Increasing Negative Examples for ITC

Our current approach utilizes Distributed Data Parallel (DDP) [1] with a batch size of 256 per GPU. With two GPUs, the combined batch size is 512, and image/text features are gathered from all devices to increase the number of negative examples, as described in VLMo [2]. This method, as demonstrated in experiments with the supervised teacher (SHRe), improves performance.

However, implementations of image-text models that leverage contrastive learning typically use much larger batch sizes, and therefore have much more negative examples available. For instance, CLIP uses a batch size of 32,768 [3]. Achieving such large batch sizes would require more GPUs, as batch sizes exceeding 256 (per device) lead to out-of-memory (OOM) errors on the GPU (NVIDIA RTX 4090).

Although adding more GPUs to our setup is costly, the training time will be reduced proportionally to the number of GPUs used. For example, using two GPUs instead of one halves the training time. This is because DDP shardes the whole training dataset between all devices, such that each device processes a different part of the dataset [1]. From a cost perspective, this is acceptable, however, we decide against this approach, because we want to keep the number of GPUs manageable. Moreover, going with more GPUs would make the success of our approach dependent on the number of GPUs one has available, which is why we search for alternatives that allow us to increase the number of negative samples without requiring more GPUs.

One intuitive approach to increasing the number of negative examples is to use a FIFO queue-based memory bank. The queue stores image and text embeddings from previous batches. With each new batch, the memory bank is updated by adding the current batch embeddings and discarding the oldest (batch). These stored embeddings, combined with the embeddings of the current batch, are then used as negative examples.

Given a batch size of N and a memory bank size of M, we can achieve $N - 1 + M$ negative samples. For instance, with a batch size of 256 and a memory bank size of 768, we can attain 1023 negative samples. This configuration effectively simulates a contrastive loss with a batch size of 1024, and is comparable to four GPUs with DDP and a batch size of 256 per GPU. However, it is important to note that this "simulation" of larger batch sizes with a memory bank only applies to the number of negative examples. The actual gradients are still computed using the effective batch size of 512 (256 for two devices/GPUs).

For an implementation the training setup remains the same, we are merely required to maintain four distinct memory banks. This is because we apply the contrastive loss to both the intermediate and output cls token [`T_CLS`]/[`I_CLS`] of the shared Transformer block, as illustrated in (TODO: cite model figure), and we need one memory bank for negative image and text examples, respectively.

	Modality	Layer	Stores negatives for:
1	Image	FFN 1	[`T_CLS`] of FFN 1
2	Text	FFN 1	[`I_CLS`] of FFN 1
3	Image	FFN 2	[`T_CLS`] of FFN 2
4	Text	FFN 2	[`I_CLS`] of FFN 2

Table 1: Each memory bank stores the representations of one modality, created by a layer, to use as negative examples for the represenations of the other modality, created by the same layer.

Illustrated in Table 2, we observed a significant drop in performance. This suggests that simply increasing the number of negative examples via a memory bank does not help in learning richer represenations.

Model	ImageNet-1K Accuracy	Retrieval MSCOCO	Retrieval Flickr30K	Batch Size	ITC # Negative Examples
CLIP [3]	**72.6**	**66.73**	**90.1**	32,768	32,767
$\text{EMKUM}_{\text{DDP}}$	26.1	66.3	42.4	512	511
EMKUM_{MB}	17.8	54.4	30.3	256	511

Table 2: CLIP

We suspect this drop in performance originates because of the following reasons: When using an actual batch size of 512, so the same approach we used before ($\text{EMKUM}_{\text{DDP}}$ in Table 2), all negative examples come from the same model with the same weights, as they are all generated during the same step. Therefore, the representations share the same latent space and are consistent with each other. A similarity measure, in our case the cosine similarity, can then provide the model with a meaning of distance between the representations, in our case an image and text.

However, when using a memory bank, the negative examples come from previous batches that were stored in the memory bank. At previous batches, or steps respectively, the model's weights were different, and therefore the information encoded in the representations. As the model's weights constantly change, especially at the beginning of training, there is a continous shift in the representation space. This shift is so pronounced that even representations from the immediate previous steps differ significantly from the current representations, and a similarity measure will not provide meaningful information to the model.

This can be thought of as a less extreme case of comparing the representations of an image-only and text-only model, which are not associated with each other. In the beginning of our experiments, we tested image-text retrieval with the Data2Vec2 image and text model, and observed that this approach is ineffective for image-text retrieval. The representations produced by both models do not have any relationship with each other, and therefore the cosine similarity does not provide any meaningful information to the model.

With a memory bank, this effect is less pronounced, as the representations are still generated by the same model, but the shift in the model's weights is still significant enough to make the representations inconsistent with each other.

Relation to Initial Memory Bank Approach

The memory bank was initially introduced by [4] as a mapping of the complete training dataset. The embedding of each sample in the dataset is stored in the memory bank (illustrated in Figure 1). For each batch, K samples are randomly drawn from the memory bank to be used as negative examples. The representations of samples that are currently in the batch are then updated in the memory bank [4]. This approach is similar to ours, but faces the same problem: The representations come from an older variant of the model with different weights. Even worse, the representation of an example in the dataset is updated when it was last seen in a batch, which can be a long time ago for large datasets. However, the authors mitigate this issue by using proximal regularization, as shown in Equation 1.

$$-\log h(i, \boldsymbol{v}_i^{t-1}) + \lambda * \|\boldsymbol{v}_i^t - \boldsymbol{v}_i^{t-1}\|_2^2 \tag{1}$$

While the term $-\log h(i, \boldsymbol{v}_i^{t-1})$ can be ignored for now, as it just denotes a form of contrastive loss, the other term $\lambda * \|\boldsymbol{v}_i^t - \boldsymbol{v}_i^{t-1}\|_2^2$ serves as the proximal regularization term. It describes the mean squared error between the representation $\boldsymbol{v}_i^t$ of a training example i, e.g. an image, which is part of the current batch, and the representation of the same training example $\boldsymbol{v}_i^{t-1}$ stored in the memory bank and updated when it was last seen, denoted as time step $t-1$.

This term enforces that the representation of a training example does not change too rapidly between updates, and allows for more stable negative examples, depending on the value of weight λ. The authors report improved results with a value of $\lambda = 30$ [4], meaning that the proximal regularization term is 30 times more important than the contrastive loss term.

This forces the model to keep the representations of the training examples in the memory bank consistent with the current batch, so that a similarity measure can provide meaningful learning signals to the model. Our approach does not take this into account.

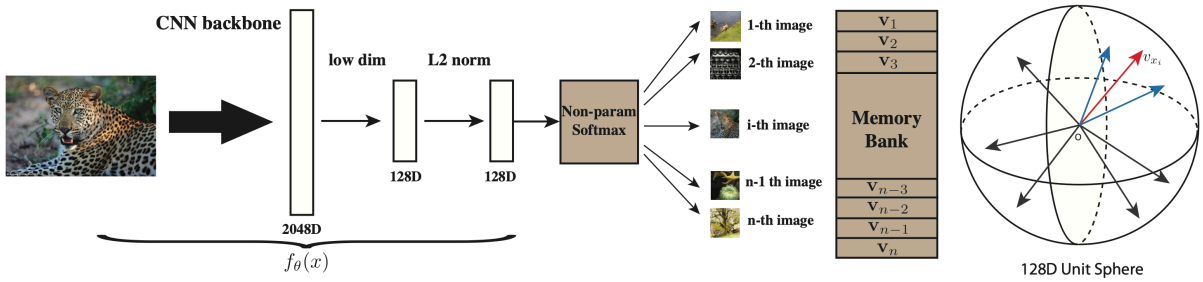


Figure 1: The memory bank, originally developed for self-supervised image representation learning, stores the 128-dimensional embedding of each training example. Contrary to what can be observed, instead of all just K samples are drawn from the memory bank in each iteration to be used as negative examples. [4]

Momentum Encoder

This problem was also identified by the authors of MoCo [5], and they employ a different approach to address this issue. They also use a queue-based memory bank, which is, similar to our approach, much smaller than the training dataset. However, in MoCo, the negative examples in the memory bank are not updated by the model that is being trained, but instead by a momentum encoder, which is an exponential moving average of the actual model weights, which is defined in Equation 2. Therefore, the negative examples do not come from the model that is trained, but only from the momentum encoder. This momentum encoder is a copy of the exact same model that is being trained, but its weights are not updated by gradients.

$$\theta_k = m * \theta_k + (1 - m) * \theta_q \tag{2}$$

With θ_k being the momentum encoder weights, θ_q the actual model weights, and m the momentum coefficient, the momentum encoder is updated very slowly. Typical values for m are usually picked between $m = 0.99$ and $m = 0.999$ [5]–[8].

The results are weights that change very slowly, which will also hold for the representations the momentum encoder produces. This approach can be seen as maintaining consistency in the model that produces the negative examples, rather than making the negative examples consistent themselves, through an additional regularization term, as in Equation 1. An application of this method for image-text contrastive learning can be seen in Figure 2.

Even though no gradients are needed to update the momentum encoder, it still requires additional GPU memory to keep it in memory, which is the disadvantage of this variant.

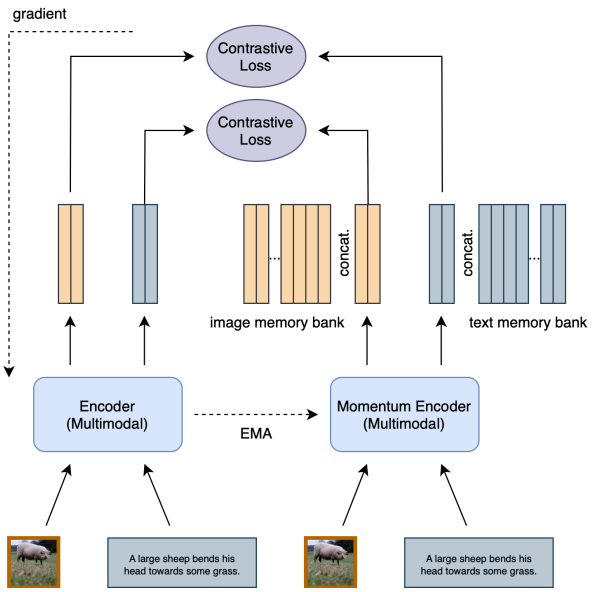


Figure 2: A momentum encoder generates negative examples for ITC, which are also stored in a memory bank that discards the representations of the oldest batch when new ones are added after every step. Figure inspired by MoCo v2 [6].

Resolution

We can't use the memory bank style of [4] since we have 3,264,868 training examples (see TODO: cite table of dataset size). Each embedding has a size of 768, and considering storing them at full precision (float32), we would need $3,264,868 * 768 * 4$ bytes > 10 GB of additional GPU memory. However, with our current setting we only have around 1.2 GB of GPU memory remaining.

We suspect that using a proximal regularization term, as in Equation 1, could also stabilize our memory bank approach. However, we cannot apply it since the term is based on the difference (MSE) between the representation of an individual training example when it was last updated in the memory bank, and its current representation in the batch. This requires the exact approach of [4], which we just recently deemed as infeasible. Our memory bank is significantly smaller than the training dataset, and older samples are dequeued, so the same training example will never be in the memory bank and the current batch simultaneously.

In conclusion:

1. We cannot use a FIFO queue-based memory bank, as representations of negative examples are inconsistent.
2. We cannot use a memory bank that maps all training examples, as it would require too much additional GPU memory.
3. Proximal regularization is not applicable to a memory bank that is smaller than the training dataset.

The only alternative is to use a momentum encoder as in MoCo [5], which is why we opt for this approach in the next experiment. Our experimental setup remains the same, but we add a momentum encoder, which is a copy of our (student) model that is trained (as described in Figure 2). Oriented on ALBEF [8], we use a memory bank of size 65,536 and a momentum factor of 0.995. Both hyperparameters also lead to good results in MoCo, where this approach was first introduced [5].

However, we encounter an OOM error, which is not surprising, considering the large memory bank size of 65k, and that we need to maintain four of those in total (see Table 1). Considering that the

size of the memory bank is crucial for performance (illustrated by MoCo [5] in Figure 3), we would like to keep it as large as possible.

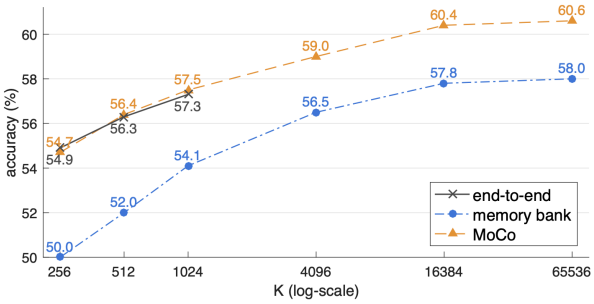


Figure 3: [5]

- we would like to keep the size of the memory bank, as this is important for performance
- therefore, we perform two optimizations:
  - we only do the contrastive loss on the last FFN layer of the shared Transformer layer, so on its cls token output
  - will reduce the GPU memory by a margin, as we only need two memory banks of size 65,536 each
  - also, while the memory bank of the last FFN layer stores embeddings of size 768, because this is the hidden dim used for our model, the memory bank of the first FFN layer stores embeddings of size 3072
    - this is because in Transformer layers the first FFN layer of the MLP expands the hidden dim by a factor of four ($4 * 768 = 3072$)
  - just removing this memory bank will save us 1.6 GB of GPU memory
  - reason: assuming embeddings are in full precision, so float32, we would need $3072 * 4B = 12,288B$, so approximately 12.3 KB per embedding
  - for one memory bank, this means $12,288 * 65,536 = 805,8$ MB of GPU memory is required
  - for two memory banks, this means $805,8 \text{ MB} * 2 \approx 1.6$ GB of GPU memory is required

We also identify a further optimization: Usually, the forward pass of the momentum encoder is done after the forward pass of the model that is trained, which is an approach MoCo [5] and ALBEF [8] follow. It follows that during the forward pass of the momentum encoder, GPU memory is already allocated to store all activations of the actual model, as they are needed for the backward pass later. Because we did not encounter an OOM error before using the momentum encoder, and we observed that the GPU memory in previous experiments was almost fully utilized (up to 98%) even without a momentum encoder, we suspect that the forward pass of the momentum encoder is the reason for the overflow.

For each step in the training loop, we therefore perform the update and forward pass of the momentum encoder before any work other work is done (i.e. forward pass of the teacher or student). This way, the activations of intermediate layers of the momentum encoder are freed before the forward pass of the actual model that is trained. This way, we avoid OOM errors while keeping the performance the same, as the work that is done per step remains the same, but is merely reordered. This is illustrated in Figure 4.

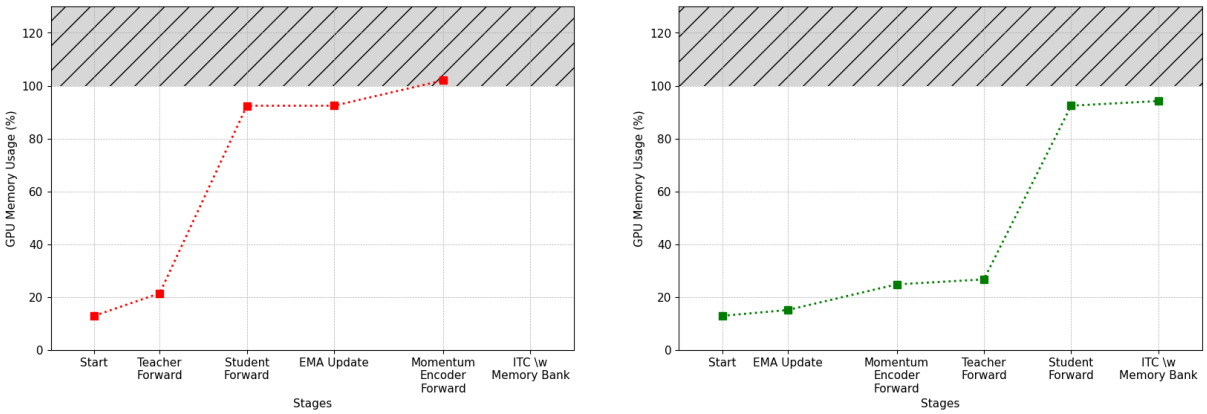
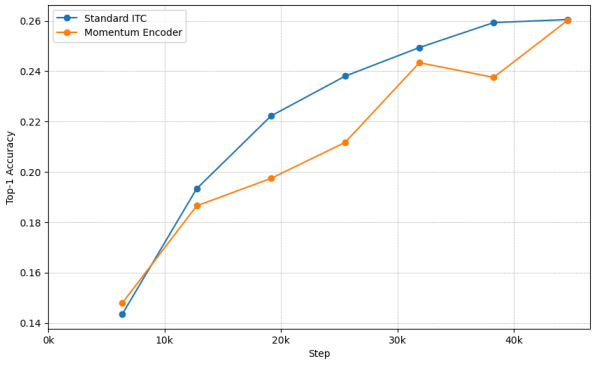


Figure 4: Doing the forward pass of the momentum encoder after the forward pass of the model, when the model's activations are already stored on the GPU memory (left), leads to a cuda OOM error. This can be avoided by reorderind the operations, so that the momentum encoder (EMA) update and forward pass are performed before the forward pass of the model (right). Results are based on NVIDIA RTX 4090 with 24 GB of GPU memory.

The result is shown in Figure 5. The additional forward pass of the momentum encoder adds approximately 5 minutes per epoch, which we cosider as marginal. However, the performance does not exceed that of the the standard gathering from all devices with just 511 negative examples (effective batch size of 512). The experiment seems more promising to achieve a higher accuracy with more epochs, compared to the previous approach, as the latter appears to saturate towards the end of training, but a longer training is both financially unsustainable for us, and lacks efficiency, which we cosider as a key aspect of our work.



Model	ImageNet-1K Accuracy	Retrieval MSCOCO	Retrieval Flickr30K
Standard ITC	26.1	66.3	42.4
Momentum Encoder	26.0	256	30.3

Figure 5: Comparison of the Standard ITC approach with momentum encoder and a memory bank of size 65,536. The momentum encoder approach does not exceed the performance of the standard ITC approach (right), even though it shows a promising trend towards the end of training (left, validation accuracy on ImageNet-1K).

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