the finetuned models (R-finetune), which shows that different language pairs generally shared N-alignment heads, which is surprising since the purpose of Nalignment heads is learning word reordering and different language pairs should have different reordering rules. Table 11 also shows that the highestaccuracy N-alignment heads are most likely from the 4th layer, i.e., the N-alignment accuracy first increases and then decreases as the layer number increases.

3.3 Head Behavior Analysis

We provide a further analysis of head behavior by comparing head accuracies in different multilingual and bilingual models. Table 12 gives the highest

¹¹We use human-annotated word alignments (Zhang and van Genabith, 2021) as the ground truth label for computing word alignment accuracies.

¹²For each language, we judge whether a word is a function word or a content word using a list of stopwords from NLTK, https://www.nltk.org/

| - | | | DeEn | | FrEn | | RoEn | | EnDe | | EnFr | | EnRo | |
|-----|-------|------------|------|--------------------|-----------------|-------------|------|--------------------|-------|--------------------|-------|--------------------|-----------------|------------------|
| S2S | obj-f | R-bi | 0.58 | | 0.40^{\times} | | 0.46 | | 0.57 | | 0.55 | | 0.53 | |
| | | R-multi | 0.42 | | 0.43^{\times} | | 0.45 | | 0.60 | | 0.49 | | 0.46^{\times} | |
| | | R-finetune | 0.46 | \triangle | 0.44 × | \triangle | 0.48 | \triangle | 0.65 | \triangle | 0.51 | \triangle | 0.54 | \triangle |
| | obj-b | R-bi | 0.46 | | 0.41 × | | 0.60 | | 0.69 | | 0.51 | | 0.61 | |
| | | R-multi | 0.41 | | 0.37^{\times} | | 0.53 | | 0.57 | | 0.55 | | 0.46 | |
| | | R-finetune | 0.44 | \triangle | 0.38^{\times} | \triangle | 0.57 | \triangle | 0.59 | \triangle | 0.56 | \triangle | 0.50 | \bigtriangleup |
| T2T | obj-f | R-bi | 0.84 | | 0.76 | | 0.69 | | 0.74 | | 0.72 | | 0.53 | |
| | | R-multi | 0.79 | | 0.76 | | 0.68 | | 0.63 | | 0.73 | | 0.52 | |
| | | R-finetune | 0.81 | \triangle | 0.78 | \triangle | 0.70 | \triangle | 0.65 | \triangle | 0.72 | \bigtriangledown | 0.55 | \triangle |
| | obj-b | R-bi | — | | — | | - | | 0.37× | | — | | — | |
| | | R-multi | — | | — | | - | | 0.38× | | - | | - | |
| | | R-finetune | _ | | — | | - | | 0.37× | \bigtriangledown | - | | - | |
| T2S | C-a | R-bi | 0.89 | | 0.88 | | 0.89 | | 0.90 | | 0.82 | | 0.87 | |
| | | R-multi | 0.88 | | 0.83 | | 0.85 | | 0.84 | | 0.79× | | 0.86 | |
| | | R-finetune | 0.88 | | 0.84 | \triangle | 0.86 | \triangle | 0.85 | \triangle | 0.80 | \triangle | 0.87 | \triangle |
| | N-a | R-bi | 0.80 | | 0.83 | | 0.79 | | 0.81 | | 0.79 | | 0.78 | |
| | | R-multi | 0.83 | | 0.83 | | 0.82 | | 0.83 | | 0.79 | | 0.78 | |
| | | R-finetune | 0.82 | \bigtriangledown | 0.83 | | 0.81 | \bigtriangledown | 0.81 | \bigtriangledown | 0.77 | \bigtriangledown | 0.78 | |

Table 12: Highest accuracy for syntactical (obj), C-alignment (C-a), and N-alignment (N-a) heads in different models. $^{\times}$ means the accuracy is not high enough to be identified as function head. \triangle (\bigtriangledown) means finetuning increased (decreased) the head accuracy (i.e., R-finetune > (<) R-multi).

accuracy of different types of function heads in the multilingual and bilingual models. As shown in Table 12, finetuning a multilingual model for a specific translation direction tended to increase accuracies of function heads (e.g., the syntactical obj heads and C-alignment heads) for the given translation direction, which is unsurprising. However, Table 12 indeed shows two interesting head behaviors in multilingual and bilingual models.

Cooperative Behavior of N-alignment Heads.

First, we find the highest N-alignment accuracy tended to decrease instead of increasing during finetuning (the average accuracy of N-alignment heads also decreased). The fact that finetuning decreased N-alignment accuracies is surprising, considering N-alignment heads are crucial for predicting the next target word. We hypothesize that this is because N-alignment heads work in a cooperative way. Since there are multiple different gold translations (reorderings) in the target language for one source sentence, the Transformer uses different heads to learn different options for predicting (aligning) the next target word. Thus, the accuracy of a single N-alignment head is less important. Table 13 gives the accuracy of at least one head from the 4th layer (the most important N-alignment layer) correctly aligning the next target word. The results show that when we consider the whole layer, the next word alignment accuracy is fairly high and the layer accuracy generally increased during finetuning. The fact that the accuracy of any individual

| | | | | EnDe | | |
|-----|------|------|------|---------------------|------|------|
| R-b | 96.8 | 97.2 | 94.7 | 96.7 96.3 | 95.9 | 94.3 |
| R-m | 96.7 | 96.9 | 95.7 | 96.3 | 95.3 | 94.3 |
| R-f | 96.8 | 96.8 | 96.0 | 96.4 | 95.4 | 95.2 |

Table 13: Layer accuracy (4th layer) for N-alignment. R-b: R-bi; R-m: R-multi; R-f: R-finetune.

N-alignment head nevertheless tended to decrease during finetuning while the overall N-alignment layer accuracy tended to increase during finetuning indicates that N-alignment heads work in a cooperative way to collect different options for word reordering.

Multilingual Interference for Head Accuracy. Second, we find that, although finetuning generally improved the accuracies of function heads, the finetuned models (R-finetune) still tended to have lower accuracy than the bilingual baseline models (R-bi), especially the C-alignment accuracy and N-alignment layer accuracy for our high-resource language pairs $De \leftrightarrow En$ and $Fr \leftrightarrow En$, as shown in Tables 12 and 13. This is surprising considering that R-finetune achieved higher translation qualities compared to R-bi, and suggests that language interference tends to cause an accuracy decrease for function heads and can be an important disadvantage of multilingual models compared to bilingual models. Regarding the reason why R-finetune generally had lower head accuracies but higher translation quality compared to R-bi for $De \leftrightarrow En$ and $Fr \leftrightarrow En$ tasks, it could be that the multilingual

pretraining helps the model to learn better representations (word embeddings) for less frequent words via the shared vocabulary.

4 Conclusion

This paper analyzes attention head functions and behaviors in multilingual Transformer translation models. We find that different language pairs, in spite of having different syntax and word orders, tend to share the same heads for the same functions, such as syntax heads and reordering heads. However, the different characteristics of different language pairs clearly cause interference in function heads and affect head accuracies, which can be an important disadvantage of multilingual models compared to bilingual models. Additionally, we reveal an interesting behavior of the Transformer cross-attention: the deep-layer crossattention heads work in a cooperative way to learn different options for word reordering, which can be caused by the nature of translation tasks having multiple different gold translations (reorderings) in the target language for one source sentence.

Limitations

Our study focuses on models trained for particular source to target language pairs. It covers six translation directions with limited typological diversity in the considered languages, due to the need for ground truth word alignments. In future work, multilingual models covering many more languages with more linguistic diversity can be investigated following our methodology.

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