Approximating Global Contrastive Losses as Optimization over Batch Assignments

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Abstract

Contrastive Learning has recently achieved state-of-the-art performance in a wide range of tasks. Many contrastive learning approaches use mined hard negatives to make batches more informative during training but these approaches are inefficient as they increase epoch length proportional to the number of mined negatives and require frequent updates of nearest neighbor indices or mining from recent batches. In this work, we provide an alternative to hard negative mining in supervised contrastive learning, Tail Batch Sampling (TBS), an efficient approximation to the batch assignment problem that upper bounds the gap between the global and training losses, $L_{Global} - L_{Train}$. TBS improves state-of-the-art performance in sentence embedding (+0.37 Spearman) and code-search tasks (+2.2% MRR), is easy to implement - requiring only a few additional lines of code, does not maintain external data structures such as nearest neighbor indices, is more computationally efficient when compared to the most minimal hard negative mining approaches, and makes no changes to the model being trained.

1 Introduction

Contrastive Learning is used ubiquitously in training large representation models and has been shown to achieve state-of-the-art performance in a wide range of unimodal and multimodal tasks across language, vision, code, and audio (Chen et al., 2020a; Gao et al., 2021; Jiang & Wang, 2022; Guo et al., 2022; Yu et al., 2022; Radford et al., 2021; Ramesh et al., 2021; Saeed et al., 2021). In supervised contrastive learning, a paired dataset $(X,Y)$, $x_i \sim y_i$ such as similar sentences, code and corresponding language descriptors, or images and their captions is first constructed. Then batches of rows are sampled from this pair of datasets and a model $f(\cdot)$ is trained to concurrently maximize inner products for outputs of similar (positive) data inputs, $f(x_i)^T f(y_i)$, and minimize inner product for outputs of dissimilar (negative) data inputs $f(x_i)^T f(y_j), i,j \in B, i \neq j$. Due to batch size constraints from hardware limitations, for a fixed batch size $k$, only $Nk$ inner products of the total $N^2$ in $f(X)f(Y)^T$ are observed in the training loss for each epoch of training. Through the rest of this paper, we will refer to this observed training loss over $Nk$ inner products as $L_{Train}$ and the total loss over $N^2$ inner products as $L_{Global}$. It has been observed, both in contrastive metric and representation learning (Saunshi et al., 2019; Iscen et al., 2018; Xuan et al., 2020; Mishchuk et al., 2017; Wu et al., 2017; Song et al., 2016; Schroff et al., 2015; Harwood et al., 2017; Ge et al., 2018), that in order for batches to be informative during training, they should be constructed to contain “hard-negatives”, or large values of $f(x_i)^T f(y_j), i \neq j$. Additionally, it has been shown that including hard negatives in batches better approximates global losses (Zhang & Stratos, 2021).

Currently, approaches for constructing batches, and controlling which inner products of the total $N^2$ should be used for training, broadly fall into one of two categories. One either uses random sampling or mines nearest neighbors of the reference sample $x_i$ in order to greedily insert hard negatives into the same batch as $x_i$. While greedily inserting hard negatives is effective in practice (Zhang et al., 2018; Xiong et al., 2021), these methods incur large costs both in time and resources as mining $l < k$ hard negatives per reference sample increases each training epoch by a factor $l$ and often requires maintaining and reranking nearest neighbor indices on expensive accelerated hardware during training. For instance, if 10

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hard negatives from $Y$ are mined for each sample in $X$ during batch construction one will increase the training time of a single epoch by a factor $10$, not including time taken for constructing and reranking nearest neighbor indices during training.

Furthermore, hard negative mining often requires frequent reranking to prevent negative anchors from being sampled from stale nearest neighbor indices and work on momentum based memory banks have found that hard negative mining is especially useful with small lookback intervals (i.e. 2-4 previous batches) (Wang et al., 2021). In this paper, we propose a global alternative to hard negative mining, Tail Batch Sampling (TBS), which seeks to efficiently learn a permutation over samples in $X$ and $Y$ to increase the likelihood of hard negatives rather than through greedy insertion. In Figure 1 above, we visually depict $L^{\text{Global}}$ and $L^{\text{Train}}$ along with the modifications on batches, and therefore the observed loss, for our proposed approach TBS.

First, we show theoretically that the upper bound on $L^{\text{Global}} - L^{\text{Train}}$, with no oversampling or assumptions on the data/model for NT-Xent losses (Sohn, 2016), the most common contrastive loss, is only dependent on batch assignments. We prove that this upper bound is minimized as a Quadratic Bottleneck Assignment Problem which seeks to maximize the number of hard negatives in batches by learning a permutation $\pi \in \Pi_N$ on the rows of $X$ and $Y$. We then formulate an $\tilde{O}(N^2)$ approximation for optimizing over this permutation, TBS, and show that it is more efficient than hard negative mining, even for $l = 1$, per training epoch. We analyze the loss behavior of TBS and show that TBS better approximates the total contrastive loss. Lastly, we empirically evaluate TBS in the context of supervised contrastive finetuning for sentence embedding (STS) and code search (CosQA, AdvTest, CodeSearchNet) and achieve state-of-the-art performance for all of these tasks.

In this work, we summarize our contributions as follows:

1. We prove that the upper bound of the gap between the total and observed losses in contrastive learning for a fixed batch size $B$ without oversampling, $L^{\text{Global}} - L^{\text{Train}}$, is constrained by a Quadratic Bottleneck Assignment Problem and can be relaxed to a Matrix Bandwidth Minimization problem.

2. We formulate a $\tilde{O}(N^2)$ approximation to the Matrix Bandwidth Minimization problem, TBS, using the Cuthill-Mckee heuristic and implement this algorithm in less than 50 lines of PyTorch.

3. We analyze the loss behavior of TBS and show that, in sentence embedding and code-search tasks, TBS better approximates the total contrastive loss.

4. We empirically evaluate TBS and achieve state-of-the-art performance on the STS taskset for sentence embeddings. Additionally, we achieve state-of-the-art performance for the CosQA, AdvTest, and CodeSearchNet tasks for joint programming language-natural language embeddings.
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The rest of this paper is organized as follows. In Section 2 we discuss related work. In Section 3, we derive upper bounds on the gap between total and observed losses and in Section 4 formulate these bounds as Quadratic Assignment Problems. In Section 5, we relax our QBAP to a Matrix Bandwidth Minimization problem, introduce our proposed method, TBS, for approximating global contrastive losses, and provide implementation details. In Section 6, we provide experimental results for sentence embedding and code search tasks using TBS. Section 7 provides discussion and Section 8 concludes the paper.

2. Related Work

2.1. Contrastive Representation Learning

Contrastive Learning has been used ubiquitously for vision, language, and audio representation learning. In vision tasks, SimCLR (Chen et al., 2020a) showed that using augmented views of the same image as positive samples and the NT-Xent objective (Sohn, 2016) improves performance of unsupervised classification, MoCo (He et al., 2020; Chen et al., 2020b) used memory banks of negative samples from recent batches to increase the effective contrastive batch size, and (Sylvain et al., 2020; Khosla et al., 2020) show improvements using supervised contrastive frameworks. For sentence embedding tasks, contrastive learning has been used both in pretraining (Logeswaran & Lee, 2018), finetuning and continuous prompt tuning settings (Gao et al., 2021; Jiang & Wang, 2022) to provide state-of-the-art performance. Additionally, contrastive learning has been used extensively to align representations across different modalities for downstream use in multimodal tasks such as those involving language/code, language/vision, and vision/decision making (Guo et al., 2022; Feng et al., 2020; Guo et al., 2021; Radford et al., 2021; Ramesh et al., 2021; Laskin et al., 2020).

2.2. Hard Negative Mining in Metric and Contrastive Learning

Selection of hard negatives during batch construction is well-studied and has been shown, both theoretically and empirically, to improve metric and contrastive learning (Saunshi et al., 2019; Iscen et al., 2018; Xuan et al., 2020; Mishchuk et al., 2017; Wu et al., 2017). Prior work in metric learning (Song et al., 2016; Schroff et al., 2015; Harwood et al., 2017; Ge et al., 2018) has observed that "hard negatives", or negatives which are difficult to discriminate against with respect to a particular query’s embedding, are beneficial for downstream classifier performance. In contrastive learning, (Zhang et al., 2018) uses Mixup to generate hard negatives in latent space. (Chuang et al., 2020) proposes a debiased contrastive loss which approximates the underlying “true” distribution of negative examples and (Yang et al., 2022) studies the effect of restricting negative sampling to regions around the query using a variational extension to the InfoNCE objective. In (Kim et al., 2020; Ho & Nvasconcelos, 2020) adversarial examples are used to produce more challenging positives and hard negatives. In (Xiong et al., 2021), nearest neighbor indices and a secondary model from prior checkpoints are used to mine hard negatives for text retrieval tasks.

(Robinson et al., 2021) reweights negative samples based on their Euclidean distance and debiases positive samples in order to control the level of difficulty in unsupervised contrastive learning. (Kalantidis et al., 2020) show that harder negative examples are needed to improve performance and training speed in vision tasks and propose adding ”synthetic” hard negatives in training batches using convex combinations of nearest neighbors.

2.3. Quadratic Assignment Problems

The Quadratic Assignment Problem (QAP), stemming from facilities locations problems (Koopmans & Beckmann, 1957), in combinatorial optimization seeks to minimize the total cost of assigning n facilities to n locations. Formally, one seeks to optimize $\min_{X \in \Pi_n} \text{trace}(WXDX^T)$ over $\Pi_n$, the set of $n \times n$ permutation matrices, for a given cost matrix $W$ and distance matrix $D$. The Quadratic Bottleneck Assignment Problem (QBAP), (Steinberg, 1961) takes a similar form but minimizes the maximum cost rather than the total cost, $\min_{X \in \Pi_n} \max_{i,j} (WXDX^T)_{i,j}$. The Graph Bandwidth Minimization Problem, seeks to minimize the dispersion of nonzero costs from the main diagonal for a sparse distance matrix $D$ and is a special case of QBAP in which the cost matrix $W$ increases proportional to $|i - j|$. In this paper, we prove that minimizing the upper bound between the total and the observed training losses $L_{Global} - L_{Train}$ over a pair of datasets $X, Y$ is bounded by Quadratic Assignment Problems and approximated by a Graph Bandwidth Minimization Problem. This connection is shown visually in Figure 1. As all of the aforementioned problems are NP-Hard, we utilize the Cuthill-McKee algorithm (Cuthill & McKee, 1969) a well-known linear time approximation for bandwidth minimization.
3. Global and Training Losses for Cross-Entropy based Contrastive Objectives

In this section, we characterize the gap between training and global losses in supervised contrastive learning for the Normalized Temperature-scaled Cross Entropy (NT-Xent) loss (Sohn, 2016). The NT-Xent loss is a ubiquitous contrastive objective used in state-of-the-art models for sentence embedding, code-language tasks and vision-language tasks (Gao et al., 2021; Jiang & Wang, 2022; Guo et al., 2022; Chen et al., 2020a; Radford et al., 2021).

Let $X, Y \in \mathcal{R}^{n \times d}$ be the output representations for two paired datasets each with $n$ samples. Consider a supervised setting where $x_i, y_i$ are considered "positive" pairs and $x_i, y_j$ are considered negative pairs $\forall i \neq j$. Note that the analysis we provide can be modified to incorporate multiple positives, such as those from class information, which will have tighter bounds in terms of the number of samples $N$ and the batch size $k$. Additionally, let $\tau \in \mathcal{R}^+$ be a tunable temperature parameter which scales logit values in the objective. When $\tau$ is small, the NT-Xent loss is a proxy for the hard maximum loss. Assume that all representations have been normalized, that is $\|x_i\|_2, \|y_i\|_2, = 1 \forall i$.

3.1. The Global and Training NT-Xent Objectives, $L_{Global}$ and $L_{Train}$

First, we provide the contrastive loss over all $N^2$ pairs of inner products between $X$ and $Y$. We call this the global objective as it contains all pairwise contrastive information and, in the absence of resource constraints, is the loss one would seek to minimize. The Global NT-Xent objective is given as follows:

**Definition 1** (Global NT-Xent objective). The Global NT-Xent objective is given as follows:

$$L_{Global} = -\frac{1}{N} \sum_{i=1}^{N} \log \left( \frac{\exp(x_i^T y_i \tau^{-1})}{\sum_{j=1}^{N} \exp(x_i^T y_j \tau^{-1})} \right) = \frac{1}{N} \sum_{i=1}^{N} (-x_i^T y_i \tau^{-1} + \log \sum_{j=1}^{N} \exp(x_i^T y_j \tau^{-1}))$$

Due to memory constraints, during training one does not make all $N^2$ comparisons over pairs in $X$ and $Y$ during a training epoch. Instead, each sample $x_i$ is only contrasted against $k$ in-batch samples in $Y$, its positive anchor $y_i$ and $k-1$ negative anchors. This observed loss during training will be strictly less than the global loss as it makes $k$ comparisons out of the total $N$ for each sample. For a fixed batch assignment $B$, let $B_i$ be the indices of rows in $Y$ contained in a batch with $x_i$. The Training NT-Xent objective is given as follows:

**Definition 2** (Training NT-Xent objective). The Training NT-Xent objective is given as follows:

$$L_{X,B} = -\frac{1}{N} \sum_{i=1}^{N} \log \left( \frac{\exp(x_i^T y_i \tau^{-1})}{\sum_{j \in B_i} \exp(x_i^T y_j \tau^{-1})} \right) = \frac{1}{N} \sum_{i=1}^{N} (-x_i^T y_i \tau^{-1} + \log \sum_{j \in B_i} \exp(x_i^T y_j \tau^{-1}))$$

3.2. Upper bounds on $L_{Global}$ and $L_{Train}$

For a fixed set of batches $B$, we will first provide upper bounds on $L_{Global}$ and lower bounds on $L_{Train}$ using Log-Sum-Exp properties (Calafiore & El Ghaoui, 2014). Using the upper bound for Log-Sum-Exp, the following upper bound on $L_{Global}$ can be obtained where equivalence is attained when all inner products have the same value.

**Lemma 3** (Upper bound on $L_{Global}$). With Log-Sum-Exp properties, $L_{Global}$ with the NT-Xent contrastive objective can be upper bounded as:

$$L_{Global} \leq \frac{1}{N} \sum_{i=1}^{N} \tau^{-1}(-x_i^T y_i \tau^{-1} + \max_j x_i^T y_j) + \log N.$$ 

Two lower bounds can be derived for $L_{Train}$, first using the standard lower bound for Log-Sum-Exp and then using the translation identity property (Nielsen & Sun, 2016).

**Lemma 4** (Lower bounds on $L_{Train}$). With Log-Sum-Exp properties, $L_{Train}$ with the NT-Xent contrastive objective can be lower bounded as:

$$L_{Train} \geq \frac{1}{N} (-\tau^{-1} x_i^T y_i + \max_j \sum_{i=1}^{N} \max_j x_i^T y_j, \min_j \sum_{i=1}^{N} \tau^{-1} x_i^T y_j + \log k))$$.
We can now bound the gap between the global and training losses of the NT-Xent objective for a fixed batch set of batches $B$. Since the diagonal terms are included in both the global and training losses, we are left with a difference over all off-diagonal elements and the off-diagonal elements within batches.

**Lemma 5** (Upper bounds on $L_{\text{Global}} - L_{\text{Train}}$). Upper bounds on $L_{\text{Global}} - L_{\text{Train}}$ for the NT-Xent objective are:

$$L_{\text{Global}} - L_{\text{Train}} \leq \frac{1}{N} \left( \sum_{i=1}^{N} \tau^{-1} \max_{y} x_i^T y_j - \max \{ \min_{i,j \in B_i} \tau^{-1} x_i^T y_j + \log \frac{N}{k}, \sum_{i=1}^{N} \sum_{j \in B_i} \tau^{-1} x_i^T y_j + \log N \} \right).$$

4. Minimizing $L_{\text{Global}} - L_{\text{Train}}$ as Quadratic Assignment over Batches

4.1. Minimizers for bounds in Theorem 5

Note that from Theorem 5 we have bounded the gap between $L_{\text{Global}} - L_{\text{Train}}$ without making any assumptions on data distribution or models. Additionally, we can see that the bounds are dependent on the batch assignments $j \in B_i$, batch size $k$, and total number of samples $N$. The minimizer of the upper bound over batch assignments, with a fixed batch size $k$ and number of samples $N$, can be written as the following optimization problems. Maximizing the first term in the $\max$ in Theorem 5 with a fixed batch size $k$, total number of samples $N$ and without oversampling, is attained by maximizing the smallest inner product over in-batch negatives: $\max_{\{B_i\}} \min_{i,j \in B_i} x_i^T y_j$. Maximizing the second term in the $\max$ of Theorem 5 with a fixed batch size $k$, total number of samples $N$ and without oversampling, is attained by maximizing the sum of inner product over in-batch negatives: $\max_{\{B_i\}} \sum_{i=1}^{N} \sum_{j \in B_i} x_i^T y_j$.

4.2. Optimizing over permutations $\pi, \pi$ with fixed $\{B\}$

We will now rewrite our optimization problems over permutations $\pi \in \Pi_N$ instead of sets of batch assignments $\{B\}$, an equivalent formulation. First, recognize that our bounds are dependent only on batch assignments of negatives $j \in B_i$. Without loss of generality assume that batches are constructed sequentially after applying a row permutation $\pi \in \Pi_N$ on $X$ and $Y$. That is, batches are constructed over $\pi(X), \pi(Y)$ such that $j \in B_i \iff \left[ \frac{i}{k} \right] = \left[ \frac{j}{k} \right]$. Recognize that this batch construction can be written as a block diagonal matrix of the form $A \in \{0,1\}^{N \times N}$ and $A_{i,j} = 1$ if $\left[ \frac{i}{k} \right] = \left[ \frac{j}{k} \right]$. Note this sequential constraint is not restrictive as it accommodates all possible batch assignments on $X, Y$ with the appropriate permutation $\pi \in \Pi_N$. When introducing a fixed sequential batching, we can rewrite the minimizer of the upper bound on $L_{\text{Global}} - L_{\text{Train}}$ from Theorem 5 as an optimization problem over permutations $\pi \in \Pi_N$ on $X, Y$ rather than explicitly on $\{B\}$. The form of these optimization problems are the Quadratic Bottleneck Assignment Problem and the Quadratic Assignment Problem (Koopmans & Beckmann, 1957). These are well-known NP-Hard combinatorial optimization problems and in the following two sections we will discuss efficient approximations and implementations in PyTorch.

4.3. Bounds related to Quadratic Bottleneck Assignment Problems

The first upper bound in Lemma 5, for the sum $(L_{X}^{\text{Global}} - L_{X}^{\text{Train}}) + (L_{Y}^{\text{Global}} - L_{Y}^{\text{Train}})$ is minimized when the smallest inner product over in-batch negatives is maximized over $\pi \in \Pi_N$. Denote $Z_{ij} \triangleq \min \{x_i^T y_j, y_i^T x_j\}$ and $\odot$ as the Hadamard product. This is a QBAP, as we are interested in the minimizing the maximum value of the elementwise product of two symmetric matrices $\pi Z \pi^T$ and $A$.

**Theorem 6** (Formulation of QBAP for first bound in Lemma 5). The following Quadratic Bottleneck Assignment Problem, minimizes the first upper bound provided in Lemma 5 summed over $X$ and $Y$:

$$\min_{\pi \in \Pi_N} \max_{i,j} -A \odot \pi Z \pi^T.$$ 

4.4. Bounds related to Quadratic Assignment Problems

The second upper bound in Lemma 5 is minimized when the sum of inner products over in-batch negatives is maximized over permutations $\pi \in \Pi_N$. This can be formulated equivalently as either the Frobenius inner product between the symmetric matrices $\pi(XY^T + YX^T) \pi^T$ and $A$ or the Trace of their product, which are QAPs.
Theorem 7 (Formulation of QAP for second bound in Lemma 5). The following Quadratic Assignment Problem minimizes the second upper bound in Lemma 5:

\[ \min_{\pi \in \Pi_N} -\text{Tr}(A\pi(XY^T + YX^T)\pi^T). \]

Note that due to \( A \) being symmetric, \( L_{\text{Global}}^X - L_{\text{Train}}^X \) and \( L_{\text{Global}}^Y - L_{\text{Train}}^Y \) will be equivalent for the second upper bound in Lemma 5. In the next section, we will formulate an approximate solution with \( \tilde{O}(N^2) \) space and time complexity to the QBAP in Theorem 6.

5. Tail Batch Sampling: Efficient approximations to the QBAP with Cuthill-McKee

In practice, when \( N \) is large it can be difficult to hold \( XY^T \) in memory and approximation algorithms for the QAP problem (Kuhn, 1955; Munkres, 1957; Edmonds & Karp, 1972; Jonker & Volgenant, 1988) have \( O(N^3) \) complexity. Therefore, in optimizing over \( \pi \in \Pi_N \) we will make two modifications in order to develop a \( O(Nk) \) space and \( \tilde{O}(N^2) \) worst-case time complexity approximation to the QBAP in Theorem 6. First, we will sparsify the matrix \( XY^T \) on a quantile \( q \) which censors values below the quantile to 0. Secondly, we use an \( \tilde{O}(N^2) \) matrix bandwidth minimization heuristic commonly used for sparse matrix multiplication and decomposition (Cuthill & McKee, 1969) to efficiently attain an assignment over batches.

5.1. Approximating the QBAP: Sparsification and Matrix Bandwidth Minimization

Previous literature (Burkard, 1984) has shown the QBAP and Matrix Bandwidth Minimization Problem to be equivalent when the cost matrix is increasing in \( |i - j| \) and (Burkard, 1984) proposes thresholding in order to reduce coefficients in the matrix \( XY^T \). First, we sparsify \( XY^T \) on a threshold quantile \( q \) as follows:

\[ (\tilde{X}Y^T)_{i,j} = \begin{cases} 1, & x_i^Ty_j > q, i \neq j \\ 0, & \text{else.} \end{cases} \]

Note that there exists a minimal quantile \( q^* \) which constructs a sparse matrix \( \tilde{XY}^T \) that achieves the same solution as the dense matrix \( XY^T \). This is due to the fact that since we are interested in maximizing the minimum inner product over in-batch negatives, the smallest values of \( XY^T \) in each row are not of interest for the batch assignment objective.

5.2. Approximating the QBAP: Cuthill-McKee Algorithm

On this sparsified matrix \( \tilde{XY}^T \), we should seek to maximize the number of nonzero values in \( \pi(\tilde{XY}^T + (\tilde{XY}^T)^T)\pi^T \odot A \) to minimize the upper bound in 6. We can show that the QBAP formulations and the Matrix Bandwidth Minimization problem are approximately equivalent due to the fixed sequential batching which assigns batches along the main diagonal of \( \pi XY^T \). Since \( \{B\} \) is comprised of blocks on the main diagonal, minimizing the dispersion of non-zero entries, after sparsification, from the main diagonal will maximize the likelihood of large inner product values within batches. As a result, our algorithm for minimizing \( 2L_{\text{Global}} - L_{X}^{\text{Train}} + L_{Y}^{\text{Train}} \), TBS, is an \( \tilde{O}(N^2) \) relaxation to the bound in Theorem 6. Above in Algorithm 1 we detail the Cuthill-Mckee algorithm for matrix bandwidth minimization (Cuthill & McKee, 1969) along with worst case runtimes for each step.
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Algorithm 1 Cuthill-McKee algorithm on sparse graph

Require: Sparse Adjacency Matrix $G \in \{0, 1\}^{N \times N}$

1. Get peripheral vertex $v_i$ with lowest degree from the vertices in $G$. Set $\pi = [v_i]$. [$O(|E|) = O((1 - q)N^2) = O(kN)$]
2. Perform Breadth First Search on the Graph $G$ rooted at $v_i$ excluding elements in $\pi$. [$O(N)$]
3. Label each vertex, other than $v_i$, on their distance from $v_i$, creating "levels". [$O(|\pi|)$]
4. Order vertices by level, tiebreaker of ascending vertex degree and append the first item to $\pi$. [$O(N\log(N))$]
5. If $|\pi| < N$, return to Step (2) and repeat this process with the most recently added vertex as the root.
6. Return permutation $\pi = [i_0, i_1, \ldots, i_n]$

Additionally, we note that the Cuthill-McKee algorithm has been extensively applied in graph bandwidth problems. In the directed unweighted graph setting, a linear graph arrangement (Feige, 2000) is applied on an adjacency matrix $G \in \{0, 1\}^{N \times N}$ such that each node is placed at the corresponding row integer value $i$ on the x-axis with edges to nodes $j$ if $G_{ij} \neq 0$. The objective in this case is to minimize the length of the longest edge. By viewing the batch assignment problem in this graphical setting, one can recognize that in our sparse implementation TBS seeks to minimize the distance between samples $x_i, y_j$ with large inner product values. This connection is visually depicted in the Figure 3 below.

Figure 3. Visual depiction of connection between minimizing graph and matrix bandwidths.

6. Experimentation

In this section, we detail experiments for sentence embedding and code-search tasks when using TBS instead of the standard Random Sampling. We find that TBS improves state-of-the-art performance for both tasks while requiring minimal code changes. Three quantiles, $\{0.99, 0.999, 0.9999\}$, for TBS were tested across all experiments; no hyperparameters were varied other than the batch size and learning rate. All experimentation was conducted on one NVIDIA A100 GPU with CUDA 11.6 and PyTorch 1.11.0. The full specification of hyperparameters are included in Appendix Section F.

6.1. Code Search Experiments

| Model          | CosQA | AdvTest | Ruby | JS   | Go    | Python | Java | PHP | CSN Avg |
|----------------|-------|---------|------|------|-------|--------|------|-----|--------|
| RoBERTa        | 60.3  | 18.3    | 58.7 | 51.7 | 85.0  | 58.7   | 59.9 | 56.0| 61.7   |
| CodeBERT       | 65.7  | 27.2    | 67.9 | 62.0 | 88.2  | 67.2   | 67.6 | 62.8| 69.3   |
| GraphCodeBERT  | 68.4  | 35.2    | 70.3 | 64.4 | 89.7  | 69.2   | 69.1 | 64.9| 71.3   |
| SYNCoBERT      | -     | 38.3    | 72.2 | 67.7 | 91.3  | 72.4   | 72.3 | 67.8| 74.0   |
| PLBART         | 65.0  | 34.7    | 67.5 | 61.6 | 88.7  | 66.3   | 66.3 | 61.1| 68.5   |
| CodeT5-base    | 67.8  | 39.3    | 71.9 | 65.5 | 88.8  | 69.8   | 68.6 | 64.5| 71.5   |
| UniXcoder      | 70.1  | 41.3    | 74.0 | 68.4 | 91.5  | 72.0   | 72.6 | 67.6| 74.4   |
| UniXcoder w/ TBS | **71.1** | **43.3** | **76.7** | **70.6** | **92.4** | **74.6** | **75.3** | **70.2** | **76.6** |

Table 1. The performance comparison of supervised models along with a comparison of the best performing model (UniXcoder) (Guo et al., 2022) when using TBS vs the standard Random Sampling. The reported score is Mean Reciprocal Rank magnified by a factor of 100. TBS improves previous best MRR when used with UniXcoder by 2.2 points achieving new state-of-the-art results (Row shaded gray).
Semantic code search is an important problem in representation learning that bridges programming and natural languages (Husain et al., 2019). In this task, one is concerned with returning relevant code when given a natural language query. This is a problem of great interest due to the potential for aiding programmers when developing code and possesses challenges in aligning highly technical and abbreviated language with the programming language modality. Recently, models for this task have been improved using contrastive learning (Guo et al., 2022) by enforcing sequence embeddings for code and their corresponding natural language comments to have large inner products relative to unrelated natural language comments. TBS provides further gains and achieves state-of-the-art performance when used with well-performing contrastive learning models, UniXcoder (Guo et al., 2022) as shown in Table 1.

### 6.2. Sentence Embedding Experiments

| Model                      | STS12 | STS13 | STS14 | STS15 | STS16 | STS-B | SICK-R | Avg |
|----------------------------|-------|-------|-------|-------|-------|-------|--------|-----|
| SBERT<sub>base</sub>       | 70.97 | 76.53 | 73.19 | 79.09 | 74.30 | 77.03 | 72.91  | 74.89|
| SBERT<sub>base</sub>-flow   | 69.78 | 77.27 | 74.35 | 82.01 | 77.46 | 79.12 | 76.21  | 76.60|
| SBERT<sub>base</sub>-whitening | 69.65 | 77.57 | 74.66 | 82.27 | 78.39 | 79.52 | 76.91  | 77.00|
| ConSEKT-BERT<sub>base</sub> | 74.07 | 83.93 | 77.05 | 83.66 | 78.76 | 81.36 | 76.77  | 79.37|
| SimCSE-BERT<sub>base</sub> | 75.30 | 84.67 | 80.19 | 85.40 | 80.82 | 84.25 | 80.39  | 81.57|
| SimCSE-BERT<sub>base</sub> w/ TBS | **75.81** | **85.30** | **81.12** | **86.58** | **81.68** | **84.80** | **80.04** | **82.19** |
| DCPCSE-BERT<sub>base</sub> | 75.58 | 84.33 | 79.67 | 85.79 | 81.24 | 84.25 | **80.79** | 81.65|
| DCPCSE-BERT<sub>base</sub> w/ TBS | 75.39 | 84.27 | 79.72 | 86.03 | **82.19** | 84.19 | 79.65  | 81.63|
| SimCSE-RoBERTa<sub>base</sub> | 76.53 | 85.21 | 80.95 | 86.03 | 82.57 | 85.83 | 80.50  | 82.52|
| SimCSE-RoBERTa<sub>base</sub> w/ TBS | 76.94 | 85.64 | 81.87 | 86.84 | 82.78 | 85.87 | 80.68  | 82.95|
| DCPCSE-RoBERTa<sub>base</sub> | 76.75 | 85.86 | 80.98 | 86.51 | 83.51 | 86.58 | 80.41  | 82.94|
| DCPCSE-RoBERTa<sub>base</sub> w/ TBS | 76.99 | 86.11 | 81.70 | 87.34 | 84.17 | 85.99 | 80.17  | 83.21|
| SimCSE-RoBERTa<sub>large</sub> | 77.46 | 87.27 | 82.36 | 86.66 | 83.93 | 86.70 | 81.95  | 83.76|
| SimCSE-RoBERTa<sub>large</sub> w/ TBS | 78.90 | 88.39 | 84.18 | **88.32** | 84.85 | 87.65 | 81.27  | 84.79|
| DCPCSE-RoBERTa<sub>large</sub> | 79.14 | 88.64 | 83.73 | 87.33 | 84.57 | **87.84** | **82.07** | 84.76|
| DCPCSE-RoBERTa<sub>large</sub> w/ TBS | **79.89** | **89.15** | **84.32** | **88.16** | **85.33** | **87.54** | 81.53  | **85.13** |

Table 2. The performance comparison of supervised models along with a comparison of the best performing models, SimCSE (Gao et al., 2021) and DCPCSE (Jiang & Wang, 2022), when using TBS vs the standard Random Sampling. The reported score is Spearman correlation magnified by a factor of 100. TBS improves previous best Spearman correlation when used with SimCSE by 1.03 points and DCPCSE by 0.37 points achieving new state-of-the-art results (Rows shaded gray).

Recently, contrastive learning approaches which enforce that pretrained sequence embeddings for mined pairs of similar sentences have large inner products relative to the inner products of random pairs of sentences have provided state of the art performance for sentence embedding tasks. TBS provides further gains and achieves state-of-the-art performance when used with well-performing contrastive learning models, SimCSE (Gao et al., 2021), DCPCSE (Jiang & Wang, 2022), as shown in Table 2.

### 7. Discussion

In this section, we analyze the loss of contrastive learning models when using TBS compared to Random Sampling. We find that Tail Batch Sampling empirically reduces the gap $L_{Global} - L_{Train}$, as intended, by 40% in Code Search Net (Ruby) experiments. Additionally, runtime for each epoch when using TBS is approximately 50% that of the most minimal Hard Negative Mining implementation.

#### 7.1. Runtime comparison for TBS, Random Sampling, and Hard Negative Mining

We provide runtime comparisons for TBS, Random Sampling and Hard Negative (1), a hard negative mining setting with minimal computational burden relative to approaches currently used in practice. We find that TBS is more efficient per epoch than this minimal implementation of Hard Negative mining. As in experimentation detailed in Section 6, runtimes were calculated for a single NVIDIA A100 GPU with CUDA 11.6 and PyTorch version 1.11.0, 52GB RAM, and 4 vCPUs. Runtime statistics for the Code Search Net (Ruby) dataset with the UniXcoder model in Table 3 and the SNLI+MNLI (entailment+hard neg) dataset for sentence embedding with the Bert-Base-Uncased model is detailed in Table 4.
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| Computation Step          | Code Search               |
|---------------------------|---------------------------|
|                           | Random Sampling | TBS | Hard Negative (1) |
| Fwd + Bkwd Pass           | 381.45          | 381.45 | 762.9 (2x batches) |
| Add’l Fwd Pass            | -              | 118.51 | 118.51 |
| Comp. Nearest Neighbors   | -              | -   | 1.19    |
| Tail Batch Sampling       | -              | 2.31 | -       |
| Total Computation         | 381.45          | 502.27 | 882.61 |

Table 3. Runtime in seconds per epoch for Random Sampling, TBS, and Hard Negative (1) for the Code Search Net (Ruby) dataset \( N = 24,927, k = 64 \) with the UniXcoder model.

| Computation Step          | Sentence Embedding           |
|---------------------------|-----------------------------|
|                           | Random Sampling | TBS | Hard Negative (1) |
| Fwd + Bkwd Pass           | 442.26          | 442.26 | 884.52 (2x batches) |
| Add’l Fwd Pass            | -              | 370.31 | 370.31 |
| Comp. Nearest Neighbors   | -              | -   | 225.99 |
| Tail Batch Sampling       | -              | 140.32 | - |
| Total Computation         | 442.26          | 965.03 | 1480.82 |

Table 4. Runtime in seconds per epoch for Random Sampling, TBS, and Hard Negative (1) for the SNLI+MNLI (entailment+hard neg) dataset \( N = 275,602, k = 256 \) for sentence embedding with the Bert-base-uncased model.

7.2. Comparison of batch loss values between TBS, Random Sampling, and Hard Negative Mining

In Figure 4, we show the loss per sample vs step number in the Code Search Net (Ruby) dataset with the UniXCoder model for Random Sampling, TBS, and mining 1 hard negative per sample at the beginning of each epoch which we denote as Hard Negative (1). This hard mining approach has a smaller computational burden compared with approaches commonly used in practice but incurs 2x the runtime of TBS and 3x the runtime of random sampling as detailed in Section 7.1.

Additionally, we compare each training step loss to the expected loss over batches calculated at the beginning of each epoch. This requires performing a forward pass at the start of each epoch, assigning batches, and then computing the loss over in-batch negatives for each sample. After the first few epochs, while the expected loss over batches for Random Sampling and TBS is well approximated by the expected loss at the epoch start, expected losses for Hard Negative Mining...
are significantly overestimated. This corroborates findings in previous literature (Wang et al., 2021; Xiong et al., 2021) which motivates the need to update nearest neighbor indices within an epoch and further increases the computational burden of Hard Negative Mining. Empirically, we find that the observed loss per sample for TBS is substantially larger than that of Random Sampling or Hard Negative (1) and, like Random Sampling but not Hard Negative (1), can be well approximated by the expected loss at the epoch start. Losses are smoothed as a running average over the previous 500 steps.

7.3. Global and Expected Training loss for TBS and Random Sampling

![Graph showing Global and Expected Training loss for TBS and Random Sampling](image)

Figure 5. $L^{Global}$ and Expected $L^{Train}$ at the start of each epoch for Random Sampling and TBS on the Code Search Net (Ruby) dataset with the UniXcoder model.

With our empirical findings that both Random Sampling and TBS losses are well approximated by the expected loss at the epoch start we empirically test our theoretical contributions which claim that Matrix Bandwidth Minimization will approximately minimize the upper bound on the gap between $L^{Global} - L^{Train}$. In order to do so, we calculate the loss for in-batch negatives and the loss over all negatives for each sample when using either Random Sampling and TBS. We conduct this experiment once again on the Code Search Net (Ruby) dataset with the UniXcoder model. As shown in Figure 5, we find that using TBS reduces the gap $L^{Global} - L^{Train}$ by 40% when compared to Random Sampling on the final epoch. Additionally, the total loss over all samples is reduced by 30% and, as shown in Section C, yields stronger validation/test performance.

8. Conclusion

In this paper, we introduced Tail Batch Sampling (TBS), a method for better approximating global losses in contrastive learning through global batch assignments. TBS is an approximation for quadratic assignment problems that we prove characterize upper bounds for the gap between global and training losses in contrastive learning. Unlike previous approaches for improving contrastive learning through hard negative mining, TBS does not increase the training time of an epoch by oversampling and is more computational efficient compared to the most minimal hard negative mining approaches. We evaluate TBS on sentence embedding and code search tasks and in both tasks we achieve state-of-the-art performance. Our method provides an efficient alternative to hard negative mining that is simple to implement, does not maintain additional data structures during training, provides strong performance, and performs global batch assignments once per training epoch.
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A. Derivation of Proofs for Theorems 6 and 7

In this section, we provide proof derivations of Theorems 6 and 7.

A.1. Proof of Theorem 6

Proof. First, we will define $L_{Global} - L_{Train}^X$ and $L_{Global} - L_{Train}^Y$. To relate the sum over these quantities to the QBAP, we need only use the fact that $\sum_{i}^{N} x_i \geq N \min_{i} x_i$.

\[
L_{Global} - L_{Train}^X \leq \frac{1}{N} \sum_{i=1}^{N} \tau^{-1}(\max_{j}^{x_i T} y_j - \min_{j \in B}^{x_i T} y_j) + \log \frac{N}{k}
\]

\[
L_{Global} - L_{Train}^Y \leq \frac{1}{N} \sum_{i=1}^{N} \tau^{-1}(\max_{j}^{y_i T} x_j - \min_{j \in B}^{y_i T} x_j) + \log \frac{N}{k}
\]

\[
\max_{B} \sum_{i=1}^{N} \min_{j \in B}^{x_i T} y_j + \min_{j \in B}^{y_i T} x_j \geq 2 \max_{B} \sum_{i=1}^{N} \min_{j \in B}^{x_i T} y_j, \min_{j \in B}^{y_i T} x_j
\]

\[
\propto \max_{B} \sum_{i=1}^{N} \min_{j \in B} Z_{ij} 
\]

\[
\geq N \max_{B} \min_{i,j \in B} Z_{ij} 
\]

\[
\propto \min_{\pi \in \Pi} -A \odot \pi Z_{\pi^T}. 
\]

(1)

A.2. Proof of Theorem 7

Proof. To relate the quantity $2L_{Global} - L_{Train}^X - L_{Train}^Y$ to the QAP, we need only use the fact that $\max_{i=1,2,...,k} x_i \geq \frac{1}{k} \sum_{i}^{k} x_i$.

\[
L_{Global} - L_{Train}^X \leq \frac{1}{N} \sum_{i=1}^{N} \tau^{-1}(\max_{j}^{x_i T} y_j - \max_{j \in B}^{x_i T} y_j) + \log N
\]

\[
\frac{1}{N} \min_{B} \sum_{i=1}^{N} -\max_{j \in B}^{x_i T} y_j \geq \frac{1}{Nk} \max_{B} \sum_{i=1}^{N} \sum_{j \in B}^{x_i T} y_j
\]

\[
= \frac{1}{Nk} \max_{\pi \in \Pi} Tr(A\pi XY^T \pi^T)
\]

\[
= \frac{1}{2Nk} \max_{\pi \in \Pi} Tr(A\pi XY^T \pi^T) + Tr((A\pi XY^T \pi^T)^T)
\]

\[
\propto \min_{\pi \in \Pi} -Tr(A\pi (XY^T + YX^T)\pi^T). 
\]

(2)

B. Expected loss values at Epoch Start for Random Sampling (10000 trials) in Code Search Net (Ruby)

We calculate the expected loss for Random Sampling over 10,000 random batch assignments and compare these loss values to TBS. The expected loss values for Random Sampling is clearly differentiated from Tail Batch Sampling even when compared with the mean over the 10,000 assignments plus 20 standard deviations as shown in Figure 6. As a result, the loss incurred by TBS is a better proxy of the global loss even compared to the largest loss incurred among 10,000 random assignments. Empirically, this shows that TBS provides improvements in Global batch assignment that are unlikely to be obtained by selecting across random assignments.
C. Validation Performance comparison for TBS, Random Sampling, and Hard Negative Mining

In this section, we provide validation and test performance for TBS, Random Sampling, and Hard Negative Mining for the Code Search Net (Ruby) dataset with the UniXcoder model. We find that TBS provides validation and test performance improvements compared to both Random Sampling and Hard Negative (1). In particular, the gap between test performance for TBS and Hard Negative (1) is greater than that of Hard Negative (1) and Random Sampling.

Figure 7. Validation and Test Performance for Random Sampling, Hard Negative (1), and TBS on the Code Search Net (Ruby) dataset with the UniXcoder model (Guo et al., 2022).
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D. Expected positive class Softmax probability at epoch start for TBS, Random Sampling, and Global

In this section, we provide the expected softmax probability at the start of each epoch across in-batch negatives when using TBS and Random Sampling and across all negative samples (i.e. Global setting) for the Code Search Net (Ruby) task with the UniXcoder model. We find that TBS better approximates the softmax probability of positive classes compared to random sampling and that random sampling results in loss saturation within a small number of epochs.

Figure 8. Expected positive anchor Softmax Probability for Code Search Net (Ruby) task using the UniXcoder model (Guo et al., 2022).

E. Complexity Analysis of Tail Batch Sampling

E.1. Quantile Estimation

First, it is necessary to compute the value at the quantile \( q \) in order to sparsify \( XY^T \). For large datasets in our experiments, this operation is estimated over chunks of \( XY^T \) and the median quantile value over the chunks is used. For each chunk of size \( l \), this requires computing values of \( XY^T \), performing a sort on these values and getting the index of the sorted values for the specified quantile. We denote matrix multiplication time complexity between two matrices as \( MM(\cdot, \cdot) \) and show that this estimation has time complexity approximately equivalent to the matrix multiplication \( XY^T \). We make the assumption that \( d \geq \log(Nl) \).

\[
\begin{align*}
\text{Space Complexity} &= N^{-1}l + NI = O(Nl) \\
\text{Time Complexity} &= 2Nl^{-1}(O(Nl \log(Nl)) + MM(Nd, ld)) = O(N^2d)
\end{align*}
\]

E.2. Optimizing over row permutations of \( X, Y \)

After estimating a value at which to sparsify, we need to get a sparsified similarity matrix \( \tilde{XY}^T \), construct a sparse adjacency matrix and run the Cuthill McKee algorithm. We assume that \( \tilde{N}(1-q) \), or the expected number of entries in each row is a
small multiple of the batch size $k$. First, we detail the space and time complexity for constructing $\tilde{X}Y^T$:

$$\text{Space Complexity} = \frac{3N^2(1 - q)}{k} = O(Nk)$$

$$\text{Time Complexity} = \frac{N^{-1}M(M(Nd,ld))}{k} = O(N^2d)$$

(4)

The space and time complexity for running the Cuthill McKee algorithm on $\tilde{X}Y^T$ is detailed below, we assume the implementation from (Chan & George, 1980) is used which provides runtime bounded by $N^2$ up to logarithmic factors.

$$\text{Space Complexity} = \frac{3N^2(1 - q)}{k} = O(Nk)$$

$$\text{Time Complexity} = \frac{O(mN \log(m))}{k} \leq O(N^2 \log(N))$$

(5)

Cuthill-McKee Runtime \leq O(N^2 \log(N))

Worst case, $m = N$

Note that $m$ is the maximum degree over nodes and for a large quantile value will typically be smaller than $N$. We find that Tail Batch Sampling incurs $O(Nk)$ space complexity and $O(N^2d)$ time complexity.

F. Hyperparameters

In Tables 5 and 6 below, we detail the hyperparameters used for the best performing sentence embedding and code search models respectively.

| Model                | Learning Rate | Batch Size | Number Epochs | Quantile q |
|----------------------|---------------|------------|---------------|------------|
| SimCSE BERT<sub>base</sub> | $3e-5$        | 256        | 5             | 0.999      |
| SimCSE RoBERTa<sub>base</sub> | $3e-5$        | 256        | 5             | 0.999      |
| SimCSE RoBERTa<sub>large</sub> | $7e-6$        | 256        | 5             | 0.9999     |
| DCPSE BERT<sub>base</sub> | $7e-3$        | 256        | 10            | 0.999      |
| DCPSE RoBERTa<sub>base</sub> | $7e-3$        | 256        | 10            | 0.999      |
| DCPSE RoBERTa<sub>large</sub> | $7e-3$        | 256        | 10            | 0.999      |

Table 5. Hyperparameters for best experimental results in Sentence Embedding tasks.

| Task      | Learning Rate | Batch Size | Number Epochs | Quantile q |
|-----------|---------------|------------|---------------|------------|
| CosQA     | $2e-5$        | 64         | 10            | 0.999      |
| AdvTest   | $2e-5$        | 64         | 10            | 0.999      |
| CSN Ruby  | $2e-5$        | 64         | 10            | 0.999      |
| CSN Go    | $2e-5$        | 64         | 10            | 0.999      |
| CSN JS    | $2e-5$        | 64         | 10            | 0.999      |
| CSN Python| $2e-5$        | 64         | 10            | 0.999      |
| CSN Java  | $2e-5$        | 64         | 10            | 0.999      |
| CSN PHP   | $2e-5$        | 64         | 10            | 0.999      |

Table 6. Hyperparameters for best experimental results in Code Search tasks for the UniXcoder model.

For Sentence Embedding tasks, hyperparameters do not vary significantly, other than the learning rate, between models and are similar to those used in the original models with random sampling (Gao et al., 2021; Jiang & Wang, 2022). For Code Search tasks, we do not vary hyperparameters from the default values from the original paper using random sampling (Guo et al., 2022) and, as a result, we use identical settings to the UniXcoder paper other than batch assignments.
G. Dataset Details

In Table 7 and Table 8, we provide details for all Sentence Embedding and Code Search datasets respectively.

| Setting | Name                          | # of samples | Source                      |
|---------|-------------------------------|--------------|-----------------------------|
| Train SNLI+MNLI (entailment+hard neg) | 275,602      | Hugging Face Download      |
| Test    | STS12                         | 3.1K         | Hugging Face Download       |
| Test    | STS13                         | 1.5K         | Hugging Face Download       |
| Test    | STS14                         | 3.7K         | Hugging Face Download       |
| Test    | STS15                         | 8.5K         | Hugging Face Download       |
| Test    | STS16                         | 9.2K         | Hugging Face Download       |
| Test    | STS-B                         | 1.4K         | Hugging Face Download       |
| Test    | SICK-R                        | 4.9K         | Hugging Face Download       |

Table 7. Description of training and evaluation datasets for sentence embedding tasks, all datasets are from (Gao et al., 2021) and further details can be found in the repository.

| Name         | Train samples | Validation | Test Samples | # of Candidates | Source                  |
|--------------|---------------|------------|--------------|-----------------|-------------------------|
| CosQA        | 20,000        | 604        | 1,046        | 1,046           | CodeBERT Repo           |
| AdvTest      | 251,820       | 9,604      | 19,210       | 19,210          | CodeBERT Repo           |
| CSN Go       | 167,288       | 7,325      | 8,122        | 28,120          | CodeBERT Repo           |
| CSN Java     | 164,923       | 5,183      | 10,955       | 40,347          | CodeBERT Repo           |
| CSN JavaScript | 58,025     | 3,885      | 3,291        | 13,981          | CodeBERT Repo           |
| CSN PHP      | 241,241       | 12,982     | 14,014       | 52,660          | CodeBERT Repo           |
| CSN Python   | 251,820       | 13,914     | 14,918       | 43,827          | CodeBERT Repo           |
| CSN Ruby     | 24,927        | 1,400      | 1,261        | 4,360           | CodeBERT Repo           |

Table 8. Description of training and evaluation datasets for code search tasks, all datasets are from (Feng et al., 2020) and further details can be found in the repository.

H. Implementation in PyTorch

In this section, we detail efficient implementation of TBS in PyTorch. Our implementation computes a permutation over samples π at the beginning of each epoch, requires less than 50 lines of code, makes no changes to the model being trained, and does not maintain external data structures after being run between epochs.

The PyTorch pseudocode for the implementation of TBS is contained below. In the case where $XY^T$ cannot be held in memory, the value of the quantile $q$ can be approximated over subsamples of entries from $XY^T$ and the sparse matrix $XY^T$ can be constructed similarly.

```python
def compute_perm_bandwidth_min(X, Y, quantile_thresh = 0.999):
    # (1) Normalize representations.
    X, Y = normalize(X), normalize(Y)

    # (2) Get value at quantile threshold on the inner product matrix.
    quantile_thresh = torch.quantile(X @ Y.T, quantile_thresh)

    # (3) Get inner product matrix hard thresholded on quantile.
    row, col, data = [], [], []
    ret = ((X @ Y.T).flatten() > quantile_thresh).nonzero
    row += ((ret - (ret % num_samples))/num_samples).tolist()
    col += (ret % num_samples).tolist()
    data += [1.0 for _ in range(len(ret))]

    # (4) Get perm which minimizes bandwidth of sparsified matrix with Cuthill-McKee.
    permutation = list(cuthill_mckee(sparse_matrix((data, (row, col)),
                                           shape=(num_samples, num_samples))))

    return permutation
```
In the next code block, we provide PyTorch pseudocode which, when inserted at the beginning of each epoch, will call the previous method and apply the permutation over samples before training. Note that the SequentialSampler is utilized to control batches after samples are reordered.

```python
## (1) At epoch start, run forward pass to get representations X, Y in the paired dataset.
model.eval()
with torch.no_grad():
    X, Y = [], []
    for batch in train_dataloader:
        X.append(model(inputs=batch[0]))
        Y.append(model(inputs=batch[1]))

## (2) Compute an approx to permutation which minimizes bandwidth of \pi XY^T \pi^T
for entries greater than quantile q.
permutation = compute_perm_bandwidth_min(X, Y, quantile=q)

## (3) Reorder the dataset on the approximate solution.
train_dataset = torch.utils.data.Subset(train_dataset, permutation)
train_sampler = SequentialSampler(train_dataset)
train_dataloader = DataLoader(train_dataset,
                             sampler=train_sampler,
                             batch_size=train_batch_size)

model.train()
## (4) Continue training.
```