Abstract

Contrastive learning has been gradually applied to learn high-quality unsupervised sentence embedding. Among the previous unsupervised methods, the latest state-of-the-art method, as far as we know, is unsupervised SimCSE (unsup-SimCSE). Unsup-SimCSE uses the InfoNCE loss function in the training stage by pulling semantically similar sentences together and pushing apart dissimilar ones. Theoretically, we expect to use larger batches in unsup-SimCSE to get more adequate comparisons among samples and avoid overfitting. However, increasing the batch size does not always lead to improvements, but instead even lead to performance degradation when the batch size exceeds a threshold. Through statistical observation, we find that this is probably due to the introduction of low-confidence negative pairs after increasing the batch size. To alleviate this problem, we introduce a simple smoothing strategy upon the InfoNCE loss function, termed Gaussian Smoothing InfoNCE (GS-InfoNCE). Specifically, we add random Gaussian noise vectors as negative samples, which act as a smoothing of the negative sample space. Though being simple, the proposed smoothing strategy brings substantial improvements to unsup-SimCSE. We evaluate GS-InfoNCE on the standard semantic text similarity (STS) task. GS-InfoNCE outperforms the state-of-the-art unsup-SimCSE by an average Spearman correlation of 1.38%, 0.72%, 1.17% and 0.28% on the base of BERT-base, BERT-large, RoBERTa-base and RoBERTa-large, respectively.

1 Introduction

A good sentence representation benefits many natural language processing tasks, so sentence representation learning has been widely studied (Logeswaran and Lee, 2018; Reimers and Gurevych, 2019). The rise of pre-trained language models has brought new improvements to many downstream tasks only through fine-tuning (Devlin et al., 2018; Liu et al., 2019). Therefore, how to produce excellent sentence representation based on pre-trained language models is worth exploring. Lack of a large amount of labeled data, researchers have been exploring to learn sentence Embedding using unsupervised methods, but recently found that directly using BERT’s pre-training embedding does not work well. In some scenarios, it is no better than averaging the Word2vec embeddings (Reimers and Gurevych, 2019; Li et al., 2020).

To tackle the problem mentioned above, contrastive learning has recently been proposed and extensively explored to learn high-quality sentence representations based on the pre-trained language models. Contrastive learning aims to learn effective representation by pulling semantically similar sentences together and pushing apart dissimilar ones (Hadsell et al., 2006), via data augmentation methods and assuming a sentence is semantically more similar to its augmented counterpart than any other sentence. Among those unsupervised sentence embedding learning methods with contrastive learning, the latest state-of-the-art method, as far as we know, is unsupervised SimCSE (unsup-SimCSE) (Gao et al., 2021). Unsup-SimCSE generates the state-of-the-art sentence embeddings by implicitly hypothesizing “dropout” acts as minimal data augmentation. Specifically, unsup-SimCSE randomly composes N sentences into a batch and then passes the batch to the pre-trained BERT twice by applying independently sampled dropout masks.
The embeddings derived from the same input sentences are “positive pairs”, while the embeddings derived from different input sentences constitute “negative pairs”. Impressively, though being simple, unsup-SimCSE works surprisingly well, performing on par with previously supervised counterparts.

Theoretically, since contrastive learning is carried out among samples within a batch, increasing the batch size will probably bring more adequate comparisons and avoid overfitting. So a potential optimization direction is to increase the batch size. However, according to the original unsup-SimCSE paper, a larger batch size does not always lead to improvements. The performance even decreases when the batch size exceeds a threshold. For example, for the unsup-Simcse model based on the bert-base-uncased, the optimal setting of the batch size is 64. Smaller or larger batch sizes will reduce the effectiveness. We assume that as the batch size increases, probably more similar samples of a sentence are introduced. However, they still constitute negative pairs with the sentence, which is detrimental to the learning of the model. To verify our assumption, we design a probing statistical experiment for different batch sizes. We use the currently best semantic textual similarity model, i.e., the supervised SimCSE-RoBERTa_{large} model published by (Gao et al., 2021), to measure the cosine similarity of a pair. Given a batch size $N$, we randomly sample a batch and measure all the similarity between any two sentences in it, i.e., the similarity of each negative pair, resulting in a $N \times N$ matrix. We sort the matrix by column in an ascending order and slice the top 4 rows, which denotes the top 4 closest neighbours for each sentence in the batch. Then we calculate the mean value of each row, getting the top 4 mean similarity values for the batch. We repeat this procedure 100 times to avoid randomness and average the 100 batches’ top 4 mean similarity values. We plot the experiment result in Figure 1, and obviously, all the top 4 similarity values increase as the batch size increases. Considering the pair construction procedure in most contrastive learning methods like unsup-SimCSE, the observation means that, in a larger batch, there will be negative pairs that are actually formed of similar sentences. When the batch size does not exceed a threshold, the top similarity scores of negative pairs will not be so high, thus the built negative pairs are good for training. But when the batch size exceeds the threshold, negative pairs with high similarity are introduced, which will mislead the model training. In some way, this explains why in the unsup-SimCSE experiments, increasing the batch size firstly improves the model performance but then degrades it. Therefore, achieving sufficient comparison for samples in a “safe” (not too large) batch is particularly important.

Label smoothing (Szegedy et al., 2016; Müller et al., 2019) is a regularization method that makes the clusters between categories more compact, increases the distance between classes, reduces the distance within classes, and avoids adversarial examples with over high confidence. But unsup-SimCSE is unsupervised, and there is no obvious boundary between positive and negative pairs. Therefore, we want to achieve the effect of smooth by modifying the loss function. So we pay attention to random Gaussian noise, which has many excellent properties and is widely used in natural language processing (Bowman et al., 2015; Makhzani et al., 2015), usually as a constraint to the posterior distribution or a data augmentation technique. As shown in the figure 1, Gaussian noise is far away from all samples and can constitute a very confident negative pair with any sample within a batch. So we introduce a Gaussian noise term to the InfoNCE loss function, termed Gaussian Smoothing InfoNCE (GS-InfoNCE). We can understand the Gaussian noise term from two perspectives. Firstly it can be regarded as a smoothing strategy. The number of negative pairs in a given batch is lim-
ited and discrete, and these pairs are used to approximate the negative distribution. We can make the distribution smoother by adding various random Gaussian noise as an extension of the negative samples. Secondly, from the perspective of the loss function, the denominator of GS-InfoNCE’s loss introduces an additional penalty term to avoid overfitting. Through experiments on the standard semantic text similarity (STS) task, GS-InfoNCE outperforms the state-of-the-art unsup-SimCSE by an average Spearman correlation of 1.38%, 0.72%, 1.17% and 0.28% on the base of BERT-base, BERT-large, RoBERTa-base and RoBERTa-large, respectively.

Our contributions can be summarized as follows: we propose GS-InfoNCE for unsup-SimCSE, by introducing random Gaussian noise as a simple smoothing strategy to alleviate the problem of negative pairs with high similarity as the batch expands. Through experimental analysis, our approach can bring substantial improvements to unsup-SimCSE with different model configurations. Moreover, GS-InfoNCE is easy to implement, and you only need to add a few extra lines to the InfoNCE code.

2 Background: Contrastive Learning

Contrastive learning is a discriminative representation learning framework, which is extensively used for unsupervised representation learning. The core idea in contrastive learning is to compare an example that is semantically similar to it (namely positive example) and an example that is not semantically similar to it (namely negative example) so that the semantically similar examples are closer in the representation space, while the semantically different examples are farther apart.

InfoNCE (Chen et al., 2020) propose to take a cross-entropy objective with in-batch negatives, namely InfoNCE objective function. It is a commonly used loss function for contrast learning by pull similar sentences closer and push dissimilar ones apart in the representation space. Specifically, given a set of sentence pairs:

$$\mathcal{D} = \{ (x_i, x_i^+) \}_{i=1}^{m}$$

, where $x_i$ and $x_i^+$ are the $i$th pair of semantically related sentences. Let $h_i$ and $h_i^+$ denote the semantical representations of $x_i$ and $x_i^+$, for a mini-batch with $N$ pairs, the training loss for $(x_i, x_i^+)$ is:

$$\ell_i = -\log \frac{e^{\text{sim}(h_i, h_i^+) / \tau}}{\sum_{j=1}^{N} e^{\text{sim}(h_i, h_j) / \tau}}$$

(2)

where $\tau$ is a temperature hyperparameter and $\text{sim}(h_i, h_j) / \tau$ is the similarity measurement function, which is typically the cosine similarity function as follows.

$$\text{sim}(h_i, h_j) = \frac{h_i^T h_j}{\|h_i\| \cdot \|h_j\|}$$

(3)

Unsupervised SimCSE The idea of unsup-SimCSE is quite simple: each positive pair takes the same sentence as input, and their embeddings only differ in dropout masks, utilizing “dropout” as minimal data augmentation. In detail, it takes a collection of sentences $\{x_i\}_{m=1}^{M}$ and use $x_i^+ = x_i$. We simply feed the same input to the encoder twice by applying different dropout masks on fully-connected layers and attention probabilities in the transformer. Through training, positive pair’s embeddings obtained in this way are similar in the representation space.

3 Gaussian Smoothing InfoNCE

We introduce a Gaussian noise term to the InfoNCE loss function, termed Gaussian Smoothing InfoNCE (GS-InfoNCE). Given a Gaussian distribution as follows:

$$G \sim N(\mu, \sigma^2)$$

(4)

whose mean is $\mu$, and the variance is $\sigma^2$, we randomly sample $M$ Gaussian noise vectors from it with the same dimensions as the sentence vector. These vectors constitute high confident negative pairs with each sample in the batch to fill and smooth the representation space. Note that these Gaussian noise vectors will not participate in the positive pair constitution. In that way, the loss function of GS-InfoNCE is denoted as follows:

$$\ell_i = -\log \frac{e^{\text{sim}(h_i, h_i^+) / \tau}}{\sum_{j=1}^{N} e^{\text{sim}(h_i, h_j) / \tau} + \lambda \cdot \sum_{k=1}^{M} e^{\text{sim}(g_k, h_i) / \tau}}$$

(5)

where $g_k$ is a random Gaussian noise vector, $M$ is the number of Gaussian noise vectors involved in the calculation, and $\lambda$ is a balance hyperparameter.
The python implementation of GS-InfoNCE is quite simple, with only three lines of codes based on the original InfoNCE implementation in unsup-SimCSE.

4 Experiments

In this section, we introduce how we verify our proposed GS-InfoNCE objective function in detail. We focus on unsup-SimCSE and replace the original InfoNCE objective loss function with GS-InfoNCE. Following (Gao et al., 2021), the main goal of sentence embeddings is to cluster semantically similar sentences. For a fair comparison, we conduct our experiments on seven standard semantic textual similarity (STS) tasks introduced below and take STS results to compare sentence embedding methods.

Semantic textual similarity tasks Semantic textual similarity measures the semantic similarity of any two sentences. STS 2012–2016 (Agirre et al., 2012, 2013, 2014, 2015, 2016) and STS Benchmark (Cer et al., 2017) are widely used semantic textual similarity benchmark datasets, which measure the relatedness of two sentences based on the cosine similarity of the corresponding sentence embeddings. After deriving the semantic similarities of all pairs in the test set, we follow unsup-SimCSE to use Spearman correlation to measure the correlation between the ranks of predicted scores and the ground-truth. For a set of size \( n \), the \( n \) raw scores \( X_i, Y_i \) are converted to its corresponding ranks \( r_{X_i}, r_{Y_i} \), then the Spearman correlation is defined as follows

\[
 r_s = \frac{\text{cov}(r_{X}, r_{Y})}{\sigma_{r_{X}} \sigma_{r_{Y}}} \tag{6}
\]

where \( \text{cov}(r_{X}, r_{Y}) \) is the covariance of the rank variables, \( \sigma_{r_{X}} \) and \( \sigma_{r_{Y}} \) are the standard deviations of the rank variables. Spearman correlation has a value between -1 and 1, which will be high when the ranks of predicted scores and the ground-truth are similar.

Training details The training details of unsup-SimCSE can be found in (Chen et al., 2020) and github\(^2\). Our experimental settings are consistent with the original method. For the Gaussian distribution, we empirically use the standard normal distribution, with \( \mu = 0, \sigma^2 = 1 \). More exploration in distribution mean and standard deviation may benefit more which is leave to our future work. Additionally, we set \( \lambda = 1 \) and \( M = 3 \times \text{batch size} \) for all experiments. As illustrated in Figure 1, we have confirmed that increasing the batch size will introduce negative pairs with high similarity, so in our experiments, we set the batch size to a moderate size of 64. This allows the samples to be extensively compared while avoiding the introduction of many negative pairs with high similarity. Following the setting of Unsup-SimCSE, we conducted experiments on four commonly used models: BERT-base, BERT-large, RoBERTa-base and RoBERTa-large. The parameter comparison is shown in Table 1:

| Model         | SimCSE | + GS-InfoNCE |
|---------------|--------|--------------|
| BERT\(_{\text{base}}\) | 64     | 64           |
| BERT\(_{\text{large}}\)  | 64     | 64           |
| RoBERTa\(_{\text{base}}\) | 512    | 64           |
| RoBERTa\(_{\text{large}}\) | 512    | 64           |

Table 1: Comparison of batch size with or without using GS-InfoNCE in unsup-SimCSE.

Main Results We list the experimental results in Table 2. On the BERT\(_{\text{base}}\) model, in terms of Pearson correlation, our GS-InfoNCE brought an average increase of 1.38% over unsup-SimCSE on seven test sets, and the maximum gain on STS-B reach 2.85%. On the BERT\(_{\text{large}}\) model, our GS-InfoNCE gave unsup-SimCSE an average improvement of 0.72% on the 7 test sets, although there was a slight decrease on the SICK15 and SICK-R data sets. On the RoBERTa\(_{\text{base}}\) and RoBERTa\(_{\text{large}}\) models, we have a similar situation, with an average improvement of 1.17% and 0.28% on the 7 test sets.

In general, the improvement brought by GS-InfoNCE to unsup-SimCSE is comprehensive and substantial. We can fully surpass the previous best model results with the same or smaller batch size in different model configurations, which well demonstrates that our smoothing strategy has played a key role. We believe that a finer search of the parameters can achieve better results and we leave it to our future work.

5 Analysis

Effect of hyperparameter \( M \) \( M \) is the number of Gaussian noise vectors involved in the GS-InfoNCE calculation. Gaussian random noise vec-
1 # ... code from original unsup-SimCSE above...
2 z1, z2 = pooler_output[:,0], pooler_output[:,1]
3 cos_sim = cls.sim(z1.unsqueeze(1), z2.unsqueeze(0))
4 reg_random = torch.normal(mean, std, size=(reg_size, hidden_size)).to(device)
5 cos_sim = cls.sim(z1.unsqueeze(1), reg_random.unsqueeze(0))
6 cos_sim = torch.cat((cos_sim, reg_cos_sim),1).to(device)
7 labels = torch.arange(cos_sim.size(0)).long().to(cls.device)
8 loss_fct = nn.CrossEntropyLoss()
9 # ... code from original unsup-SimCSE below...

Listing 1: Codes in red are regularization modifications to the original InfoNCE loss

| Model               | STS12  | STS13  | STS14  | SICK15 | STS16  | STS-B  | SICK-R  | Avg.  |
|---------------------|--------|--------|--------|--------|--------|--------|--------|-------|
| SimCSE-BERTbase♣    | 68.40  | 82.41  | 74.38  | 80.91  | 78.56  | 76.85  | 72.23  | 76.25 |
| + GS-InfoNCE        | 70.12  | 82.57  | 75.21  | 82.89  | 80.23  | 79.70  | 72.70  | 77.63 |
| SimCSE-BERT.large♣  | 70.88  | 84.16  | 76.43  | 84.50  | 79.76  | 79.26  | 73.88  | 78.41 |
| + GS-InfoNCE        | 73.75  | 85.09  | 77.35  | 84.44  | 79.88  | 79.94  | 73.48  | 79.13 |
| SimCSE-RoBERTabase♣ | 70.16  | 81.77  | 73.24  | 81.36  | 80.65  | 80.22  | 68.56  | 76.57 |
| + GS-InfoNCE        | 71.12  | 83.24  | 75.00  | 82.61  | 81.36  | 81.26  | 69.62  | 77.74 |
| SimCSE-RoBERTa.large♣ | 72.86 | 83.99  | 75.62  | 84.77  | 81.80  | 81.98  | 71.26  | 78.90 |
| + GS-InfoNCE        | 71.76  | 84.91  | 76.79  | 84.35  | 81.74  | 82.97  | 71.71  | 79.18 |

Table 2: Sentence embedding performance on semantic textual similarity (STS) test sets in terms of Spearman’s correlation. ♣: results from the official published model by the unsup-SimCSE.

We show the performance changing trend in Figure 2 and the performance statistics in Table 3. As $M$ becomes larger, the performance of GS-InfoNCE on the validation set and test set slowly improves. When $M = 3$, the best performance is reached, after which the model performance begins to decline. When $M = 16$, the model performance on the validation set and the test set is inconsistent. We argue that this is because the noise scale greatly exceeded the real data scale. We list the specific numerical changes on the test set in Table 3. When $M = 16$, the model’s performance on the test set is even worse than that of the model trained without noise. In general, GS-InfoNCE is not particularly sensitive to the choice of $M$, which makes it easier to adjust parameters in practical applications. We recommend the reference value of $M$ should be no larger than 8.

6 Related Work

With millions or even billions of parameters, deep and wide models are prone to overfitting, and thus regularization strategies are important to improve their generalization ability. Among them, smoothing is a very commonly used method. (Szegedy et al., 2016; Müller et al., 2019) propose to use label smoothing as a regularization method that makes

![Figure 2: The changing trend of model performance when M increases.](image-url)
the clusters between categories more compact, increases the distance between classes, reduces the distance within classes, and avoids adversarial examples with high confidence. Text smoothing (Wu et al., 2020; Zhu et al., 2019) also seems to be able to bring further improvements in tasks such as text classification and machine translation by smoothing the one-hot representation of the input text into the probability distribution representation of the dictionary. Our GS-InfoNCE can also be regarded as a smoothing strategy. The number of negative samples in a fixed-size batch is limited and discrete. We can make the distribution of negative samples smoother by introducing multiple random Gaussian noise vectors as an extension of the negative examples. From the perspective of the loss function, the denominator of GS-InfoNCE’s loss introduces an additional penalty term so that the positive sample avoids overfitting to the view added to its data, which is very similar to the function of label smoothing. However, compared with the first two smoothing methods, GS-InfoNCE directly use the standard Gaussian distribution for sampling, saving computational costs largely.

## 7 Conclusion and Future Work

In this paper, we propose GS-InfoNCE for the unsup-SimCSE method by introducing random Gaussian noise as regularization, to alleviate the problem of negative pairs with high similarity as the batch size expands. In the future, we will explore how to improve the generalization capability of GS-InfoNCE and verify its effectiveness on more contrastive learning methods. In addition, we will explore whether using the VAE-based method can learn Gaussian distribution directly from training data to improve GS-InfoNCE further.

## References

Eneko Agirre, Carmen Banea, Claire Cardie, Daniel Cer, Mona Diab, Aitor Gonzalez-Agirre, Weiwei Guo, Rada Mihalcea, German Rigau, and Janyce Wiebe. 2014. Semeval-2014 task 10: Multilingual semantic textual similarity. In Proceedings of the 8th international workshop on semantic evaluation (SemEval 2014), pages 81–91.

Eneko Agirre, Carmen Banea, Claire Cardie, Daniel Cer, Mona Diab, Aitor Gonzalez Agirre, Rada Mihalcea, German Rigau Claramunt, and Janyce Wiebe. 2016. Semeval-2016 task 1: Semantic textual similarity, monolingual and cross-lingual evaluation. In SemEval-2016. 10th International Workshop on Semantic Evaluation; 2016 Jun 16-17; San Diego, CA. Stroudsburg (PA): ACL; 2016. p. 497-511. ACL (Association for Computational Linguistics).

Eneko Agirre, Daniel Cer, Mona Diab, and Aitor Gonzalez-Agirre. 2012. Semeval-2012 task 6: A pilot on semantic textual similarity. In * SEM 2012: The First Joint Conference on Lexical and Computational Semantics–Volume 1: Proceedings of the main conference and the shared task, and Volume 2: Proceedings of the Sixth International Workshop on Semantic Evaluation (SemEval 2012), pages 385–393.

Eneko Agirre, Daniel Cer, Mona Diab, Aitor Gonzalez-Agirre, and Weiwei Guo. 2013. * sem 2013 shared task: Semantic textual similarity. In Second joint conference on lexical and computational semantics (* SEM), volume 1: proceedings of the Main conference and the shared task: semantic textual similarity, pages 32–43.

Samuel R Bowman, Luke Vilnis, Oriol Vinyals, Andrew M Dai, Rafal Jozefowicz, and Samy Bengio. 2015. Generating sentences from a continuous space. arXiv preprint arXiv:1511.06349.

Daniel Cer, Mona Diab, Eneko Agirre, Inigo Lopez-Gazpio, and Lucia Specia. 2017. Semeval-2017 task 1: Semantic textual similarity-multilingual and cross-lingual focused evaluation. arXiv preprint arXiv:1708.00055.

Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. 2020. A simple framework for contrastive learning of visual representations. In International conference on machine learning, pages 1597–1607. PMLR.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2018. Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805.

| bs=64 | 0× | 0.5× | 1× | 2× |
|-------|----|------|----|----|
| BERT<sub>base</sub> | 76.25 | 76.96 | 76.90 | 77.11 |
| bs=64 | 3× | 4× | 8× | 16× |
| BERT<sub>base</sub> | **77.63** | 76.94 | 76.94 | 75.57 |

Table 3: Effect of the hyperparameter M on BERT<sub>base</sub>. We set M as a multiple of batch size (bs=64). 0× means the original SimCSE without using GS-InfoNCE.
Tianyu Gao, Xingcheng Yao, and Danqi Chen. 2021. Simcse: Simple contrastive learning of sentence embeddings. arXiv preprint arXiv:2104.08821.

Raia Hadsell, Sumit Chopra, and Yann LeCun. 2006. Dimensionality reduction by learning an invariant mapping. In 2006 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR’06), volume 2, pages 1735–1742. IEEE.

Bohan Li, Hao Zhou, Junxian He, Mingxuan Wang, Yiming Yang, and Lei Li. 2020. On the sentence embeddings from pre-trained language models. arXiv preprint arXiv:2011.05864.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. 2019. Roberta: A robustly optimized bert pretraining approach. arXiv preprint arXiv:1907.11692.

Lajanugen Logeswaran and Honglak Lee. 2018. An efficient framework for learning sentence representations. arXiv preprint arXiv:1803.02893.

Alireza Makhzani, Jonathon Shlens, Navdeep Jaitly, Ian Goodfellow, and Brendan Frey. 2015. Adversarial autoencoders. arXiv preprint arXiv:1511.05644.

Rafael Müller, Simon Kornblith, and Geoffrey Hinton. 2019. When does label smoothing help? arXiv preprint arXiv:1906.02629.

Nils Reimers and Iryna Gurevych. 2019. Sentence-bert: Sentence embeddings using siamese bert-networks. arXiv preprint arXiv:1908.10084.

Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jon Shlens, and Zbigniew Wojna. 2016. Rethinking the inception architecture for computer vision. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 2818–2826.

Xing Wu, Yibing Liu, Xiangyang Zhou, and Dianhai Yu. 2020. Distilling knowledge from pre-trained language models via text smoothing. arXiv preprint arXiv:2005.03848.

Jinhua Zhu, Fei Gao, Lijun Wu, Yingce Xia, Tao Qin, Wengang Zhou, Xueqi Cheng, and Tie-Yan Liu. 2019. Soft contextual data augmentation for neural machine translation. arXiv preprint arXiv:1905.10523.