IOT: Instance-wise Layer Reordering for Transformer Structures

Abstract

With sequentially stacked self-attention, (optional) encoder-decoder attention, and feed-forward layers, Transformer achieves big success in natural language processing (NLP), and many variants have been proposed. Currently, almost all these models assume that the *layer order* is fixed and kept the same across data samples. We observe that different data samples actually favor different orders of the layers. Based on this observation, in this work, we break the assumption of the fixed layer order in Transformer and introduce instance-wise layer reordering into model structure, which leads to enlarged model capacity under the constraint of almost same number of parameters, and we name it Instance-wise Ordered Transformer (IOT). To achieve this, we introduce a light predictor with negligible cost to decide the most capable and favorable layer order for any input sequence. Experiments on 3 tasks (neural machine translation, abstractive summarization, and code generation) and 9 datasets demonstrate consistent improvements of our method. We further show that our method can also be applied to other architectures beyond Transformer. Our code is released at Github[1].

1 Introduction

Transformer (Vaswani et al., 2017) has been the dominant architecture in deep learning models (Hassan et al., 2018; Ng et al., 2019; Carion et al., 2020; Radford et al., 2019; Dai et al., 2019; Lee et al., 2019; Devlin et al., 2018; Yang et al., 2019; Cai & Lam, 2019). A Transformer model is stacked by several identical blocks, and each block consists of sequentially ordered layers: the self-attention (*SA*), encoder-decoder attention (*ED*) (decoder only) and feed-forward (*FF*) layer. Recently, various modifications have been proposed, where the focus is on replacing or inserting some components (e.g., attention layer/layer norm/position encoding) in standard Transformer (Wu et al., 2019; Lu et al., 2019; Shaw et al., 2018; So et al., 2019; Ahmed et al., 2017).

Despite these Transformer alternatives have achieved improved performances, one critical element is almost neglected in current models, which is how to arrange the components within a Transformer network, i.e., the *layer order* also matters. As pointed by He et al. (2016b), different orders of ReLU, BN and residual connection significantly affect the performance of ResNet (He et al., 2016a). Towards this direction, we ask: What if we reorder the sequential layers in Transformer (e.g., *SA→FF* or *FF→SA* of encoder, *SA→FF→ED* or *FF→ED→SA* of decoder)? What is the best order for the layers?

We first conduct preliminary experiments. We vary the three layers in decoder with all six variants (each with a unique order of the three layers) and train these models. Results on IWSLT14 German→English translation are reported in Table 1. As we can see, their performances are similar and no one is outstanding. The corpus BLEU variance is only 0.0045, which means that simply reordering the layers and training over the whole corpus impacts little. Press et al. (2019) also reported this for machine translation, but they stopped here.

Order	De→En	Ratio
1:SA→ED→FF	34.64	17.9%
2:FF→SA→ED	34.60	17.9%
3:ED→FF→SA	34.75	16.5%
4:ED→SA→FF	34.67	17.5%
5:SA→FF→ED	34.76	14.1%
6:FF→ED→SA	34.78	16.1%
Variance	0.0045	-

Table 1: Results for different decoder orders on IWSLT14 De→En translation.

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[1] https://github.com/instance-wise-ordered-transformer/IOT

Reference	and just like that , the iceberg shows you a different side of its personality .	BLEU↑	TER↓
Order 1 Trans	and just so , the iceberg shows a different side of its personality .	77.11	18.75
Order 2 Trans	and just like that , the iceberg shows you a different side of its personality .	100.00	0.00
Order 3 Trans	and just so , the iceberg gives you another side of his personality .	0.00	37.50
Order 4 Trans	and just like this , the iceberg gives you another side of its personality .	38.71	25.00
Order 5 Trans	ans so simply , the iceberg shows another side of his personality .	30.33	50.00
Order 6 Trans	and just like this , the iceberg shows you another side of his personality .	36.61	25.00

Table 2: Translations (*Trans*) from all ordered decoders of Transformer for one example sentence.

This seems to be a negative answer. However, we take a further step and ask one more question: Does different data favor different ordered layers? That is, we investigate whether each specific data has its own preference for one particular order. Intuitively, putting various data patterns in one order should not be the best choice. For example, harder samples may favor a particular order while easier ones favor another one. Thus, for each order, we count the ratio of samples that achieve the best score with that order. In Table 1, we find they almost lie on a uniform distribution (e.g., 17.9% samples achieve the best BLEU with order $SA{\rightarrow}ED{\rightarrow}FF$). Besides, we calculate the BLEU variance for each sample, and average all these variances, the result is 114.76, which is much larger than above corpus variance (0.0045). These both mean the data indeed has its own preference to different orders. In Table 2, we present translations from all decoders for on example with BLEU and TER score to give an evidence.

Motivated by above observations, in this work, we present Instance-wise Ordered Transformer (IOT), in which the layer order is determined by the specific data through instance-wise learning. To achieve this, we utilize a light predictor to predict the confidence for each order, given the corresponding classification losses as training signals. However, directly training the predictor with conventional (i.e., NMT) loss tends to quickly converge to a bad order, and ignore explorations on others. Thus, we introduce two auxiliary losses to make an effective training while keeping an unambiguous prediction for each data. As a result, the best order for each data is decided by the predictor during inference.

We evaluate our approach on 3 sequence generation tasks, including neural machine translation (NMT), abstractive summarization (ABS) and code generation (CG). For NMT, we work on 8 IWSLT and 2 WMT tasks, both on low-resource and rich-resource scenarios. Our method can consistently obtain 1.0 BELU score improvements over Transformer. For ABS, IOT also outperforms Transformer and other baselines on Gigaword dataset. For CG tasks, the results on 2 large-scale real-world code datasets (Java and Python) collected from Github surpass the state-of-the-art performances. These all demonstrate the effectiveness of our IOT. Furthermore, we provide detailed studies to verify that the instance-wise learning and order selection make a reasonable and necessary modeling.

The contributions of this work can be summarized as follows:

- We are the first to leverage instance-wise learning for layer order selection in a Transformer model (with shared parameters), and we demonstrate the instance-wise learning is critical.

- We demonstrate our learning approach can be universally applied to other structures beside Transformer (e.g., Dynamic Convolutions), as long as there are multiple different layers.

- Experiments on 3 sequence generation tasks and 9 datasets verify the effectiveness of IOT with consistent performance improvements.

2 RELATED WORK

Architecture Exploration Inventing novel architectures by human designing or automatic searching plays an important role in deep learning. Specific to Transformer structures, various modifications have been proposed. For example, human knowledge powered designs include DynamicConv (Wu et al., 2019), Macaron Network (Lu et al., 2019), Reformer (Kitaev et al., 2020) and others (Fonollosa et al., 2019; Ahmed et al., 2017; Shaw et al., 2018). As for automatic searching, neural architecture search can discover networks with state-of-the-art performances but always with complicated computation, i.e., Evolved Transformer (So et al., 2019). The underlying principle is to add or replace some components of Transformer. For instance, Wu et al. (2019) replace self-attention with dynamic convolution, So et al. (2019) add a separate convolution layer in a new branch. Different from them, we, instead, only focus on the order of layers to enlarge model capacity without a heavy modification. Besides, our approach is structure agnostic, which can be universally applied to other structures, only if multiple different layers exist.

Figure 1: The IOT framework. *Pred* means the light predictor introduced in 3.1 for order selection. We show two ordered encoders/decoders here. After taking X_1, X_2, X_3, the selected order for Y_2, Y_3 is the lower encoder and upper decoder, while for Y_1 is the upper encoder and lower decoder.

Instance-wise Learning Deep learning models are trained over large-scale datasets, and data samples are often treated equally without modeling the difference between them. Some works attempt to weight each data with different importance (Ren et al., 2018; Hu et al., 2019; Chang et al., 2017) or feed data with curriculum learning according to its difficulty (Bengio et al., 2009; Fan et al., 2018). However, they often explicitly manipulate the data during training only, while no distinction exists in inference, and under one fixed model. Elbayad et al. (2020) take a step further and propose the depth-adaptive Transformer, which can forecast different depths (layers) of the network by predicting the required computation for a particular data. Similarly, Liu et al. (2020) propose a sample-wise adaptive mechanism to dynamically calculate the number of required layers so that samples with varying complexity perform efficient inference. They both aim at reducing the computation cost and speed up the inference. Instead, we pay attention to explore the model capacity and perform instance-wise order selection in order to boost the Transformer performance.

The most related work is Press et al. (2019), which manually generates randomly ordered Transformer encoders and finds the *Sandwich Transformer* can slightly reduce the perplexity of language modeling. However, they find that Sandwich Transformer pattern has no effect on NMT task. Besides, it still performs over the whole corpus without considering each specific data. We, instead, investigate on various sequence-to-sequence generation tasks and greatly improve the task performances through instance-wise learning, so as to discover the optimal ordered Transformer for each particular data.

3 INSTANCE-WISE ORDERED TRANSFORMER

The overall framework of IOT is presented in Figure 1. In comparison with the standard Transformer, IOT only incorporates light-weighted predictors and reorders the encoder/decoder with weight tying, under the constraint of almost same number of parameters and exempt from heavy modifications. In this section, we introduce the details of IOT, including training, inference and discussions.

Notations Sequence-to-sequence learning aims to map one sequence $x = [x_1, x_2, ..., x_{T_x}]$ into another sequence $y = [y_1, y_2, ..., y_{T_y}]$, where x_i, y_j denotes the i-th and j-th token of x and y, T_x and T_y are the corresponding lengths. Given one sentence pair (x, y) and a learning model $\mathcal{M}$, we can define the training objective as minimizing the cross-entropy loss $\mathcal{L}_{\mathcal{M}} = -\sum_{j=1}^{T_y} \log P(y_j|y_{<j}, x)$. Besides, $D_{KL}(\mathbb{P}\|\mathbb{Q})$ denotes the Kullback-Leibler (KL) divergence between distributions $\mathbb{P}$ and $\mathbb{Q}$.

3.1 INSTANCE-WISE ENCODER/DECODER

IOT intends to break the fixed order of layers in Transformer. As shown in introduction, simply reordering the layers w.r.t the whole corpus impacts little, while each data has its own preference to orders. Therefore, IOT incorporates instance-wise learning to adjust the favorable order for each data.

As shown in Figure 1, both encoder and decoder in IOT consist of several blocks of SA, ED, FF layer with dynamic order, and we assume there are M (e.g., $M = 2$) ordered encoders and N (e.g., $N = 6$) ordered decoders (with shared weights). Inspired by the fact that lower training loss implies the higher proficiency confidence for candidate orders, we utilize the cross-entropy loss as signals to learn the confidence. That is, we calculate confidence γ_m and λ_n for each encoder enc_m, decoder dec_n (resulted model $\mathcal{M}^{m,n}$), and use them to weight the training loss $\mathcal{L}_{\mathcal{M}}^{m,n}$. To calculate the confidence, we add a simple predictor to help distinguish the orders, with only negligible time cost.

Training Given one source sequence $x = [x_1, x_2, ..., x_{T_x}]$, we first map each token into word embedding $e = [e_1, e_2, ..., e_{T_x}]$, where $e_i \in \mathbb{R}^d$, and then apply one light encoder predictor π_{enc} to predict the confidence of encoder orders using sentence embedding $s_e = \frac{1}{T_x} \sum_{i=1}^{T_x} e_i$. Concretely, π_{enc} takes s_e as input and predicts γ_m for enc_m by Gumbel-softmax (Jang et al., 2016):

$$\gamma_m = \frac{\exp\left(\left(\log\left(\pi_{\text{enc}_m}\right) + g_m\right)/\tau_e\right)}{\sum_{k=1}^{M} \exp\left(\left(\log\left(\pi_{\text{enc}_k}\right) + g_k\right)/\tau_e\right)}, \quad \pi_{\text{enc}} = \text{softmax}\left(s_e W_e\right), \tag{1}$$

where g_m is sampled from Gumbel distribution: $g_m = -\log(-\log U_m), U_m \sim \text{Uniform}(0, 1)$, $W_e \in \mathbb{R}^{d \times M}$ is the weight matrix, τ_e is a constant temperature to control the distribution to be identical approximation with categorical distribution. Simultaneously, the token embeddings e will feed to the encoders to get hidden states $h = [h_1, h_2, ..., h_{T_x}]$, then we can calculate decoder order confidence λ_n by one predictor π_{dec} in the same way as π_{enc}:

$$\lambda_n = \frac{\exp\left(\left(\log\left(\pi_{\text{dec}_n}\right) + g_n\right)/\tau_d\right)}{\sum_{k=1}^{N} \exp\left(\left(\log\left(\pi_{\text{dec}_k}\right) + g_k\right)/\tau_d\right)}, \quad \pi_{\text{dec}} = \text{softmax}\left(s_d W_d\right), \tag{2}$$

where $s_d = \frac{1}{T_x} \sum_{i=1}^{T_x} h_i$ and W_d is the weight matrix. For each ordered path through enc_m and dec_n, we can obtain the training loss $\mathcal{L_M}^{m,n}$, and the final cross-entropy loss is weighted by confidence γ_m and λ_n with $\mathcal{L_M}^{m,n}$, formulately as:

$$\mathcal{L_C} = \sum_{m=1}^{M} \sum_{n=1}^{N} (\gamma_m \cdot \lambda_n)\mathcal{L_M}^{m,n}. \tag{3}$$

Inference During inference, we directly replace the Gumbel-softmax used in training with argmax, in order to choose the most capable encoder and decoder for each sequence x:

$$\text{enc} = \text{argmax}\left(s_e W_e\right), \quad \text{dec} = \text{argmax}\left(s_d W_d\right). \tag{4}$$

Discussion The decoding process is almost the same as standard Transformer, with only little overhead for order predictions. One may concern the training cost is increased through our training. As we present in Appendix B.1, the cost is actually acceptable with a fast convergence. Currently, we reorder the layers of the encoder/decoder block and stack the same ordered block L times (see Figure 1). A complex extension is to reorder all L blocks of encoder/decoder and we take it as future work.

3.2 Auxiliary Losses

As we can see, the predictors are trained in an unsupervised way, and we observe they lean to be lazy so that all samples quickly converge to one same order during training, without a senseful learning. Thus, to make an effective training and inference, we introduce two auxiliary losses in our framework.

(1) First, we explore the diverse capability of all orders with help of a loss $\mathcal{L_D}$ to encourage all orders to participate in training. The spirit is the same as to encourage exploration in reinforcement learning. The expected softmax probability $\mathbb{E}_x\left[\pi_x\right]$ (encoder/decoder) from the predictor should approximate the uniform distribution $\mathbb{Q} = [\frac{1}{N}, \frac{1}{N}, \ldots, \frac{1}{N}]$ (e.g., decoder orders), and we achieve this by minimizing KL-divergence between the statistical average $\mathbb{E}_x\left[\pi_x\right]$ and $\mathbb{Q}$:

$$\mathcal{L_D} = D_{KL}(\mathbb{Q}\|\mathbb{E}_x\left[\pi_x\right]) = -\frac{1}{N} \sum_{n=1}^{N} \log(\mathbb{E}_x\left[(\pi_x)_n\right]) - \log N, \tag{5}$$

where $(\pi_x)_n$ is the probability of n-th decoder order for data x. For encoder order, it is $(\pi_x)_m$ processed in a same way as decoder.

(2) Different from $\mathcal{L_D}$ to keep all orders effectively trained, during inference, the output distribution π_x for each data should be able to make an unambiguous argmax selection. We then introduce another loss $\mathcal{L_S}$ to constrain each π_x to be far away from the uniform distribution $\mathbb{Q}$. Concretely, we maximize the KL-divergence between each probability π_x and $\mathbb{Q}$:

$$\mathcal{L_S} = -\mathbb{E}_x\left[D_{KL}(\mathbb{Q}\|\pi_x)\right] = -\mathbb{E}_x\left[-\frac{1}{N} \sum_{n=1}^{N} \log(\pi_x)_n - \log N\right]. \tag{6}$$

Note that we clamp the value of probability π_x since the KL value is theoretically unbounded. With above auxiliary losses, the final training objective is to minimize:

$$\mathcal{L} = \mathcal{L}_{\mathcal{C}} + c_1 \mathcal{L}_{\mathcal{D}} + c_2 \mathcal{L}_{\mathcal{S}}, \tag{7}$$

where c_1 and c_2 are coefficients to make a trade-off between $\mathcal{L}_{\mathcal{D}}$ and $\mathcal{L}_{\mathcal{S}}$. In this way, we can achieve effective training, while keeping the ability to distinguish the favorable order for each data.

Discussion $\mathcal{L}_{\mathcal{D}}$ and $\mathcal{L}_{\mathcal{S}}$ aim to keep effective training and unambiguous inference. There are several alternatives. The first is to simply decay the temperature τ in Equation (1) and (2), and remove the auxiliary losses. However, we do not notice obvious gain. Second is to linearly decay c_1 only and remove $\mathcal{L}_{\mathcal{S}}$, which is able to fully train all orders at the beginning and loose this constraint gradually. We find this is also beneficial, but our two losses method performs better.

4 Experiments

We conduct experiments on 3 sequence generation tasks: neural machine translation (both low-resource and rich-resource), code generation and abstractive summarization. The main settings of each experiment are introduced here, and more details can be found in Appendix A.

4.1 Dataset

Neural Machine Translation For the low-resource scenario, we conduct experiments on IWSLT14 English↔German (En↔De), English↔Spanish (En↔Es), IWSLT17 English↔French (En↔Fr), English↔Chinese (En↔Zh) translations. The training data includes $160k$, $183k$, $236k$, $235k$ sentence pairs for each language pair respectively. For the rich-resource scenario, we work on WMT14 En→De and WMT16 Romanian→English (Ro→En) translations. For WMT14 En→De, we filter out $4.5M$ sentence pairs for training and concatenate newstest2012 and newstest2013 as dev set, newstest2014 as test set. For WMT16 Ro→En, we concatenate the $0.6M$ bilingual pairs and $2.0M$ back translated data[2] for training, newsdev2016/newstest2016 serve as dev/test set.

Code Generation Code generation aims to map natural language sentences to programming language code. We work on one Java (Hu et al., 2018) and one Python dataset (Wan et al., 2018), following Wei et al. (2019) to process the two datasets. The Java dataset is collected from Java projects on Github, and the Python dataset is collected by Barone & Sennrich (2017). We split each dataset with ratio $0.8 : 0.1 : 0.1$ as training, dev and test set.

Abstractive Summarization Abstractive summarization is to summarize one long sentence into a short one. The dataset we utilized is a widely acknowledged one: Gigaword summarization, which is constructed from a subset of Gigaword corpus (Graff et al., 2003) and first used by Rush et al. (2017). The training data consists of $3.8M$ article-headline pairs, while the dev and test set consist of $190k$ and $2k$ pairs respectively.

4.2 Model and Optimization

For IWSLT translation tasks, we use `transformer_iwslt_de_en` setting as model configuration. The number of block, embedding size and feed-forward network (FFN) size are 6, 512, 1024. WMT tasks use `transformer_vaswani_wmt_en_de_big` configuration, with 6 blocks, embedding size 1024 and FFN size 4096. Optimization and learning scheduler are the default settings in Vaswani et al. (2017). For code generation, block number/embedding size/FFN size are 3, 256, 1024 respectively. Others are the same as NMT. For summarization, we take `transformer_wmt_en_de`, with 6 blocks, embedding size 512 and FFN size 2048. Dropout (Srivastava et al., 2014) is set to be 0.3. Other settings are also the same as NMT task. Implementation is developed on Fairseq (Ott et al., 2019). We first grid search c_1, c_2 on IWSLT14 De→En dev set, and then apply them on other tasks. The best setting is $c_1 = 0.1$, $c_2 = 0.01$, and the importance study of c_1, c_2 is shown in Appendix B.2.

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[2]http://data.statmt.org/rsennrich/wmt16_backtranslations/ro-en/.

Table 3: Preliminary results of varied orders on IWSLT14 De→En task.

(a) Results of encoder, decoder orders, and combinations on IWSLT14 De→En translation.

	De→En
Transformer	34.64
Encoder ($M = 2, N = 1$)	35.18
Decoder ($M = 1, N = 6$)	35.60
Encoder×Decoder ($M = 2, N = 6$)	35.24
Encoder×Decoder ($M = 2, N = 4$)	35.30
Encoder×Decoder ($M = 2, N = 2$)	35.25

(b) Results of varied decoder orders on IWSLT14 De→En translation.

	De→En
Transformer	34.64
IOT ($M = 1, N = 6$)	35.60
IOT ($M = 1, N = 5$)	35.65
IOT ($M = 1, N = 4$)	35.62
IOT ($M = 1, N = 3$)	35.58
IOT ($M = 1, N = 2$)	35.32

Table 4: BLEU scores of IOT on eight IWSLT low-resource translation tasks.

	En→De	De→En	En→Fr	Fr→En	En →Zh	Zh→En	En→Es	Es→En
Transformer	28.57	34.64	35.9	36.1	26.3	18.4	39.0	40.6
IOT	29.52	35.62	37.2	37.8	27.2	19.3	40.1	41.7

Table 5: Results on IWSLT14 De→En translation task (a), Java and Python code generation tasks (b).

(a) Results on IWSLT14 De→En translation.

Method	BLEU
Transformer	34.64
IOT	**35.62**
Adversarial MLE (Wang et al., 2019a)	35.18
DynamicConv (Wu et al., 2019)	35.20
Macaron Network (Lu et al., 2019)	35.40
MADL (Wang et al., 2019c)	35.56

(b) Results on Java and Python code generations.

Method	Java		Python	
	BLEU	PoV	BLEU	PoV
Transformer	24.58	74.44%	13.20	61.89%
IOT	**25.51**	**77.30**%	**14.05**	**63.14**%
Wei et al. (2019)	17.17	27.4%	12.09	51.9%

4.3 EVALUATION

We use `multi-bleu.perl` to evaluate IWSLT14 En↔De and all WMT tasks for a fair comparison with previous works. For other NMT tasks, we use `sacre-bleu` for evaluation. During inference, we follow Vaswani et al. (2017) to use beam size 4 and length penalty 0.6 for WMT14 En→De, beam size 5 and penalty 1.0 for other tasks. For code generation, the evaluation is based on two metrics, the sentence BLEU computes the n-gram precision of a candidate sequence to the reference, and the percentage of valid code (PoV) that can be parsed into an abstract syntax tree (AST). As for summarization, the generated summarization is evaluated by ROUGE-1/2/L F1 score (Lin, 2004).

4.4 MAIN RESULTS

Encoder/Decoder Orders Encoder block only contains SA and FF layers, the resulted max number of encoder layer orders M is 2, while for decoder, the max order variants N is 6. Therefore, we first evaluate the utilization of encoder orders, decoders orders, and both orders on IWSLT14 De→En translation, in order to see the impacts of different number of order candidates and their combinations. In Table 3 (a), we can see that 2 ordered encoders improve the result, and 6 ordered decoders achieve more gain. This meets our expectation, since the search space is limited when there are only 2 ordered encoders. However, if we train both encoder and decoder orders (e.g., $M = 2, N = 6$), the results (e.g., 35.30) can not surpass the 6 decoders only (35.60). We suspect the search space is too large so that training becomes hard, and decoder orders play a more important role than encoder orders for sequence generation. Therefore, we turn to investigate different decoder order candidates (refer to Appendix A.3 for detailed combinations) in Table 3 (b). Results show that $N = 4, 5, 6$ achieve similar strong performances (results on other tasks/datasets are in Appendix A.4). Thus, considering the efficiency and improvements, we utilize $N = 4$ ordered decoders (order 1, 2, 4, 6 in Table 1) to reduce training cost in later experiments.

NMT Results BLEU scores on 8 IWSLT low-resource tasks are shown in Table 4. As we can see, IOT achieves more than 1.0 BLEU points improvement on all tasks (e.g., 1.7 on Fr→En). The consistent gains on various language pairs well demonstrate the generalization and effectiveness of our method. We then present comparison with other works on IWSLT14 De→En task in Table 5 (a), and IOT is also better than several human designed networks. The results of WMT14 En→De and WMT16 Ro→En are reported in Table 6. We also compare with existing works, such as the unsupervised Ro→En based on pre-trained cross-lingual language model (Lample & Conneau, 2019). Similarly, our method outperforms them and shows our framework can work well on rich-resource scenario.

Code Generation Results The results are shown in Table 5(b). It is observable that Transformer can obtain better results than the LSTM-based work (Wei et al., 2019). Compared with Transformer, IOT can further improve the quality of generated code. Specifically, IOT boosts Transformer with 0.93 BLEU/2.86% PoV gain on Java generation and 0.75 BLEU/1.25% PoV gain on Python respectively. Again, these results well demonstrate the effectiveness of our method.

Abstractive Summarization Results The IOT performances on summarization task are shown in Table 7. From the results, we can see IOT achieves a good performance on Gigaword summarization and obtains 0.8, 0.7 and 1.0 scores gain of ROUGE-1, ROUGE-2 and ROUGE-L metrics over standard Transformer. IOT also surpasses other works such as reinforcement learning based method (Wang et al., 2018), which again verifies our approach is simple yet effective.

Method	En→De
Transformer⋆	29.12
IOT	**30.03**
Shaw et al. (2018)	29.20
Ott et al. (2018)	29.30
Wu et al. (2019)	29.70
So et al. (2019)	29.80

Method	Ro→En
Transformer⋆	37.73
IOT	**38.83**
Sennrich et al. (2016)	33.90
Lample & Conneau (2019)	38.50

Table 6: WMT14 En→De and WMT16 Ro→En translation results. ⋆stands for our reproduced result.

Method	ROUGE-1	**ROUGE-2**	ROUGE-L
Transformer (Vaswani et al., 2017)	35.59	17.74	32.98
IOT	36.37	**18.46**	33.89
RNNSearch+MRT (Ayana et al., 2016)	36.54	16.59	33.44
Concept pointer+DS (Wang et al., 2019b)	37.01	17.10	34.87
RNNSearch+select+MTL+ERAML (Li et al., 2018)	35.33	17.27	33.19
CGU (Lin et al., 2018)	36.30	18.00	33.80
Reinforced-Topic-ConvS2S (Wang et al., 2018)	36.92	18.29	34.58

Table 7: ROUGE-1/2/L F1 scores for Gigaword summarization.

5 STUDY AND ANALYSIS

5.1 CASE VERIFICATION

We perform a study with $N = 3$ to verify that IOT has made a necessary instance-wise order selection. We first split IWSLT14 En↔De dev set into 3 subsets according to the prediction of π_{dec}, and then we decode each subset use all 3 ordered decoders, and report the BLEU results. As shown in Figure 2, each subset indeed achieves the best score on the corresponding predicted order (outperforms other orders by 0.2-0.4 BLEU). We also do the same study on the test set, and the predicted order outperforms others by 0.7-0.8 BLEU. These well prove that IOT makes a reasonable prediction.

Besides, we find that the predicted orders correlate to different sentence difficulties. In our case, the set 1 sentences belong to decoder 1 achieve highest BLEU than other sets, which means set 1 is relatively simple to translate, and vice versa for samples in set 2. These imply that different difficulty sentences have different structure preferences. We provide statistics and examples in Appendix B.3.

5.2 APPLY ON ANOTHER STRUCTURE (DYNAMICCONV)

As we discussed, our instance-wise layer reordering is structure agnostic. In this subsection, we evaluate this by applying our approach on DynamicConv network (Wu et al., 2019) beyond standard

(a) BLEU scores on IWSLT14 En→De.   (b) BLEU scores on IWSLT14 De→En.

Figure 2: BLEU scores of three subsets (divided by predicted decoder) on all decoders.

Transformer, which replaces the self-attention with dynamic convolution. We train layer ordered DynamicConv on $N = 2, 3, 4$ decoders and test the performances. The BLEU score of standard DynamicConv is 35.20, and with our instance-wise order learning, we achieve $35.60, 35.82, 35.87$ for $N = 2, 3, 4$ ordered decoders respectively (near 0.7 point gain). Therefore, this study verifies our claim that our approach can be applied to other structures, as long as multiple different layers exist.

5.3   DISCUSSIONS

Ensemble Since our framework involves multiple orders (with shared parameters), which is also done in ensemble framework, we make a comparison with ensemble. The ensemble method trains multiple models with different parameters separately in an independent way. While our work trains orders in a joint way with an intention to make them more diverse. More importantly, from the view of time and memory cost, the ensemble framework increases N times which is totally different from ours. In this sense, our method can be combined with ensemble to further boost performance. The competitive results on test set are shown in Table 8. We can clearly conclude that IOT and ensemble are complementary and beneficial to each other.

Ensemble Models	En→De	De→En
1-model (standard)	28.57	34.67
2-model (standard)	29.71	35.92
3-model (standard)	30.08	36.40
4-model (standard)	30.18	36.54
1-model (IOT)	29.52	35.62
2-model (IOT)	30.38	36.80
3-model (IOT)	30.93	37.25
4-model (IOT)	31.02	37.38

Table 8: Ensemble performances of standard Transformer and IOT.

Regularization IOT consists of different ordered blocks in a weight tying method, which may looks like a parameter regularization to some extent. However, we show that IOT is more than regularization and can be complementary with other regularization methods. We first train a Transformer model on IWSLT14 De→En task with all ordered decoders, but without instance-wise learning, and test the performance with each order. We find the BLEU scores on test set are near 34.80 for each order, much worse than IOT, which means that simply regularizing the shared parameters for different orders is not the main contribution to performance improvement, and verifies our instance-wise learning is critical. Another experiment is that we train Transformer with LayerDrop (Fan et al., 2019), a dropout technique to regularize the layer parameters. The test BLEU is 35.40, which achieves about 0.8 score improvement over Transformer. After applying IOT with LayerDrop, we obtain further gains than IOT only (35.62) to reach a BLEU score 36.13. Therefore, this demonstrates IOT is not only regularization and can be smoothly integrated with other regularization methods.

6   CONCLUSION

In this work, we propose Instance-wise Ordered Transformer, which leverages instance-wise learning to reorder the layers in Transformer for each data. Compared with standard Transformer, IOT only introduces slightly increased time cost. Experiments on 3 sequence generation tasks and 9 datasets demonstrate the effectiveness of IOT. We also verify that our approach can be universally applied to other structures, such as DynamicConv. In future, we plan to work on more complicated reordering in each block, as well as other tasks such as multi-lingual translation and text classification.

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A EXPERIMENTAL SETTINGS AND MORE RESULTS

A.1 DETAILED DATA SETTINGS

Neural Machine Translation Following the common practice (Ott et al., 2019), we lowercase all words for IWSLT14 En↔De. For IWSLT14 En↔De, En↔Es, IWSLT17 En↔Fr, we use a joint source and target vocabulary with $10k$ byte-pair-encoding (BPE) (Sennrich et al., 2015) operations, and for IWSLT17 En↔Zh, we use a seperate source and target vocabulary. For all WMT tasks, sentences are encoded by a joint source and target vocabulary of $32k$ tokens.

Code Generation In the Java dataset, the numbers of training, validation and test sequences are $69, 708$, $8, 714$ and $8, 714$ respectively, and the corresponding numbers for Python are $55, 538$, $18, 505$ and $18, 502$. All samples are tokenized. We use the downloaded Java dataset without further processing, and use Python standard AST module to further process the python code. The source and target vocabulary sizes in natural language to Java code generation are $27k$ and $50k$, and those for natural language to Python code generation are 18k and $50k$. In this case, following Wei et al. (2019), we do not apply subword tokenization like BPE to the sequences.

Abstractive Summarization The Gigaword corpus represents for a headline generation task, each source article contains about 31.4 tokens on average, while the target headline contains near 8.3 tokens per sentence. The training data consists of $3.8M$ article-headline pairs, while the validation and test set consist of $190k$ and $2k$ pairs respectively. We preprocess the dataset in a same way as NMT task. The words in the source article and target headline are concatenated to make a joint BPE vocabulary. After preprocessing, there are $29k$ subword tokens in the vocabulary.

A.2 DETAILED MODEL/TRAINING CONFIGURATIONS

Model Configuration The detailed model configurations are as follows:

- `transformer_iwslt_de_en` setting: 6 blocks in encoder and decoder, embedding size 512, feed-forward size 1024, attention heads 4, dropout value 0.3, weight decay 0.0001.

- `transformer_vaswani_wmt_en_de_big` setting: 6 blocks in encoder and decoder, embedding size 1024, feed-forward size 4096, attention heads 16, dropout value 0.3, attention dropout 0.1, relu dropout 0.1.

- `transformer_wmt_en_de_big` setting: 6 blocks in encoder and decoder, embedding size 0124, feed-forward size 4096, attention heads 16, dropout value 0.3.

Optimization We adopt the default optimization setting in Vaswani et al. (2017). Adam (Kingma & Ba, 2014) optimizer with $\beta_1 = 0.9, \beta_2 = 0.98$ and $\epsilon = 10^{-9}$. The learning rate scheduler is `inverse_sqrt` with warmup steps $4, 000$, default learning rate is 0.0005. Label smoothing (Szegedy et al., 2016) is used with value 0.1. As introduced, to learn the predictors, we clamp the `softmax` output with value 0.05.

A.3 RESULTS OF ORDER COMBINATIONS

We show in the paper that different number of orders (e.g., $N = 4$ or $N = 5$) have varied performances. Therefore, one necessary point is about the different combinations of these N decoders. Here, we work on $N = 5$ IOT model to show the results of different order candidates.

We first present each ordered decoder in Table 9 again (same as in Table 1). For the $N = 5$ ordered decoders with IOT model, we show the performances with 5 combined orders selected from all six variants on dev set of IWSLT14 De→En and En→De translations. The results are reported in Table 10. We can see the different combinations achieve similar strong performances, which shows that our

Code	1	2	3	4	5	6
Order	SA→ED→FF	FF→SA→ED	ED→FF→SA	ED→SA→FF	SA→FF→ED	FF→ED→SA

Table 9: Each numbered code for one specific ordered decoder.

IOT ($N = 5$)	12345	12346	12356	12456	13456	23456
En→De	30.64	30.65	30.53	30.58	30.70	30.67
De→En	36.71	36.67	36.72	36.79	36.74	36.75

Table 10: BLEU scores for IWSTL14 De→En and En→De translations on dev set. '12345' represents the combinations of order $1, 2, 3, 4, 5$ decoders.

approach is robust towards different order combinations. This also demonstrate that the importance of IOT is the diversity among order candidates that can help each data distinguish them. For other N ordered decoders, the patterns are similar. Therefore, here we only report the N combinations used for IOT experiments in the paper as follows: IOT ($N = 2$) is combined by order $4, 6$ (*ED→SA→FF* and *FF→ED→SA*), and IOT ($N = 3$) is order $1, 4, 6$, IOT ($N = 4$) is order $1, 2, 4, 6$, and IOT ($N = 5$) is order $1, 2, 4, 5, 6$.

A.4 RESULTS OF DIFFERENT NUMBER OF DECODERS

The results of $N = 4$ ordered decoders (order $1, 2, 4, 6$) are mainly reported in the paper. Here, we also show results of other N decoders for all tasks, along with the Transformer baseline.

The results of different N decoders for WMT14 En→De and WMT16 Ro→En translations, code generation task, and Gigaword summarization are reported in Table 12, Table 13 and Table 14 respectively. As we can see, more ordered decoders can bring better performance, which supports the effectiveness of our framework and demonstrates the data has its own favor towards different orders. Considering the efficiency, we do not perform experiments with more than 4 decoders for these tasks.

Model	En→De	De→En	En→Fr	Fr→En	En →Zh	Zh→En	En→Es	Es→En
Transformer	28.57	34.64	35.9	36.1	26.3	18.4	39.0	40.6
IOT ($N = 6$)	29.48	35.60	37.4	37.7	27.1	19.2	40.2	41.5
IOT ($N = 5$)	29.51	35.65	37.2	37.6	27.2	19.2	40.2	41.9
IOT ($N = 4$)	29.52	35.62	37.2	37.8	27.2	19.3	40.1	41.7
IOT ($N = 3$)	29.43	35.58	37.0	37.6	27.0	19.1	39.7	41.5
IOT ($N = 2$)	29.18	35.32	36.6	37.1	26.8	18.9	39.6	41.0

Table 11: BLEU scores on 8 IWSLT tasks with different N ordered decoders (with shared weights).

Model	WMT14 En→De	WMT16 Ro→En
Transformer	29.12	37.73
IOT ($N = 2$)	29.71	38.57
IOT ($N = 3$)	29.89	38.79
IOT ($N = 4$)	30.05	38.83

Table 12: BLEU scores for WMT14 En→De and WMT16 Ro→En translation tasks of different N ordered decoders in IOT.

B MORE STUDIES

B.1 INFERENCE/TRAINING COST

As stated in the paper, our approach only increases negligible time cost and parameters. Here we compare the inference time and model size of our framework to the standard Transformer. The detailed parameter numbers and inference time on IWSLT14 En↔De test set are shown in Table 15. Since we only add one linear layer and softmax layer as the predictor, the number of extra parameters is $M \times hidden\_size$ (encoder predictor) or $N \times hidden\_size$ (decoder predictor), which is negligible compared to other model parameters. Therefore, IOT achieves enlarged model capacity

	Java		Python	
Method	BLEU	PoV	BLEU	PoV
Transformer	24.58	74.44%	13.20	61.89%
IOT ($N = 2$)	25.44	77.88%	13.97	62.22%
IOT ($N = 3$)	25.51	75.83%	14.00	62.04%
IOT ($N = 4$)	25.51	77.30%	14.05	63.14%

Table 13: BLEU and PoV scores for Java and Pyton code generation results of different N ordered decoders in IOT.

Model	ROUGE-1	ROUGE-2	ROUGE-L
Transformer	35.59	17.87	32.98
IOT ($N = 2$)	36.14	18.37	33.61
IOT ($N = 3$)	36.15	18.48	33.81
IOT ($N = 4$)	36.37	18.46	33.89

Table 14: ROUGE F1 scores for Gigaword abstractive summarization results of different N ordered decoders in IOT.

	En$\rightarrow$De		De$\rightarrow$En	
	Inference time (s)	#parameters	Inference time (s)	#parameters
Transformer	1487.19	36741120	1432.03	36741120
IOT ($N = 2$)	1496.70	36742144	1429.26	36742144
IOT ($N = 3$)	1470.40	36742656	1480.83	36742656
IOT ($N = 4$)	1505.83	36743168	1444.74	36743168
IOT ($N = 5$)	1491.40	36743680	1424.10	36743680
IOT ($N = 6$)	1479.20	36744192	1464.00	36744192

Table 15: Inference time and model parameters counted for Transformer and our framework on IWSLT14 En$\leftrightarrow$De. The study is performed on Tesla P100 GPU card.

and performance, but under the constraint of almost the same number of parameters. As for the inference time, the only difference is from the one-pass order prediction and the cost is low compared with the heavy autoregressive generation process, which can be seen from Table 15.

As one may concern about the training cost since IOT trains multiple orders in one model, we provide several statistics here. Jointly optimizing different orders indeed introduces the training cost, for example, one epoch costs $189s$, $302s$ and $417s$ for $N = 1$, $N = 2$ and $N = 3$ orders respectively on IWSLT14 De$\leftrightarrow$En dataset. However, with the shared parameters between these orders, the model convergence also becomes faster, which converges at about 80+, 40+ and 30+ epochs for $N = 1$, $N = 2$ and $N = 3$ orders. Therefore, the training cost is actually acceptable with a fast convergence, without much increase.

B.2 IMPACT OF WEIGHTED AUXILIARY LOSSES

We conduct another study on IWSLT14 De$\rightarrow$En dev set to investigate the impact of our proposed auxiliary losses controlled by weight c_1 and c_2. The values of c_1 and c_2 are varied between $[0.0, 0.05, 0.1, 0.5]$ and $[0.0, 0.005, 0.01, 0.05]$ respectively, and the results are presented in Table 16. It can be seen that the best configuration is $c_1 = 0.1$ and $c_2 = 0.01$. Therefore, we report the leading results in the paper with $c_1 = 0.1, c_2 = 0.01$. The results also clearly demonstrate that the two additional losses are necessary to make our framework effective.

c_1/c_2		0.0	0.005	0.01	0.05
IOT ($N = 2$)	**0.0**	35.97	36.36	36.46	36.42
	0.05	36.35	–	36.58	–
	0.1	36.31	36.56	**36.60**	36.54
	0.5	36.39	–	36.40	–
IOT ($N = 3$)	**0.0**	36.16	36.44	36.66	36.51
	0.05	36.47	–	36.47	–
	0.1	36.35	36.48	**36.79**	36.57
	0.5	36.44	–	36.62	–

Table 16: BLEU scores for IWSLT14 De→En dev set. The performances are varied by different weighted auxiliary losses controlled by c_1 and c_2 value.

Set	S_i	T_i	D_i	F_i	$BLEU_{Avg}$
$i = 1$	$2,404$	$56,036$	$4,557$	0.3693	32.49
$i = 2$	$2,093$	$49,077$	$4,897$	0.3234	27.92
$i = 3$	$2,786$	$66,226$	$4,699$	0.3668	30.28

Table 17: Statistics of each English valid subset on IWSLT14 En→De translation.

Set 1	i will come to it later .
	i wasn 't very good at reading things .
Set 2	this is a very little known fact about the two countries .
	it 's why they leave lights on around the house .
Set 3	and how can we do that ?
	it 's our faith , and we will be lo@@ y@@ al to it .

Table 18: Samples of each English valid subset on IWSLT14 En→De translation.

B.3 DATA EXAMPLES VERIFICATION

As discussed in Section 5.1, the data split by the corresponding predicted order is in different pattern. For example, the difficulty of each set is different. We therefore analyze the split data and calculate some statistics among these subsets. Specifically, we first count the sentence number S, the tokens T, and the distinct vocabulary D_i in each subset. We show these numbers in Table 17, along with corresponding averaged BLEU score (see Figure 2). We can see that the vocabulary size of set 1 is the smallest, and set 2 is the largest, which means there are more distinct words in set 2. This leads the generation of set 2 to be harder than set 1, which maps the BLEU score ranking among these sets. Besides, we also calculate the token frequency f_{ij} for token j in each own subset i, and sum the frequency of top 20 tokens in each subset, $F_i = \sum_{j=1}^{20} f_{ij}$, to give another evidence. The results also show that F_1 is the highest, which means the tokens in set 1 contains most frequent words to make an easy learning, while set 2 is harder since F_2 is small.

We further take a look at the data and find the sentences in set 1 are mostly "simple sentences", and set 2 contains many "emphatic sentences", while set 3 is somehow mixed. In Table 18, we provide some sentence examples belong to each subset to give more clarifications.

B.4 ROBUSTNESS

An impact of IOT training besides performance gain is that the model can be more robust compared to one order only. In Table 19, we provide one example to prove the robustness. We train one Transformer model by decoder order *1*, and to decode the sentences with all orders in inference. Obviously, only decoding with order *1* leads to good performance, while other orders can not achieve

Order	Transformer	IOT
1⋆	35.84	36.42
2	27.96	36.45
3	8.05	36.47
4	5.11	36.38
5	1.32	36.46
6	0.35	36.41

Table 19: Robustness study on IWSTL14 De→En translation task on dev set. ⋆ is the order trained by Transformer.

reasonable scores since the layer order is changed and the feature exaction becomes incorrect. As for IOT, the generated sequences remain stable and high results for each order.