Improving Contrastive Learning of Sentence Embeddings with Case-Augmented Positives and Retrieved Negatives

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ABSTRACT
Following SimCSE, contrastive learning based methods have achieved the state-of-the-art (SOTA) performance in learning sentence embeddings. However, the unsupervised contrastive learning methods still lag far behind the supervised counterparts. We attribute this to the quality of positive and negative samples, and aim to improve both. Specifically, for positive samples, we propose switch-case augmentation to flip the case of the first letter of randomly selected words in a sentence. This is to counteract the intrinsic bias of pre-trained token embeddings to frequency, word cases and subwords. For negative samples, we sample hard negatives from the whole dataset based on a pre-trained language model. Combining the above two methods with SimCSE, our proposed Contrastive learning with Augmented and Retrieved Data for Sentence embedding (CARDS) method significantly surpasses the current SOTA on STS benchmarks in the unsupervised setting.

CCS CONCEPTS
• Information systems → Similarity measures.

KEYWORDS
Text retrieval, data augmentation, natural language understanding, hard negatives, intrinsic bias, RoBERTa

1 INTRODUCTION
It is a standard paradigm in natural language understanding to pre-train large-scale models, and adapt them to various downstream tasks [28, 32]. Recently, a contrastive learning framework called SimCSE [18] is proposed to finetune the pre-trained BERT [13] and RoBERTa [30] to learn sentence embeddings, with performance significantly surpassing previous results [41]. In the unsupervised setting, SimCSE encodes the same sentence twice with independent dropout noises to produce a positive pair of sentence embeddings. Meanwhile, it treats other samples from the same batch as negatives. SimCSE is further enhanced in follow-up studies by carefully designed data augmentation methods [48, 51], momentum contrast [48], and prompt tuning [22]. Despite its success, there is still a significant gap between the performance of SimCSE trained using unlabelled English Wikipedia dataset and that using labelled SNLI+MNLI dataset [7, 46], where the latter has manually designed entailed and contradictory sentence pairs treated as positive and negative samples respectively (see Tab. 2). We attribute the gap to the higher quality of positive and negative samples in SNLI+MNLI than those produced by dropout and found in the same batch. Thus, to narrow down the gap, we attempt to improve the quality of both positive and negative samples in the unsupervised setting.

Data augmentation is arguably the most straightforward approach to improve sample quality. However, it is known to be challenging for language data, possibly due to their discrete nature [15]. Existing rule-based methods, such as word insertion, deletion, swap [44] and crop [31], may alter the semantic meaning of sentences, e.g., even deleting one word hurts the performance in the SimCSE framework [18]. Back-translation [36, 39] or other syntactic/semantic transformations [26, 33] can generate plausible samples, but may involve other models like GPT2 [37]. Adversarial training [11, 29, 54] tends to incur a large computational cost [52]. Is it possible to obtain positive samples with minimal semantic alternation and computational overhead? A promising answer, proposed by ESimCSE [48], is to augment a sentence by randomly repeating some words/sub-words in it. However, token repetition may introduce unlikely samples. In natural language generation studies, token repetition is often considered as a degenerate property of Transformer-based models trained with the maximum likelihood objective [21, 45]. On the other hand, token embeddings in the pre-trained BERT and RoBERTa models are biased towards token frequency, word case and subwords [22, 25, 53] (see Fig.1). The performance of using the average of token embeddings as the sentence embedding can be significantly improved by simply removing top frequent tokens, subwords and uppercase tokens [22].
We argue this may still not be effective, as the majority of sentences we change the frequency of tokens used, and in many cases, the 1) - all is done without affecting much the meaning of the sentences negative retrieval, comprise our unsupervised learning method provide enough informative information due to the diversity of conduct a comprehensive evaluation of CARDS on seven STS tasks for its hard negatives.

Inspired by this, we propose switch-case augmentation: by flipping the case of the first letter of randomly selected words in a sentence, we change the frequency of tokens used, and in many cases, the tokenization of words and thus the length of sentence ids (see Tab. 1) - all is done without affecting much the meaning of the sentences from the human perspective.

As for negative samples, the in-batch local negatives may not mitigate the bias towards word frequency [53]. Of last few layers) of pre-trained BERT, and additional data fails to biases exist in contextualized token embeddings (the hidden states of last few layers) of pre-trained RoBERTa large, biased towards token frequency, word case (green), upper-case (blue) and sub-tokens (red); Fig. 1b shows the first token of a word the beginning token, and the rest subordi-

The above two optimizations, switch-case augmentation and negative retrieval, comprise our unsupervised learning method coined Contrastive learning with Augmented and Retrieved Data for Sentence embedding (CARDS). In the following sections, we conduct a comprehensive evaluation of CARDS on seven STS tasks for sentence embedding learning.

Table 1: Effects of switch-case on RoBERTa tokenization.

| Type         | Tokenization1                      | Percentage2 |
|--------------|------------------------------------|-------------|
| Substitution | natural-istic → Natural-istic       | 69.9        |
| Division     | Chart-ing → chart-ing               | 15.0        |
| Fusion       | interpret → Inter-pret             | 6.2         |
| Regrouping   | Neigh-bor → ne-igh-bor             | 3.9         |
|              | recomm-ended → Recommended         | 1.8         |
|              | Ser-ious → serious                 | 1.3         |
|              | urg-ency → Ur-gency                | 1.2         |
|              | O-ng-oint → ong-oint               | 1.0         |

1 The tokens of a word are connected by hyphens. 2 The percentage of occurrence is calculated on WiKi-1m, a subset of Wikipedia corpus used in SimCSE [18].

2 METHODS

We first briefly present contrastive learning and SimCSE, then explain our proposed CARDS method in details.

2.1 Contrastive Learning and SimCSE

Contrastive learning is a general self-supervised learning framework. It works by maximizing the agreement between differently augmented views of the same data example, while separating the views of different examples [9]. In the context of sentence embedding, each data example is a sentence \( x_i \). We denote \( f_0 \) as the language encoder, and \( h_i = f_0(x_i, \overline{T}) \) as the embedding of \( x_i \) with augmentation \( \overline{T} \). SimCSE uses the following training objective:

\[
\ell_i = - \log \frac{\exp(\cos(h_i, h'_j)/\tau)}{\sum_{j \neq i} \exp(\cos(h_i, h'_j)/\tau)}
\]

where in unsupervised setting, the positive sample pair \((h_i, h'_j)\) is obtained by passing \( x_i \) to the encoder twice with different dropout masks as data augmentation; for \( h_i \), the \( N - 1 \) negative samples \( h_{j=1:N, j\neq i} \) are simply from the same batch; the embedding similarity is measured using cosine operation and \( \tau \) is the temperature.

2.2 Switch-case augmentation

Previous studies find that the token embeddings of pre-trained BERT and RoBERTa are biased towards token frequency, word case and subword tokenization [22, 25]. In Fig. 1, we visualize the token embeddings of the pre-trained RoBERTa large model, where we call the first token of a word the beginning token, and the rest subordinate tokens or sub-tokens. For example, ‘ne-igh-bor’ is tokenized into one beginning token ‘ne’ and two sub-tokens ‘igh’ and ‘bor’. Fig. 1a shows an almost clear separation of embeddings for lower-case (green), upper-case (blue) and sub-tokens (red); Fig. 1b shows gradual change from rare token (light green) regions to frequent token (dark blue) regions for each cluster of tokens. Moreover, these biases exist in contextualized token embeddings (the hidden states of last few layers) of pre-trained BERT, and additional data fails to mitigate the bias towards word frequency [53].

We propose switch-case augmentation to alleviate the biases. The idea is simple: we randomly select words in a sentence with a fixed probability \( p_{se} \) and flip the case of the first letter of these words. There are four possible consequences (see Tab. 1):
(1) Substitution. Only the beginning token is replaced with a case-switched token; the sub-tokens are not affected.

(2) Division. The case-switched subword istokenized into two or more tokens, thus the total number of tokens $N$ increases.

(3) Fusion. The case-switched subword is combined with other tokens into one, thus $N$ decreases.

(4) Regrouping. The case-switched subword is regrouped with other tokens, and $N$ may increase, decrease or remain the same.

Tab. 1 also lists the occurring proportion of each consequence when applying switch-case to sentences in Wiki-1m dataset, a subset of Wikipedia corpus used in SimCSE study [18]. In about 85% of the cases, the beginning token is replaced with another token of probably different frequency. In 14% of the cases, the total number of tokens varies. ESimCSE [48] randomly repeats some tokens to avoid the trivial solution of using sentence length to distinguish the negative pairs from the positives. We achieve this with a negligible influence on the sentence semantics (see Tab. 2 for an example).

### 2.3 Hard negative retrieval

The in-batch negatives, sampled uniformly from the training corpus, may not be hard enough due to the diversity of natural sentences [38, 43]. Inspired by text retrieval studies [49, 50], we propose to retrieve top $k$ hard negatives in the training corpus for each sample $x_i$ in the current batch, uniformly sample $s = 1$ from them to get $x_i^r$, and use it in the training objective:

$$
\ell_i = -\log \frac{\exp(\cos(h_i, h_i^r)/\tau)}{\sum_j \exp(\cos(h_i, h_j^r)/\tau) + \exp(\cos(h_i, h_j)/\tau)}
$$

(2)

Note $x_i^r$ will be treated as a random negative for other samples in the batch. To do retrieval, we first build the index, or the representation of each sentence in the training corpus, by passing each one to the same pre-trained language model to be finetuned in contrastive learning. Then the hardness is measured as cosine similarity between each pair of representations. See Tab. 2 for examples of retrieved and random negatives.

### 3 EXPERIMENTS

#### 3.1 Evaluation Setup

For sentence embedding learning, we follow the same process as SimCSE-related studies [18, 22, 48, 51] to evaluate our proposed CARDS framework, and compare it against SimCSE [18], ESimCSE [48], VaSCL [51] and PromptBERT [22]. Later in Appendix A, we also evaluate switch-case on DeBERTa$_{1,5B}$ and the GLUE benchmark to show its generality as a data augmentation approach.

**Datasets.** We use Wiki-1m from SimCSE as our training set, which consists of 1 million sentences randomly drawn from the English Wikipedia corpus. We use STS12-STS16 [1–5] and STS-B [8] from the SentEval toolkit [12] as our evaluation sets. For each STS task, the standard evaluation pipeline from SentEval is used.

**Implementation details.** We finetune the pre-trained checkpoints of RoBERTa$_{base}$ and RoBERTa$_{large}$ on Wiki-1m for one epoch. The maximum number of tokens in a sentence is confined to 32. Meanwhile, we evaluate the models on STS-B development dataset every 125 steps to select the best intermediate model for test. For switch-case, we select $p_{sc}$ in $[0.05, 0.1, 0.15]$ and fix dropout rate at 0.1. For hard negative retrieval, we adopt Faiss library$^1$ [23] to efficiently build the index and do similarity search. The index or sentence representations for retrieval are calculated using the pre-trained checkpoints before any finetuning and shared across all experiments. For each sample, the number of hard negatives $k$ to retrieve (excluding itself) is selected from $[8, 64]$. We also deduplicate the Wiki-1m dataset and remove sentences with less than three words. This does not affect much the final performance but significantly stabilize the training in the late stages. Our code$^2$ is implemented based on the HuggingFace Transformers library$^3$ [47].

#### 3.2 Main Results

As shown in Tab. 3, the proposed CARDS significantly improve over SimCSE, ESimCSE and VaSCL on almost all STS tasks and the average STS scores for both RoBERTa$_{base}$ and RoBERTa$_{large}$ models. Moreover, adding either switch-case or retrieval to SimCSE could achieve comparable average STS scores to ESimCSE and VaSCL. It is interesting to note that combining switch-case and negative retrieval in CARDS achieves even a bigger improvement than simply summing up their respective improvements together, showing that the two methods may strengthen the effects of each other. Although on RoBERTa$_{base}$, CARDS does not perform as good as Prompt-RoBERTa, we argue that Prompt-RoBERTa is an orthogonal method in that it finetunes RoBERTa with prompts, and may be combined with CARDS.

#### 3.3 Ablation studies

In this section, we investigate how the performance of CARDS on STS tasks is influenced by design and hyper-parameters of the proposed switch-case and negative retrieval.

For switch-case, Fig. 2a shows that it adds a negligible overhead to the training walltime and increasing the switch-case probability $p_{sc}$ above 0.15 will deteriorate the average STS score. In Tab. 4, we test whether ignoring the upper-case words (by switching them to lower case) during training and/or evaluation affects the

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$^1$https://github.com/facebookresearch/faiss

$^2$https://github.com/alibaba/SimCSE-with-CARDS.

$^3$https://github.com/huggingface/transformers

$^4$Note the walltimes also depend on hardware and code implementation. They are shown here for a rough illustration of the method complexity and should not be used to verify user implementation.
we consider two augmentation approaches: (1) substitution - do substitution only for words of the substitution type (see Tab. 1) to remove the effects of varied sequence length; (2) re-tokenization - for division and regrouping-type words, switch their case, keep the changed tokenization, then switch their case back and do tokenization again, so that their case is not changed but tokenization of certain long words. Given this, the performance drop when raising $p_{sc}$ above 0.15 in Fig. 2a may be caused by the increasing difficulty of associating more tokens with their re-tokenized version. At last, we show in Appendix A that switch-case is a general data augmentation approach applicable to DeBERTaL3B on GLUE tasks.

Regarding negative retrieval, Fig. 2b shows that it increases roughly 40% of the training time, partially because negative retrieval doubles the number of negative samples. Increasing the number of retrieved negatives do not vary the training time too much, possibly due to the efficient implementation of retrieval in Faiss, but decreasing it below 32 ($= 2^5$) significantly deteriorates the performance. We further investigate the effects of the number of sampled negatives $s$ from the retrieved ones and the type of negatives used in contrastive learning. For the latter one, we consider three types: (1) the default used in CARDS, denoted as $\mathbb{R}_{\text{uniform}}$; samples $s$ negatives uniformly from $k$ retrieved ones; (2) $\mathbb{R}_{\text{top}}$ selects only the top $s$, or $s$ hardest negatives from the retrieved ones; and (3) $\mathbb{D}_{\text{uniform}}$ samples $s$ negatives uniformly from the whole training set. Fig. 3 shows that both increasing $s$ beyond 1 in $\mathbb{R}_{\text{uniform}}$ and selecting the $s$ hardest negatives in $\mathbb{R}_{\text{top}}$ significantly deteriorate the performance, possibly due to the increasingly adverse impact of false negatives. On the other hand, sampling uniformly from the whole dataset only helps when $s$ is large, which, however, incurs a considerable computational cost due to more negative samples. Currently, we sample uniformly from $k$ retrieved ones to balance the difficulty of hard negatives and the impact of false negatives. We suspect filtering out false negatives [10] may further help, and leave this for future work.

Interestingly, BPE-dropout generally hurts the performance across different hyper-parameter settings in our SimCSE framework, but ignoring BPE-dropout for the most frequent words hurts less.

### Table 3: Test performance of unsupervised sentence embedding on STS tasks.

| Base Model | STS12 | STS13 | STS14 | STS15 | STS16 | STS-B | SICK-R | Avg  |
|------------|-------|-------|-------|-------|-------|-------|--------|-----|
| SimCSE [1] | 70.16 | 81.77 | 73.24 | 81.36 | 80.65 | 80.22 | 68.56  | 76.57 (−0.43) |
| ESimCSE [48] | 69.90 | 82.50 | 74.68 | 83.19 | 80.30 | 80.99 | 70.54  | 77.44 (−0.44) |
| VaSCL [51] | 69.08 | 81.95 | 74.64 | 82.64 | 80.57 | 80.23 | 71.23  | 77.19 (−0.19) |
| Prompt-RoBERTa [22] | **73.94** | **84.74** | **77.28** | **84.99** | 81.74 | 81.88 | 69.50  | **79.15** (−0.15) |
| CARDS | 73.30 | 84.58 | 77.16 | 84.89 | 81.78 | 82.90 | 71.88  | 79.50 (−0.50) |

### Table 4: Test performance of SimCSE-RoBERTa large with upper-case ignored during training/evaluation.

| Baseline | Ignoring upper-case during | Training | Evaluation | Train. & Eval. | Switch-case |
|----------|-----------------------------|----------|------------|----------------|-------------|
| SimCSE [1] | 72.86 | 83.99 | 75.62 | 84.77 | 81.80 | 81.98 | 71.26 | 78.90 |
| ESimCSE [48] | 73.20 | 84.93 | 76.88 | 84.86 | 81.21 | 82.79 | 72.27 | 79.45 (−0.55) |
| VaSCL [51] | 74.34 | 83.35 | 76.79 | 84.37 | 81.46 | 82.86 | **73.23** | 79.48 (−0.58) |
| Prompt-RoBERTa [22] | **74.63** | **86.27** | **79.25** | **85.93** | **83.17** | **83.86** | **72.77** | **80.84** (−0.74) |

1. Results obtained from GitHub checkpoints: https://github.com/princeton-nlp/SimCSE. 
2. Prompt-RoBERTa results are not officially released. Upon paper submission, we were unable to achieve promising results using its code and manually designed prompts. 
3. Our reproduced SimCSE results are different from that of SimCSE GitHub. We use the higher ones as baseline to calculate the relative improvements of each method in brackets. 
4. CARDS = SimCSE + switch-case + retrieval.
Table 5: Average STS test scores of RoBERTa$_{base}$ with three switch-case variants (default, substitution and re-tokenization) and BPE-dropout.

| Variants   | STS Avg. |
|------------|----------|
| Baseline   | 77.00    |
| Default    | 77.78    |
| Substit    | 77.43    |
| Re-token   | 77.70    |
| BPE-drop.  | 76.74    |

Figure 3: Effects of number of sampled negatives on average STS test scores using RoBERTa$_{base}$ and negative retrieval variants. The baseline is shown in dashed line.

3.4 Negative results

Below we briefly describe two ideas that did not look promising in our initial experiments:

1. We applied switch-case to BERT$_{large}$-case and BERT$_{large-uncase}$. However, switch-case cannot be applied to uncased models such as BERT$_{large-uncase}$.

2. Note that [49, 50] propose to update the index during training to get “dynamic” hard negatives. However, we tried various update strategies but none improved over the static one. We suspect that, with training going on, the false negatives become more frequently retrieved and deteriorate the training. Thus, we only build the index once before training and do the retrieval using fixed sentence embeddings, and leave “dynamic” hard negatives retrieval for future study.

4 CONCLUSIONS

In this study, we propose Contrastive learning with Augmented and Retrieved Data for Sentence embedding (CARDS), which introduces switch-case augmentation and hard negative retrieval to improve the positive and negative samples respectively in the SimCSE framework. We show that CARDS works towards closing the gap between unsupervised and supervised training of SimCSE.

We believe that following our work, more data augmentation methods could be tailored to further close this gap.

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A SWITCH-CASE EXPERIMENTS ON GLUE

A.1 Evaluation Setup

To show switch-case is a general data augmentation approach applicable beyond RoBERTa models and sentence embedding learning tasks, we evaluate it on DeBERTa$_{3B}$ [20] and the General Language Understanding Evaluation (GLUE) benchmark [42].

Datasets. GLUE contains eight tasks covering natural language inference (MNLI, RTE and QNLI), semantic similarity (MRPC, QQP and STS-B), sentiment classification (SST-2), and linguistic acceptability classification (CoLA). The evaluation metrics are Matthews correlation for CoLA, Spearman correlation for STS-B, the MNLI-match accuracy for MNLI, and accuracy for the rest. We also report the average of metrics of these eight tasks as the overall performance standard.

Baselines. We follow the framework of R-drop [27], which shares a similar idea with SimCSE. R-drop passes the same batch to the encoder twice with different dropout masks, and calculates the distance of the two output representations using the symmetric KL-divergence. The distance is used as a regularization loss added to the original task objective. We apply switch-case augmentation to one side of R-drop, i.e., dropout to create one view, dropout+switch-case for the other, and compare it against the R-drop baseline.

Appendices
Table 6: Performance of DeBERTa\textsubscript{1.5B} with R-drop and switch-case on GLUE development set.

| Task        | Dataset size | MNLI-m | QQP | QNLI | SST-2 | CoLA | STS-B | MRPC | RTE | Avg. |
|-------------|--------------|--------|-----|------|-------|------|-------|------|-----|------|
| DeBERTa\textsubscript{1.5B} | 392k         | 91.7   | 92.7| 96.0 | 97.2  | 72.0 | 92.9  | 92.0 | 93.5| 90.7 |
| + R-drop    | 363k         | 91.9   | 92.9| 96.1 | 97.2  | 73.8 | 93.2  | 93.1 | 93.7| 91.2 |
| + R-drop + switch-case | 108k         | 92.0   | 93.0| 96.3 | 97.2  | 75.5 | 93.6  | 93.9 | 94.2| 91.7 |

Implementation Details. We adopt the pretrained DeBERTa\textsubscript{1.5B} model as the encoder. With 1.5 billion parameters, it surpasses a majority of pre-trained models on GLUE benchmark with a large margin. A simple linear classification or regression head is placed on top of the encoder to handle each GLUE task, and the overall model is trained in a supervised manner. We mainly follow the hyper-parameter settings of the original DeBERTa paper [20], except that we train the model for 20 epochs on small tasks (CoLA, MRPC, STS-B and RTE) to alleviate the large variance [34], and 4 epochs for the rest tasks. We select the weight of the R-drop KL-divergence loss in \(\{1, 2, 3, 4\}\), and switch-case probability \(p_{sc}\) in \(\{0.05, 0.1, 0.15\}\). All GLUE scores are reported based on the development dataset.

A.2 results

As shown in Tab. 6, switch-case can be used as a data augmentation method to further improve R-drop’s performance on natural language understanding tasks. Specifically, when applied on DeBERTa\textsubscript{1.5B}, R-drop improves the average GLUE score from baseline’s 90.7 to 91.2, while the proposed switch-case further increases it to 91.7. As with many data augmentation methods (including dropout in R-drop), switch-case is most effective on small tasks, e.g., CoLA and MRPC. Switch-case is not effective on SST-2, perhaps because sentiment analysis relies more on the understanding of a few keywords than the whole sentence. We also note that (1) DeBERTa\textsubscript{1.5B} uses Sentencepiece tokenizer [24] with a 128k vocabulary, rather than RoBERTa’s BPE tokenizer [40] with 50k vocabulary, showing that switch-case works across different tokenizer settings. (2) DeBERTa\textsubscript{1.5B} has a much larger model size (1.5B) than RoBERTa\textsubscript{large} (355M), showing that the bias of pretrained word embeddings still exists in larger models.