Abstract

Fine-tuning pre-trained language models (PTLMs), such as BERT and its better variant RoBERTa, has been a common practice for advancing performance in natural language understanding (NLU) tasks. Recent advance in representation learning shows that isotropic (i.e., unit-variance and uncorrelated) embeddings can significantly improve performance on downstream tasks with faster convergence and better generalization. The isotropy of the pre-trained embeddings in PTLMs, however, is relatively under-explored. In this paper, we analyze the isotropy of the pre-trained [CLS] embeddings of PTLMs with straightforward visualization, and point out two major issues: high variance in their standard deviation, and high correlation between different dimensions. We also propose a new network regularization method, isotropic batch normalization (IsoBN) to address the issues, towards learning more isotropic representations in fine-tuning. This simple yet effective fine-tuning method yields about 1.0 absolute increment on the average of seven benchmark NLU tasks.

1 Introduction

Pre-trained language models (PTLMs), such as BERT (Devlin et al., 2019) and RoBERTa (Liu et al., 2019b), have revolutionized the area of natural language understanding (NLU). Fine-tuning PTLMs has advanced performance on many benchmark NLU datasets such as GLUE (Wang et al., 2018a). The most common fine-tuning method is to continue training pre-trained model parameters together with a few additional task-specific layers. The PTLMs and task-specific layers are usually connected by the embeddings of [CLS] tokens, which are regarded as sentence representations.

Recent works on text representation (Arora et al., 2016; Mu et al., 2018; Gao et al., 2019; Wang et al., 2020) have shown that regularizing word embeddings to be more isotropic (i.e., rotational invariant) can significantly improve their performance on downstream tasks. An ideally isotropic embedding space has two major merits: a) all dimensions have the same variance and b) all dimensions are uncorrelated with each other. These findings align with conventional feature normalization techniques (Cogswell et al., 2015; Ioffe and Szegedy, 2015; Huang et al., 2018), which aim to transform input features into normalized, uncorrelated representations for faster convergence and better generalization ability.

It, however, remains an open question that how isotropic the representations of PTLMs are. Particularly, we want to understand the isotropy of pre-trained [CLS] embeddings in PTLMs, and how we can improve it towards better fine-tuning for downstream tasks. In this paper, we first analyze the isotropy of the pre-trained [CLS] embeddings. There are two essential aspects of an isotropic embedding space: unit-variance and uncorrelatedness. Thus, we start our analysis by visualizing the standard deviation and Pearson correlation coefficient of pre-trained [CLS] embeddings in BERT and RoBERT on several NLU datasets.

Our visualization and quantitative analysis in Section 2 finds that: 1) the [CLS] embeddings have very different variance (Sec. 2.1); 2) the [CLS] embeddings construct a few large clusters of dimensions that are highly correlated with each other (Sec. 2.2). Both findings indicate that pre-trained contextualized word embeddings are far from being isotropic, i.e., normalized and uncorrelated. Therefore, these undesired prior bias from PTLMs may result in sub-optimal performance in fine-tuning for target tasks.

Given that pre-trained [CLS] embeddings are

1https://github.com/INK-USC/IsoBN/
very anisotropic, a natural research question is then: how can we regularize the fine-tuning process towards more isotropic embeddings?

There are two common methods for improving the isotropy of feature representations: whitening transformation and batch normalization (Ioffe and Szegedy, 2015). However, both are not practically suitable in the scenario of fine-tuning PTLMs. Whitening transformation requires calculating the inverse of the covariance matrix, which are ill-conditioned in PTLMs’ embeddings. Unfortunately, calculating the inverse is thus numerically unstable, computationally expensive, and incompatible in half-precision training. Batch normalization is proposed to alleviate the inverse-computation issue by assuming that the covariance matrix is diagonal, which in turn completely ignores the influence of correlation between dimensions.

Motivated by the research question and limitations of existing works, we propose a new network regularization method, isotropic batch normalization (IsoBN) in Section 3. The proposed method is based on our observation that the embedding dimensions can be seen as several groups of highly-correlated dimensions. Our intuition is thus to assume that the absolute correlation coefficient matrix is a block-diagonal binary matrix, instead of only a diagonal matrix. The dimensions of the same group have an absolute correlation coefficient of 1 (duplicate of each other), and dimensions in different group of 0 (uncorrelated).

This method greatly reduces the computation efforts in calculating the inverse, and better models the characteristics of the pre-trained [CLS] embeddings. Our experiments (Sec. 4) show that the IsoBN indeed improves both BERT and RoBERTa in fine-tuning, yielding about 1.0 absolute increment on average of a wide range of 7 GLUE benchmark tasks. We also empirically analyze the isotropy increment brought by IsoBN via explained variance, which clearly shows that IsoBN produces much more isotropic embeddings than conventional batch normalization method.

To the best of our knowledge, this work is the first one in studying the isotropy of the pre-trained [CLS] embeddings. We believe our findings and the proposed IsoBN method will inspire interesting future research directions in improving pre-training language models as well as better fine-tuning towards more isotropy of PTLMs.

2 How isotropic are [CLS] embeddings?

The [CLS] embeddings of PTLMs, regarded as sentence representations, are directly used for fine-tuning (e.g., BERT and RoBERTa) towards a wide range of downstream tasks. Given its impact in fine-tuning, we want to understand their isotropy. As we know unit-variance and uncorrelatedness are two essential aspects of an isotropy space, we start our investigation by analyzing the standard deviation and Pearson correlation coefficient.
Figure 2: Absolute Pearson correlation coefficients between dimensions of pre-trained [CLS] embeddings. We show the results of BERT-base-cased and RoBERTa-Large on four NLU datasets. Note that the dimension indexes of the matrices are re-arranged by the clustering results. Ideally, an isotropic embedding space should be 1 (darkest blue) on the diagonal and 0 on (white) other cells. A dark block in a matrix means a cluster of features that are highly correlated with each other.

Specifically, we take the corpus of four popular NLU tasks (MRPC, RTE, COLA, and STS-b) from the GLUE benchmark datasets (Wang et al., 2018b) and then analyze their pre-trained [CLS] embeddings in terms of standard deviation (Section 2.1) and correlation (Section 2.2) respectively.

2.1 Analysis of Standard Deviation

To visualize the standard deviation of embeddings, we take the input sentences of the whole training dataset to PTLMs, then calculate the standard deviation on their [CLS] embeddings, and finally obtain the distribution.

The standard deviation of a nearly isotropic embedding space should concentrate on a very small range of values. Simply put, an ideally isotropic embedding space should have a small variance of the distribution of their standard deviation, i.e., all dimensions of [CLS] embeddings should have almost the same standard deviation.

As shown in Figure 1, we can see that both BERT and RoBERTa do not have such desired property for pre-trained [CLS] embeddings. The standard deviations of the embeddings vary in a very wide range of values (e.g., \([10^{-10}, 1]\) in BERT for MRPC). Interestingly, we can see that RoBERTa is evidently better than BERT from this perspective (e.g., usually ranging in \([0.01, 1]\)). However, the [CLS] embeddings of RoBERTa are still far from being isotropic, as there is no significantly dominant centering standard deviation value.

2.2 Analysis of Correlation Coefficient

Correlation between different dimensions of [CLS] embeddings is an essential aspect of isotropy. Embeddings with low correlation between dimensions usually show better generalization on downstream applications (Cogswell et al., 2015). It, however, is relatively ignored by many neural network regularization methods, such as batch normalization (Ioffe and Szegedy, 2015).

In order to better visualize the Pearson correlation coefficient of [CLS] embeddings, we cluster the dimensions by their pairwise coefficient, and then re-arrange the dimension index, such that highly correlated dimensions locate near each other. The absolute value of correlations are shown in Figure 2, where darker cells means higher correlation.

We can see that both BERT and RoBERTa usually have very high correlations between different dimensions (i.e., most cells are in dark blue), although the situation is less severe in a few cases such as BERT on CoLA and RoBERTa on RTE. We find that BERT’s embeddings have several large clusters of correlated features, while RoBERTa tends to have a single extreme large cluster.

In either case, such high correlation between embedding dimensions is harmful to future fine-tuning. Recall that the [CLS] embeddings are usually connected to a linear classifier which is
uniformly initialized. In the beginning of the fine-
tuning process, the classifier will be biased to these
features since they gain more importance in back-
propagation. This undesired prior prevents models
to exploit other potentially value features, and thus
require more training data or epochs to converge and generalize in downstream tasks.

2.3 Summary of the Analysis
Based on our analysis and visualization, we find
that the pre-trained [CLS] embeddings of both
BERT and RoBERTa have:
- high variance in the distribution of dimensions
  on their standard deviation.
- large clusters of dimensions that are highly
correlated with each other.

We argue that these two findings together indi-
cate that pre-trained language models are far from
being isotropic (i.e., normalized and uncorrelated),
and thus undesired prior bias may result in sub-
optimal model performance for fine-tuning.

3 Approach
Based on our analysis in Section 2, we propose
a new regularization method, isotropic batch nor-
malization towards learning more isotropic repre-
sentations of the [CLS] tokens for better fine-
tuning PTLMs. We first introduce some back-
ground knowledge about whitening and conven-
tional batch normalization (Section 3.1), then for-
mally introduce the proposed IsoBN (Section 3.2),
and finally show the implementation details (Sec-
tion 3.3).

3.1 Whitening and Batch Normalization
To improve the isotropy of feature representations,
there are two widely-used methods: 1) whitening
transformation and 2) batch normalization (Ioffe
and Szegedy, 2015).

Whitening transformation changes the input
vector into a white noise vector, and can be defined
as a transformation function as follows:
\[ \hat{h} = \Sigma^{-\frac{1}{2}} (h - \mu \cdot 1^T), \]
where \( \Sigma \in \mathbb{R}^{d \times d} \) is the covariance matrix of
the input \( h \in \mathbb{R}^{d \times N} \), \( \mu \in \mathbb{R}^d \) is the mean of
\( h \). Thus, the transformation is a mapping from
\( \mathbb{R}^{d \times N} \rightarrow \mathbb{R}^{d \times N} \). This transformation produces
a perfectly isotropic embedding space, where the
dimensions are uncorrelated and have the same
variance. It can be applied in either feature pre-
processing (Rosipal et al., 2001) or neural network
training (Huang et al., 2018). A similar method is
to remove a few top principal components from the
embedding (Arora et al., 2016; Mu et al., 2018).

However, these methods are hard to apply in
fine-tuning pre-trained language models, as they
require calculating the inverse of the covariance
matrix. As shown in Section 2.2, the embeddings
in PTLMs contain groups of highly-correlated di-
mensions. Therefore, the covariance matrices are
ill-conditioned, and calculating the inverse is thus
numerically unstable. In addition, calculating the
inverse is computationally expensive and incompat-
ible in half-precision training.

Batch normalization (BN) aims to simplify the
inverse-computation problem by assuming that the
covariance matrix is diagonal, thus the whitening
function becomes:
\[ \hat{h} = \Lambda^{-1} (h - \mu \cdot 1^T), \]
where \( \Lambda = \text{diag}(\sigma_1, ..., \sigma_d) \) is a diagonal matrix
consisting the standard deviation of each input di-
menion. Batch normalization greatly improves the
stability and model performance in training deep
neural networks.

However, it completely ignores the influence of
correlation in the embeddings, and thus not suitable
for our interested [CLS] embeddings, where high
correlation is a critical issue that needs to be ad-
dressed. We seek to design a novel normalization
method specially for fine-tuning PTLMs, which
can be efficiently computed yet still improve repre-
sentations towards isotropy property.

3.2 Isotropic Batch Normalization
Recall Figure 2, from the correlation matrix of
pre-trained embeddings, we observe that on most
datasets, the correlation matrix is nearly block-
diagonal\(^3\). That is, the embedding dimensions
form several clusters of highly-correlated di-
mensions. Dimensions within the same cluster have an
absolute correlation coefficient of nearly 1, while
dimensions from different clusters are almost un-
correlated. Inspired by this, we propose an en-
hanced simplification of the covariance matrix.

We assume that the absolute correlation coeffi-
cient matrix is a block-diagonal binary matrix.

\(^3\)A block diagonal matrix is a block matrix that is a square
matrix such that the main-diagonal blocks are square matrices
and all off-diagonal blocks are zero matrices.
That is, the embedding dimensions can be clustered into $m$ groups $G_1, \ldots, G_m$, where dimensions of the same group have an absolute correlation coefficient of 1 (duplicate of each other), and dimensions in different group have a correlation coefficient of 0 (uncorrelated). This assumption is illustrate in Figure 3 as a conceptual comparison. Comparing with the conventional batch normalization, our assumption takes accounts of correlations and thus is an more accurate approximation of the realistic correlation coefficient matrices. Thereby, instead of whitening the correlation matrix, we want the influence of each group of dimensions similar in the fine-tuning process.

We first normalize each dimension to unit-variance, similar to batch normalization, for convenience of further derivation. This makes the dimensions in the same group exactly same to each other. Then, for dimension $i \in G_{g(i)}$, it is repeated in embeddings by $|G_{g(i)}|$ times. Therefore, the normalization transformation becomes:

$$\hat{h}^{(i)} = \frac{1}{\sigma_i \cdot |G_{g(i)}|} (h^{(i)} - \mu_i \cdot 1^T). \quad (3)$$

The dimensions of embeddings, however, are not naturally separable into hard group divisions. Thus, we create a soft version of computing the size of a feature-group $|G_{g(i)}|$ via the correlation coefficient matrix $\rho$:

$$|G_{g(i)}| \xrightarrow{\sim} \gamma_i = \sum_{j=1}^{d} \sigma_{ij}^2. \quad (4)$$

This equation produces the same result as $|G_{g(i)}|$ when our assumption holds in real correlation matrix. Finally, our transformation can be written as:

$$\hat{h}^{(i)} = \frac{1}{\sigma_i \cdot \gamma_i} (h^{(i)} - \mu_i \cdot 1^T). \quad (5)$$

The major difference between our method and conventional batch normalization is the introduction of the $\gamma$ term, as a way to explicitly consider correlation between feature dimensions. As shown in our experiments (Section 4), $\gamma$ can greatly improve the isotropy of embedding. We name our proposed normalization method as isotropic batch normalization (IsoBN), as it is towards more isotropic representations during fine-tuning.

### 3.3 Implementation Details

We use IsoBN before the classifier in fine-tuning PTLMs. In experiments, we find that the original form of IsoBN performs poorly on some tasks. We observe that:

- Subtracting the mean $\mu$ from $[CLS]$ embedding hurts fine-tuning performance on datasets with unbalanced class labels. We hypothesize that $\mu$ is related to the learning of the bias of the classifier. Removing the mean will slow down the learning of classifier bias.
- The optimal normalization strength varies from model and datasets.
- The scale of computed scaling term $(\sigma \cdot \gamma)^{-1}$ is very small, which causes the transformed embedding close to 0.

To solve the above problems, we remove the bias term from normalization. For the scaling term, we add a hyper-parameter $\beta$ to control its normalization strength, and re-normalize it to make the sum of variances in transformed embeddings unchanged. The final transformation function is defined as:

$$\theta_i = (\sigma_i \cdot \gamma_i + \epsilon)^{-\beta}, \quad (6)$$

$$\bar{\theta} = \frac{\sum_{i=1}^{d} \sigma_i^2 \theta^2_i}{\sum_{i=1}^{d} \sigma_i^2 \theta_i}, \quad (7)$$

$$\hat{h} = \bar{\theta} \odot h. \quad (8)$$

In IsoBN, we use the covariance matrix and standard deviation to calculate the scaling factor. We maintain their moving statistics and update them in training. The whole process is shown in Algorithm 1. Compared to decorrelated batch normalization, our method does not calculate the inverse matrix, which is more efficient in training speed.

### 4 Evaluation

In this section, we first present the setup of our experiments (i.e. the datasets, frameworks, and hyper-parameters), then discuss the empirical results, and finally evaluate the isotropy gain through the lens of explained variance.
Table 1: Empirical results on the dev sets of seven GLUE tasks. We run 5 times with different random seeds and report median and the std. IsoBN consistently improves the performance around 1.0 absolute increment on Avg.

4.1 Experiment Setup

Our implementation of PTLMs is based on HuggingFace Transformer (Wolf et al., 2019). The model is fine-tuned with AdamW (Loshchilov and Hutter, 2017) optimizer using a learning rate in the range of \(1 \times 10^{-5}, 2 \times 10^{-5}, 5 \times 10^{-5}\) and batch size in \{16, 32\}. The learning rate is scheduled by a linear warm-up (Goyal et al., 2017) for the first 6% of steps followed by a linear decay to 0. The maximum number of training epochs is set to 10. For IsoBN, the momentum \(\alpha\) is set to 0.95, the \(\epsilon\) is set to 0.1, and the normalization strength \(\beta\) is chosen in the range of \{0.25, 0.5, 1\}.

We apply early stopping according to task-specific metrics on the dev set. We select the best combination of hyper-parameters on the dev set. We fine-tune the PTLMs with 5 different random seeds and report the median and standard deviation of metrics on the dev set.

4.2 Experimental Results

We evaluate IsoBN on two PTLMs (BERT-base-cased and RoBERTa-large) and seven NLU tasks from the GLUE benchmark (Wang et al., 2018b). The experiments results are shown in Table 1. Using IsoBN improves the evaluation metrics on all datasets. The average score increases by 1% for BERT-base and 0.8% for RoBERTa-large. For small datasets (MRPC, RTE, CoLA, and STS-B), IsoBN obtains an average performance improvement of 1.6% on BERT and 1.3% on RoBERTa. For large datasets (MNLI, QNLI, and SST-2), IsoBN obtains an average performance improvement of 0.15% on BERT and 0.25% on RoBERTa. This experiment shows that by improving the isotropy of embeddings, our IsoBN results in better fine-tuning performance.

4.3 Experiments of EV\(_k\) Metric

To quantitatively measure the isotropy of embeddings, we propose to use explained variance (EV) as the metric for isotropy, which is defined as:

\[
EV_k(h) = \frac{\sum_{i=1}^{k} \lambda_i^2}{\sum_{j=1}^{d} \lambda_j^2},
\]

where \(h \in \mathcal{R}^{N \times d}\) is the [CLS] embeddings, \(\sigma_i\) is the \(i^{th}\) largest singular value of the matrix \(h\). Note that \(N\) is the number of sentences in a certain corpus, and \(d\) is the dimension of hidden states in the last layer of a pre-trained language model.

This metric measures the difference of variance in different directions of the embedding space. Intuitively, if the \(EV_k\) value is small, the variations of embedding tend to distribute equally in all directions and lead to more angular symmetric representation. If the \(EV_k\) value is large, most of the variations will concentrate on the first few directions, and the embedding space will degrade to a narrow cone. Thus, the \(EV_k\) is a good metric of the isotropy of embedding space.
We use $EV_k$ as the isotropy metric because it enjoys two beneficial properties:

- It is invariant to the magnitude of the embeddings, and thus comparisons between different models and datasets is more fair.
- It is also invariant to the mean value of the embeddings, aligning with sentence classification/regression tasks of our interest.

We compute the $EV_k$ metric on two PTLMs (BERT-base-case and RoBERTa-large) and four NLU tasks (MRPC, RTE, CoLA, STS-B). For IsoBN, the normalization strength $\beta$ is set to 1. We show the first three $EV_k$ value ($EV_1$, $EV_2$, and $EV_3$) in Table 2.

We observe that before normalization, the pre-trained [CLS] embeddings have very high $EV_k$ value. The average $EV_3$ value is around 0.86 for both BERT-base and RoBERTa-large. For some datasets (e.g. STS-b), the top three principal components already explain over 90% of the variance. Batch normalization can only reduce the $EV_k$ value by a small margin (0.025 for BERT and 0.148 for RoBERTa on $EV_3$), because it ignores the correlations among embedding dimensions. Our proposed IsoBN greatly reduces the $EV_k$ value (0.123 for BERT and 0.425 for RoBERTa on $EV_3$).

We also visualize the distribution of $EV_k$ values in Figure 4. We choose the first 50 $EV_k$ value for BERT-base and first 200 $EV_k$ value for RoBERTa-large. We observe that with IsoBN, we can decrease the $EV_k$ value of pre-trained embeddings. This experiment shows that compared to batch normalization, IsoBN can further improve isotropy of [CLS] embedding of PTLMs.

### Table 2: The explained variance on BERT-base and RoBERTa-large. Compared to batch normalization, our method can greatly reduce the explained variance and thus improve the isotropy of embeddings.

|       | $EV_1$ | $EV_2$ | $EV_3$ | $EV_1$ | $EV_2$ | $EV_3$ | $EV_1$ | $EV_2$ | $EV_3$ |
|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| BERT-base | 0.76/0.87/0.89 | 0.88/0.93/0.95 | 0.49/0.58/0.64 | 0.89/0.94/0.96 |
| BERT-base+BN | 0.74/0.84/0.86 | 0.70/0.89/0.93 | 0.37/0.59/0.63 | 0.69/0.88/0.92 |
| BERT-base+IsoBN | 0.37/0.68/0.77 | 0.49/0.72/0.85 | 0.25/0.37/0.48 | 0.41/0.69/0.85 |
| RoBERTa-L | 0.86/0.90/0.91 | 0.53/0.66/0.70 | 0.83/0.88/0.90 | 0.87/0.90/0.92 |
| RoBERTa-L+BN | 0.64/0.73/0.76 | 0.36/0.50/0.57 | 0.61/0.70/0.75 | 0.65/0.72/0.77 |
| RoBERTa-L+IsoBN | 0.18/0.36/0.43 | 0.15/0.29/0.37 | 0.21/0.38/0.49 | 0.17/0.32/0.45 |

5 Related Work

**Normalization techniques.** Normalizing inputs (Montavon and Müller, 2012; He et al., 2016; Szegedy et al., 2017) and gradients (Schraudolph, 1998; Bjorck et al., 2018) has been known to be beneficial for training deep neural networks. Batch normalization (Ioffe and Szegedy, 2015) is the first technique to normalize neural activation us-
ing statistics (mean, standard deviation) calculated on mini-batches. One drawback of batch normalization is that the batch size must be sufficiently large for accurate estimation of batch statistics. To address this problem, some attempts focus on substituting the mean and standard deviation with more stable statistics (Yan et al., 2020; Shen et al., 2020).

Another drawback of batch normalization is that it ignores the correlations between input dimensions. Some methods (Huang et al., 2018, 2019) seek to calculate the full whitening transformation. However, computing the whitening matrix requires singular value decomposition (SVD), which is computationally expensive. Moreover, whitening transformation will encounter severe numerical issues when the covariance matrix is ill-conditioned. Compared to existing methods, our normalization method considers the correlations among embedding dimensions but is much more efficient.

Fine-tuning Language Models Pre-trained language models (Devlin et al., 2019; Liu et al., 2019b) achieve the state-of-the-art performance on various natural language understanding tasks. For text classification tasks, the common practice to fine-tune BERT is taking the [CLS] embedding of the last layer and predicting the label with a simple softmax classifier. However, this method will cause over-fitting, especially on small datasets. Various methods including adversarial training (Zhu et al., 2020; Jiang et al., 2019), gradual unfreezing (Howard and Ruder, 2018; Peters et al., 2019), multi-tasking (Clark et al., 2019; Liu et al., 2019a) are proposed to improve fine-tuning performance. To our best knowledge, our method is the first attempt to improve fine-tuning performance by improving isotropy of embeddings.

6 Conclusion

Our major contributions in this paper are two-fold:

- This work studies the isotropy of the pre-trained [CLS] embeddings. Our analysis based on straightforward visualization about standard deviation and correlation coefficient.
- The proposed regularization method, IsoBN, stably improves the fine-tuning of BERT and RoBERTa towards more isotropic representations, yielding an absolute increment around 1.0 point on 7 popular NLU tasks.

We hope our work points to interesting future research directions in improving pre-training language models as well as better fine-tuning towards more isotropy of PTLMs.

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