An Effective Post-training Embedding Binarization Approach for Fast Online Top-K Passage Matching

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Abstract

With the rapid development of Natural Language Understanding for information retrieval, fine-tuned deep language models, e.g., BERT-based, perform remarkably effective in passage searching tasks. To lower the architecture complexity, the recent state-of-the-art model ColBERT employs Contextualized Late Interaction paradigm to independently learn fine-grained query-passage representations. Apart from the architecture simplification, embedding binarization, as another promising branch in model compression, further specializes in the reduction of memory and computation overheads. In this concise paper, we propose an effective post-training embedding binarization approach over ColBERT, achieving both architecture-level and embedding-level optimization for online inference. The empirical results demonstrate the efficaciousness of our proposed approach, empowering it to perform online query-passage matching acceleration.

1 Introduction

The Information Retrieval community has witnessed an emerging slew of BERT (Devlin et al., 2018)-based deep ranking models that achieves performance superiority in various retrieval benchmarks (Dai and Callan, 2019b; MacAvaney et al., 2019; Nogueira and Cho, 2019; Yilmaz et al., 2019). Despite their advantage in learning deeply-contextualized semantic representations, a major issue however is the heavy computational complexity. A recent model ColBERT (Khattab and Zaharia, 2020) detaches the query-passage contextual encoding in the proposed Contextualized Late Interaction mechanism, achieving substantial progress in optimizing the runtime resource footprints.

Orthogonal to architecture simplification, embedding binarization, i.e., another model compression technique, has received growing attention across various applications (Lin et al., 2017; Zhang and Zhu, 2019; Qin et al., 2020; Chen et al., 2022a). Despite the promising advantages, it usually suffers from large performance degradation even with adequate training supports (Bai et al., 2021), in which the crux generally lies in:

- **Inevitable semantic erosion.** Compared to the original embeddings, binarized targets are naturally less informative to represent the semantics. Consequently, this leads to a degraded model capability in distinguishing and ranking passages for query-based requests.

- **Inaccurate gradient estimation.** Due to the non-differentiability of binarizer sign(·), several gradient estimators are proposed (Darabi et al., 2018; Yang et al., 2019; Liu et al., 2019; Qin et al., 2020; Gong et al., 2019). However, these estimators usually are based on visually similar simulation to sign(·), but not necessarily are theoretically relevant to it, which may lead to inaccurate gradient estimation in backpropagation.

To tackle these issues, we propose an effective post-training binarization approach by introducing:

1. **Semantic diffusion** technique to “distribute” informative latent semantics to the embedding matrix more uniformly (instead of to the condensed sub-areas) to hedge the binarization information erosion (§ 3.1).

2. **Approximation of Unit Impulse Function** to approximate the derivatives of sign(·) more rigorously to provide the consistent optimization direction in both forward and backward propagation of the model training workflow (§ 3.2).

Related work & Future directions. There exist several other methods to close the performance disparity, such as knowledge distillation (Hinton et al., 2015; Anil et al., 2018), multi-bit quantization (Li et al., 2016), and various augmentation strategies (Ning et al., 2020; Jang and Cho, 2021). In this paper, we base on ColBERT (2020) to evaluate the proposed post-training binarization approach, and will study its generalization to other appropriate deep language models as future work.
2 Preliminaries

ColBERT (Khattab and Zaharia, 2020). It comprises: (1) a query encoder \( f_Q \), (b) a passage encoder \( f_D \), and (3) a query-passage score predictor. Specifically, given a query \( q \) and a passage \( d \), \( f_Q \) and \( f_D \) encode them into a bag of fixed-size embeddings \( E_q \) and \( E_d \) as follows:

\[
E_q := \text{Normalize} (\text{CNN}(\text{BERT}(\text{"[Q]"} q_0 q_1 \cdots q_t \# \# \# \# \) ) ) ) ,
E_d := \text{Filter} (\text{Normalize} (\text{CNN}(\text{BERT}(\text{"[D]"} d_0 d_1 \cdots d_n \# \# \# \# \) ) ) ) ,
\]

where \( q \) and \( d \) are tokenized into tokens \( q_0 q_1 \cdots q_t \) and \( d_0 d_1 \cdots d_n \) by BERT-based WordPiece (Wu et al., 2016), respectively. \([Q] \) and \([D]\) indicate the sequence types and \# denotes the special padding token when a query has fewer tokens than a pre-defined token number.

**Embedding Binarization and Optimization.** The conventional methods (Gersho and Gray, 2012; Courbariaux et al., 2016; Lin et al., 2017; Chen et al., 2021) generally adopt \( \text{sign}(\cdot) \) function for binarization mainly because of its \( O(1) \) simplicity. However, as \( \text{sign}(\cdot) \) is non-differentiable, previous **visually similar** gradient estimators (2018; 2019; 2020; 2019) are not necessarily **theoretically relevant** to \( \text{sign}(\cdot) \). For example, estimator \( \text{1} - \tanh^2(\cdot) \) provides executable gradient estimation, which however is the factual derivative of \( \tanh(\cdot) \) (Qin et al., 2020; Gong et al., 2019).

This may distract the main direction of the factual gradient for model optimization in forward and backward propagation, which thus leads to performance degradation of downstream tasks.

3 Bi-ColBERT Methodology

To tackle the aforementioned issue, we propose Bi-ColBERT by introducing two effective and lightweight techniques: (1) semantic diffusion to hedge the information loss against embedding binarization, and (2) approximation of Unit Impulse Function (Dirac, 1927; Bracewell and Bracewell, 1986) for more accurate gradient estimation.

3.1 Semantic Diffusion

Binarization with \( \text{sign}(\cdot) \) inevitably smooths the embedding informativeness into the binarized space, e.g., \([-1, 1]^d \) regardless of its original values. Thus, intuitively, we want to avoid condensing and gathering informative latent semantics in (relatively-small) sub-structures of embedding bags, e.g., \( E_q \); in other words, we seek to **diffuse the embedded semantics in all embedding dimensions as one effective strategy to hedge the inevitable information loss caused by the numerical binarization and retain the semantic uniqueness after binarization as much as possible.**

Recall in singular value decomposition (SVD), singular values and vectors reconstruct the original matrix; normally, large singular values can be interpreted to associate with major semantic structures of the matrix (Wei et al., 2018). Hence, based on this observation, we can achieve semantic diffusion via normalizing singular values for equalizing their respective contributions in constituting latent semantics. To achieve this, **Power Normalization** (Li et al., 2017; Koniusz et al., 2016) is one of the solutions that tackle related problems such as feature imbalance in image processing (Koniusz et al., 2018; Quattoni and Torralba, 2009). Inspired by the recent approximation attempt (Yu et al., 2020), we introduce a lightweight semantic diffusion technique as follows.

Concretely, let \( I \) denote the identity matrix, we start from generating a standard normal random vector \( p(0) \sim \mathcal{N}(0, I) \) where \( p(0) \in \mathbb{R}^d \). Based on the embedding matrix for semantic diffusion, e.g., \( E_q \), we compute the **diffusion vector** \( p(h) \) by iteratively performing \( p(h) = E_q^T E_q p(h-1) \). Next we can obtain the projection matrix \( P_q \) of \( p \) via:

\[
P_q = \frac{p(h) p(h)^T}{||p(h)||^2_2}.
\]

Then we have the **semantic-diffused** embedding bag with the hyper-parameter \( \epsilon \in (0, 1) \) as:

\[
\tilde{E}_q = E_q (I - \epsilon P_q).
\]

We conduct similar operations to passage embedding bags, e.g., \( E_d \), for semantic diffusion. Compare to the unprocessed embedding bag, i.e., \( E_q \), embedding \( \tilde{E}_q \) presents a diffused semantic structure with a more balanced spectrum (distribution of singular values) in expectation. We theoretically explain this by Theorem 1 in Appendix A and illustrate a visual comparison in Figure 1.
which implies that:
\[
\frac{\partial \text{sign}(t)}{\partial t} \approx \frac{2\gamma}{\sqrt{\pi}} \exp(- (\gamma t)^2).
\]  
(7)

As shown in Figure 2, hyper-parameter $\gamma \in \mathbb{R}^+$ determines the curve sharpness to approximate $\text{sign}(\cdot)$. Intuitively, this estimator in Equation (7) follows the main direction of factual gradients of $\text{sign}(\cdot)$, which produces a coordinated embedding optimization for inputs with diverse value ranges. Its performance superiority over other recent estimators is demonstrated in experiments later.

### 3.2 Gradient Estimation

**Rescaled Binarization.** After obtaining the semantic-diffused embedding bag, e.g., $\tilde{E}_q$, we conduct the *rescaled embedding binarization* for each one embedding of the contextualized bag as:

\[
B_{q_i} := \omega_{q_i} \cdot \text{sign}(\tilde{E}_{q_i}), \text{ where } \omega_{q_i} = \frac{||\tilde{E}_{q_i}||_1}{c}.
\]  
(4)

Here $i \in ||\tilde{E}_q||$ and $c$ denotes the embedding dimension. The binarized embedding bag $B_q$ sketches the original embeddings via (1) binarized codes (i.e., $\{\{-1, 1\}\}$) and (2) embedding scaler (i.e., $\omega_{q_i} \in \mathbb{R}^+$), both of which collaboratively reveal the value range of original embedding entries. Moreover, such rescaled binarization supports the bit-wise operations for computation acceleration in matching prediction, which will be introduced later.

**Approximation of Unit Impulse Function.** Although previous gradient estimators are visually similar (e.g., $\text{tanh}(\cdot)$) (Gong et al., 2019; Qin et al., 2020) to provide an executable gradient flow, it however may lead to the inconsistent optimization direction in forward and backward propagation. This is because, the integral of the approximation function (e.g., derivatives of $\text{tanh}(\cdot)$) may not be consistent with $\text{sign}(\cdot)$. To tackle this issue and furnish the accordant gradient estimation, we utilize the approximation of *Unit Impulse Function* (Dirac, 1927; Bracewell and Bracewell, 1986) as follows.

It has been proved that *Unit Impulse Function* defined in the right-hand side of Equation (5) is the derivatives of Unit Step function $u(t)$\(^1\), where $u(t) = 0$ for $t \leq 0$ and $u(t) = 1$ otherwise.

\[
\frac{\partial u(t)}{\partial t} = \begin{cases} 0 & t \neq 0 \\ \infty & t = 0 \end{cases}.
\]  
(5)

It is obvious to take a translation by $\text{sign}(t) = 2u(t) - 1$, and theoretically $\frac{\partial \text{sign}(t)}{\partial t} = 2u(t)$. Furthermore, $\frac{\partial u(t)}{\partial t}$ can be introduced with zero-centered Gaussian probability density function as:

\[
\frac{\partial u(t)}{\partial t} = \lim_{\beta \to \infty} \frac{|\beta|}{\sqrt{\pi}} \exp\left(-\left(\beta t\right)^2\right),
\]  
(6)

\(^1\)https://en.wikipedia.org/wiki/Heaviside_step_function

### 3.3 Online Query-passage Matching

Similarly to ColBERT (Khattab and Zaharia, 2020), we employ its proposed *Late Interaction Mechanism* for matching score computation, which is implemented by a sum of maximum similarity computation with embedding dot-products:

\[
S_{q,d} := \sum_{i \in ||B_q||} \max_{j \in ||B_d||} B_{q_i} \cdot B_{d_j}^T.
\]  
(8)

Which can be equivalently implemented with bit-wise operations as follows:

\[
S_{q,d} := \sum_{i \in ||B_q||} \max_{j \in ||B_d||} \text{count}(\text{xnor}(\text{sign}(B_{q_i}) \cdot \text{sign}(B_{d_j}^T))).
\]  
(9)

Equation (9) replaces most of floating-point arithmetics with bit-wise operations, providing the potentiality of online computation acceleration. We plan to develop hardware-adapted computation operators (e.g., "bit-wise tensors") in future. Lastly, Bi-ColBERT adopts the training paradigm of ColBERT (2020) that is optimized via the pairwise softmax cross-entropy loss over the computed scores of positive and negative passage samples.

### 4 Experimental Evaluation

We now evaluate our approach with the aim of answering the following research questions:

- **RQ1.** How does Bi-ColBERT perform in the fine-grained Top-K passage searching task?

- **RQ2.** Is the proposed semantic diffusion technique effective to hedge the information loss?

- **RQ3.** How does the proposed gradient estimator compare to the previous counterparts?

We implement our embedding binarization approach directly on pretrained ColBERT, denoted as ColBERT\(\text{pretrain}\). To give a fair comparison, we use the same dataset (i.e., MS MARCO) and evaluation metric (i.e., MRR@10) with ColBERT. Detailed experimental setups and baseline introduction are attached in Appendix B.
Table 1: Top-1000 Reranking results on MS MARCO.

| Model                  | MRR@10 |
|------------------------|--------|
| BM25_{official} (Robertson et al., 1995) | 16.7   |
| KNRM (Xiong et al., 2017; Dai et al., 2018) | 19.8   |
| Duet (Mitra et al., 2017) | 24.3   |
| FT+ConvKNRM (Hofstätter et al., 2019) | 29.0   |
| BERT_{base} (Nogueira and Cho, 2019) | 34.7   |
| BERT_{large} (Nogueira and Cho, 2019) | 36.5   |
| ColBERT_{official} (Khattab and Zaharia, 2020) | 34.9   |
| ColBERT_{pretrain}     | 32.8   |
| Bi-ColBERT             | 31.7   |

4.1 Overall Performance (RQ1)

Similar to ColBERT (2020), we evaluate the fine-grained searching capability via the official Top-1000 reranking on MS MARCO w.r.t. MRR@10. From Table 1, we have the following observations:

1. Bi-ColBERT works better than prior non-BERT-based models, owing to the power of fine-tuned BERT-based methods in learning deep contextualized semantic representations.

2. Furthermore, ColBERT and Bi-ColBERT make the tradeoff between passage searching quality and retrieval cost, where ColBERT aims to simplify the neural architecture and our proposed methods focus on effective embedding binarization. We use $r_s$ and $r_t$ to denote the ratios of Bi-ColBERT over ColBERT w.r.t. embedding size compression and online score computation acceleration on CPUs (details are in Appendix B). Considering the advantages in memory reduction and inference acceleration, i.e., $r_s=15.1 \times$, $r_t=7.3 \times$, Bi-ColBERT provides an alternative option for ColBERT, especially in resource-limited scenarios.

3. Despite the performance gap between ColBERT and our approach, we argue that it is mainly caused by the inevitable information loss in numerical binarization, which is unfortunately common in prior work (Lin et al., 2017; Darabi et al., 2018; Gong et al., 2019; Qin et al., 2020). To narrow the gap, as briefly introduced in § 1, several independent yet advanced methods can be further studied and deployed for model improvement. We provide a detailed discussion later in § 5.

4.2 Analysis of Semantic Diffusion (RQ2)

In this section, we study the effectiveness of our proposed semantic diffusion (SD) by setting two groups of ablation experiments. From Table 2(A),

1. We first disable the embedding binarization (EB) and check the effect of SD on our model. Results show that simply using SD will not negatively affect the holistic model performance. This validates our analysis in Appendix A that SD aims to balance the spectrum of embedding matrix (e.g.,

Table 2: (A) Ablation study of Semantic Diffusion. (B) Gradient estimator comparison.

| Components          | Results |
|---------------------|---------|
| SD ($f$) + EB ($\frac{1}{s}$) | 32.8    |
| SD ($f$) + EB ($\frac{1}{t}$) | 32.9    |
| SD ($f$) + EB ($\frac{1}{r}$) | 30.3    |
| SD ($f$) + EB ($\frac{1}{s}$) | 31.7    |

2. In the second experiment group, we trigger EB and the results demonstrate that SD together with our proposed gradient estimation can effectively approach our target to hedge the information loss for representation binarization.

4.3 Gradient Estimator Comparison (RQ3)

Lastly, the experimental results in Table 2(B) show the consistent performance superiority of our proposed gradient estimator over all prior counterparts. This generally follows our observation explained in § 2. On the contrary, our approach to approximate Unit Impulse Function follows the main optimization direction of factual gradients with sign$(\cdot)$; and different from previous solutions, this guarantees the coordination in both forward and backward propagation of model optimization.

5 Discussion for Future Work

We summarize five promising future directions.

1. It is pragmatic to evaluate the adaptability of our approach to other BERT-based models.

2. A promising direction could be using embedding binarization for other scenarios with efficiency demands (Zhang and Zhu, 2020; Chen et al., 2022b; Zhang et al., 2022; Chen et al., 2022c; Yang et al., 2021).

3. ColBERT also employs faiss (Johnson et al., 2019), a tool for large-scale vector-similarity search. Thus, it is worth developing a similar index-based data structure specifically for retrieval in the discrete embedding space.

4. Data augmentation, e.g., feature-based augmentation (Wang et al., 2019), is another effective technique to boost embedding informativeness before and after the binarization.

5. If the training resource is adequate, quantization-aware training (Zafrir et al., 2019) resembles the standard fine-tuning and thus is promising to compensate for the performance degradation.
A Semantic Diffusion Analysis

**Theorem 1** (Semantic Diffusion). For each pair of unprocessed and processed embedding bags, i.e., \((E, E')\), \(E = U \Sigma V^T\), where \(U\) and \(V\) are unitary matrices and descending singular value matrix \(\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_d)\). Then \(E(E) = U \Sigma \Sigma \mu V^T\) where \(\Sigma_{\mu} = \text{diag}(\mu_1, \mu_2, \ldots, \mu_d)\) \(0 < \mu_1 \geq \ldots \geq \mu_d < 1\) is in the ascending order.

**Proof.** Conducting SVD decomposition on \(E\), we have \(E = U \Sigma V^T\), where \(U\) and \(V\) are unitary matrices of singular vectors. Then following \(p_{(h)} = (E^T E)^{h-1} p_{(0)}\), we shall have \(p_{(h)} = (E^T E)^{h} p_{(0)}\). Replacing \(E\) with its SVD decomposition, we get the following equation:

\[
p_{(h)} = (V \Sigma^{2h} V^T) p_{(0)}. \tag{10}
\]

Then we transform the projection matrix computed in Equation (2) as follows:

\[
P = p_{(h)} p_{(h)}^T = (V \Sigma^{2h} V^T) p_{(0)} (V \Sigma^{2h} V^T) p_{(0)}^T = V \Sigma^{2h} V_{(h)} p_{(0)} (V \Sigma^{2h} V^T) p_{(0)}^T = V \Sigma^{2h} V p_{(0)}^T V_{(h)} \tag{11}
\]

Let \(t = V^T p_{(0)}\), we can further simplify the above equation to:

\[
P = V \Sigma^{2h} t (t^T)^{-1} V^T \tag{12}
\]

where scalar \(t^T \Sigma^{2h} t\) is defined as:

\[
t^T \Sigma^{2h} t = \sum_{j=1}^{d} t_j^2 \sigma_j^{4h} \tag{13}
\]

Recalling that \(E = E(I - \epsilon P)\), \(E(\hat{E}) = E - \epsilon \cdot E(E P)\). Then we focus on the term \(E(E P)\):\n
\[
E(E P) = \frac{1}{t^T \Sigma^{h}} U \Sigma^{h+1} t \cdot \Sigma^{2h} V^T. \tag{14}
\]

Since \(p_{(0)} \sim \mathcal{N}(0, I)\) and \(V\) is a unitary matrix, thus \(t \sim \mathcal{N}(0, I)\). This indicates that each element of \(t\), e.g., \(t_j \in t\), is i.i.d. random variable. Thus, \(E(t_j \cdot t_k) = 0\) for \(j \neq k\) and \(E(t^T t)\) is a diagonal matrix, i.e., \(E(t^T t) = \text{diag}(t_1^2, t_2^2, \ldots, t_d^2)\). We then have:

\[
E(E P) = U \cdot \text{diag}(\sigma_1 t_1^2 \sigma_1^{4h}, \ldots, \sigma_d t_d^2 \sigma_d^{4h}) \cdot V. \tag{15}
\]

Therefore,

\[
E(\hat{E}) = U \cdot \text{diag}(\sigma_1 - \epsilon \sigma_1 t_1^2 \sigma_1^{4h}, \ldots, \sigma_d - \epsilon \sigma_d t_d^2 \sigma_d^{4h}) \cdot V. \tag{16}
\]

Let \(\mu_k = 1 - \epsilon \sigma_k t_k^2 \sigma_k^{4h}\), with \(\epsilon \in (0, 1)\), obviously, \(0 < \mu_k < 1\). Furthermore, \(\gamma_k \geq k_2\), we have:

\[
\mu_k - \mu_k = \epsilon \sigma_k t_k^2 \sigma_k^{4h} \sum_{j=1}^{d} \frac{t_j^2 \sigma_j^{4h}}{t_k^2 \sigma_k^{4h}} \geq \epsilon \sigma_k t_k^2 - \frac{t_k^2 \sigma_k^{4h}}{t_k^2 \sigma_k^{4h}} = 0, \tag{17}
\]

as \(\sigma_k \geq \sigma_k^{4h}\) and \(t_{k_1}\) and \(t_{k_2}\) are i.i.d. random variables with same normal distribution. Equation (17) proves that \(\mu_k\) is monotone non-decreasing in expectation, which completes the proof. \(\square\)

Intuitively, given the same orthonormal bases, compared to unprocessed embedding bag \(E\), it is harder in expectation to reconstruct \(\hat{E}\) with informative semantics being diffused out in larger matrix sub-structures, which however hedges the information loss in numerical binarization.

B Experiment Setup

**Dataset and Metric.** Similar to work (2019a; 2019b; 2020), we evaluate our model on the MS-MARCO Ranking (2016) dataset. It is a collection of 8.8M passages from 1M real-world queries to Bing. Each query is associated with sparse relevance judgments of one (or a small number of) documents marked as relevant and no documents explicitly marked as irrelevant. Similar to ColBERT (2020), we use metric MRR@10 for performance evaluation.

**Baselines.** We include baselines for comparison from prior (1) learn-to-rank models, i.e., BM25 (official) (1995), KNRM (2018; 2017), Duet (2017), FastText+ConvKNRM (2019) (denoted as FT-ConvKNRM), and (2) BERT-based models, i.e., BERTbase (2019), BERTlarge (2019) and ColBERT (2020). We use subscripts, i.e., official- and large-, to denote respective referred versions. ColBERTpretrain denotes the pretrained version.

**Implementations.** Our model is implemented under Python 3.7 and PyTorch 1.6.0. We initialize our model by using the pretrained ColBERT model under its reported default settings, i.e., ColBERTpretrain. Then we fine-tune our proposed model with: the same learning rate - \(3 \times 10^{-6}\), the batch size - 32, and embedding dimension - 128, iteration number for diffusing vector computation - \(h = 2\), and hyper-parameter \(\gamma = 0.5\). For other evaluation settings, we directly follow ColBERT (2020). We train our model in a Linux machine with 4 GPUs, each of which is a NVIDIA V100 GPU, 4 Intel Core i7-8700 CPUs, 32 GB of RAM with 3.20GHz. For Top-K reranking tasks, we use CPUs per query for the passage retrieval. To evaluate the embedding compression ratio \(r_s\), we measure the size of embeddings produced by Bi-ColBERT and ColBERT per query. For embeddings from ColBERT, we use float32 as the default. Then to measure online score computation time cost ratio \(r_T\), based on the computed embeddings, we conduct experiments on CPUs with the vanilla NumPy (2022) implementation.
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