Enhancing the Nonlinear Mutual Dependencies in Transformers with Mutual Information

Anonymous ACL submission

Abstract

The predictive uncertainty problem exists in Transformers. We present that pre-trained Transformers can be further regularized by employing mutual information to alleviate such issues in neural machine translation (NMT). In this paper, to enhance the representation, we explicitly capture the nonlinear mutual dependencies existing in two types of attention in the decoder to reduce the model uncertainty. Specifically, we employ mutual information to measure the nonlinear mutual dependencies of token-token interactions during attention calculation. Moreover, we resort to InfoNCE for mutual information estimation to avoid the intractable problem. By maximizing the mutual information among tokens, we capture more knowledge concerning token-token interactions from the training corpus to reduce the model uncertainty. Experimental results on WMT'14 En→De and WMT'14 En→Fr demonstrate the consistent effectiveness and evident improvements of our model over the strong baselines. Quantifying the model uncertainty again verifies our hypothesis. The proposed plug-and-play approach can be easily incorporated and deployed into pre-trained Transformer models. Code will be released soon[1].

1 Introduction

Predictive uncertainty ubiquitously exists in deep learning or machine learning based models (Ott et al., 2018a; Xiao and Wang, 2019; Wang et al., 2019; Abdar et al., 2020; Xiao and Wang, 2021). It consists of data uncertainty (aleatoric uncertainty) and model uncertainty (epistemic uncertainty). Data uncertainty mainly results from the noise during the data collection. In practice, model uncertainty depicts whether the model can best describe the data distribution, and model uncertainty significantly attributes to the poor fitting of the data distribution (Wang et al., 2019). Model uncertainty can be reduced by feeding more data or knowledge to the model. Researchers capture and quantify uncertainties to better interpret models and enhance the representation.

	Token-token interactions	Uncertainty	
		Token	Token-token
Transformer	linear	↑	↓ (implicitly)
Our model	linear + nonlinear	↑	↓ (explicitly)

Table 1: Comparison between the vanilla Transformer and our model on the interaction style between tokens and how to deal with the uncertainty. Both models employ the label smoothed cross entropy to properly raise the uncertainty (↑) of determining a single token across the vocabulary. In addition, we **explicitly** reduce the uncertainty (↓) in the dimension of token-token interactions within a certain context to address the predictive uncertainty problem (Xiao and Wang, 2021). Definitions of some terms can be found in the Appendix.

Recently, almost all research fields of artificial intelligence have been deeply influenced by the Transformer (Vaswani et al., 2017). State-of-the-art neural machine translation (NMT) models are mostly built upon Transformers (Ott et al., 2018b; Dehghani et al., 2018; So et al., 2019; Zhou et al., 2020a; Liu et al., 2020). However, Transformer models also inevitably suffer from the uncertainty problem (Ott et al., 2018a; Wei et al., 2020; Xiao and Wang, 2021; Shelmanov et al., 2021). Xiao and Wang (2021) and Wei et al. (2020) handle with such problem outside of the model[2]. Namely, feeding more unseen samples or augmented data to the model to reduce the model uncertainty. By contrast, we address the issue inside the model. We enhance

[1] Anonymous: https://github.com/self-attention-MI/UE

[2] Note that, the word 'uncertainty' is somewhat heavily reused in the literature. For instance, Xiao and Wang (2021) incorporated uncertainty into the decoding process to reduce the hallucination. In practice, the introduced uncertainty enables the model to see otherwise unseen cases to reduce the model uncertainty in a certain context. Wei et al. (2020) employed the similar presentation. It should be appropriately distinguished from the data uncertainty and the model uncertainty in the literature (Kochkina and Liakata, 2020).

the model representation by introducing additional knowledge, namely feeding the model more relationships concerning token-token interactions in terms of nonlinear mutual dependencies.

In this paper, we aim to explicitly capture the nonlinear mutual dependencies among tokens during the attention calculation (self-attention and encoder-decoder attention in decoder) and reduce the uncertainty residing in the token-token interactions as shown in Table 1. In particular, we employ mutual information to measure the nonlinear mutual dependencies between pairs of tokens regarding the token-token interactions. Mutual information is a good measure of nonlinear relationships between random variables. To avoid the intractable feature of problems by using mutual information, we resort to InfoNCE for mutual information estimation (Logeswaran and Lee, 2018; van den Oord et al., 2019; Gutmann and Hyvärinen, 2012). InfoNCE is a mature framework for unsupervised contrastive learning. It has the theoretical and practical guarantee that a reliable lower bound can be obtained by maximizing it.

Therefore, we can explicitly obtain nonlinear mutual dependencies by regularizing the pre-trained Transformer models with maximizing mutual information. We dub the regularization of the token-token interactions in attention calculation *capturing the nonlinear mutual dependencies*. These dependencies are heavily overlooked in the vanilla Transformer, which can be employed as the additional knowledge fed to the model and reduce the model uncertainty. Experiments on WMT'14 En→De and WMT'14 En→Fr present that the performance of our model has achieved competitive results over the strong baselines and other counterparts. By contrast, to reach the same performance, contrast models either consume extra training corpus or more trainable parameters.

Contributions and highlights are as follows:

- The proposed idea is simple and makes little change to the model. It can potentially generalize to other pre-trained models leveraging self-attention.
- We explicitly capture nonlinear mutual dependencies between pairs of tokens in attentions of the decoder to reduce the model uncertainty.
- We adopt an unsupervised contrastive learning framework to estimate the mutual information, which serves in the NMT problem.
- We present a detailed analysis of the variants of the model uncertainty before and after enhancing the mutual dependencies.

2 Preliminary

2.1 Mutual Information

Mutual information in discrete distributions is generally described as Equation 1:

$$\begin{aligned} I(X;Y) &= D_{\mathrm{KL}}(p(X,Y)\|p(X)p(Y)) \\ &= \sum_{y\in Y}\sum_{x\in X} p(x,y)\log\left(\frac{p(x,y)}{p(x)p(y)}\right) \\ &= \mathbb{E}_{p(x,y)}\left[\log\frac{p(x,y)}{p(x)p(y)}\right], \end{aligned} \tag{1}$$

where, X, Y denote two random variables. x, y indicate concrete samples in X and Y. $p(\cdot)$ and $p(\cdot,\cdot)$ represent marginal probability and joint probability respectively. D_{KL} is the Kullback–Leibler divergence (also known as the *relative entropy*) (Kullback and Leibler, 1951).

2.2 Contrastive Learning

Following Kong et al. (2019), we employ InfoNCE to estimate the mutual information under the contrastive learning framework. InfoNCE maximizes the mutual information to obtain a lower bound, which in practice is a good estimation of mutual information:

$$\begin{aligned} &I(X,Y) \geq \\ &\mathbb{E}_{p(X,Y)}\left[f_{\boldsymbol{\theta}}(x,y) - \mathbb{E}_{q(\tilde{\mathcal{Y}})}\left[\log\sum_{\tilde{y}\in\tilde{\mathcal{Y}}}\exp f_{\boldsymbol{\theta}}(x,\tilde{y})\right]\right] \\ &+\log|\tilde{\mathcal{Y}}|, \end{aligned} \tag{2}$$

where, x is the positive sample token of the source sentence and y is the positive sample token of the target sentence. f_θ is a measure of relevance between x and y. Usually, a similarity score function is adopted. $\tilde{\mathcal{Y}}$ is the negative sample set of y, note that it contains the positive sample. $q(\cdot)$ is a distribution proposal function offering the specific rule to build the negative sample set. $\tilde{y}$ is a random sample from the negative sample set.

The following part of Equation 2 is the crucial component when we incorporate the contrastive learning framework into the NMT problem:

$$\mathbb{E}_{p(X,Y)}\left[f_{\boldsymbol{\theta}}(x,y) - \log\textstyle\sum_{\tilde{y}\in\mathcal{Y}}\exp f_{\boldsymbol{\theta}}(x,\tilde{y})\right]. \tag{3}$$

3 Methodology

3.1 Motivation to Reduce the Model Uncertainty

As mentioned in Ott et al. (2018a), a well-trained model still spreads too much probability mass across sequences. In other words, model distribution is too spread in hypothesis spaces in that it has to cater to the uncertainty brought by the data distribution. Also, as stated in Xiao and Wang (2021), unsuitable tokens attaining considerable probability mass attribute to the uncertainty of the token prediction. Moreover, Wang et al. (2019); Zhou et al. (2020b) present that lower model uncertainty indicates a better fitting of the data distribution. Therefore, in a certain context, the model uncertainty should be reasonably and appropriately reduced.

The widely adopted training paradigm is token-level teacher-forcing in NMT, which notoriously leads to the discrepancy between training and inference, namely, the exposure bias problem (Xie et al., 2016; Ranzato et al., 2016; Norouzi et al., 2016). Exposure bias partially accounts for the model uncertainty. During inference, model distribution dominates the decoding process. However, high model uncertainty directly indicates unsatisfactory fitting of the data distribution (Zhou et al., 2020b; Xiao and Wang, 2019). Canonical auto-regressive generation can be formulated as Equation 4:

$$p(Y \mid X;\theta) = \prod_{t=1}^{N+1} p\left(y_t \mid y_{<t}, x_{1:M};\theta\right), \quad (4)$$

where, θ denotes the parameters modeling the language model. M is the length of the source sentence and N is the length of the target sentence.

At each time step, clues on the next token are all from previously generated tokens. In other words, it depends on *how much uncertainty on the next token can be reduced by knowing partially generated prefix tokens*. Vanilla Transformer implicitly reduces the uncertainty of token-token interactions during decoding. By contrast, we aim to explicitly reduce the uncertainty of the token-token interactions during the next token generation.

3.2 Contrastive Learning Framework Construction in NMT

Methods to Build the Training Samples: Contrastive learning needs an effective and efficient relevance measure of two tokens. Specifically, a clear distinction should be presented between the similarity score of a positive sample a and a positive sample b and the similarity score of a positive sample a and a negative sample $\tilde{b}$. However, the cosine-based similarity measure solely cannot properly reflect the subtle difference in this context[3]. Therefore, we elaborately design a simple but effective method as Equation 5 and Equation 6:

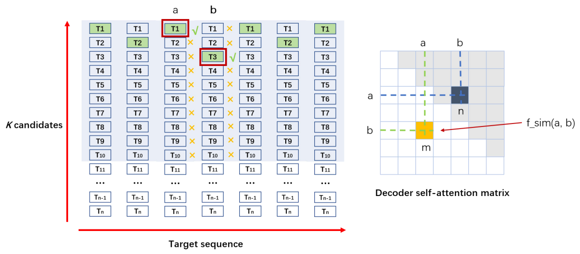

Figure 1: Graphical illustration of how to calculate $f_\theta(a,b)$. a and b denote two positions (tokens) in target sentence. In this context, T is an abbreviation for "Top", which should be distinguished from the notation of "the number of forward passes". Suppose T_1 and T_3 are ground-truth targets of position a and b respectively. There are two critical components composing $f_\theta(a,b)$, namely $f\_sim(a,b)$ and $logit(b)$ for the pair of a and positive b while $f\_sim(a,b)$ and $logit(\tilde{b})$ for the pair of a and negative sample $\tilde{b}$ from top k candidates. The value of $f\_sim(a,b)$ can be directly fetched from the self-attention matrix. In the left subfigure, negative samples are from the top k candidates in position b marked by '$\times$' or marked by '$\checkmark$', which offer $logit(\cdot)$. Causal self-attention matrix is demonstrated in the right sub-figure. Due to the property of symmetry, there are two $f\_sim(a,b)$ scores of the same value. However, position m is taken into account rather than position n in view of the causal relationship.

$$f_\theta(x,y) = f\_sim(x,y) + f\_logit(y), \quad (5)$$

where, $f\_sim(x,y)$ is the cosine similarity score between x and y as usual. $f\_logit(y)$ is the logit (score before $softmax$) by the most confident prediction of y (during inference) or the logit corresponding to the ground-truth token of y (during training).

$$f_\theta(x,\tilde{y}) = f\_sim(x,y) + f\_logit(\tilde{y}), \quad (6)$$

[3] The vanilla cosine similarity does not elaborately distinguish the positive samples and the negative samples in this context. No matter the positives or negatives, it calculates a score. The score can be very close to each other due to the candidates from top ranking. For NMT problems under contrastive learning, we need to be deliberate in distinguishing them. Therefore, we add an explicit factor to the original cosine similarity to enhance its representation.

Model	BLEU	
	En→De	En→Fr
GNMT+RL Wu et al. (2016)	25.20	40.50
ConvS2S Gehring et al. (2017)	25.16	40.46
Transformer (base) Vaswani et al. (2017)	27.30	38.10
Transformer (big) Vaswani et al. (2017)	28.40	41.80
Evolved Transformer (big) So et al. (2019)	29.80 / 29.20	41.30
Transformer (ADMIN init) Liu et al. (2020)†	30.10 / 29.50	43.80 / 41.80
Uncertainty-Aware SANMT Wei et al. (2020)	30.29	42.92
Baseline (WMT only) Ott et al. (2018b)	29.30 / 28.60	43.20 / 41.40
Baseline (WMT+Paracrawl) Ott et al. (2018b)	29.80 / 29.30	42.10 / 40.90
Baseline (Reproduced)††	29.75 / 29.30	43.16 / 41.06
Baseline + finetuning (Contrast group)‡	29.89 / 29.40	43.17 / 41.06
Ours (Baseline+$\{L_{3,4,5}$+DS+ED$\}$)	$30.45^{**}/29.80^{**}$	$43.67^{*}/41.51^{*}$

† The model has approx. 40M more parameters than ours.
†† Our reproduced results are from the provided pre-trained checkpoints.
‡ This is for a fair comparison. Results by directly finetuning fail to pass the significance tests.

Table 2: Performance comparison between different models on WMT'14 dataset. Our results are based on the reproduced results. Default values are case-sensitive *tokenized* BLEU scores and otherwise a pair of (case-sensitive *tokenized* BLEU) / (*detok.* sacreBLEU). BLEU scores are based on newstest2014 for WMT'14 English-German (En→De) and WMT'14 English-French (En→Fr). Checkpoint averaging is not used in our results. For WMT'14 En→De, we use the general configuration of $L_{3,4,5}$+DS+ED and $k = 40$. For WMT'14 En→Fr, we use the general configuration of $L_{3,4,5}$+DS+ED and $k = 50$. $L_{3,4,5}$ indicates regularization on the layer 3,4,5 of the decoder. The definitions and usage of DS and ED can be found in Equation 8. '$*/**$': significantly better than the baselines ($p < 0.05$ / $p < 0.01$) tested by bootstrap resampling. Note that, our results also significantly outperform the contrast groups ($p < 0.05$).

where, the first part of the right-hand side is exactly the same with Equation 5. Difference between Equation 5 and Equation 6 relies on $f\_logit(\cdot)$. Figure 1 depicts how to calculate the concrete value of $f_\theta(a, b)$.

Due to the steady state of the pre-trained NMT model, the component f_logit can take up most of the constituent that well distinguishes a legal pair of tokens with contrastive pairs. Moreover, this divergence can be further amplified due to the monotonicity of $softmax$ operation. This is a key point our idea leverages to distinguish positive sample pairs from contrastive sample pairs.

Leveraging the Pre-trained Self-attention Logits: To fetch $f\_sim(x, y)$ from multi-head attention, we need a rational strategy. According to Michel et al. (2019); Voita et al. (2019); Rogers et al. (2020), it is non-trivial to partition these heads into groups. Therefore, we take as similarity scores the average of all heads as follows[4]:

$$F\_sim(X, Y) = \text{Average}\left(\text{head}_1, \ldots, \text{head}_\text{h}\right), \quad (7)$$

where, X and Y are a set of tokens. Average is the average operation on similarity scores over all attention heads. head_* is a collection of similarity scores from attention heads. h is the number of attention heads. $F\_sim(X, Y)$ contains all pairs of similarity scores between tokens and other tokens to be attended. The value of $f\_sim(x, y)$ can be indexed by (x, y).

Combination objective: The overall objective consists of the label smoothed cross entropy and another two custom objectives based on mutual information maximization constraints as follows:

$$\begin{aligned} loss = &(1 - \alpha - \beta) \times lce\_loss \\ &+ \alpha \times ED \\ &+ \beta \times DS, \end{aligned} \quad (8)$$

where, lce_loss indicates the label smoothed cross entropy loss, ED represents the regularization on encoder-decoder attention and DS denotes the regularization on decoder self-attention. Both of them are defined and estimated as Equation 2. α and β are hyperparameters to balance the label smoothed cross entropy loss and two custom losses.

[4]We employed other methods to do such work, say MAX operation. However, the average operation meets our expectation.

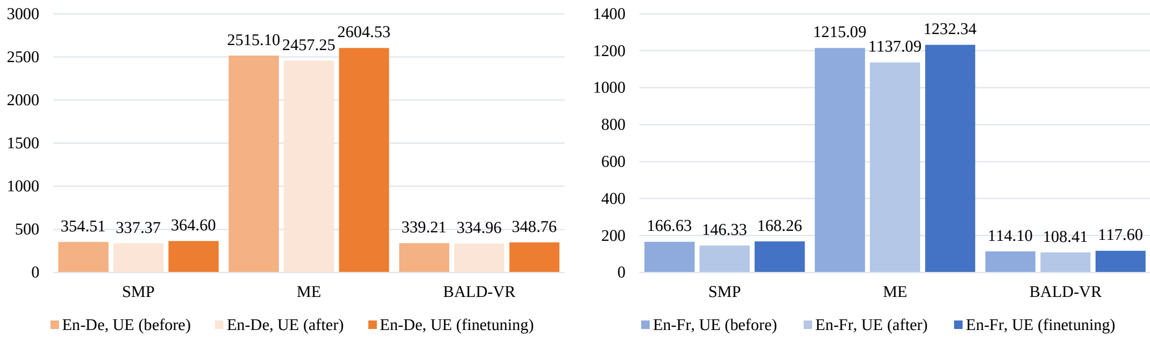

Figure 2: Variation of the model uncertainty before regularization and after regularization. The vertical axis is the model uncertainty. We employ Monte Carlo Dropout on all layers. We adopt three Uncertainty Estimation (UE) methods, namely, sampled maximum probability (SMP), mean entropy (ME) and BALD-VR to investigate the variations. The number of forward passes T is 10. The results are not normalized over the number of tokens. We add a control group for a fair comparison. We can infer that our method (histogram in the middle) reliably reduces the model uncertainty after regularization. However, directly finetuning the baselines introduces more uncertainty (histogram in the right).

4 Experiments

In this section, we describe the details of our experiments. We evaluate our model on WMT'14 En→De and WMT'14 En→Fr datasets. Moreover, we conduct ablation studies to assess the effectiveness of different objectives and hyperparameters setup.

4.1 Experimental Setup

We implement our model based on the official Fairseq toolkit implemented by PyTorch[5] (Ott et al., 2019) and report statistical significance tests by using compare-mt (Neubig et al., 2019)[6] and sacreBLEU [7].

Dataset and Metric We train our model on WMT'14 En→De (4.5M)[8] and WMT'14 En→Fr (36M). For WMT'14 En→De, we validate our model on newstest13 and test on newstest2014. Following Ott et al. (2018b), we use byte pair encoding (BPE) (Sennrich et al., 2016) to prepare the joint vocabulary of 32K symbols. For WMT'14 En→Fr, we validate our model on newstest12+13 and test on newstest14. The joint vocabulary is 40K. We employ two BLEU metrics to evaluate our performance, namely, case-sensitive *tokenized* BLEU and *detokenized* sacreBLEU. We report BLEU scores with a beam size of 4 and a length penalty of 0.6.

[5]https://github.com/pytorch/fairseq

[6]https://github.com/neulab/compare-mt

[7]https://github.com/mjpost/sacreBLEU

[8]To be consistent with the baseline and other counterparts, we use WMT'16 En→De to train our model and report results on the WMT'14 test set.

Model and Hyperparameters Our model leverages the pre-trained baseline model, which is an extension of the Transformer big model ($d_{model} = d_{hidden} = 1024$, $n_{layer} = 6$, $n_{head} = 16$) (Vaswani et al., 2017). We adopt Adam (Kingma and Ba, 2015) to optimize our model by setting $\beta_1 = 0.90$, $\beta_2 = 0.98$ and $\epsilon = 1e\text{-}08$. We finetune our model from a pre-trained checkpoint with the learning rate 3e-04 for En→De and 5e-04 for En→Fr. Our criterion to configure 'ntokens' and 'update-freq' is that, neither hitting the OOM nor the threshold of the loss scale. 'ntokens' is 10240 for En→De and 9216 for En→Fr. 'update-freq' is 1 for En→De and 4 for En→Fr. The maximum epoch for En→De is 20 and 10 for En→Fr. Embeddings are shared in all positions. We tune hyperparameters on the validation set.

All experiments are conducted on a machine with 8 NVIDIA TITAN RTX GPU and a memory-efficient version of FP16 half-precision training. The proposed method has a relatively low computational overhead, taking roughly 6-7 hours for the WMT'14 En→De dataset. For the WMT'14 En→Fr dataset, it takes about two days.

4.2 Main Results

Table 2 demonstrates the performance comparison of our model and the baseline models along with other SOTA models on the WMT'14 dataset. We utilize a general setup of $L_{3,4,5}$+DS+ED to conduct the experiments. To facilitate comparison with the results of different studies, we depict both the case-sensitive *tokenized* BLEU and *detokenized*

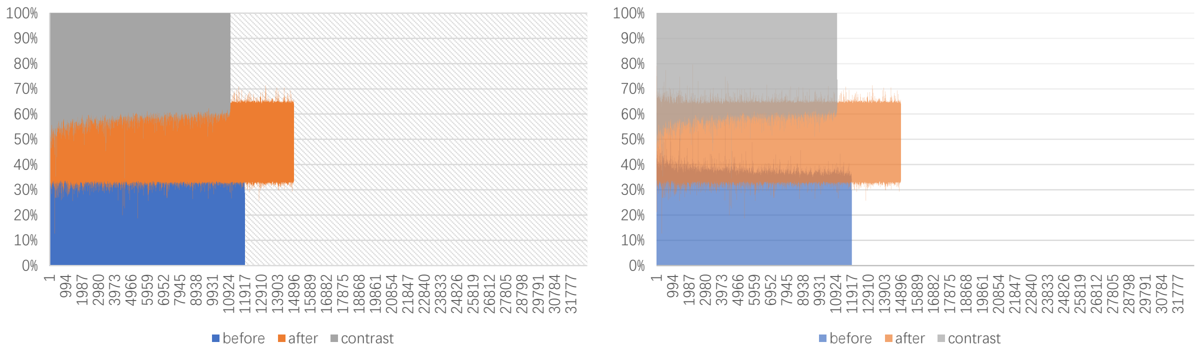

Figure 3: Comparison between the probability mass distribution across the token vocab regarding different models (before regularization, after regularization and the contrast group). The vertical axis is the percentage of probability mass. The horizontal axis is the index of the vocab. The right figure enhances the contrast of the percentage of each of the three models to present a more intuitive visual. The experiments are conducted on the WMT'14 En→De dataset. A subset of the test set is randomly selected and employed to report the results. From the figure, it can be seen that the regularized model has a reasonable distribution of probability mass, which makes sense and is as anticipated. The contrast group is obtained by directly finetuning the pre-trained checkpoint to the same steps. However, the probability mass of the contrast group becomes inflated. From Figure 2, the contrast group introduces more uncertainty. As aforementioned, unsuitable tokens attaining considerable probability mass account for the uncertainty of the token prediction. By contrast, after regularization, our model has lower model uncertainty, and its probability mass approaches to shrink, which indicates the probability mass is properly balanced over different tokens.

SacreBLEU (Post, 2018)[9]. Morever, to make a fair comparison, we also directly finetune the pre-trained checkpoints to the same steps and employ them as the contrast groups.

As shown in Table 2, it can be seen that our model achieves a compelling improvement over the strong baselines and other competitive SOTA models. Besides, our model significantly outperforms both the baseline and the contrast groups. However, the contrast group fails to pass the significance test. Therefore, we can infer that the proposed regularization method has a positive effect on the performance of the model. And our hypothesis of reducing model uncertainty by enhancing nonlinear mutual dependencies as additional knowledge is partially verified by model performance improvement. To further support our view that the performance improvement is related to the model uncertainty and dissect the relationship between the model uncertainty and the probability mass distribution across the vocab, we present more analysis in the following sections.

Since our method does minute change to the baseline models, the improvements are reasonable and justified. Additional contrast groups make our results even more convincing and credible. Moreover, it is easy to incorporate our approach to existing models leveraging Transformer models. In practice, our method avoids the requirements of additional considerations for actual deployment.

[9]SacreBLEU hash: BLEU+case.mixed+lang.en-de+ numrefs.1+smooth.exp+test.wmt14/full+tok.13a+version.1.4.14

4.3 Analysis

Variation of Model Uncertainty: We employ a combination of BALD (Bayesian Active Learning Disagreement) (Houlsby et al., 2011; Hazra et al., 2021) and Variation Ratio (Kochkina and Liakata, 2020) to conceptually form a new metric BALD-VR. Along with BALD-VR, we also use Mean Entropy (Kochkina and Liakata, 2020) and Sampled Maximum Probability (Shelmanov et al., 2021) to evaluate the model uncertainty, results are shown in Figure 2. From Figure 2, we can infer that the proposed method reduces the model uncertainty to some extent, which verifies our hypothesis. By contrast, the contrast group introduces more uncertainty to the model. More details are depicted in the appendix.

Variation of the Probability Mass As aforementioned in Section 3.1, high model uncertainty is potentially related to unsuitable probability mass distribution. We have presented that our model reduces the uncertainty and achieves better performance. However, we should unravel the relationship between the model uncertainty and the probability mass variation we assumed. To explore

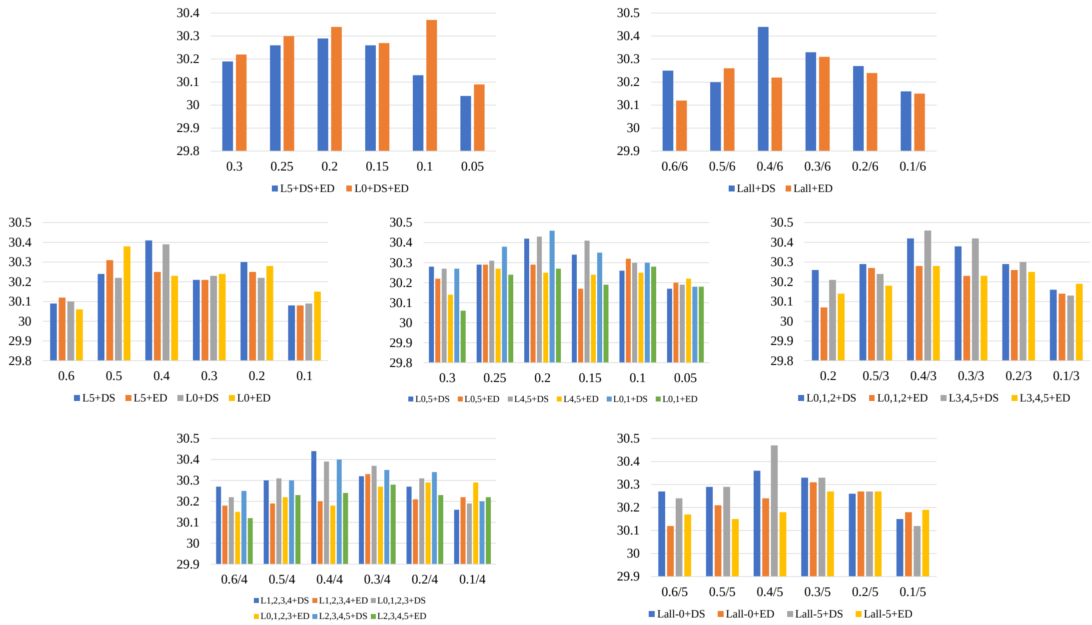

Figure 4: Ablation studies on the layer-level performance. The vertical axis is the BLEU value and the horizontal axis is the value of α and β. L_* denotes certain layers. To simplify the experiments, we employ the same value of α and β. We try to cover those representative cases and leave the rest for future work. Experiments are conducted on WMT'14 En→De. To reduce the overheads of training, we ignore the influence of k and set $k = 10$ in these experiments. The definitions of DS and ED can be found in Equation 8. From these results, we can infer that 'DS' has a slight better performance compared with 'ED'. Employing either 'DS' or 'ED' on all layers of the decoder is somewhat over-constraint. In a certain range, appropriately adding regularization can be effective in improving performance. Detailed results are presented in the Appendix.

the variation of model probability mass, we further analyze the probability mass distribution across token vocab dimensions with different models on the same test data. Figure 3 shows the comparison of probability mass over the three models. It can be seen that our model softens the distribution of probability mass and shrinks the probability mass of several tokens. By contrast, the probability mass distribution of the contrast group is further bloated, and within a certain range, the allocated probability mass increases. The experimental results are consistent in our model and the contrast group, including the model before regularization that the high uncertainty model has an inflated probability mass distribution, while the low uncertainty model has a relatively shrinking and more reasonable probability mass distribution.

Correlation with the Label Smoothed Cross Entropy: There is no conflict between the widely adopted label smoothed cross entropy (raising uncertainty) and the proposed idea (reducing uncertainty) in that they perform in the different dimensions. For clarity, label smoothing loosens a one-hot label to a soft alternative, which occurs from the viewpoint of a single token across the vocabulary. It aims to penalize the over-confidence of the model, namely raising the model uncertainty towards a single token decision. While our approach reduces the uncertainty existing in the interactions between token and token in a certain context. It occurs from the perspective of token-token interactions, especially when a certain context is held during decoding. By contrast, our model pays attention to the inevitably introduced uncertainty that takes up non-negligible probability mass (Ott et al., 2018a). Therefore, the proposed idea is a companion to the label smoothed cross entropy rather than a replacement or alternative.

4.4 Ablation Study

Contribution of Different Objectives: We employ two hyperparameters α and β to balance different losses as shown in Equation 8. We validate the effectiveness of the proposed mutual information constraints by setting the hyperparameter $1-\alpha-\beta$ from 0.4 to 0.9. When it comes to the case of multiple layers, α and β are equally divided by the number of layers. Results are depicted in Figure 4. From Figure 4, it is intuitive to infer that both cus-

k	1	2	3	4	5	10	20	30	40	50	100	200
BLEU	27.52	27.63	27.77	27.79	27.86	27.79	27.89	27.85	27.92	27.89	27.91	-

Table 3: The impact of different choices of k (regarding the capacity of a negative sample set) on performance. The experiment is conducted on the WMT'14 En→De valid set. A combination of two regularizations (ED+DS) is adopted. Here, the metric 'BLEU' indicates case-sensitive *tokenized* BLEU. In the case of $k = 200$, the model hits the OOM under the same setup of other configurations. We use $k = 40$ to report the final result of WMT'14 En→De. Similarly, we use $k = 50$ to report the final result of WMT'14 En→Fr.

tom objectives have a positive impact on the model performance. 'DS' performs slightly better than 'ED'. The boundary cases are considered as contrast groups.

Impact of the Proposed Regularization Methods on Different Layers of the Decoder: We conduct ablation experiments of regularization on layer-level performance in this section. Results are presented in Figure 4. From Figure 4, it can be inferred that there is no consistently positive relationship between the increase in performance and the increase in regularization on more layers. To a certain extent, appropriately adding regularization can be effective in improving performance. However, too much regularization can lead to performance degradation. We speculate that it is caused by over-regularization. Therefore, considering the performance and the overhead, we recommend that the number of regularization layers should be less than 3.

Hyperparameter k in Contrastive Learning Framework Construction: According to Kong et al. (2019), the larger the capacity of the negative sample set, the more accurate the framework is to estimate the lower bound of mutual information. Also, as we demonstrated in Equation 2 and Equation 3, the lower bound becomes even tighter when the number of tokens in the negative sample set is large enough. We conduct experiments with different hyperparameter k as shown in Table 3, in which we can infer that capacity of a negative sample set has a positive impact on performance in a certain range. In the case of $k = 1$, model performance is not far from satisfactory, which is due to the pre-trained nature of the NMT model. In other words, a pre-trained NMT model itself is a competent distribution proposal function.

5 Conclusion

In this paper, we propose a novel regularization method based on the maximization of mutual information. We implement our ideas under the unsupervised contrastive learning framework to capture and enhance nonlinear mutual dependencies among tokens, which reduces the model uncertainty. Experiments and ablation studies demonstrate the consistent effectiveness of our approach. Besides, analysis of model uncertainty quantification again verifies our hypothesis.

Limitation and Future Work: To simplify the ablation studies, we employ the same weights on 'DS' and 'ED'. Whether there will be further performance gains when taking into account regularization on different encoder layers, we will leave in the future work. Besides, our idea is based on the self-attention mechanism, which serves plenty of pre-trained language models. Nonlinear mutual dependencies may potentially have a positive influence on these models for downstream tasks. This is the first step we take to investigate how to incorporate the model uncertainty analysis into the NMT problem.

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Appendix

A Terminology

Token-token interactions We refer to 'token-token interactions' as the process of a token attending to the other token and formulating its representation by linear interpolation (vanilla Transformer) of relative candidates. There are three types of attention in a Transformer model. The behavior of token-token interactions is different in each attention. We concentrate on the attention mechanism in the decoder, namely the self-attention in the decoder and the encoder-decoder attention in the decoder. Given the causal feature of the self-attention in the decoder, we should value the masking mechanism. The architecture of the vanilla Transformer model is shown in Figure 5.

Maximizing mutual information Mathematically, mutual information is a good measure of nonlinear relationships between random variables. Mutual information quantifies the information on one token to be predicted given previous generated one in the context of sequence generation. By maximizing mutual information among tokens during token-token interactions, we can capture more nonlinear mutual dependencies. We name the process of maximizing mutual information during fine-tuning regularization. We refer to 'enhancing the nonlinear mutual dependencies' as the process of regularization, in other words, maximizing mutual information. The nonlinear mutual dependencies we captured can be seen as additional knowledge extracted from the training corpus. Extra training corpus or knowledge is capable of reducing the model uncertainty. We propose our method to reduce the model uncertainty in terms of feeding this knowledge from the existing training corpus. From the perspective of linguistics, the enhanced representation can reinforce token-token connections in some contexts.

Enhancing nonlinear mutual dependencies Enhancing or capturing nonlinear mutual dependencies is equal to maximizing mutual information among tokens or regularization on attention calculation in the decoder. Why *nonlinear*? Linear interpolation of representation is intrinsic in the attention mechanism of vanilla Transformer models. Compared with nonlinear, linear interpolation has a feature of limited expressiveness. Why *mutual information*? Mutual information captures such nonlinear relationships. What are the *dependencies*? Relationships or connections of tokens.

Model uncertainty Model uncertainty is also known as epistemic uncertainty. It describes whether the model we employ can well fit the data distribution. Model design and selection accounts for the model uncertainty. Model uncertainty can

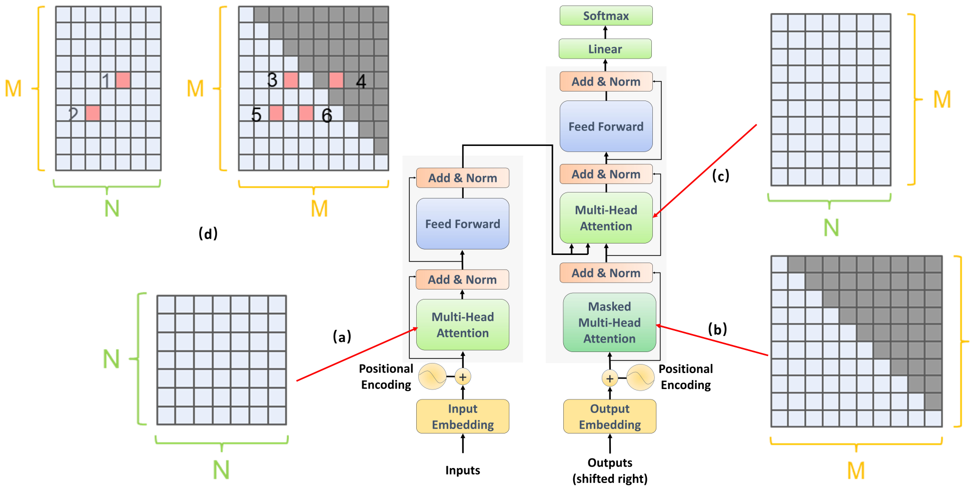

Figure 5: Transformer model and self-attentions. (a) Self-attention in the encoder. Queries, keys, and values are the same. It is a symmetric matrix. The outputs of the last layer serve as the keys and values of the encode-decoder attention in the decoder. (b) Decoder self-attention. Queries, keys, and values are the same as the outputs of the decoder step by step. It is also a square matrix. Only positions of the lower triangular region are legal. Black blocks indicate those positions masked to keep the causal property. (c) Encoder-decoder attention in the decoder. Queries are from outputs of decoder self-attention. Due to the different lengths between the source and target sentence, this is generally a non-square matrix. In (d), Mark 1 or Mark 2 indicate a target token (indexed by row number) attends to a source token (indexed by column number) in encoder-decoder attention in the decoder, respectively. It is also a convenient lookup table to fetch the cosine similarity score of pairs of tokens employed in calculating mutual information. In (d), a token can attend to Mark 3 but not Mark 4 due to its causal nature. By contrast, Mark 5 and Mark 6 can be attended by tokens indexed by the row number.

be reduced by feeding more data or knowledge to the model. Both model uncertainty and data uncertainty affect the prediction. In this work, we concentrate on the *model* uncertainty. Following Shelmanov et al. (2021); Zhou et al. (2020b); Xiao and Wang (2019); Wang et al. (2019), we employ Monte Carlo Dropout (Gal and Ghahramani, 2016) to approximate Bayesian inference to conduct the Uncertainty Estimation (UE). Specifically, we demonstrate the quantification of model uncertainty before and after the regularization to investigate the variation:

$$UE(\boldsymbol{\theta}) = \frac{1}{N}\sum_{n=1}^{N} \mathrm{Var}\left[P\left(y^n \mid x^n, \hat{\boldsymbol{\theta}}^t\right)\right]_{t=1}^{T}, \tag{9}$$

where, θ is the set of model parameters. x and y are training samples. N indicates the number of samples. T is the number of stochastic passes. $\left\{\hat{\theta}^1, ..., \hat{\theta}^T\right\}$ are sampled parameters during stochastic passes. To be consistent with Wang et al. (2019), we calculate the uncertainty after the prediction process is done in that we do not employ the model uncertainty to improve the model prediction, instead, we quantify the model uncertainty.

Data uncertainty Data uncertainty is also named aleatoric uncertainty. For NLP problems, the semantically equivalent transformation of sentences or tokens attributes to the data uncertainty. Besides, noisy data generated during the collection of training corpus can also introduce data uncertainty.

Reducing the model uncertainty High model uncertainty indicates the poor fitting of the data distribution, which results in worse model performance. Either feeding more data or additional knowledge can reduce the model uncertainty. We regard these nonlinear mutual dependencies extracted by regularizing the model as additional knowledge fetched from the training corpus. Besides, reducing the model uncertainty is roughly equal to raising the model confidence of decision-making in a certain context. Why we would like to *reduce* the model uncertainty? And is there any correlation between model uncertainty and translation quality? There are at least two perspectives to analyze these questions. For instance, as we mentioned in Table 1 and also in the Section "Correlation with the Label Smoothed Cross Entropy". In some cases, an appropriate **increase** in the model uncertainty can generalize the model performance. A good example is that the widely employed label smoothed cross entropy properly raises the uncertainty of determining a **single** token across the vocabulary. Because the generalization capability of the model is enhanced, the translation quality becomes better. From another perspective of **token-token** interactions, our approach **reduces** the uncertainty existing in the interactions between token and token in a certain context. The model uncertainty can be reduced by feeding more data or knowledge to the model. Therefore, we employ more knowledge in terms of nonlinear relationships to reduce the model uncertainty. Please note that our method is based on enhancing the model representation of token-token interactions, in other words, it occurs in a certain context. Intuitively, the model could be more confident when making decisions in certain contexts. This is reasonable and makes sense. From this point of view, an appropriate reduction of model uncertainty can increase the quality of the translation.

B Motivation and Connection Between Different Terms

In this section, we further clarify our motivation and describe some inner connections between newly introduced concepts.

We found in the literature that the use of uncertainty reduction can help solve other NLP problems. And the famous Transformer model in the NMT problem has the predictive uncertainty problem. Therefore, we aim to introduce a certain approach to reduce such predictive uncertainty in Transformer. Most existing research concentrates on feeding more data to the model to reduce the model uncertainty. By contrast, we would like to enhance the model representation by introducing additional knowledge, namely feeding the model more relationships between token-token interactions.

The interactions among two tokens in a sentence are obtained by a weighted summation in a linear fashion. We would like to capture more relationships among tokens beyond what we know. Therefore, **mutual information** occurs to us. We employ InfoNCE to approximate the mutual information. To facilitate problem-solving, we also formulate the whole problem under the framework of contrastive learning. We can maximize the mutual information by InfoNCE to obtain a lower bound.

So far, we have established **the relationship between the NMT problem and the mutual information**. We suppose that maximizing the mutual information could be helpful in the NMT system from the perspective of reducing the model uncertainty.

To this end, on one hand, we evaluate the performance of translation in the form of the widely employed BLEU value. On the other hand, we also verify our hypothesis by quantifying the model uncertainty before regularization and after regularization. Besides, given that there are relatively few relevant studies in this research, we also provide some abbreviated analyses of the analytical methods.

C Detailed Experimental Results

Some detailed experimental results are presented in Table 4, Table 5, Table 6, and Table 7 for further reference.

D Hyperparameters in MC Dropout Inference

Two key factors that affect the MC dropout inference. Namely, the number of forward passes T and the dropout ratio p. We investigate such factors in this section. We conduct ablation experiments and demonstrate the results in Figure 6. From Figure 6, we can infer that $T = 10$ and $p = 0.3$ meet the requirements.

	Models†					
$1-\alpha-\beta$	0.4	0.5	0.6	0.7	0.8	0.9
α, β	0.6/2	0.5/2	0.4/2	0.3/2	0.2/2	0.1/2
L_5+DS+ED	30.19/29.50	30.26/29.60	30.29/29.60	30.26/29.60	30.13/29.50	30.04/29.40
L_0+DS+ED	30.22/29.50	30.30/29.60	30.34/29.60	30.27/29.60	30.37/29.80	30.09/29.50
α, β	0.6	0.5	0.4	0.3	0.2	0.1
L_5+DS	30.09/29.40	30.24/29.50	30.41/29.70	30.21/29.60	30.30/29.70	30.08/29.50
L_5+ED	30.12/29.40	30.31/29.60	30.25/29.50	30.21/29.60	30.25/29.70	30.08/29.50
L_0+DS	30.10/29.40	30.22/29.50	30.39/29.70	30.23/29.60	30.22/29.60	30.09/29.50
L_0+ED	30.06/29.40	30.38/29.70	30.23/29.50	30.24/29.60	30.28/29.70	30.15/29.50
α, β	0.6/2	0.5/2	0.4/2	0.3/2	0.2/2	0.1/2
$L_{0,5}$+DS	30.28/29.60	30.29/29.60	30.42/29.70	30.34/29.70	30.26/29.60	30.17/29.60
$L_{0,5}$+ED	30.22/29.50	30.29/29.60	30.29/29.60	30.17/29.50	30.32/29.70	30.20/29.60
$L_{4,5}$+DS	30.27/29.60	30.31/29.60	30.43/29.70	30.41/29.70	30.30/29.70	30.19/29.60
$L_{4,5}$+ED	30.14/29.40	30.27/29.60	30.25/29.60	30.24/29.60	30.25/29.70	30.22/29.70
$L_{0,1}$+DS	30.27/29.60	30.38/29.70	30.46/29.70	30.35/29.70	30.30/29.70	30.18/29.60
$L_{0,1}$+ED	30.06/29.30	30.24/29.60	30.27/29.60	30.19/29.60	30.28/29.70	30.18/29.60
α, β	0.6/3	0.5/3	0.4/3	0.3/3	0.2/3	0.1/3
$L_{0,1,2}$+DS	30.26/29.60	30.29/29.60	30.42/29.70	30.38/29.70	30.29/29.70	30.16/29.60
$L_{0,1,2}$+ED	30.07/29.40	30.27/29.60	30.28/29.60	30.23/29.60	30.26/29.70	30.14/29.60
$L_{3,4,5}$+DS	30.21/29.50	30.24/29.50	30.46/29.70	30.42/29.70	30.30/29.70	30.13/29.60
$L_{3,4,5}$+ED	30.14/29.50	30.18/29.50	30.28/29.60	30.23/29.60	30.25/29.70	30.19/29.60
α, β	0.6/4	0.5/4	0.4/4	0.3/4	0.2/4	0.1/4
$L_{1,2,3,4}$+DS	30.27/29.60	30.30/29.60	30.44/29.70	30.32/29.70	30.27/29.70	30.16/29.60
$L_{1,2,3,4}$+ED	30.18/29.50	30.19/29.60	30.20/29.50	30.33/29.70	30.21/29.60	30.22/29.70
$L_{0,1,2,3}$+DS	30.22/29.50	30.31/29.60	30.39/29.70	30.37/29.70	30.31/29.70	30.19/29.60
$L_{0,1,2,3}$+ED	30.15/29.40	30.22/29.50	30.18/29.50	30.27/29.60	30.29/29.70	30.29/29.60
$L_{2,3,4,5}$+DS	30.25/29.50	30.30/29.60	30.40/29.70	30.35/29.70	30.34/29.70	30.20/29.60
$L_{2,3,4,5}$+ED	30.12/29.40	30.23/29.60	30.24/29.60	30.28/29.70	30.23/29.70	30.22/29.60
α, β	0.6/5	0.5/5	0.4/5	0.3/5	0.2/5	0.1/5
L_{all-0}+DS	30.27/29.60	30.29/29.60	30.36/29.60	30.33/29.70	30.26/29.60	30.15/29.60
L_{all-0}+ED	30.12/29.40	30.21/29.60	30.24/29.60	30.31/29.70	30.27/29.70	30.18/29.60
L_{all-5}+DS	30.24/29.50	30.29/29.60	30.47/29.70	30.33/29.70	30.27/29.70	30.12/29.60
L_{all-5}+ED	30.17/29.50	30.15/29.50	30.18/29.50	30.27/29.60	30.27/29.70	30.19/29.60
α, β	0.6/6	0.5/6	0.4/6	0.3/6	0.2/6	0.1/6
L_{all}+DS	30.25/29.50	30.20/29.60	30.44/29.70	30.33/29.70	30.27/29.60	30.16/29.60
L_{all}+ED	30.12/29.40	30.26/29.60	30.22/29.50	30.31/29.70	30.24/29.70	30.15/29.60

† We tune the parameters on the validation set, and report these results on the test set. Values in this table may be susceptible to different setups that we did not thoroughly explore. However, we do not aim to provide the best situations of all cases, instead, we offer analysis of possible trends. We ignore the influence of k and set $k = 10$ in these experiments.

Table 4: Ablation studies on the layer-level performance. 'DS' indicates the proposed regularization approach applied on the decoder self-attention. 'ED' means the proposed regularization approach applied on the encoder-decoder attention in the decoder. To simplify the experiments, we adopt the same value of α and β to balance 'DS' and 'ED'. For instance, if the weight on the label smoothed cross entropy is w, then $\alpha, \beta = (1-w)/2$, when 'DS' and 'ED' are applied on a single layer of the decoder. Similarly, $\alpha, \beta = (1-w)/6$, when 'DS' or 'ED' are applied on all layers of the decoder, and so on. Different contributions of 'DS' or 'ED' in the combination fashion of 'DS+ED', we leave them in the future work. L_0 means the first layer in the decoder. L_5 means the last layer. $L_{0,5}$ means the first layer and the last layer. $L_{4,5}$ means the last two layers. $L_{0,1}$ means the first two layers. $L_{0,1,2}$ means the first three layers. $L_{3,4,5}$ means the last three layers. L_{all-0} means all layers except the first layer. L_{all-5} means all layers except the last layer. We average the last 5 checkpoints to report these results. Experiments are conducted on WMT'14 En→De. From these results, we can infer that 'DS' has slight better performance compared with 'ED'. Employing either 'DS' or 'ED' on all layers of the decoder is somewhat over-constraint. In a certain range, appropriately adding regularization can be effective in improving performance.

Dropout Type	Model Acquisition	En→De		En→Fr	
		UE (before)	UE (after)	UE (before)	UE (after)
MC-all	Sampled max. probability	354.5077	337.3681	166.6318	146.3338
MC-all	Mean entropy	2515.1008	2457.2503	1215.0922	1137.0944
MC-all	BALD-VR	339.2128	334.9575	114.1011	108.4149

Table 5: Variation of the model uncertainty before regularization and after regularization. 'MC-all' means 'Monte Carlo Dropout' employed on all layers. We employ three Uncertainty Estimation (UE) methods, namely, Sampled max. probability, Mean Entropy and BALD-VR to investigate the variations. The number of forward passes T is 10. The results are not normalized over the number of tokens.

Num. of T	1	2	3	4	5	6
SMP	338.0088 / 319.5488	347.5487 / 329.9464	350.2366 / 333.0439	351.9552 / 334.9495	353.7504 / 335.7504	353.4781 / 336.2595
ME	2403.5835 / 2341.8491	2460.3462 / 2400.5967	2479.6318 / 2421.1494	2492.6663 / 2435.1404	2500.8201 / 2441.8916	2504.8918 / 2445.9519
BALD-VR	0 / 0 †	154.9255 / 150.7553	214.0106 / 210.4574	251.8404 / 246.7234	275.8936 / 270.2872	294.9787 / 288.6808
Num. of T	**7**	**8**	**9**	**10**	**20‡**	**30‡**
SMP	353.6949 / 336.5727	353.9379 / 336.8132	354.3253 / 337.1445	354.5077 / 337.3681	176.3070 / 168.1396	87.0544 / 83.3469
ME	2507.3079 / 2449.6633	2509.6550 / 2451.1414	2512.8601 / 2454.7310	2515.1008 / 2457.2503	1249.8004 / 1224.1233	615.8340 / 605.8625
BALD-VR	307.9149 / 303.4787	321.2128 / 315.9893	331.2021 / 326.0425	339.2128 / 334.9575	193.9734 / 192.5053	101.8218 / 101.2766

† Zero values are due to the calculation of variance towards a single value.
‡ In the case of $T = 20$ and $T = 30$, results seem to be disproportionate to other cases. This is due to the setup of batch size during inference in order to avoid OOM.

Table 6: The impact of the number of forward passes T on MC dropout inference. We show the variations of the three metrics. 'SMP' for 'sampled maximum probability'; 'ME' for 'mean entropy'; 'BALD-VR' for a combination of 'Bayesian Active Learning by Disagreement' and 'variation ratio'. The values presented here are UE (before) / UE (after). Experiments are conducted on WMT'14 En→De. Dropout ratio p is the default value 0.3. We can infer that as the value T increases, the gap between two UEs tends to decrease. However, UE (after) is consistently smaller than UE (before). Considering the practical situation and following the common literature, we choose $T = 10$ throughout the experiments.

dropout ratio p	0.1	0.2	0.3†	0.4	0.5
SMP	302.3890 / 286.0438	323.7969 / 306.6345	354.5077 / 337.3681	403.9660 / 388.3170	~~495.5341 / 485.3623~~
ME	2057.5542 / 1990.6696	2240.8325 / 2173.9890	2515.1008 / 2457.2503	2962.1492 / 2926.7832	~~3779.8779 / 3796.4238~~
BALD-VR	234.0745 / 231.3511	285.9575 / 282.3511	339.2128 / 334.9575	406.0213 / 403.2021	~~529.4787 / 537.0319~~
dropout ratio p	**0.6**	**0.7**	**0.8**	**0.9**	**1.0**
SMP	~~698.8461 / 703.8344~~	~~890.4090 / 887.0627~~	~~940.6628 / 943.8118~~	~~955.7371 / 955.7843~~	~~868.1199 / 868.6059~~
ME	~~5537.7705 / 5691.3364~~	~~7761.6455 / 7963.3516~~	~~9321.2520 / 9468.3799~~	~~9783.8789 / 9785.2402~~	~~5698.2153 / 5684.1841~~
BALD-VR	~~803.1170 / 823.4362~~	~~954.4681 / 955.8192~~	~~957.7553 / 957.7553~~	~~957.7553 / 957.7553~~	~~0 / 0~~

† There are three main types of dropout operation in the implementation of Transformer model, namely, dropout for layer output, dropout for attention weights and dropout for activation in FFN. Here, we refer 'dropout' to the first case. Note that, 0.3 is the default value for WMT'14 En→De model.

Table 7: The impact of the dropout ratio p on MC dropout inference. We show the variations of the three metrics. 'SMP' for 'sampled maximum probability'; 'ME' for 'mean entropy'; 'BALD-VR' for a combination of 'Bayesian Active Learning by Disagreement' and 'variation ratio'. The values presented here are UE (before) / UE (after). Experiments are conducted on WMT'14 En→De. The number of forward passes T is 10. From the results above, we can infer that the appropriate value of the dropout ratio p is no more than 0.4, which is in line with our expectations. Bad cases are marked by ~~strikethrough~~.

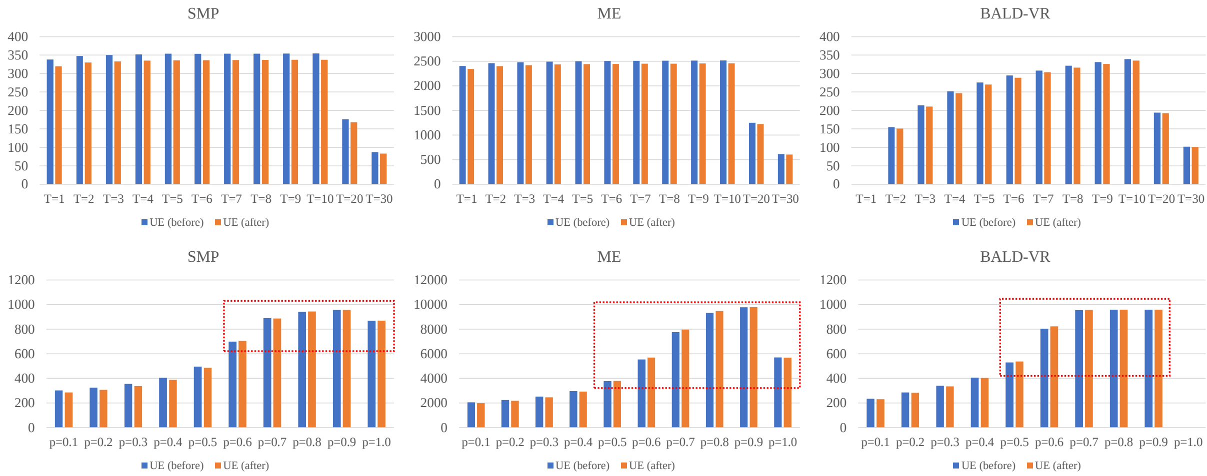

Figure 6: Experiments on the selection of hyperparameters in uncertainty estimation. The vertical axis is the unnormalized model uncertainty score and the horizontal axis is the number of forward pass T in the figures of the first row, and the dropout ratio p in the figures of the second row. Bad cases are marked by red boxes. From these ablation results, we can infer that the number of T has little impact on performance in our work. Following the general literature, we employ $T = 10$ throughout the experiments. However, the dropout ratio p matters a lot. From the results shown above, we should use a value less than 0.4. Therefore, we adopt $p = 0.3$ throughout the experiments.