R-Drop: Regularized Dropout for Neural Networks

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Abstract

Dropout is a powerful and widely used technique to regularize the training of deep neural networks. In this paper, we introduce a simple regularization strategy upon dropout in model training, namely R-Drop, which forces the output distributions of different sub models generated by dropout to be consistent with each other. Specifically, for each training sample, R-Drop minimizes the bidirectional KL-divergence between the output distributions of two sub models sampled by dropout. Theoretical analysis reveals that R-Drop reduces the freedom of the model parameters and complements dropout. Experiments on 5 widely used deep learning tasks (18 datasets in total), including neural machine translation, abstractive summarization, language understanding, language modeling, and image classification, show that R-Drop is universally effective. In particular, it yields substantial improvements when applied to fine-tune large-scale pre-trained models, e.g., ViT, RoBERTa-large, and BART, and achieves state-of-the-art (SOTA) performances with the vanilla Transformer model on WMT14 English

German translation (30.91 BLEU) and WMT14 English→French translation (43.95 BLEU), even surpassing models trained with extra large-scale data and expert-designed advanced variants of Transformer models. Our code is available at GitHub¹.

1 Introduction

In recent years, deep learning has achieved remarkable success in various areas, e.g., natural language processing, computer vision, speech/audio processing, etc. When training a deep neural network, regularization techniques [59, 62, 26, 3, 71, 60, 22, 75] are indispensable to prevent over-fitting and improve the generalization ability of deep models. Among them, the dropout technique [23], the most widely used one, aims to avoid co-adapting and performs implicit ensemble by simply dropping a certain proportion of hidden units from the neural network during training.

In this paper, we introduce a simple regularization technique upon dropout, named as R-Drop. Different from most of the previous regularization methods that work on the hidden units of each layer (e.g., the standard dropout [23]) or model parameters (e.g., dropconnect [62]), R-Drop works on the output of sub models sampled by dropout. Concretely, in each mini-batch training, each data sample goes through the forward pass twice, and each pass is processed by a different sub model by randomly dropping out some hidden units. R-Drop forces the two distributions for the same data sample outputted by the two sub models to be consistent with each other, through minimizing the bidirectional Kullback-Leibler (KL) divergence between the two distributions. That is, R-Drop regularizes the outputs of two sampled sub models for each data sample in model training. Compared with conventional neural network training, R-Drop only adds a KL-divergence loss without any structural modifications.

https://github.com/dropreg/R-Drop

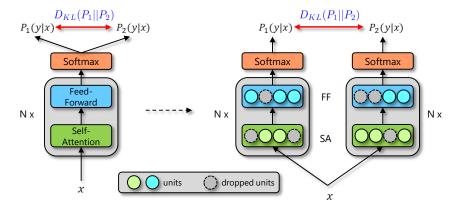


Figure 1: The overall framework of our proposed R-Drop. We take Transformer [61] structure for illustration. The left picture shows that one input x will go through the model twice and obtain two distributions \mathcal{P}_1 and \mathcal{P}_2 , while the right one shows two different sub models produced by dropout.

We theoretically analyze the regularization effect of R-Drop from the optimization perspective and show that R-Drop implicitly regularizes the freedom of the parameter space, thus reducing the complexity of the model space and enhancing the generalization of the obtained model.

Though R-Drop regularization is simple, we find it is surprisingly effective through extensive experiments on 5 tasks with 18 datasets, spanning from natural language processing, including language modeling, neural machine translation, abstractive summarization, and language understanding, to computer vision, i.e., image classification. It creates new records on multiple datasets, such as 30.91 BLEU score on WMT14 English \rightarrow German and 43.95 on WMT14 English \rightarrow French translation tasks while only be simply applied to the training of the vanilla Transformer, and also achieves SOTA results on the CNN/DailyMail summarization dataset. These universal improvements clearly demonstrate the effectiveness of R-Drop.

Our main contributions are summarized as follows:

- We propose R-Drop, a simple yet effective regularization method built upon dropout, which can be universally applied to train different kinds of deep models.
- We theoretically show that our R-Drop can reduce the freedom of model parameters, which
 is complementary with other regularization methods that work on the hidden units or the
 model weights.
- Through extensive experiments on 4 NLP and 1 CV tasks with total 18 datasets, we show that R-Drop achieves extremely strong performances, including multiple SOTA results.

2 Approach

The overall framework of our R-Drop regularization method is shown in Figure 1. Before elaborating on the details, we first present some necessary notations. Given the training dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, the goal of the training is to learn a model $\mathcal{P}^w(y|x)$, where n is the number of the training samples, (x_i, y_i) is the labeled data pair. x_i is input data and y_i is the label. For example, in NLP, x_i can be the source language sentence in machine translation, and y_i is the corresponding target language sentence. In CV, x_i can be one image, and y_i is the categorical class label. The probability distribution of the mapping function is also denoted as $\mathcal{P}^w(y|x)$, and the Kullback-Leibler (KL) divergence between two distributions \mathcal{P}_1 and \mathcal{P}_2 is represented by $\mathcal{D}_{KL}(\mathcal{P}_1||\mathcal{P}_2)$. In the following, we will explain our proposed R-Drop, training algorithm, and theoretical analysis, respectively.

2.1 R-Drop Regularization

We introduce our simple regularization method in this part. Given the training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, one basic learning objective for a deep learning model is to minimize the negative log-likelihood loss

function, which is as follow:

$$\mathcal{L}_{nll} = \frac{1}{n} \sum_{i=1}^{n} -\log \mathcal{P}^{w}(y_i|x_i). \tag{1}$$

Since the deep neural networks are prone to over-fitting, regularization methods such as dropout [59] are usually adopted during training to reduce the generalization error of the model. Specifically, dropout randomly drops part of units in each layer of the neural network to avoid co-adapting and over-fitting. Besides, dropout also approximately performs to combine exponentially many different neural network architectures efficiently [59], while model combination can always improve the model performance. Based on above characteristics and the randomness of the structure brought by dropout, we propose our R-Drop to further regularize the output predictions of sub models from dropout.

Concretely, given the input data x_i at each training step, we feed x_i to go through the forward pass of the network twice. Therefore, we can obtain two distributions of the model predictions, denoted as $\mathcal{P}_1^w(y_i|x_i)$ and $\mathcal{P}_2^w(y_i|x_i)$. As discussed above, since the dropout operator randomly drops units in a model, the two forward passes are indeed based on two different sub models (though in the same model). As shown in the right part of Figure 1, the dropped units in each layer of the left path for the output prediction $\mathcal{P}_1^w(y_i|x_i)$ are different from that of the right path for output distribution $\mathcal{P}_2^w(y_i|x_i)$. Thus the distributions of $\mathcal{P}_1^w(y_i|x_i)$ and $\mathcal{P}_2^w(y_i|x_i)$ are different for the same input data pair (x_i,y_i) . Then, at this training step, our R-Drop method tries to regularize on the model predictions by minimizing the bidirectional Kullback-Leibler (KL) divergence between these two output distributions for the same sample, which is:

$$\mathcal{L}_{KL}^{i} = \frac{1}{2} (\mathcal{D}_{KL}(\mathcal{P}_{1}^{w}(y_{i}|x_{i})||\mathcal{P}_{2}^{w}(y_{i}|x_{i})) + \mathcal{D}_{KL}(\mathcal{P}_{2}^{w}(y_{i}|x_{i})||\mathcal{P}_{1}^{w}(y_{i}|x_{i}))). \tag{2}$$

With the basic negative log-likelihood learning objective \mathcal{L}^i_{NLL} of the two forward passes:

$$\mathcal{L}_{NLL}^{i} = -\log \mathcal{P}_{1}^{w}(y_{i}|x_{i}) - \log \mathcal{P}_{2}^{w}(y_{i}|x_{i}), \tag{3}$$

the final training objective is to minimize \mathcal{L}^i for data (x_i, y_i) :

$$\mathcal{L}^{i} = \mathcal{L}_{NLL}^{i} + \alpha \cdot \mathcal{L}_{KL}^{i} = -\log \mathcal{P}_{1}^{w}(y_{i}|x_{i}) - \log \mathcal{P}_{2}^{w}(y_{i}|x_{i}) + \frac{\alpha}{2} [\mathcal{D}_{KL}(\mathcal{P}_{1}^{w}(y_{i}|x_{i})||\mathcal{P}_{2}^{w}(y_{i}|x_{i})) + \mathcal{D}_{KL}(\mathcal{P}_{2}^{w}(y_{i}|x_{i})||\mathcal{P}_{1}^{w}(y_{i}|x_{i}))],$$
(4)

where α is the coefficient weight to control \mathcal{L}^i_{KL} . In this way, our R-Drop further regularizes the model space beyond dropout and improves the generalization ability of a model. Compared Equation (1) with Equation (4), our R-Drop only adds a KL-divergence loss \mathcal{L}^i_{KL} based on two forward passes in training. Note that our regularization methodology can be universally applied on different model structures if there exists randomness in a model (e.g., dropout) that can produce different sub models or outputs. We leave further explorations as future work.

2.2 Training Algorithm

The overall training algorithm based on our R-Drop is presented in Algorithm 1. As introduced before, at each training step, Line 3-5 show that we go forward the model twice and obtain output distributions $\mathcal{P}_1^w(y|x)$ and $\mathcal{P}_2^w(y|x)$, then Line 6-7 calculate the negative log-likelihood and the KL-divergence between the two distributions. Finally, the model parameters are updated (Line 8) according to the loss of Equation (4). The training will continue over the data epochs till convergence. For implementation, to save the training cost, we do not forward the data twice, instead, we repeat the input x once and concatenate them ([x;x]) in the same mini-batch to forward once. Compared to the conventional training, our implementation is similar to enlarge the batch size to be double, and one potential limitation is that the computational cost of R-Drop increases at each step. As we show in Section 4.1, similar to other regularization methods (e.g., training w/ or w/o dropout), though R-Drop needs more training to converge, the final optimum is much better with a superior performance. We also show another study of baseline with doubled batch size in Appendix C.1.

2.3 Theoretical Analysis

We analyze the regularization effect of R-Drop in this subsection. Let $h^l(x) \in \mathbb{R}^d$ denote the output of the l-th layer of a neural network with input vector x, and let $\xi^l \in \mathbb{R}^d$ denote a random vector,

Algorithm 1 R-Drop Training Algorithm

Input: Training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$.

Output: model parameter w.

- 1: Initialize model with parameters w.
- 2: while not converged do
- 3: randomly sample data $(x_i, y_i) \sim \mathcal{D}$,
- 4: forward the data one time and obtain the output distribution $\mathcal{P}_1^w(y_i|x_i)$,
- 5: forward the data one more time and obtain the output distribution $\mathcal{P}_2^w(y_i|x_i)$,
- 6: calculate the negative log-likelihood loss \mathcal{L}_{NLL}^{i} by Equation (3),
- 7: calculate the KL-divergence loss \mathcal{L}_{KL}^i by Equation (2),
- 8: update the model parameters by minimizing loss \mathcal{L}^i of Equation (4).
- 9: end while

each dimension of which is independently sampled from a Bernoulli distribution B(p):

$$\xi_{i}^{l} = \begin{cases} 1, & \text{with probability } p, \\ 0, & \text{with probability } 1\text{-}p. \end{cases}$$

Then the dropout operation on $h^l(x)$ can be represented by $h^l_{\xi^l}(x) = \frac{1}{p} \xi^l \odot h^l(x)$, where \odot denotes the element-wised product. Hence, the output distribution of the neural network with parameter w after applying dropout is $\mathcal{P}^w_{\xi}(y|x) := \mathtt{softmax}(\mathtt{linear}(h^L_{\xi^L}(\cdots (h^1_{\xi^1}(x_{\xi^0})))))$, where $\xi = (\xi^L, \cdots, \xi^0)$.

The R-Drop enhanced training can be formulated as solving the following constrained optimization problem:

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\xi} \left[-\log \mathcal{P}_{\xi}^{w}(y_i|x_i)\right],\tag{5}$$

s.t.
$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\xi^{(1)}, \xi^{(2)}} [\mathcal{D}_{KL}(\mathcal{P}_{\xi^{(1)}}^{w}(y_i|x_i)||\mathcal{P}_{\xi^{(2)}}^{w}(y_i|x_i)))] = 0.$$
 (6)

More precisely, R-Drop optimizes the constrained optimization problem in Equation (9) and Equation (10) in a stochastic manner, i.e., it samples two random vectors $\xi^{(1)}$ and $\xi^{(2)}$ (corresponding to two dropout instantiations) from Bernoulli distribution and one training instance (x_i, y_i) , and updates the parameter w according to the stochastic gradient $\nabla_w \mathcal{L}^i$ from Equation (4).

Compared with the loss without dropout $\mathcal{L} = \frac{1}{n} \sum_{i=1}^{n} -\log \mathcal{P}^{w}(y_{i}|x_{i})$, it has been shown that optimizing the loss \mathcal{L}_{NLL} constrains the model complexity by controlling the Jacobian matrix of the model $\mathcal{P}^{w}_{\xi}(\cdot)$ [66]. The following proposition shows that the constraint in Equation (10) further constrains the model complexity by reducing the freedom of the parameters.

Proposition 2.1. For a fully-connected neural network $\mathcal{P}^w(y|x)$, e.g., multilayer perceptron and Transformer, the constraint in Equation (10) is equivalent to constraining all the parameters of the network to be equal.

Remark: Actually, constraining the KL-divergence of any two sub structures of the neural network brings a constraint on the freedom of the parameters of the neural network. Therefore, optimizing the constrained optimization problem in Equation (9) and (10) turns to seek a model that can minimize the loss \mathcal{L}_{NLL} with the smallest freedom of the parameters, hence avoiding over-fitting and improving the generalization ability. Detailed discussions and proofs on the regularization effect can be found in Appendix B.

3 Experiments

To evaluate our approach and show its universal impact, we conduct experiments on 5 different tasks, including 4 natural language processing (NLP) and 1 computer vision (CV) tasks, which are neural machine translation (NMT) (6 datasets), abstractive summarization (1 dataset), language understanding (8 datasets), language modeling (1 dataset), and image classification (2 datasets). For convenience, we utilize 'RD' to represent R-Drop in the tables of experimental results hereinafter. More details of experimental settings for each dataset can be found in Appendix A.

Model	En→De	De→En	En→Fr	Fr→En	En→Zh	Zh→En	En→Es	Es→En Avg
Transformer [61]	28.57	34.64	35.9	36.1	26.3	18.4	39.0	40.6 32.44
Transformer + RD	30.72	37.25	38.0	38.9	28.1	19.5	41.8	43.2 34.68

Table 1: BLEU scores on 8 IWSLT machine translation tasks.

3.1 Application to Neural Machine Translation

We first evaluate the NMT tasks, which is very important in NLP. To best show the effectiveness of our method, experiments are conducted on both low-resource and rich-resource translation tasks.

Datasets The datasets of low-resource scenario are from IWSLT competitions, which include IWSLT14 English↔German (En↔De), English↔Spanish (En↔Es), and IWSLT17 English↔French $(En \leftrightarrow Fr)$, English \leftrightarrow Chinese $(En \leftrightarrow Zh)$ translations. The rich-resource datasets come from the widely acknowledged WMT translation tasks, and we take the WMT14 English \rightarrow German and English \rightarrow French tasks. The IWSLT datasets contain about 170k training sentence pairs, 7k valid pairs, and 7k test pairs. The WMT data sizes are 4.5M, 36M for En \rightarrow De and En \rightarrow Fr respectively, valid and test data are from the corresponding newstest data.

Model & Training We take the most popular Transformer [61] network as our model structure. The transformer_iwslt_de_en and transformer_vaswani_wmt_en_de_big are the configurations for IWSLT and WMT translations respectively. The weight α is set as 5 for all translation tasks. Implementation is developed on Fairseq [48].

Results We calculate the BLEU scores on these tasks for evaluation, following [80]. The IWSLT resource WMT results are in Table 2. First, we En \rightarrow Fr machine translation tasks. can see that our R-Drop achieves more than 2.0

Method	$En{\rightarrow}De$	$En{\rightarrow}Fr$	
Transformer [61]	29.12	42.69	
MUSE [77]	29.90	43.50	
Depth Growing [70]	30.07	43.27	
Transformer-Admin [37]	30.10	43.80	
Data Diversification [46]	30.70	43.70	
BERT-fused NMT [80]	30.75	43.78	
Transformer + RD	30.91	43.95	

performances are shown in Table 1 and the rich- Table 2: BLEU scores on WMT14 En→De and

BLEU score improvements on 8 IWSLT translation tasks, which clearly shows the effectiveness of our method. Specially, for the well known IWSLT14 De→En translation, R-Drop obtains 37.25 BLEU score with 2.6 points improvements, which is the best result². The results on WMT translations are more impressive. After applying our simple method on the basic Transformer network, we achieve the state-of-the-art (SOTA) BLEU score on WMT14 En \rightarrow De (30.91) and En \rightarrow Fr (43.95) translation tasks, which surpass current SOTA models, such as the BERT-fused NMT [80] model that leverages large-scale monolingual data, and the Data Diversification [46] method trained with many translation models. Note that R-Drop is complementary to the above methods, and we believe stronger results can be achieved if we apply R-Drop on their methods and better backbone models beyond Transformer.

3.2 Application to Language Understanding

Dataset We further evaluate our proposed approach on the language understanding tasks by finetuning the pre-trained models³, which are the standard development sets of GLUE [63] benchmark. The GLUE benchmark includes 8 different text classification or regression tasks, which are MNLI, MRPC, QNLI, QQP, RTE, SST-2, STS-B (regression), CoLA. The detailed statistics can be found in Appendix A.4.

Model & Training We take the BERT-base [9] and strong RoBERTa-large [38] pre-trained models as our backbones to perform fine-tuning, which are publicly available. For each task, different random seeds and parameter settings are required, thus we dynamically adjust the coefficient α among $\{0.1, 0.5, 1.0\}$ for each setting. Other configurations are following the previous works [9, 38].

²Cutoff [58], a data augmentation approach, achieves 37.6 BLEU. Our method is complementary to theirs, and Cutoff + RD achieves 37.88 BLEU, which is also SOTA.

³We apply our R-Drop on the fine-tuning stage only in this work. R-Drop can also be applied during pre-training. Due to the computational cost, we leave this as future work.

Model	MNLI	MRPC	QNLI	QQP	RTE	SST-2	STS-B	CoLA	Avg
BERT-base [9]	83.8	85.3	90.8	91.0	68.2	92.4	89.3	62.3	82.85
BERT-base + RD	85.5	87.3	92.0	91.4	71.1	93.0	89.6	62.6	84.06
RoBERTa-large [38] XLNet-large [72] ELECRTA-large [7]	90.2 90.8 90.9	90.9 90.8 90.8	94.7 94.9 95.0	92.2 92.3 92.4	86.6 85.9 88.0	96.4 97.0 96.9	92.4 92.5 92.6	68.0 69.0 69.1	88.93 89.15 89.46
RoBERTa-large + RD	90.9	91.4	95.2	92.5	88.4	96.9	92.5	70.0	89.73

Table 3: Fine-tuned model performances on GLUE language understanding benchmark.

For the regression task STS-B, we use MSE instead of KL-divergence to regularize the outputs (see Appendix A.4 for MSE regularization details).

Results The evaluation metrics for above 8 tasks are as follows: The result for STS-B is the Pearson correlation; Matthew's correlation is used for CoLA; Other tasks are measured by Accuracy. The results are presented in Table 3. We can see that R-Drop achieves 1.21 points and 0.80 points (on average) improvement over the two baselines BERT-base and RoBERTa-large, respectively, which clearly demonstrate the effectiveness of R-Drop. Specifically, our RoBERTa-large + RD also surpasses the other two strong models: XLNet-large [72] and ELECTRA-large [7], which are specially designed with different model architecture and pre-training task.

3.3 Application to Summarization

Dataset Abstractive summarization task is to summarize the long sentence/document into a short sequence/sentence (through generation) with the main content remained. For this generation task, we use the CNN/Daily Mail dataset originally introduced by Hermann et al. [21] to evaluate our method. This dataset contains news documents (source), and their corresponding highlights (target) crawled from CNN and Daily Mail website. It contains 287,226 documents for training, 13,368 documents for validation and 11,490 documents for test. We follow [34] to preprocess the dataset.

Model & Training To mostly show the effectiveness, we take the super strong pre-trained sequence-to-sequence BART [34] model as our backbone and fine-tune it using our method. In this task, the coefficient weight α is set as 0.7 to control the KL-divergence. For other hyper-parameters, we follow the setting of the original paper [34] without modification.

Results The performance is evaluated by ROUGE F1 score [36]. Specifically, we report the unigram ROUGE-1 (RG-1) and bigram ROUGE-2 (RG-2) overlap to assess the informativeness, and the longest common subsequence ROUGE-L (RG-L) score to assess the fluency. The results are shown in Table 4. We can see that R-Drop based training outperforms the fine-tuned BART model by 0.3 points on RG-1 and RG-2 score and achieves the SOTA performance. Specifically, our result also surpasses the PEGASUS method [74], which brings a novel self-supervised paradigm carefully designed for summarization, and the previous best work BART+R3F [1], which introduces a paramet-

Method	RG-1	RG-2	RG-L
Transformer [61]	39.50	16.06	36.63
ProphetNet [52]	44.02	21.17	41.30
BART [34]	44.16	21.28	40.90
PEGASUS [74]	44.17	21.47	41.11
BART + R3F [1]	44.38	21.53	41.17
BART + RD	44.51	21.58	41.24

Table 4: ROUGE results on CNN/Daily Mail summarization dataset. RG-1, RG-2, RG-L stand for ROUGE-1, ROUGE-2, and ROUGE-L scores.

ric noise sampled from normal or uniform distributions. Instead, our R-Drop does not introduce any extra parameters or model structure changes during training.

3.4 Application to Language Modeling

Dataset We also evaluate our approach on another widely acknowledged NLP task: language modeling. The dataset we choose for this task is the commonly adopted Wikitext-103 dataset [40], which is the largest available word-level language modeling benchmark with long-term dependency. WikiText-103 contains about 103M training tokens from 28K articles on Wikipedia, and the average length of tokens per article is about 3.6K. The data is preprocessed by following [48].

Model & Training We take two models to conduct the language modeling task. One is the basic Transformer decoder [61], another is the more advanced one: Adaptive Input Transformer [5], which introduces adaptive input embeddings into the Transformer model. We use the open-source Fairseq [48] toolkit, and the corresponding model configurations are transformer_lm_gpt and transformer_lm_wiki103 for Transformer and Adaptive Input Transformer. We set $\alpha=1.0$ for Transformer and 0.5 for Adaptive Input Transformer. Other configurations are same as [48] and [5].

Results The evaluation metric for language modeling is perplexity, which can well measure the probability of a sentence. Same as [5], we report the perplexity on both valid and test sets. The results are shown in Table 5. From the table, we can see that our R-Drop based training improves the perplexity on both two different model structures, e.g., 0.80 perplexity improvement on test set over Adaptive Input Transformer. Besides, more improvement can be achieved when the baseline model is not so strong, e.g., 1.79 perplexity gain on valid set and 1.68 on test set above the Transformer baseline.

Method	Valid	Test
Transformer [61] Transformer + RD	25.76 23.97	26.62 24.94
Adaptive [5] Adaptive + RD	18.94 18.18	18.87 18.07

Table 5: Perplexity results on Wikitext-103 language modeling task. Adaptive refers to Adaptive Input Transformer [5].

3.5 Application to Image Classification

Dataset For image classification, we conduct experiments on two widely acknowledged benchmark datasets, i.e., CIFAR-100 [31] and the ILSVRC-2012 ImageNet dataset [8] (denoted as ImageNet for short). CIFAR-100 dataset consists of 60k images of 100 classes, and there are 600 images per class with 500 for training and 100 for testing. The ImageNet dataset consists of 1.3M image samples of 1,000 categorical classes. We utilize the same data preprocessing strategies with [11], where the details are given in [29].

Model & Training We choose the recent strong and popular Vision Transformer (ViT) [11] model as our backbone. More specifically, we take the two publicly released pre-trained models, ViT-B/16 and ViT-L/16, with 86M and 307M parameters respectively, and we conduct model fine-tuning on the CIFAR-100 and ImageNet datasets. During fine-tuning, the weight α is set as 0.6 for both models, and we set other hyper-parameters/training details to be same as [11].

Results The classification performance is measured by Accuracy, and the results are presented in Table 6. For CIFAR-100, we achieve about 0.65 accuracy improvement over ViT-B/16 baseline, and 0.41 points over ViT-L/16 model. Similarly, on the large-scale ImageNet dataset, consistent improvements are also obtained. These observations demonstrate that our R-Drop can still benefit the model performance even the baseline is powerful. In a word, through the above NLP tasks and this image classification task, we clearly show R-Drop is effective and can be universally applied.

Method	CIFAR-100	ImageNet
ViT-B/16 [11]	92.64	83.97
ViT-B/16 + RD	93.29	84.38
ViT-L/16 [11]	93.44	85.15
ViT-L/16 + RD	93.85	85.57

Table 6: Accuracy on CIFAR-100 and ImageNet classification tasks.

4 Study

Beyond the superior experimental results, in this section, we conduct extensive studies on different perspectives to better understand our R-Drop method. The analysis experiments are performed on the IWSLT14 De→En translation task. More studies can be found in Appendix C.

4.1 Regularization and Cost Analysis

We first show the regularization effect of our R-Drop and study the potential limitation of training cost (as discussed in Section 2.2). Hence, we plot the curves of training/valid loss and valid BLEU along the training update number for Transformer and Transformer + RD models. Besides, we also plot the corresponding curves along the training time (minutes). The curves are shown in Figure 2. We can observe: 1) Along with the training, Transformer quickly becomes over-fitting, and the gap

between train and valid loss of Transformer is large, while R-Drop has a lower valid loss. This well proves that R-Drop can provide persistent regularization during training. 2) At the early training stage, Transformer improves the BLEU score quickly but converges to bad local optima soon. In comparison, R-Drop gradually improves the BLEU score and achieves a much superior performance. Though it needs more training to converge, the final optimum is better. This is same as other regularization methods (e.g., training w/ or w/o dropout). R-Drop indeed increases the training cost at each step since it requires repeating input x for another computation in a mini-batch. Note that this is similar to batch size doubled training without KL-divergence. In Appendix C.1, we conduct this training and show that R-Drop increases negligible cost but with a much stronger performance.

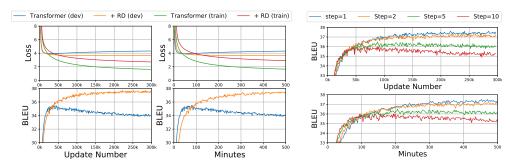


Figure 2: Loss/BLEU curves along with model training.

Figure 3: R-Drop with different step.

4.2 k-step R-Drop

The above study shows that R-Drop can achieve much stronger performance, but with a lower convergence, thus we study another training strategy that is to perform R-Drop every k steps to improve the training efficiency, instead of applying at each step. We vary k in $\{1, 2, 5, 10\}$ to see the difference, where k=1 is the current training strategy. The valid BLEU curves along with training update number and training time are presented in Figure 3. From the curves, we can conclude that though the convergence is faster with larger k, the training fails to fall into good optima, which quickly over-fits, and the BLEU scores become worse and worse when we increase k. This proves that our R-Drop at each step can well regularize the training and obtain superior performances.

4.3 m-time R-Drop

Our method regularizes the model output between two distributions $P_1^w(y|x)$ and $P_2^w(y|x)$, and it is also interesting to see whether more improvements can be achieved if we regularize m distributions for the same input data, where m=2 is the current setting. Therefore, we extend our R-Drop to regularize the output distributions when m=3 for a feasible implementation. The BLEU score for IWSLT14 De \rightarrow En test set is 37.30 when m=3, which is similar to that when m=2 (37.25 BLEU score). This reflects that R-Drop already has a strong regularization effect between two distributions, without the necessity of stronger regularization.

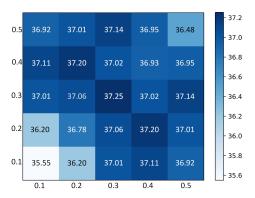


Figure 4: R-Drop with two different dropout rate combinations. Among the 25 numbers, 15 are different since the table is symmetric and triangular.

4.4 Two Dropout Rates

Besides the above studies, we investigate R-Drop from another perspective, i.e., the dropout values. In current training, the two distributions are based on the same dropout value (e.g., 0.3 for IWSLT translations). In this study, we utilize two different dropout values for the two output distributions during training (e.g., 0.1 for $P_1^w(y|x)$, 0.3 for $P_2^w(y|x)$) to see the difference. We choose the two dropout rates from $\{0.1, 0.2, 0.3, 0.4, 0.5\}$ with total 15 (C_5^2 for two different rates + C_5^1 for two

same rates) combinations. The results are shown in Figure 4. Among these different results, we can see that: 1) Dropout rates with the same value (0.3,0.3) is the best choice (current setting), 2) R-Drop can stably achieve strong results when the two dropout rates are in a reasonable range $(0.3 \sim 0.5)$ without a big performance difference. One interesting point is that even the two dropout values are both 0.5, which means half of the units are expected to be dropped, R-Drop can still obtain a satisfied result (36.48 BLEU) compared with the baseline Transformer (34.64 BLEU). These results all confirm the advantage of our R-Drop, and we are interested in studying more in the future.

4.5 Effect of Weight α

Finally, we investigate the impact of the KL-divergence loss weight α . As mentioned in Section 3.1, we set $\alpha=5$ for NMT experiments. Here we vary the α in $\{1,3,5,7,10\}$ and conduct experiments. As shown in Table 7, small α (e.g., 1) can not perform as good as large α (e.g., 5), which means we should pay more attention to the KL-divergence regularization. However, too much regularization ($\alpha=10$) is also not good, and the best balanced choice is $\alpha=5$. Note that the choice of α is distinct for different tasks (e.g., NMT, language understanding), which depends on how easy the over-fitting happens caused by the specific data size and model size of each task.

α	Transformer + RD
$\alpha = 1$	36.05
$\alpha = 3$	36.85
$\alpha = 5$	37.25
$\alpha = 7$	37.20
$\alpha = 10$	36.95

Table 7: BLEU scores with different α .

5 Related Work

Regularization Methods Bigger models always tend to have better performance, especially for various large-scale pre-trained models, e.g., Vision Transformer [11], Swin Transformer [39], GPT families [53, 54, 6], BERT [9], BART [34], Switch Transformers [14], etc. With millions and even billions of parameters, these deep models are prone to over-fitting, thus requiring regularization strategies to improve their generalization ability [33]. To tackle with over-fitting, many regularization techniques have been proposed, e.g., weight decay [32, 30, 27, 67], dropout [23, 62, 4, 64, 59], normalization [26, 55, 3, 25, 71], adding noise [24, 50], layer-wise pre-training and initialization [12, 20], label-smoothing [60], and so on. Among which, dropout and its variants are most popular owing to its effectiveness and moderate cost as well as good compatibility with other regularization methods [44], which has been successfully applied to regularize a wide range of neural network architectures [49], e.g., convolutional neural network layers [68, 10], recurrent neural networks [17, 56, 41], Transformer [73, 79, 69]. The success of dropout methods can be interpreted by preventing co-adaptation of neurons and performing an implicit ensemble of sub models from dropout. Owing to the effect in promoting sparsity of weights and stochastic nature, dropout methods are also adapted to other applications, e.g., neural network compression [43, 45] and model uncertainty estimation [16].

Unlike previous researches of designing specific dropout variants or adapting dropout to different applications, we consider to further regularize the model on the success of dropout. Specifically, any two sub models sampled from dropout are encouraged to produce consistent model prediction for an input data by utilizing KL-divergence in the training stage. That is, we conduct regularization on the model output level. In doing so, the sub model outputs produced by the randomness of dropout are regularized to reduce the parameter freedom, which will enhance generalization in inference.

Self-distillation Minimizing the KL-divergence between the output distributions of two different models correlates with knowledge distillation [22, 15, 2, 35, 13, 78], where the two models refer to teacher and student, respectively. In our setting, the teacher and student are the dropout instantiations of the same model, thus it resembles self-knowledge distillation [42] scenario. Different from existing method that exploits dark knowledge from the model itself [19, 18] or distills knowledge between different layers [75], our strategy can be regarded as an instance-wise self-knowledge distillation, i.e., each pair of sampled sub models perform distillation between each other for the same input, which also relates to mutual learning [76] but ours is much more efficient without extra parameters.

6 Conclusions and Future Work

In this paper, we proposed a simple yet very effective regularization method built upon dropout, namely R-Drop, which minimizes the bidirectional KL-divergence of the output distributions of any pair of sub models sampled from dropout in model training. Experimental results on 18 popular deep learning datasets show that not only can our R-Drop effectively enhance strong models, e.g., ViT, BART, Roberta-large, but also work well on large-scale datasets and even achieve SOTA performances when combined with vanilla Transformer on WMT14 English—German and English—French translations. Due to the limitation of computational resources, for pre-training related tasks, we only tested R-Drop on downstream task fine-tuning in this work. We will test it on pre-training in the future. In this work, we focused on Transformer based models. We will apply R-Drop to other network architectures such as convolutional neural networks.

References

- [1] Armen Aghajanyan, Akshat Shrivastava, Anchit Gupta, Naman Goyal, Luke Zettlemoyer, and Sonal Gupta. Better fine-tuning by reducing representational collapse. *arXiv preprint* arXiv:2008.03156, 2020.
- [2] Zeyuan Allen-Zhu and Yuanzhi Li. Towards understanding ensemble, knowledge distillation and self-distillation in deep learning. *arXiv* preprint arXiv:2012.09816, 2020.
- [3] Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. *arXiv preprint* arXiv:1607.06450, 2016.
- [4] Lei Jimmy Ba and Brendan Frey. Adaptive dropout for training deep neural networks. In *Proceedings of the 26th International Conference on Neural Information Processing Systems-Volume* 2, pp. 3084–3092, 2013.
- [5] Alexei Baevski and Michael Auli. Adaptive input representations for neural language modeling. In *International Conference on Learning Representations*, 2018.
- [6] Tom B Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *arXiv preprint arXiv:2005.14165*, 2020.
- [7] Kevin Clark, Minh-Thang Luong, Quoc V Le, and Christopher D Manning. Electra: Pre-training text encoders as discriminators rather than generators. In *International Conference on Learning Representations*, 2019.
- [8] Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In 2009 IEEE conference on computer vision and pattern recognition, pp. 248–255. Ieee, 2009.
- [9] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pp. 4171–4186, 2019.
- [10] Terrance DeVries and Graham W Taylor. Improved regularization of convolutional neural networks with cutout. *arXiv preprint arXiv:1708.04552*, 2017.
- [11] Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. In *International Conference on Learning Representations*, 2021.
- [12] Dumitru Erhan, Pierre-Antoine Manzagol, Yoshua Bengio, Samy Bengio, and Pascal Vincent. The difficulty of training deep architectures and the effect of unsupervised pre-training. In *Artificial Intelligence and Statistics*, pp. 153–160. PMLR, 2009.

- [13] Zhiyuan Fang, Jianfeng Wang, Lijuan Wang, Lei Zhang, Yezhou Yang, and Zicheng Liu. Seed: Self-supervised distillation for visual representation. *International Conference on Learning Representations*, 2021.
- [14] William Fedus, Barret Zoph, and Noam Shazeer. Switch transformers: Scaling to trillion parameter models with simple and efficient sparsity. *arXiv* preprint arXiv:2101.03961, 2021.
- [15] Tommaso Furlanello, Zachary Lipton, Michael Tschannen, Laurent Itti, and Anima Anandkumar. Born again neural networks. In *International Conference on Machine Learning*, pp. 1607–1616. PMLR, 2018.
- [16] Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pp. 1050–1059. PMLR, 2016.
- [17] Yarin Gal and Zoubin Ghahramani. A theoretically grounded application of dropout in recurrent neural networks. *Advances in neural information processing systems*, 29:1019–1027, 2016.
- [18] Akhilesh Gotmare, Nitish Shirish Keskar, Caiming Xiong, and Richard Socher. A closer look at deep learning heuristics: Learning rate restarts, warmup and distillation. In *International Conference on Learning Representations*, 2019.
- [19] Sangchul Hahn and Heeyoul Choi. Self-knowledge distillation in natural language processing. In *Proceedings of the International Conference on Recent Advances in Natural Language Processing (RANLP 2019)*, pp. 423–430, 2019.
- [20] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In *Proceedings of the IEEE international conference on computer vision*, pp. 1026–1034, 2015.
- [21] Karl Moritz Hermann, Tomáš Kočiskỳ, Edward Grefenstette, Lasse Espeholt, Will Kay, Mustafa Suleyman, and Phil Blunsom. Teaching machines to read and comprehend. *arXiv preprint arXiv:1506.03340*, 2015.
- [22] Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. Distilling the knowledge in a neural network. *arXiv preprint arXiv:1503.02531*, 2015.
- [23] Geoffrey E Hinton, Nitish Srivastava, Alex Krizhevsky, Ilya Sutskever, and Ruslan R Salakhutdinov. Improving neural networks by preventing co-adaptation of feature detectors. *arXiv* preprint arXiv:1207.0580, 2012.
- [24] Sepp Hochreiter and Jürgen Schmidhuber. Simplifying neural nets by discovering flat minima. In *Advances in neural information processing systems*, pp. 529–536, 1995.
- [25] Lei Huang, Xianglong Liu, Bo Lang, Adams Yu, Yongliang Wang, and Bo Li. Orthogonal weight normalization: Solution to optimization over multiple dependent stiefel manifolds in deep neural networks. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018.
- [26] Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In *International conference on machine learning*, pp. 448–456. PMLR, 2015.
- [27] Guoliang Kang, Jun Li, and Dacheng Tao. Shakeout: A new regularized deep neural network training scheme. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 30, 2016.
- [28] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
- [29] Alexander Kolesnikov, Lucas Beyer, Xiaohua Zhai, Joan Puigcerver, Jessica Yung, Sylvain Gelly, and Neil Houlsby. Big transfer (bit): General visual representation learning. *arXiv* preprint arXiv:1912.11370, 6(2):8, 2019.

- [30] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. Advances in neural information processing systems, 25:1097– 1105, 2012.
- [31] Alex Krizhevsky et al. Learning multiple layers of features from tiny images. 2009.
- [32] Anders Krogh and John A Hertz. A simple weight decay can improve generalization. In *Advances in neural information processing systems*, pp. 950–957, 1992.
- [33] Alex Labach, Hojjat Salehinejad, and Shahrokh Valaee. Survey of dropout methods for deep neural networks. *arXiv preprint arXiv:1904.13310*, 2019.
- [34] Mike Lewis, Yinhan Liu, Naman Goyal, Marjan Ghazvininejad, Abdelrahman Mohamed, Omer Levy, Veselin Stoyanov, and Luke Zettlemoyer. Bart: Denoising sequence-to-sequence pretraining for natural language generation, translation, and comprehension. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pp. 7871–7880, 2020.
- [35] Kevin J Liang, Weituo Hao, Dinghan Shen, Yufan Zhou, Weizhu Chen, Changyou Chen, and Lawrence Carin. Mixkd: Towards efficient distillation of large-scale language models. *International Conference on Learning Representations*, 2021.
- [36] Chin-Yew Lin and Eduard Hovy. Manual and automatic evaluation of summaries. In *Proceedings* of the ACL-02 Workshop on Automatic Summarization, pp. 45–51, 2002.
- [37] Xiaodong Liu, Kevin Duh, Liyuan Liu, and Jianfeng Gao. Very deep transformers for neural machine translation. *arXiv preprint arXiv:2008.07772*, 2020.
- [38] Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. Roberta: A robustly optimized bert pretraining approach. *arXiv* preprint arXiv:1907.11692, 2019.
- [39] Ze Liu, Yutong Lin, Yue Cao, Han Hu, Yixuan Wei, Zheng Zhang, Stephen Lin, and Baining Guo. Swin transformer: Hierarchical vision transformer using shifted windows. *arXiv preprint arXiv:2103.14030*, 2021.
- [40] Stephen Merity, Caiming Xiong, James Bradbury, and Richard Socher. Pointer sentinel mixture models. *arXiv preprint arXiv:1609.07843*, 2016.
- [41] Stephen Merity, Nitish Shirish Keskar, and Richard Socher. Regularizing and optimizing lstm language models. In *International Conference on Learning Representations*, 2018.
- [42] Hossein Mobahi, Mehrdad Farajtabar, and Peter L Bartlett. Self-distillation amplifies regularization in hilbert space. *arXiv preprint arXiv:2002.05715*, 2020.
- [43] Dmitry Molchanov, Arsenii Ashukha, and Dmitry Vetrov. Variational dropout sparsifies deep neural networks. In *International Conference on Machine Learning*, pp. 2498–2507. PMLR, 2017.
- [44] Reza Moradi, Reza Berangi, and Behrouz Minaei. A survey of regularization strategies for deep models. *Artificial Intelligence Review*, 53(6):3947–3986, 2020.
- [45] Kirill Neklyudov, Dmitry Molchanov, Arsenii Ashukha, and Dmitry Vetrov. Structured bayesian pruning via log-normal multiplicative noise. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pp. 6778–6787, 2017.
- [46] Xuan-Phi Nguyen, Shafiq Joty, Kui Wu, and Ai Ti Aw. Data diversification: A simple strategy for neural machine translation. In *Advances in Neural Information Processing Systems*, pp. 10018–10029, 2020.
- [47] Myle Ott, Sergey Edunov, David Grangier, and Michael Auli. Scaling neural machine translation. In Proceedings of the Third Conference on Machine Translation: Research Papers, pp. 1–9, 2018.

- [48] Myle Ott, Sergey Edunov, Alexei Baevski, Angela Fan, Sam Gross, Nathan Ng, David Grangier, and Michael Auli. fairseq: A fast, extensible toolkit for sequence modeling. In NAACL-HLT (Demonstrations), 2019.
- [49] Hieu Pham and Quoc V Le. Autodropout: Learning dropout patterns to regularize deep networks. *arXiv preprint arXiv:2101.01761*, 2021.
- [50] Ben Poole, Jascha Sohl-Dickstein, and Surya Ganguli. Analyzing noise in autoencoders and deep networks. *arXiv* preprint arXiv:1406.1831, 2014.
- [51] Matt Post. A call for clarity in reporting bleu scores. In *Proceedings of the Third Conference on Machine Translation: Research Papers*. Association for Computational Linguistics, 2018.
- [52] Weizhen Qi, Yu Yan, Yeyun Gong, Dayiheng Liu, Nan Duan, Jiusheng Chen, Ruofei Zhang, and Ming Zhou. Prophetnet: Predicting future n-gram for sequence-to-sequence pre-training. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: Findings*, pp. 2401–2410, 2020.
- [53] Alec Radford, Karthik Narasimhan, Tim Salimans, and Ilya Sutskever. Improving language understanding by generative pre-training.
- [54] Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.
- [55] Tim Salimans and Diederik P Kingma. Weight normalization: a simple reparameterization to accelerate training of deep neural networks. In *Proceedings of the 30th International Conference on Neural Information Processing Systems*, pp. 901–909, 2016.
- [56] Stanislau Semeniuta, Aliaksei Severyn, and Erhardt Barth. Recurrent dropout without memory loss. In *Proceedings of COLING 2016, the 26th International Conference on Computational Linguistics: Technical Papers*, pp. 1757–1766, 2016.
- [57] Rico Sennrich, Barry Haddow, and Alexandra Birch. Neural machine translation of rare words with subword units. In *Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 1715–1725, 2016.
- [58] Dinghan Shen, Mingzhi Zheng, Yelong Shen, Yanru Qu, and Weizhu Chen. A simple but tough-to-beat data augmentation approach for natural language understanding and generation. *arXiv* preprint arXiv:2009.13818, 2020.
- [59] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1):1929–1958, 2014.
- [60] Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jon Shlens, and Zbigniew Wojna. Rethinking the inception architecture for computer vision. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 2818–2826, 2016.
- [61] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pp. 6000–6010, 2017.
- [62] Li Wan, Matthew Zeiler, Sixin Zhang, Yann Le Cun, and Rob Fergus. Regularization of neural networks using dropconnect. In *International conference on machine learning*, pp. 1058–1066. PMLR, 2013.
- [63] Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel Bowman. Glue: A multi-task benchmark and analysis platform for natural language understanding. In *Proceedings of the 2018 EMNLP Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP*, pp. 353–355, 2018.
- [64] Sida Wang and Christopher Manning. Fast dropout training. In *international conference on machine learning*, pp. 118–126. PMLR, 2013.

- [65] Yue Wang, Yuting Liu, and Zhi-Ming Ma. The scale-invariant space for attention layer in neural network. *Neurocomputing*, 392:1–10, 2020.
- [66] Colin Wei, Sham Kakade, and Tengyu Ma. The implicit and explicit regularization effects of dropout. In *International Conference on Machine Learning*, pp. 10181–10192. PMLR, 2020.
- [67] Wei Wen, Chunpeng Wu, Yandan Wang, Yiran Chen, and Hai Li. Learning structured sparsity in deep neural networks. In *Proceedings of the 30th International Conference on Neural Information Processing Systems*, pp. 2082–2090, 2016.
- [68] Haibing Wu and Xiaodong Gu. Towards dropout training for convolutional neural networks. *Neural Networks*, 71:1–10, 2015.
- [69] Hongqiu Wu, Hai Zhao, and Min Zhang. Not all attention is all you need. *arXiv preprint* arXiv:2104.04692, 2021.
- [70] Lijun Wu, Yiren Wang, Yingce Xia, Fei Tian, Fei Gao, Tao Qin, Jianhuang Lai, and Tie-Yan Liu. Depth growing for neural machine translation. In *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pp. 5558–5563, 2019.
- [71] Yuxin Wu and Kaiming He. Group normalization. In *Proceedings of the European conference on computer vision (ECCV)*, pp. 3–19, 2018.
- [72] Zhilin Yang, Zihang Dai, Yiming Yang, Jaime Carbonell, Russ R Salakhutdinov, and Quoc V Le. Xlnet: Generalized autoregressive pretraining for language understanding. Advances in Neural Information Processing Systems, 32:5753–5763, 2019.
- [73] Lin Zehui, Pengfei Liu, Luyao Huang, Junkun Chen, Xipeng Qiu, and Xuanjing Huang. Dropattention: A regularization method for fully-connected self-attention networks. *arXiv* preprint arXiv:1907.11065, 2019.
- [74] Jingqing Zhang, Yao Zhao, Mohammad Saleh, and Peter Liu. Pegasus: Pre-training with extracted gap-sentences for abstractive summarization. In *International Conference on Machine Learning*, pp. 11328–11339. PMLR, 2020.
- [75] Linfeng Zhang, Jiebo Song, Anni Gao, Jingwei Chen, Chenglong Bao, and Kaisheng Ma. Be your own teacher: Improve the performance of convolutional neural networks via self distillation. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp. 3713–3722, 2019.
- [76] Ying Zhang, Tao Xiang, Timothy M Hospedales, and Huchuan Lu. Deep mutual learning. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp. 4320–4328, 2018.
- [77] Guangxiang Zhao, Xu Sun, Jingjing Xu, Zhiyuan Zhang, and Liangchen Luo. Muse: Parallel multi-scale attention for sequence to sequence learning. arXiv preprint arXiv:1911.09483, 2019.
- [78] Helong Zhou, Liangchen Song, Jiajie Chen, Ye Zhou, Guoli Wang, Junsong Yuan, and Qian Zhang. Rethinking soft labels for knowledge distillation: A bias-variance tradeoff perspective. *International Conference on Learning Representations*, 2021.
- [79] Wangchunshu Zhou, Tao Ge, Furu Wei, Ming Zhou, and Ke Xu. Scheduled drophead: A regularization method for transformer models. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: Findings*, pp. 1971–1980, 2020.
- [80] Jinhua Zhu, Yingce Xia, Lijun Wu, Di He, Tao Qin, Wengang Zhou, Houqiang Li, and Tieyan Liu. Incorporating bert into neural machine translation. In *International Conference on Learning Representations*, 2019.

A Detailed Experimental Settings

We provide more detailed settings for the experiments of each task in this part.

A.1 Neural Machine Translation

For all the NMT tasks, we use the public datasets from IWSLT competitions⁴ and WMT competitions⁵. We tokenize all the datasets with byte-pair-encoding (BPE) [57] approach with the dictionary built jointly upon the source and target sentence pairs except the IWSLT17 En \leftrightarrow Zh translation dataset that is built separately. After tokenization, the resulted vocabularies for IWSLT datasets are near 10k, while for WMT datasets, the vocabulary size is about 32k.

To train the Transformer based NMT models, we use transformer_iwslt_de_en configuration for IWSLT translations, which has 6 layers in both encoder and decoder, embedding size 512, feed-forward size 1,024, attention heads 4, dropout value 0.3, weight decay 0.0001. For the WMT experiments, the transformer_vaswani_wmt_en_de_big setting has 6 layers in encoder and decoder, embedding size 1,024, feed-forward size 4,096, attention heads 16, dropout value 0.1, attention dropout 0.1 and relu dropout 0.1. The training is optimized with Adam [28] with $\beta_1 = 0.9, \beta_2 = 0.98, \epsilon = 10^{-9}$. The learning rate scheduler is inverse_sqrt with default learning rate 0.0005 and warmup steps 4,000. Label smoothing [60] is adopted with value 0.1. Our code implementation is based on open-source Fairseq⁶. We train the IWSLT translations on 1 GEFORCE RTX 3090 card and the WMT translations on 8 GEFORCE RTX 3090 cards.

To evaluate the performance, we use multi-bleu.perl⁷ to evaluate IWSLT14 En \leftrightarrow De and all WMT tasks for a fair comparison with previous works [80, 47]. For other NMT tasks, we use sacre-bleu⁸ [51] for evaluation. When inference, we follow [61] to use beam size 4 and length penalty 0.6 for WMT14 En \rightarrow De, beam size 5 and penalty 1.0 for other tasks.

A.2 Abstrative Summarization

For summarization, we take the pre-trained BART [34] model as backbone and fine-tune on the CNN/DailyMail dataset⁹. BART is a pre-trained sequence-to-sequence model based on the masked source input and autoregressive target output, which contains 12 layers of Transformer encoder and 12 layers of Transformer decoder, the embedding size is 1,024, and the feed-forward size is 4,096. Dropout value is 0.1. During fine-tuning, we follow the hyper-parameters used in [34]. The pre-trained model and the backbone implementations are all from Fairseq¹⁰. The training is conducted on 8 GEFORCE RTX 3090 GPU cards.

A.3 Language Modeling

For language modeling, we train on the Transformer decoder [61] and Adaptive Input Transformer [5] models. The configuration for Transformer is $transformer_lm_gpt$, which contains 12 layers with embedding size 768 and feed-forward size 3, 072, attention heads 12. Dropout and attention dropout are 0.1. For Adaptive Input Transformer, the configuration is $transformer_lm_wiki103$ with 16 layers, embedding size 1,024, feed-forward size 4,096, attention heads 16, dropout 0.3, attention dropout 0.1, gelu dropout 0.1 and adaptive softmax dropout 0.2. We train Transformer model for 50k steps and Adaptive Input Transformer for 286k steps. The development is based on the code base Fairseq¹¹. The training is on 8 Tesla V100 GPU cards.

⁴https://iwslt.org/

⁵https://www.statmt.org/wmt14/translation-task.html

⁶https://github.com/pytorch/fairseq/tree/master/examples/translation

Thttps://github.com/moses-smt/mosesdecoder/blob/master/scripts/generic/multi-bleu.perl

⁸https://github.com/mjpost/sacrebleu

⁹https://github.com/abisee/cnn-dailymail

¹⁰ https://github.com/pytorch/fairseq/tree/master/examples/bart

¹¹https://github.com/pytorch/fairseq/tree/master/examples/language_model

Hyper-parameter	CoLA	MRPC	RTE	SST-2	MNLI	QNLI	QQP	STS-B
Learning Rate	1e-5	1e-5	1e-5	1e-5	1e-5	1e-5	1e-5	1e-5
Max Update	5336	2296	3120	20935	123873	33112	113272	3598
Max Sentence (Batch)	16	16	8	32	32	32	32	16
Dropout	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Coefficient α	0.5	1.0	1.0	1.0	0.5	1.0	0.5	1.0

Table 8: Hyper-parameters when fine-tuning our models on GLUE benchmark.

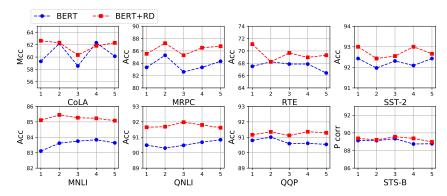


Figure 5: Results on 8 GLUE tasks with different random seed.

A.4 Language Understanding

For language understanding tasks, we follow the popular pre-training and fine-tuning methodology, and the fine-tuned sets are the GLUE [63] benchmark. We follow previous works [7, 38] to work on the 8 tasks, including singe-sentence classification tasks (CoLA, SST-2), sentence-pair classification tasks (MNLI, QNLI, RTE, QQP, MRPC), and sentence-pair regression task (STS-B). The detailed data statistics can be found from the original paper [63].

The pre-trained BERT-base model is the Transformer [61] encoder network, which contains 12 layers with embedding size 768, feed-forward size 3,072 and attention heads 12. Correspondingly, the Roberta-large model contains 24 layers with embedding size 1,024, feed-forward size 4,096 and attention heads 16. During fine-tuning, we use Adam [28] as our optimizer with $\beta_1 = 0.9$, $\beta_2 = 0.98$, $\epsilon = 10^{-6}$, and L_2 weight decay of 0.01. We select the learning rate in range $\{5 \times 10^{-6}, 10^{-5}\}$ and batch size in $\{8, 16, 32\}$. Other hyper-parameter settings are mostly same as previous works [38]. The pre-trained model and the backbone implementations are all from Huggingface Transformers 12. We report the specific settings of several important hyper-parameters in Table 8, including the dropout value. The fine-tuning experiments are conducted on 1 GEFORCE RTX 3090 GPU card.

Further, to give a clear comparison of our R-Drop based fine-tuning and vanilla fine-tuning, we plot the performance changes from different random seeds over the pre-trained BERT model on each GLUE task. The curves are shown in Figure 5. We can see that consistent improvements are achieved on different random seeds, which means our R-Drop can robustly help improve the mode generalization and model performance.

MSE Regularization Our R-Drop is presented under the KL-divergence between two distributions. To extend our method into the regression task, such as STS-B in GLUE, we introduce the MSE-based regularization. For input data (x, y), we forward the x two times similarly as in classification and obtain the two predicted values y_1' and y_2' . Then we regularize these two predicted values with MSE as follow:

$$\mathcal{L}_{mse_r} = ||y_1' - y_2'||_2,\tag{7}$$

¹²https://github.com/huggingface/transformers

and we add \mathcal{L}_{mse_r} with conventional MSE loss: $\mathcal{L}_{mse} = ||y - y_1'||_2 + ||y - y_2'||_2$. The final optimization objective is:

$$\mathcal{L} = \mathcal{L}_{mse} + \alpha \mathcal{L}_{mse_r}. \tag{8}$$

A.5 Image Classification

The image classification task is evaluated with the recent popular Vision Transformer (ViT) [11] model, which is the same as Transformer but with the image patch data as input. We take the two publicly released models 13 , ViT-B/16 and ViT-L/16, which are pre-trained on ImageNet-21k [8] dataset with 21k classes and 14M images in total. ViT-B/16 is a Transformer model with 12 Transformer encoder layers, embedding size 768, feed-forward size 3,072 and attention heads 12, while ViT-L/16 with 24 layers, 1,024 embedding size, 4,096 feed-forward size and 16 attention heads. We only conduct the fine-tuning stage experiments on CIFAR-100 and ImageNet. Note that the ImageNet results are computed without additional techniques (Polyak averaging and 512 resolution images) used to achieve results in [11]. During fine-tuning, the dropout values are 0.1 for both models. Fine-tuning is on 8 GEFORCE RTX 3090 GPU cards.

B Theoretical Discussion of R-Drop

For self-contained, we reformulate the constrained optimization problem as:

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\xi} \left[-\log \mathcal{P}_{\xi}^{w}(y_i|x_i) \right], \tag{9}$$

s.t.
$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\xi^{(1)}, \xi^{(2)}} [\mathcal{D}_{KL}(\mathcal{P}_{\xi^{(1)}}^{w}(y_i|x_i)||\mathcal{P}_{\xi^{(2)}}^{w}(y_i|x_i)))] = 0.$$
 (10)

For a multi-layer perceptron (MLP) with dropout, its output is represented as:

$$\mathcal{P}_{\xi}(y|x) = \text{softmax}(vh_{\xi^L}^L); \quad h_{\xi^l}^l = \xi^l \odot \sigma(w^l h_{\xi^{l-1}}^{l-1}), l = 1, \cdots, L; \quad h_{\xi^0}^0 = \xi_0 \odot x, \qquad (11)$$

where $\sigma(\cdot)$ is the activation function.

We also consider the MLP with skip/residual connections (which is more popular than plain MLP), whose output after dropout is represented as:

$$\mathcal{P}_{\xi}^{res}(y|x) = \operatorname{softmax}(vh_{\xi^L}^L); \quad h_{\xi^l}^l = \xi^l \odot \sigma(w^l h_{\xi^{l-1}}^{l-1}) + h_{\xi^{l-1}}^{l-1}, l = 1, \cdots, L; \quad h_{\xi^0}^0 = \xi_0 \odot x. \tag{12}$$

For a Transformer model, the output can be represented as:

$$z = SA(Q, K, V) = \operatorname{softmax}\left(\frac{(Qw_1)(Kw_2)^T}{\sqrt{d}}\right) Vw_3, \tag{13}$$

$$f(z) = v_2 \max(0, v_1 z), \tag{14}$$

where v_1, v_2, w_1, w_2, w_3 are learnable parameters, $SA(\cdot)$ stands for self-attention operation, and $f(\cdot)$ is the position-wise feed-forward network as described in Transformer [61]. We only consider dropout inside the self-attention layer, i.e.,

$$z_{\xi} = SA(Q, K, V) = \left(\xi_2 \odot \operatorname{softmax}\left(\frac{((\xi_1 \odot Q)w_1)((\xi_1 \odot K)w_2)^T}{\sqrt{d}}\right)\right)((\xi_1 \odot V)w_3), \quad (15)$$

$$f(z_{\xi}) = v_2 \max(0, (v_1 z_{\xi_1})), \tag{16}$$

$$\mathcal{P}_{\varepsilon}^{TF}(y|x) = \text{softmax}(f(z_{\varepsilon})), \tag{17}$$

where the size of random matrix ξ_1 equal to the size of Q^{14} , and the size of ξ_2 equal to the size of the value after softmax.

Now we provide the proof for the next proposition. Here, we consider a sampling strategy called dropout₂, which randomly samples p portion of hidden neurons at each layer. Thus, this strategy can keep the width for the sampled sub-structure and avoid extremely thin sub-structures.

¹³https://github.com/jeonsworld/ViT-pytorch

¹⁴Please note that for self-attention, Q = K = V.

Proposition B.1. For a fully-connected neural network $\mathcal{P}^w(y|x)$, e.g., multilayer perceptron and Transformer, the constraint in Equation (10) is equivalent to constraining all the parameters of the network at the same layer to be equal.

Proof: We consider two sub-structures \mathcal{P}_1 and \mathcal{P}_2 that differ from each other at only one hidden node. Without loss of generality, we suppose the hidden node that is only contained in \mathcal{P}_1 as h_i^l and the hidden node that is only contained in \mathcal{P}_2 as h_i^l .

Since we constrain the $KL(\mathcal{P}_1||\mathcal{P}_2)=0, \forall x$, which is equivalent to $\mathcal{P}_1(y|x)=\mathcal{P}_2(y|x), \forall x$. Then we have $h_i^l=h_j^l, \forall x$. If not, we can construct an $x\in\mathbb{R}^d$ to make their final output unequal¹⁵. Because the two sub-structures share the other hidden nodes, the inputs of h_i^l and h_j^l are the same, i.e., $h_i^l=\sigma(\tilde{w}_i^l\tilde{h}^{l-1}), h_j^l=\sigma(\tilde{w}_j^l\tilde{h}^{l-1}),$ where w_i denotes the ingoing weights of h_i^l and we use the subscript to denote the hidden output and weight matrix after the dropout. Then, we have $\tilde{w}_i^l=\tilde{w}_j^l$. Traversing all the paired sub-structures (produced by dropout₂) that differ at only one hidden node, we can get that all the parameters at the same layer are equal.

Similarly, for the Transformer model, we can also get the results in the above Proposition, but it is established by removing the redundancy in weights. In detail, the weights w_1 and w_2 have redundant freedom due to the scaling invariant property of $Qw_1(Kw_2)^T$ [65], i.e., If we regard w_1 and w_2 as two linear layers of MLP, the ingoing weights of one hidden node are multiplying a scalar c and its outgoing weights are dividing by c, the resulted output will not change. To remove the redundancy, we fix the first column in w_1 (one ingoing weight for each hidden node) to have the same value. Then Proposition B.1 is established for w_1, w_2, w_3 .

Remark: Although Proposition B.1 is established for a different sampling strategy with original dropout, it will approach to the result for original dropout **with high probability** because the mean portion of the sampled neurons will be closed to p according to central limit theorem.

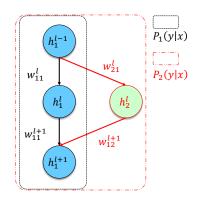


Figure 6: Example of MLP in 1).

Proposition B.1 can be regarded as a result of original dropout in the sense of high probability. Next, we briefly discuss what will happen if we consider the original sampling strategy in dropout. Since the original strategy contains more sub-structures, it actually brings a much stronger restriction to the model. For example, the model has the chance to degenerate to a zero mapping.

1) For MLP: If we consider the original sampling strategy in dropout, the constraint of Equation (4) is equivalent to constraining one layer of the MLP to be zero. We can consider an extreme sub-structure that there is only one hidden node after dropout and denote its output as:

$$\mathcal{P}_1(y|x) = \mathtt{softmax}(vh_1^L); \quad h_1^l = \sigma(w_{11}^l h_1^{l-1}), l = 1, \cdots, L; \quad h_1^0 = x_1,$$

where h_1^l denotes the 1-th hidden node at layer l and w_{11}^l denotes the weights that connects h_1^{l-1} and h_1^l . Then we consider another sub-structure $\mathcal{P}_2(y|x)$ which has one more hidden node at layer l (denoted as h_2^l) than $\mathcal{P}_1(y|x)$, i.e.,

$$h_2^l = \sigma(w_{21}^l h_1^{l-1}); h_1^{l+1} = \sigma(w_{11}^{l+1} h_1^l + w_{12}^{l+1} h_2^l),$$

and other computations are the same as the calculation of $\mathcal{P}_1(y|x)$ (see the example in Figure 6). Therefore, the sub-structure \mathcal{P}_2 has two additional parameters w_{12}^{l+1} and w_{21}^{l} compared with the sub-structure \mathcal{P}_1 , and they share weights on w_{11}^{l} , $l=1,\cdots,L$. Because we constrain the $KL(\mathcal{P}_1||\mathcal{P}_2)=0, \forall x$, which is equivalent to $\mathcal{P}_1(y|x)=\mathcal{P}_2(y|x), \forall x$. Therefore, we need $\sigma(w_{11}^{l+1}h_1^l+w_{12}^{l+1}h_2^l)=\sigma(w_{11}^{l+1}h_1^l), \forall x$. Then we must have $w_{12}^{l+1}=0$ or $w_{21}^{l}=0$. Similarly, we can traverse all such extreme cases to get the results.

2) For MLP with skip/residual connections: Using the similar technique in 1), if we consider the MLP with skip connection $\mathcal{P}^{res}_{\xi}(y|x)$ and the original sampling strategy in dropout, the constraint in

¹⁵Here, we suppose the activation function σ satisfies that $w^2\sigma(w^1x)=\tilde{w^2}\sigma(\tilde{w}^1x), \forall x$ if and only if $w^2=\tilde{w^2}, w_1=\tilde{w}^1$.

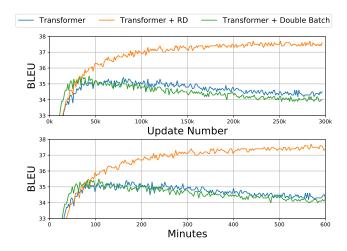


Figure 7: Results of R-Drop and Transformer with double batch.

Equation (4) is equivalent to constraining all the parameters equals zero. The network will degenerate to an identity mapping of x.

C More Studies

C.1 Batch Size Doubled Training

As discussed in Section 2.2, we implement the algorithm by repeating input data x once and concatenate the x with repeated one in the same mini-batch to forward once. This is similar to enlarge the batch size to be double size at each step. The difference is that half of the data are the same as the other half, while directly doubling the batch size, the data in the same mini-batch are all different. Therefore, we are still interested in the result of directly doubling the batch size to and the batch size is enlarged from 4,096 to be 8,192. The result is 34.93 BLEU score. We can see that though slight improvement is achieved (compared to baseline 34.64), it falls far behind our strong performance 37.25. For the detailed training cost for each step, we represent the number here: Transformer + Double Batch costs near 9ms per step, while Transformer + DR costs about 10ms per step. The additional cost is from the KL-divergence loss backward computation. We can see the cost is 1.1 times, which is a negligible cost. We also plot the valid BLEU curves along with the training for this study. The curves are shown in Figure 7. Compare to this batch size doubled training and our R-Drop, we can clearly see the advantage of R-Drop. With similar training cost, R-Drop gradually improves the performance to a much stronger one. In the figures, we also plot the curve for Transformer with the original batch size training (e.g., 4,096) for a better comparison.

C.2 Importance of KL-divergence

Our method introduces a KL-divergence between the two distributions from the same sample. In this study, we specifically investigate the importance of KL-divergence loss. Thus, this ablation removes the \mathcal{L}_{KL} loss between the two distributions and only keeps the \mathcal{L}_{NLL} loss for training. Similar to other studies, we work on IWSLT14 De \rightarrow En translation, and the model is Transformer. The result is also 34.93 BLEU score (same as above enlarge batch size), which is slightly better than the Transformer baseline (34.64), but far worse from our R-Drop based training result 37.25 BLEU score. This result well demonstrates the importance and effectiveness of our introduced KL-divergence loss.