UNDER REVIEW

RESCIENCE C

Replication / Representation Learning

[Re] Bootstrap Your Own Latent: A new approach to self-supervised learning

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Sections marked with an ‡ are identical or exhibit substantial similarity to corresponding sections in our companion reproduction paper [1] on "A Simple Framework for Contrastive Learning of Visual Representations" [2]. This duplication is a consequence of the shared challenges and common methodologies inherent in the reproduction of the two closely related methods.

1 Reproducibility Summary

1.1 Scope of Reproducibility‡

In the course of our research, we undertook the task of reimplementing several methods of self-supervised learning of visual representations. This report details our efforts to reproduce parts of the article "Bootstrap Your Own Latent: A new approach to self-supervised learning" [3], which introduced BYOL in 2020. The core concept of these self-supervised approach is to learn meaningful representations by forcing similar embeddings for pairs of similar synthetic views of images. The ultimate goal of these representations is to transfer effectively to downstream tasks. Consequently, the evaluation of the representations involves linear evaluation, few-shot learning, and transfer learning. In this report, our focus is solely on reproducing the results related to the linear evaluation protocol on CIFAR10 and ImageNet. Additionally, we developed a code that is easily extensible, as well as adapted for high-performance computing.

1.2 Methodology‡

As for all the methods we reimplemented, we began by re-implementing BYOL using the CIFAR10 dataset for preliminary feedback, as it is a small dataset, before transitioning to the ImageNet dataset.

Throughout the development process, we heavily relied on the information provided in the original paper, which explains the approach in detail, as well as various code bases, including the official one[1], developed in Jax and Haiku. Additionally, we benefited from tutorials provided by the Jean Zay[2] cluster for the HPC (High-Performance Computing) aspects.

For the implementation, we utilized PyTorch as the machine learning framework, with support for multi-GPU and multi-node computation on the Slurm partition cluster of Jean Zay. We also ensured the code could run on single GPU and CPU setups. This proved useful during debugging processes on personal computers. Numerous experiments and runs were performed throughout the process, totaling around 20,000 GPU hours[3].

[1]https://github.com/deepmind/deepmind-research/tree/master/byol
[2]http://www.idris.fr/eng/jean-zay/jean-zay-presentation-eng.html
[3]In the following, *real hours* is used in opposition to *GPU hours* (which is the number of real hours times the number of GPU).

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The authors have declared that no competing interests exists.

1.3 Results

We made considerable efforts to reimplement BYOL, ensuring compatibility with the Jean Zay supercomputer. However, our results slightly trail behind the official implementation across our experiments, and the reason for this minor discrepancy remains unclear.

1.4 What was easy‡

The original method was well-described in the article, making it easy to implement various aspects such as the architecture, hyperparameters, data augmentation policy, and the overall training procedure.

1.5 What was difficult‡

First, the optimizer used by these methods, including BYOL, is not readily available in PyTorch, and existing repositories lack control over certain parameters, thus, it required its own reproduction.

Then, although the article provides significant precision and details, it still lacks some tips and tricks that were found either in the source code or in the implementations of other related methods in the literature. That was particularly a challenge as those implementation details belonged to unknown unknowns.

Finally, adapting the code for the Slurm (workload manager) infrastructure was challenging. Ensuring multi-node and multi-GPU support and respecting the HPC standards was far from straightforward.

1.6 Communication with original authors‡

We did not seek to contact the authors of the original article. As mentioned, the details provided in the article were sufficiently clear for us to re-implement the method when presented. Our most significant challenge was adapting the methods for high-performance computing, and we believed that seeking help from the authors would have not been particularly relevant for this specific aspect.

2 Introduction‡

The objective of self-supervised representation learning methods, such as BYOL [3], is to pre-train a model without human supervision and enable it to learn meaningful features [2, 4, 5, 6]. These representations must fulfill two key requirements [7]: they should contain information relevant to downstream tasks (typically object recognition), which are unknown at training time, and they should possess a simple structure, to ensure that the representations can be easily utilized (either with a lightweight architecture model and/or with limited labeled data). Additionally, these representations should be applicable to out-of-domain datasets. As a result, the models should demonstrate good performance in linear evaluation, few-shot learning, and transfer to other datasets or tasks. For more comprehensive details on the current state-of-the-art methods and how the representations are evaluated, we recommend referring to [8].

3 Reproduced Method (BYOL)

BYOL, introduced in "Bootstrap Your Own Latent: A new approach to self-supervised learning" [3], offers a novel approach to self-supervised visual representation learning. Its position in the SSL (Self-Supervised Learning) landscape is unique, primarily because it diverges from the contrastive learning paradigm by eliminating the use of negative pairs.

The model uses two neural networks: the *online* network, which includes a projection head and a predictor, and the *target* network, which is an updated version of the online network, without the predictor. When processing two different augmentations of an image, one view goes through the online network, while the other goes through the target network. During training, BYOL aims to make the representations from these networks for each augmentation similar. By utilizing augmentations that alter the image at the pixel level without changing its semantic content, the model ensures that the learned representations capture meaningful aspects of the data.

More formally, let t and t' signify two augmentations drawn from separate distributions of augmentations $\mathcal{T}_1$ and $\mathcal{T}_2$. Two distinct views of a given image $\boldsymbol{x}$ are created as $\boldsymbol{v}_i = t(\boldsymbol{x})$ and $\boldsymbol{v}_j = t'(\boldsymbol{x})$. For N original images, we obtain a batch of $2N$ views. The first N correspond to one view $\boldsymbol{v}_i$, and the remaining N correspond to another view $\boldsymbol{v}_j$ for each image. We denote by f_θ the online network encoder parameterized by θ that generates representations from images. This online network also contains a projection head g_ϕ and a predictor q_ψ. And we note $f_{\overline{\theta}}$ the target encoder and $g_{\overline{\phi}}$ the target projection head, where $\overline{\theta}$ and $\overline{\phi}$ are simply momentum-based moving average of the online parameters θ and ϕ, with τ the momentum parameter. Consequently, the representations for the views are $\boldsymbol{h}_i = f_\theta(\boldsymbol{v}_i)$ and $\boldsymbol{h}_j = f_{\overline{\theta}}(\boldsymbol{v}_j)$. After passing through the projection head and the predictor, the embeddings are defined as $\boldsymbol{z}_i = q_\psi(g_\phi(\boldsymbol{h}_i))$ and $\boldsymbol{z}_j = g_{\overline{\phi}}(\boldsymbol{h}_j)$. The objective of BYOL is to reduce the difference between $\boldsymbol{z}_i$ and $\boldsymbol{z}_j$, while the gradient is only backpropagated through the online network, defining the loss for the positive pair (i, j) as:

$$\ell_{i,j} = 2 - 2 \times \text{sim}(\boldsymbol{z}_i, \boldsymbol{z}_j) \tag{1}$$

where $\text{sim}(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a}^\top \boldsymbol{b} / (\|\boldsymbol{a}\| \|\boldsymbol{b}\|)$ is the cosine similarity. Ultimately, the aggregate model loss is calculated using Eq. 1, considering all pair combinations, specifically both (i, j) and (j, i), within the batch.

Evaluating the representations learned by BYOL typically involves a linear evaluation, where the learned embeddings are frozen and a linear classifier is trained on top of them. Likewise, its efficiency in using labels is often tested through few-shot learning, and the generalizability of these embeddings is evaluated by their transfer performance on datasets different from the training set. This report narrows its focus solely on the linear evaluation aspect.

4 Reproducibility Objectives‡

The objective of this reproduction was to develop a flexible and modifiable version of BYOL, among other SSL methods, for studying the incorporation of an equivariance module to enhance perfor-

mance of recent SSL approaches [9]. Therefore, our primary focus was on replicating similar results for the linear evaluation on CIFAR10 and ImageNet, which is a widely used protocol in the literature for comparing existing methods. Additionally, since this project utilized the computational resources provided by the supercomputer Jean Zay, we designed our code to be scalable and specifically optimized for Jean Zay's HPC system.

5 Difficulties encountered

5.1 Difficulties related to recent SSL

LARS with parameter exclusion‡ — The recent SSL methods rely on using large batch sizes, either to prevent collapse by requiring numerous negative pairs or to accelerate the training process [2, 4, 5, 6]. However, training with such large batch sizes using stochastic gradient descent can lead to instability. To mitigate this, it is common to utilize the LARS (Layer-wise Adaptive Rate Scaling) optimizer [10]. During the training process of these methods, certain parameters should be excluded from the LARS adaptation, as well as from weight decay. However, existing PyTorch implementations of LARS lack the flexibility for such control. One workaround is to employ SGD (Stochastic Gradient Descent) for the parameters that are excluded from LARS adaptation, but this requires managing two separate optimizers, leading to additional complications. To overcome these challenges, we've chosen to develop our custom LARS implementation. This version introduces a weight parameter to regulate the strength of the LARS adaptation applied (i.e., a value of 0.0 signifies the use of SGD, while 1.0 represents the original LARS). This parameter can be set for a group of parameters, enabling the straightforward exclusion of certain parameters from the LARS adaptation.

No bias before batch normalization‡ — An often omitted detail, as in the original article, yet observed in many codebases (including the official one), is the absence of bias in layers followed by a BN (Batch Normalization) [11]. While this is already implemented in PyTorch's version of ResNets, it must also be applied to the projection head. The reasoning behind this is that the batch normalization layer will center back the data, canceling the bias [11]. Thus, it does not improve the computational capacity of the model, while it adds an extra parameter, which subsequently complicates the optimization process.

Interpolation mode of the resize augmentation‡ — Another detail we uncovered by reviewing various codebases, together with the official one, is that the interpolation method used in the resize augmentation is not the default one. These codebases appeared to predominantly use bicubic interpolation, which yielded superior results in our experiments.

Zero-initializing the residual branches‡ — Lastly, another unmentioned technique involves initializing to zero the last BN layer of the residual branches for the ResNet backbone. We discovered this strategy in the official codebase, as well as in some other implementations, and found that it enhances performance.

5.2 Difficulties related to HPC

PyTorch's slow cosine similarity‡ — The native cosine operation provided by PyTorch is slow and used to be a significant bottleneck. This issue was addressed by executing the computation using PyTorch's primitives. This process involves the normalization of the embeddings matrix, followed by the matrix multiplication of this matrix with its transpose.

Batch norm multi-node synchronization‡ — Analogous to the previous section, the batch normalization computation requires the entire batch to be accurately performed. Thankfully, PyTorch offers a solution by providing a way to convert all existing batch normalization layers of a model to synchronized batch normalization, effectively solving this issue. This problem was highlighted in

the original paper, which also proposed other, more complex solutions. It's important to mention that the batch normalization of the target network must also be synchronized.

Jobs too long and checkpoints‡ — A final, yet significant issue, relates to the quality-of-service offered by the Jean Zay supercomputer. Due to the large number of GPUs and nodes required for such experiments, the only suitable quality-of-service allows for jobs with a maximum duration of 20 real hours. However, typical ImageNet training takes approximately 170 real hours. Therefore, the jobs had to be split multiple times during a single training session. This necessitated the implementation of a checkpoint system to resume training after each job interruption. The system had to handle the saving and loading of the epoch, model (both online and target), optimizer, and learning rate scheduler.

6 Experimental settings

6.1 Datasets‡

We began our experiments by working with the CIFAR10 dataset [12], which was provided via the torchvision package. We chose to start with this dataset because of its small size, which allowed for quick iterations during our reimplementation. CIFAR10 consists of 50,000 training images and 10,000 test images, all of which are 32×32 pixels in size. The images are categorized into 10 classes, representing various animals and vehicles.

Next, we conducted additional experiments using the ImageNet dataset [13], which was made available through Jean Zay. ImageNet is the standard benchmark for comparison in visual representation learning, and thus, is used in the original article. This dataset comprises 1,000 classes of natural images with varying resolutions. It consists of 1.28 million training images and 100,000 test images.

It is worth noting that throughout the process of learning representations, the labels of the data were not used, as the objective was to achieve self-supervised learning.

6.2 Architectures‡

The architectures vary depending on the dataset, but in all cases, utilize a ResNet [14] as the backbone. For CIFAR10, a ResNet18 architecture is used with the usual CIFAR10 modifications: the first convolutional layer has a 3×3 kernel with a stride of 1, and the max-pooling layer is removed. On the other hand, for the ImageNet dataset, a standard ResNet50 architecture is employed. It's important to note that for both cases, the final linear layer is replaced by a projection head and predictor. Each consists of two fully connected layers, with the first layer incorporating a BN and a ReLU activation function.
For the ResNet, we based our implementation on the torchvision library, which provides a convenient way to instantiate ResNet models. We then modified these models' architectures as previously described.

6.3 Hyperparameters‡

When available, we use the original implementation's hyperparameters, therefore, the models are trained for 1000 epochs using a cosine decay learning rate schedule and 10 warm-up epochs. A batch size of 4096 is used for ImageNet and 512 for CIFAR10, with an initial learning rate of 3.2 for ImageNet and 2.0 for CIFAR10. For the optimizer, the momentum is set to 0.9 and the weight decay to 1.5×10^{-6} on ImageNet but 10^{-6} on CIFAR10. The dimensions of the embedding space have been set to 256. For the target network, τ is set to 0.996 at the start, but follows a cosine decay. Finally, the LARS [10] optimizer is used for all experiments, although biases and BN parameters were removed from both weight decay and LARS adaptation.

6.4 Augmentation policy‡

We reimplemented the distinct augmentation policies for the CIFAR10 and ImageNet datasets. Note that all these augmentations are provided by the torchvision library.

For the CIFAR10 dataset, a random resized crop is applied, which generates output images of 32×32 pixels. This transformation features a scale parameter ranging from 0.2 to 1.0 and an aspect ratio that varies from $3/4$ to $4/3$. As previously noted in the challenges section, bicubic interpolation is utilized for the resizing operation. Subsequently, the cropped image undergoes a potential horizontal flip, determined probabilistically with a 50% likelihood. This was followed by a color jitter transformation with 80% probability, altering the brightness, contrast, saturation, and hue parameters by up to 0.4, 0.4, 0.2, and 0.1 respectively. Images were also converted to grayscale with a 20% probability. Then, regarding the views, the augmentations diverge. First view was followed by a Gaussian blur transformation using a kernel size that is 10% of the image's dimensions, and sigma ranging from 0.1 to 2.0, while second view had this blur with probability 10% and a solarize operation with probability of 20%. The final step was the normalization of image tensors using mean $(0.4914, 0.4822, 0.4465)$ and standard deviation $(0.247, 0.243, 0.261)$.

For the ImageNet dataset, the training augmentations was similar to the one used for CIFAR10, but with a few key differences. The random resized crop generated images of size 224×224 pixels, with scale ranging from 0.08 to 1.0. And the final normalization step used mean $(0.485, 0.456, 0.406)$ and standard deviation $(0.229, 0.224, 0.225)$.

6.5 Linear evaluation‡

The linear evaluation of the trained models is performed using SGD optimizer with Nesterov momentum and cross-entropy loss. The learning rate is initialized to 0.2 and follows a cosine scheduler to adjust it over the 90 epochs of learning. The batch size for this phase is 256. The momentum parameter is set to 0.9 and no weight decay is applied, reflecting a standard configuration in such scenarios.

For this evaluation phase, the augmentation policies are also modified for both CIFAR10 and ImageNet datasets. For CIFAR10 during the training phase, color, grayscale, solarize, and blur transformations are removed, and the lower bound of the scale parameter in the random resized crop operation is reduced to 0.08. For the testing phase, the random resized crop and random horizontal flip are replaced by a resize operation to 36 pixels, followed by a center crop to 32 pixels.

In the case of ImageNet, that training phase also sees the removal of color, grayscale, solarize, and blur transformations. For the testing phase, similar to CIFAR10, transformations are replaced, this time by a resize operation to 256 pixels, and a subsequent center crop to 224 pixels.

6.6 Resources, setup, and code‡

Experiments were conducted using the Jean Zay supercomputer, which employs Slurm for cluster management. The code, written in Python, leverages PyTorch 1.10.0 and TorchVision 0.11.0, CIFAR10 experiments were executed on a single node equipped with 2 Tesla V100 32GB GPUs for approximately 4 real hours of training, while ImageNet experiments utilized 8 nodes, each with 4 Tesla V100 32GB GPUs during 170 real hours of training.

7 Detailed results

7.1 Results reproducing original paper

Tab. 1 presents the results from various datasets, comparing them to the original findings. While the original paper doesn't provide results for CIFAR10, an unofficial GitHub implementation[4] does.

[4] https://github.com/DonkeyShot21/essential-BYOL

It claims achievements of 91.1% for top 1 and 99.8% for top 5, which we've included in Tab. 1.

Our initial efforts were directed towards the CIFAR10 dataset. As depicted in Tab. 1, while our reimplementation displayed small variations from the unofficial reference results, it was quite aligned.
Moreover, when we expanded our experiments to ImageNet, we observed a better alignment. Our performance on this dataset was remarkably close to the original, with only slight deviations in both Top-1 and Top-5 accuracy metrics. Nonetheless, given that these results arise from a single run, due to computational constraint, the slight discrepancies could stem from statistical noise inherent to the stochastic nature of the model initialization.

Taken together, our findings corroborate the efficiency of BYOL. They also suggest that our reimplementation, optimized for the Jean Zay supercomputer, is successful.

Implementations	CIFAR10		ImageNet	
	Top-1	Top-5	Top-1	Top-5
Original	91.1	99.8	74.3	91.6
Our	91.92	99.69	74.03	91.51

Table 1. Linear Evaluation; BYOL's implementations top-1 and top-5 accuracies (in %) under linear evaluation on CIFAR10 and ImageNet.

8 Conclusion

In this document, we have detailed our efforts in re-implementing BYOL, aiming to match the original's benchmarked linear evaluation results, all the while optimizing our code for the Jean Zay supercomputer.

In our initial tests with the CIFAR10 dataset, we noted small discrepancies between our results and those of the original paper. Upon advancing to the more intricate ImageNet dataset, we managed to narrow this difference, although our results still fell slightly short of the original. These minor variations could simply be due to statistical noise caused by the stochastic nature of the model initialization.

It is crucial to acknowledge that these methodologies are computationally demanding, requiring the simultaneous utilization of numerous GPUs for extensive periods. Without the support of Jean Zay, carrying out this work would have been unfeasible. In addition to our gratitude towards Jean Zay, we take pride in contributing to the scientific community by sharing the weights of our trained models (while the official ones of BYOL are available on the official GitHub). This gesture is aimed at sparing others the significant costs, time, and energy that would otherwise be needed to replicate these computationally intense training processes.

9 Acknowledgements

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