# Scaling Deep Contrastive Learning Batch Size with Almost Constant Peak Memory Usage

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of negatives improve the quality of supervisedly or unsupervisedly learned encoders and representations [1, 7, 8]. This leads to 1) the

use of in-batch negatives where other anchors' positives (and hard

negatives) targets will be shared with current anchor as negatives,

2) scaling of the batch size to raise the total number of negatives.

Though in-batch negatives reuse representations to lower encoding

cost, computing loss and updating model parameters with respect

to it still require encoding all batch data as well as storing all activa-

## **ABSTRACT**

Contrastive learning has been applied successfully to learn numerical vector representations of various forms of data, such as texts and images. Learned encoders exhibit versatile transfer capabilities to many downstream tasks. Representation based search is highly efficient with state-of-the-art performance. Previous researches demonstrated that learning high-quality representations requires a large number of negatives in contrastive loss. In practice, the technique of in-batch negative is used, where for each example in a batch, other batch examples' positives will be taken as its negatives, avoiding encoding extra negatives. This, however, still conditions each example's loss on all batch examples and requires fitting the entire large batch into GPU memory.

This paper introduces a re-computation technique that decouples back propagation between contrastive loss and the encoder, removing encoder backward pass data dependency along the batch dimension. As a result, gradients can be computed for one subset of the batch at a time, leading to an almost constant peak GPU memory usage for batches of different sizes.

## **ACM Reference Format:**

## 1 INTRODUCTION

Contrastive learning learns to encode data into an embedding space such that related data points have closer representations and unrelated ones have further apart ones. Common recent contrastive losses such as noise contrastive estimation (NCE) and its derivatives operate in a batch-wise fashion, where each batch contains a number of data points separated into two groups, anchors and targets. Each batch anchor element is paired with a related target positive as well as zero or a few unrelated target hard (to distinguish) negatives. The similarities between anchor to positive and to all negatives are normalized into probability, and the negative log likelihood of the positives is used as a loss [14]. This attempts to estimate and raise the probability of positive against the full collection. Intuitive results demonstrated in many recent works is that a larger number

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tion. Therefore batch size is limited by total available GPU memory. The gradient accumulation technique, splitting a batch into chunks and summing gradients, cannot emulate a large batch as each chunk will be smaller and have fewer negatives. In this paper, we detail a technique that thresholds peak memory usage for contrastive learning to almost constant regardless of the batch size. We observe that we can separate the back-propagation process for contrastive learning loss into two parts, loss to representation, and representation to model parameter, with the latter being independent across batch examples given the former, detailed in subsection 3.2. We adopt the philosophy of trading computation for memory [2] and propose to run an additional forward without gradient tracking at the beginning of each update to build up all representations. The first part of back propagation is then run based on the representations to generate and store representations' gradient vectors into a Representation Gradient Cache. We then run one sub-batch at a time to fit into GPU memory and perform

encoder model forward-backward passes for each with the cached

representation gradients, casting the second part into a gradient

accumulation problem. Experiments show that with a small sacri-

fice in FLOPs, our technique enables a single consumer-grade GPU

to run experiments that used to require eight professional GPUs.

## 2 RELATED WORK

Contrastive Learning. Contrastive learning learns data representations by comparing the similarities of positive and negative data pairs and forcing the positive pairs to be more similar in the embedding space. Such a mechanism has been used in both unsupervised and supervised fashion. Unsupervised contrastive learning usually uses a data point's different augmentations as mutual positives and aims at pre-training a strong encoder [1, 6, 14]. Supervised contrastive learning has been applied to learn effective task-specific model as well as embedding space for representation based search [4, 7, 8]. As learning is not the focus of this paper, we refer readers to a survey paper we found helpful by Le-Khac et al. [10] for more information.

Deep Network Memory Reduction. Many early work has been done on reducing peak memory usage for training deep neural networks. Lots of them focus on the deepness of the model and

reduce memory usage along the depth dimension. The well-known gradient checkpoint method attempts to emulate training deep networks by training shallower layers and connecting them with gradient checkpoints and re-computation [2]. Some methods also attempted to use reversible activation functions, allowing internal activation in the network to be recovered over the course of back propagation [5, 11]. However, their effectiveness as part of contrastive encoders has not been confirmed. Recent work also attempts to remove the redundancy in optimizer tracked parameters on each GPU [13]. Another line of research focuses on reducing per floating number memory usage to store model parameters and/or activation and introduces techniques such as half or lower precision training and mixed precision training. These methods all reduce a model's memory usage by a factor and helps with training larger models. They can also be used to increase the batch size by the same factor. However, they are not designed to scale batch size for loss with data dependency and cannot further scale batch size beyond that factor.

## **METHODOLOGIES**

In this section, we first provide a mathematical analysis of properties of contrastive loss in subsection 3.2, based on which we describe the Gradient Cache technique in subsection 3.3. Then subsection 3.4 describes how the technique can be extended to multi GPUs.

## **Contrastive Learning Preliminaries**

Under a general formulation, given two classes of data  $S, \mathcal{T}$ , we want to learn encoders f and g for each such that, given  $s \in \mathcal{S}$ ,  $t \in$  $\mathcal{T}$ , encoded representations f(s) and g(t) are close if related and far apart if not related by some distance measurement. For large  ${\cal S}$ and  $\mathcal{T}$  and deep neural network based f and g, direct training is not tractable and a common approach is to use noise contrastive estimation (NCE) loss: sample anchors  $S \subset S$  and targets  $T \subset T$  as a training batch, where each element  $s_i \in S$  has a related element  $t_{r_i} \in T$  as well as zero or more specially sampled hard negatives. The rest of the random samples in T will be used as in-batch negatives. Define loss based on dot product as follows:

$$\mathcal{L} = -\frac{1}{|S|} \sum_{s_i \in S} \log \frac{exp(f(s_i)^\intercal g(t_{r_i})/\tau)}{\sum_{t_j \in T} exp(f(s_i)^\intercal g(t_j)/\tau)} \tag{1}$$

where each summation term depends on the entire set T and requires fitting all of them into memory.

We set temperature  $\tau = 1$  in the following discussion for simplicity as in general it only adds a constant multiplier to the gradient. As a side note, though to make it concrete we analyze NCE form loss, the technique to be introduced in subsection 3.2 is loss agnostic and can be applied to margin based loss such as Hinge as well.

#### **Analysis of Computation** 3.2

In this section, we give a mathematical analysis of NCE loss computation and its gradient. We will show that the back propagation process can be divided into two parts, loss to representation, and representation to encoder model; the separation then enables us to

devise a technique that removes data dependency in encoder parameter update. As an extra notation, denote normalized similarity,

$$p_{ij} = \frac{exp(f(s_i)^{\mathsf{T}}g(t_j))}{\sum_{t \in T} exp(f(s_i)^{\mathsf{T}}g(t))}$$
(2)

Suppose the function f is parameterized with  $\Theta$  and g with  $\Lambda$ .

$$\frac{\partial \mathcal{L}}{\partial \Theta} = \sum_{s_i \in S} \frac{\partial \mathcal{L}}{\partial f(s_i)} \frac{\partial f(s_i)}{\partial \Theta}$$
 (3)

$$\frac{\partial \mathcal{L}}{\partial \Lambda} = \sum_{t_i \in T} \frac{\partial \mathcal{L}}{\partial g(t_j)} \frac{\partial g(t_j)}{\partial \Lambda}$$
(4)

We note that the summation term for a particular  $s_i$  or  $t_i$  is a function of the batch, as,

$$\frac{\partial \mathcal{L}}{\partial f(s_i)} = -\frac{1}{|S|} \left( g(t_{r_i}) - \sum_{t_i \in T} p_{ij} g(t_j) \right), \tag{5}$$

$$\frac{\partial \mathcal{L}}{\partial g(t_j)} = -\frac{1}{|S|} \left( \epsilon_j - \sum_{s_i \in S} p_{ij} f(s_i) \right), \tag{6}$$

where

$$\epsilon_j = \begin{cases} f(s_k) & \text{if } \exists \ k \text{ s.t. } r_k = j \\ 0 & \text{otherwise} \end{cases}$$
 (7)

which prohibits the use of gradient accumulation.

We give two observations here:

- The partial derivative  $\frac{\partial f(s_i)}{\partial \Theta}$  depends only on  $s_i$  and  $\Theta$  while
- $\frac{\partial g(t_j)}{\partial \Lambda}$  depends only on  $t_j$  and  $\Lambda$ ; and Computing partial derivative  $\frac{\partial \mathcal{L}}{\partial f(s_i)}$  and  $\frac{\partial \mathcal{L}}{\partial g(t_j)}$  require only encoded representations and not  $\Theta$  or  $\Lambda$ .

This means we can run back propagation of  $f(s_i)$  for data point  $s_i$  independently with its own computation graph if we know the numer*ical* value of the partial derivative  $\frac{\partial \mathcal{L}}{\partial s_i}$ . Meanwhile the derivation of  $\frac{\partial \mathcal{L}}{\partial s_i}$  requires only *numerical* values of two set of representation vectors  $F = \{f(s_1), f(s_2), ..., f(s_{|S|})\}\$  and  $G = \{g(t_1), g(t_2), ..., g(t_{|T|})\}.$ A similar argument holds true for g, where we can use representation vectors to compute  $\frac{\partial \mathcal{L}}{\partial t_i}$  and back propagate for each  $g(t_j)$ independently. In the next section, we detail a technique to scale up batch size by pre-computing these representation vectors.

## 3.3 Gradient Cache Technique

Given a large batch, which does not fit into the available GPU memory for training, we first divide it into a set of sub-batches each of which can fit into memory for gradient computation, denoted as  $\mathbb{S} = {\hat{S}_1, \hat{S}_2, ...}, \mathbb{T} = {\hat{T}_1, \hat{T}_2, ...}$ . The full-batch gradient update is computed with the following steps.

Step1: Graph-less Forward. Before gradient computation, we first run an extra encoder forward pass for each batch instance to get their representations. Importantly, this forward pass will run without constructing the computation graph. It is possible to use larger sub-batches in this forward pass. Aligning the sub-batches with ones previously defined, on the other hand, allows recovery of models' stochastic behaviors such as dropout in a second forward

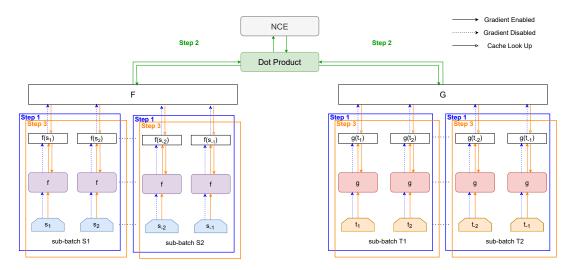


Figure 1: A illustration of our method. Up-going arrows corresponds to forward computation and down-going gradient back-propagation. For simplicity, we show size 2 sub-batch. Step 1 (blue) and Step 3 (yellow) run one sub-batch (box in figure) at a time, while Step 2 (green) process all representations F and G together.

Step2: Representation Gradient Computation and Caching. All representations computed are collected. We then compute the NCE loss for the batch based on the representation and have a corresponding computation graph constructed. A backward pass is then run to populate gradients for each representation. Note that the encoder is not included. Let  $\mathbf{u}_i = \frac{\partial \mathcal{L}}{\partial f(s_i)}$ ,  $\mathbf{v}_i = \frac{\partial \mathcal{L}}{\partial g(t_i)}$ , we take these gradient tensors and store them as a Representation Gradient Cache,  $[\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{v}_1, \mathbf{v}_2, ...]$ .

Step3: Sub-batch Gradient Accumulation. For each sub-batch defined, we run encoder sequentially to compute representations and build the corresponding computation graph. We take the sub-batch's representation gradients from the cache and run back propagation through the encoder. Gradients are accumulated for encoder parameters across all sub-batches. Effectively for f we have,

$$\frac{\partial \mathcal{L}}{\partial \Theta} = \sum_{\hat{S}_i \in \mathbb{S}} \sum_{s_i \in \hat{S}_i} \frac{\partial \mathcal{L}}{\partial f(s_i)} \frac{\partial f(s_i)}{\partial \Theta} = \sum_{\hat{S}_i \in \mathbb{S}} \sum_{s_i \in \hat{S}_i} \mathbf{u}_i \frac{\partial f(s_i)}{\partial \Theta}$$
(8)

where the outer summation enumerates each sub-batch and the entire internal summation corresponds to one step of accumulation. Similarly, for g, gradients accumulate based on,

$$\frac{\partial \mathcal{L}}{\partial \Lambda} = \sum_{\hat{T}_i \in T} \sum_{t_i \in \hat{T}_i} \mathbf{v}_i \frac{\partial g(t_i)}{\partial \Lambda}$$
 (9)

*Step4: Optimization.* When all sub-batches are processed, we can step the optimizer as if the full batch is processed in a single forward-backward pass.

Compared to directly updating with the full batch, which requires memory linear to the number of examples, our method fixes the number of examples in each model parameter gradient computation to be the size of sub-batch and therefore requires constant

memory for encoder forward-backward pass. The extra data pieces introduced by our method that remain persistent across steps are the representations and their corresponding gradients with the former turned into the latter after representation gradient computation. Consequently, in a general case with data from S and T each represented with d dimension vectors, we need to store (|S|d+|T|d) floating points on top of the computation graph in the cache, hence the almost constant peak memory usage.

Our method is non-intrusive to deep learning frameworks: in the second forward pass, forward-backward computation is applied for each sub-batch sequentially with gradients accumulated on model parameters in an additive manner. It can be combined easily with techniques such as automatic mixed precision. Meanwhile, this largely avoids compatibility issues and the need for adjusting the deep learning framework to optimize computation efficiency, eliminating the need for extra packages.

## 3.4 Multi-GPU Training

Illustrated in Figure 2, to exploit all examples across GPUs, we need to compute the gradients with all examples across all GPUs. This requires a single additional cross GPU communication after Step1 when all representations are computed. We use an all-gather operation to make all representations available on all GPUs. Denote  $F^n, G^n$  representations on n-th GPU and a total of N device. Step2 runs with gathered representations  $F^{\rm all} = F^1 \cup ... \cup F^N$  and  $G^{\rm all} = G^1 \cup ... \cup G^N$ . While  $F^{\rm all}$  and  $G^{\rm all}$  are used to compute loss, the n-th GPU only computes gradient of its local representations  $F^n, G^n$  and stores them into cache. No communication happens in Step3, when each GPU independently computes gradient for local representations. Step4 will then perform gradient reduction across GPUs as with standard parallel training.

<sup>&</sup>lt;sup>1</sup>Despite the mathematical derivation in the last section, automatic differentiation system is used in actual implementation, which automatically supports other variations of contrastive loss.

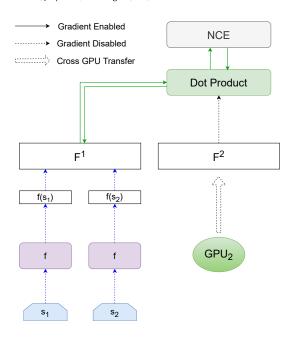


Figure 2: Multi-GPU: a 2 GPU setup where we show data flow in Step1 and Step2 for encoder f on the first GPU. For simplicity, we show only two examples.

#### 4 EXPERIMENTS

## 4.1 Setups

Task. As a concrete example, we take the training of representation based passage retriever and measure the efficiency of our proposed method. With queries as  $\mathcal S$  and passages as  $\mathcal T$ , the learning objective is to encode query, passage, and their relatedness with representation similarity in a supervised fashion (with relevance judgments). Text applications have much lower data processing/transfer overhead, allowing us to examine the actual compute time. We train a retriever with standard NCE loss using queries as anchors and pair each with a positive passage, a hard negative, and all in-batch negatives.

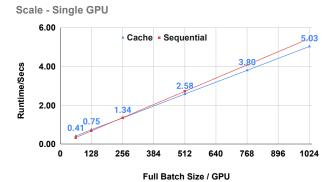
*Tests.* We introduce three tests to examine our method's efficiency and reliability in the existing deep learning framework. Let *max batch* denote the largest batch that fit into GPU memory,

- Scaling test: we compare scaling batch size to a  $\beta$  multiple of max batch using our method, to running sequentially as  $\beta$  training steps. We test with  $\beta = 1, 2, 4, 8, 12, 16$ .
- Small batch test: we take batch of β fraction max batch size and compare runtime with and without using gradient cache.
   Note that in these tests, using cache is not necessary but for measuring extra cost. We test with β = 1, ½, ¼, ½.
- Accuracy test: For verification, we also implement our method into dense passage retriever (DPR) code released by Karpukhin et al. [7] and compare accuracy to the original model trained on 8 V100 GPUs.

Data. Scaling and small batch tests use queries of length 16 and passages of length 128 common for web search. We only split

passage batch as short queries do not cause memory issues. The accuracy test uses the Natural Questions dataset [9].

Implementations. We initialize our encoder with deep Transformer model BERT-base [3] and implement the pipeline with Pytorch [12]. Models are trained in mixed precision. Multi-GPU tests are implemented with Distributed Data Parallel (DDP) with an NCCL backend. Note that DDP reduces gradients on each backward call (in Step3) and therefore incurs extra overheads. Single GPU tests run on one RTX 2080 ti and multiple GPU tests on four within a single node. Our GPU can fit 64 passages batch for training in scaling and small batch tests. A code snippet that supports multi GPU and mixed precision training can be found in subsection A.1. Accuracy test follows DPR training hyperparameters, using a 128 batch size and 256 max text length. It runs on a single RTX 2080 ti with mixed precision training and a sub-batch size of 16 for questions and 8 for passages <sup>2</sup>.



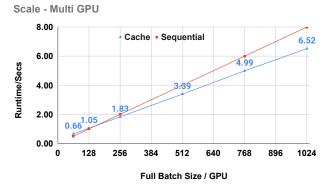
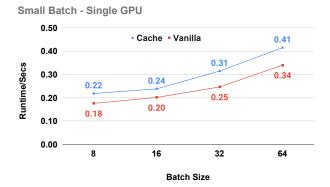


Figure 3: Scaling Tests: We compare runtime of a large batch between scaling batch size using cache (Blue) to running as small batches sequentially (Red).

#### 4.2 Results

Results for scaling test are plotted in Figure 3: we observe a roughly linear growth in update time against batch size, with our method's growth ratio being lower than sequential processing for both single and multi GPU cases. As it reaches four times batch size at 256, our method starts to show a margin of speed advantage. The reason

<sup>&</sup>lt;sup>2</sup>Detail can be found in our released code https://github.com/luyug/GC-DPR.



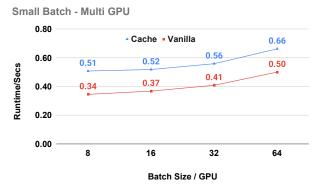


Figure 4: Small Batch Tests: We compare direct update (Vanilla, Red) with updates using gradient cache (Cache, Blue) runtime per batch with various small batch sizes.

Method	Top-20	Top-100	Runtime
DPR	78.4	85.4	~ 1day
Ours	79.9	86.1	40 hrs

Table 1: Accuracy Test: We compare top-20/100 hit accuracy and runtime reported by DPR authors using 8 GPUs and our implementation with Gradient Cache using 1 GPU. DPR runtime is a rough estimation taken from its github page.

is that though our method requires an additional representation computation, it has less (a single) optimizer step compared to the sequential case. The trade-off between weight update and extra forward computation here results in our method having larger throughput of examples compared to the vanilla sequential updates.

Figure 4 shows the result for small batch test. Our method incurs roughly 20% increase in time for a single GPU and 30% for multiple GPUs due to the extra computation. Meanwhile, similar to the vanilla update, our method also has under utilization issue when batch sizes are small, suggesting that one should use as large a sub-batch size as possible.

Accuracy test results are shown in Table 1. We observe only small differences in accuracy due to randomness in training. Thanks to its non-intrusive nature, we are able to combine our gradient cache technique with mixed precision training and train the model in less

than two times time with GPU resource of 23 times less memory and 8 times less FLOPS without accuracy compromise.

#### 5 EXTEND TO DEEP DISTANCE FUNCTION

Previous discussion assumes a simple parameter-less dot product similarity. In general it can also be deep distance function  $\Phi$  richly parameterized by  $\Omega$ , formally,

$$d_{ij} = d(s_i, t_j) = \Phi(f(s_i), g(t_j))$$
 (10)

This can still scale by introducing an extra *Distance Gradient Cache*. In the first forward we collect all representations as well as all distances. We compute loss with  $d_{ij}s$  and back propagate to get  $w_{ij} = \frac{\partial \mathcal{L}}{\partial d_{ij}}$ , and store them in Distance Gradient Cache,  $[w_{00}, w_{01}, ..., w_{10}, ...]$ . We can then update  $\Omega$ , in a sub-batch manner<sup>3</sup>,

$$\frac{\partial \mathcal{L}}{\partial \Omega} = \sum_{\hat{S} \in \mathbb{S}} \sum_{\hat{T} \in \mathbb{T}} \sum_{s_i \in \hat{S}} \sum_{t_j \in \hat{T}} w_{ij} \frac{\partial \Phi(f(s_i), g(t_j))}{\partial \Omega}$$
(11)

Additionally, we *simultaneously* compute with the constructed computation graph  $\frac{\partial d_{ij}}{\partial f(s_i)}$  and  $\frac{\partial d_{ij}}{\partial g(t_j)}$  and accumulate across batches,

$$\mathbf{u}_{i} = \frac{\partial \mathcal{L}}{\partial f(s_{i})} = \sum_{j} w_{ij} \frac{\partial d_{ij}}{\partial f(s_{i})}$$
(12)

and,

$$\mathbf{v}_{j} = \frac{\partial \mathcal{L}}{\partial g(t_{j})} = \sum_{i} w_{ij} \frac{\partial d_{ij}}{\partial g(t_{j})}$$
(13)

with which we can build up the Representation Gradient Cache. When all representations' gradients are computed and stored, encoder gradient computed with Step3 described in subsection 3.3. In philosophy this is essentially using gradient checkpoint to link up two caches. Note this covers early interaction f(s) = s, g(t) = t as a special case.

### 6 BROADER IMPACT

Today's use of cloud computing offers the flexibility to scale up hardware to a certain extent. When possible, higher-capacity hardware offers the most effective way of scaling training batch size. However, when a set of hardware is already built, it could take non-trivial efforts to grow further. Our technique enables scaling batch size for contrastive learning far beyond the limitation of GPU memory. With it, researchers can validate ideas without waiting for hardware updates and push the research boundary of large batch training, designing better models, objectives, and optimizers.

More importantly, we observe that for many university research groups (and small startup companies), the use of consumer-grade hardware usually caps the deep learning machine at 4 GPU systems with roughly 40G of GPU memory in total. In comparison, the popular DGX workstation in the industry offers 8 cards with about 240G of GPU memory, not to mention the cloud TPUs at Google. Our technique removes the memory limitation and alleviates the hardware gap. It allows experiments to be conducted at a larger scale under an academic setup: in particular, university researchers can replicate experiments done with higher capacity hardware. Meanwhile, adaptations of a pre-trained model for task and/or domain

<sup>&</sup>lt;sup>3</sup>It is not required to have same sub-batch splits for the two caches.

transfer does not need to compromise in batch size. In general, we make it possible for more people to work on and contribute to the problem and the application of contrastive learning.

The results of the scaling test show that merging batches with our methods can lower total computation time by reducing the number of optimizer steps. With optimization techniques [15, 16] that can use a large batch to produce an equal or better result with *equal or less* data than a small batch, our method provides a means to reduce the total computation time for limited resource learning.

#### 7 CONCLUSION

In this paper, we introduce a technique that breaks GPU memory limitations for contrastive learning. We adopt the philosophy of trading compute for memory and construct a representation gradient cache that removes in-batch data dependency in encoder optimization. We detail one non-intrusive implementation of the technique and cast the method into gradient accumulation. We show that the implementation is efficient for both single and multi-GPU training.

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#### A APPENDICES

## A.1 Code Snippet

Here we provide a Pytorch style code for our method. The code supports mixed precision training, gradient accumulation and multi GPU parallelism. In practice, one can make adjustments to cater actual setups such as model signature. The **train\_step** function can then be used in a training loop or a trainer class such as Lightning or Huggingface trainer.

```
import torch
import torch.nn.functional as F
from torch import Tensor, nn
from torch import distributed as dist
from torch.utils.checkpoint import get_device_states, set_device_states
from torch.cuda.amp import GradScaler, autocast
from typing import Iterable
CHUNK_SIZE_S = 16
CHUNK_SIZE_T = 8
class RandContext:
    Context manager that records device random state in first forward
    and restore it in the second forward
    def __init__(self, *tensors: Iterable[Tensor]):
        self.fwd_cpu_state = torch.get_rng_state()
        self.fwd_gpu_devices, self.fwd_gpu_states = get_device_states(*tensors)
    def __enter__(self):
        self._fork = torch.random.fork_rng(
            devices=self.fwd_gpu_devices,
            enabled=True
        )
        self._fork.__enter__()
        torch.set_rng_state(self.fwd_cpu_state)
        set_device_states(self.fwd_gpu_devices, self.fwd_gpu_states)
    def __exit__(self, exc_type, exc_val, exc_tb):
        self._fork.__exit__(exc_type, exc_val, exc_tb)
        self._fork = None
class Gatherer:
    Gatherer that gathers tensors from all GPUs in distributed training
    def __init__(self):
        assert dist.is_available()
        self.world_size = dist.get_world_size()
        self.rank = dist.get_rank()
    def gather_tensor(self, t: Tensor):
        all_tensors = [torch.empty_like(t) for _ in range(self.world_size)]
        dist.all_gather(all_tensors, t)
        all_tensors[self.rank] = t
        all_tensors = torch.cat(all_tensors, dim=0)
        return all_tensors
```

```
def encode(
        model: nn.Module,
        chunk: Tensor,
        fp16: bool
):
    with torch.no_grad():
        if fp16:
            with autocast():
                reps = model(chunk)
        else:
            reps = model(chunk)
    return reps
def encode_and_compute_grad(
        model: nn.Module,
        chunk: Tensor,
        grad: Tensor,
        fp16: bool
):
    if fp16:
        with autocast():
            reps = model(chunk)
            # apply gradient based on chain rule
            surrogate = torch.dot(reps.flatten(), grad.flatten())
    else:
        reps = model(chunk)
        # apply gradient based on chain rule
        surrogate = torch.dot(reps.flatten(), grad.flatten())
    return surrogate
def train_step(
        model_s: nn.Module,
        model_t: nn.Module,
        S: Tensor,
        T: Tensor,
        target: Tensor,
        accumulate_steps: int = 1,
        fp16: bool = False,
        scaler: GradScaler = None
):
    s_rand_contexts = []
    t_rand_contexts = []
    s_reps = []
    t_reps = []
    gatherer = Gatherer()
    # split into sub-batches
    s_chunks = S.split(CHUNK_SIZE_S)
    t_{chunks} = T.split(CHUNK_SIZE_T)
    # run first forward and record random states
    for chunk in s_chunks:
        s_rand_contexts.append(RandContext())
```

```
reps = encode(model_s, chunk, fp16)
    s_reps.append(reps)
s_reps = torch.cat(s_reps)
for chunk in t_chunks:
    t_rand_contexts.append(RandContext())
    reps = encode(model_t, chunk, fp16)
    t_reps.append(reps)
t_reps = torch.cat(t_reps)
# gather representations across GPUs
s_reps = gatherer.gather_tensor(s_reps)
t_reps = gatherer.gather_tensor(t_reps)
# compute representation gradient cache
s_reps = s_reps.detach().requires_grad_()
t_reps = t_reps.detach().requires_grad_()
loss = F.cross_entropy(torch.matmul(s_reps, t_reps.transpose(∅, 1)), target)
loss = loss / accumulate_steps
loss.backward()
s_grads = s_reps.grad.view(
    gatherer.world_size,
    -1,
    s_reps.size(1)
)[gatherer.rank].split(CHUNK_SIZE_S)
t_grads = t_reps.grad.view(
    gatherer.world_size,
    -1,
    t_reps.size(1)
)[gatherer.rank].split(CHUNK_SIZE_T)
# accumulate gradients across S sub-batches
for chunk_id, chunk in enumerate(s_chunks):
    # restore random state and compute gradient
   with s_rand_contexts[chunk_id]:
        surrogate = encode_and_compute_grad(
            model_s, chunk, s_grads[chunk_id], fp16)
    if fp16:
        scaler.scale(surrogate).backward()
    else:
       surrogate.backward()
# accumulate gradients across T sub-batches
for chunk_id, chunk in enumerate(t_chunks):
    # restore random state and compute gradient
    with t_rand_contexts[chunk_id]:
        surrogate = encode_and_compute_grad(
            model_t, chunk, t_grads[chunk_id], fp16)
    if fp16:
        scaler.scale(surrogate).backward()
    else:
        surrogate.backward()
# optimizer will be stepped on last accumulation step after function call
```