Feature diversity in self-supervised learning

Pranshu Malviya *
Department of Computer and Software Engineering
Mila - Quebec AI Institute
École Polytechnique de Montréal
Montréal, Canada

Arjun Vaithilingam Sudhakar *
Department of Computer Science and Operations Research
Mila - Quebec AI Institute
Université de Montréal
Montréal, Canada

Abstract

Many studies on scaling laws consider basic factors such as model size, model shape, dataset size, and compute power. These factors are easily tunable and represent the fundamental elements of any machine learning setup. But researchers have also employed more complex factors to estimate the test error and generalization performance with high predictability. These factors are generally specific to the domain or application. For example, feature diversity was primarily used for promoting syn-to-real transfer by Chen et al. (2021a). With numerous scaling factors defined in previous works, it would be interesting to investigate how these factors may affect overall generalization performance in the context of self-supervised learning with CNN models. How do individual factors promote generalization, which includes varying depth, width, or the number of training epochs with early stopping? For example, does higher feature diversity result in higher accuracy held in complex settings other than a syn-to-real transfer? How do these factors depend on each other? We found that the last layer is the most diversified throughout the training. However, while the model’s test error decreases with increasing epochs, its diversity drops. We also discovered that diversity is directly related to model width.

1 Introduction

In recent years, self-supervised learning (SSL) has achieved exceeding empirical success (He et al., 2019) and also a method of pretraining neural networks (Caron et al., 2020). A major advantage of SSL as compared to supervised learning is the ability to scale since SSL requires no manual labeling process. Goyal et al. (2019) scales the dataset and difficulty of the problem for this study. They found that the results matched and even surpassed those of supervised learning techniques. They also released a benchmark for 9 different datasets and tasks for evaluation. Once trained, these models can be used to learn new tasks more data-efficiently by finetuning (Chen et al., 2021a).

Contrastive learning is a type of SSL technique that pulls representations of the anchor image and its transformations closer and pushes the images from the different classes farther. Jaiswal et al. (2021) and Le-Khac et al. (2020) discuss about contrastive learning’s superior performance and the inductive bias of self-supervised algorithms.

With the growing interest in techniques like contrastive learning and invariant predictions (Mitrovic et al., 2020), it is imperative to discover the factors promoting generalization and scaling laws of state-of-the-art CNN models under the SSL setup (Goyal et al., 2022).

Generalization plays a key role to measure the performance of the model. The importance of the role of diversity of learned feature embedding in terms of generalization is studied by Chen et al. (2021a) and Liu et al. (2018b). The lack of diversity in the representation learned by the model makes the prediction sensitive to natural fluctuations in the real world. Hence, it is essential to understand what factors promote generalization in the CNN architecture. We investigate whether increased feature diversity leads to improved accuracy and generalization in complex self-supervised algorithms.

Liu et al. (2018b) regularized the neural network by minimum hyperspherical energy (MHE) in order to avoid undesired representation because of the over-parametrization. Also, Xie et al. (2017) proposed a regularization based on the uncorrelations and evenness that promotes diversity. This will promote the components to be uncorrelated and to have equal roles in data modeling.

Diversity in representation makes the learned self-supervised models resilient to natural variations in the real world. Hence, in this work, we investigate how specific characteristics like depth, width, or the number of training epochs...
attribute generalization through diversity. We also perform experiments to analyze how test loss relates to the diversity metric. Does higher feature diversity result in better performance? In order to estimate the diversity of each component, we use hyperspherical potential energy.

2 APPROACH

2.1 SELF-SUPERVISED LEARNING

Self-supervised learning receives supervisory signals from the data itself, mostly utilizing the data’s underlying structure (Liu et al., 2020). SimCLR (Chen et al., 2020) is an approach based on contrastive learning to learn the visual representation. The representations are learned from the input data by maximizing the agreement between augmented images of the same image through contrastive loss in the latent space.

The loss function for the SimCLR is defined as,

$$L_{SimCLR}^{(i,j)} = -\log \frac{\exp(\text{sim}(z_i, z_j) / \tau)}{\sum_{k=1}^{2N} \delta_{k \neq i} \exp(\text{sim}(z_i, z_k) / \tau)}$$

where, $z_i = g(h_i)$, $z_j = g(h_j)$ and $\delta_{k \neq i}$ acts as an indicator function, returning 1 if $k \neq i$ is present, and 0 otherwise. In the above equation, $\text{sim}(\cdot)$ represents the cosine similarity. This loss is based on $g(\cdot)$ representation’s extra projection layer. Also, $h$ representation is used only for the downstream task.

We also used other self-supervised learning algorithms like DeepCluster-V2 (Caron et al., 2018) which acts as an end-to-end system where the parameters of the network and the clustering assignments of the features are learned. In JigSaw (Noroozi & Favaro, 2016) the pretext task to learn the representations is jigsaw puzzles. (tiles are taken from the images and shuffled). We also used RotNet (Gidaris et al., 2018), which learns the image representation by using CNN to predict the 2D rotations of the input images. This approach will help the model learn the semantic information in the image without any labeled data. In NPID (Wu et al., 2018) (Non-Parametric Instance Discrimination) is also a self-supervised algorithm that is based on the non-parametric classification approach. Finally, PIRL (Misra & van der Maaten, 2019) based on the pretext task, the invariant representations are learnt. The most commonly used pretext task is solving jigsaw puzzles.

2.2 ESTIMATING FEATURE DIVERSITY BY MINIMUM HYPERSPHERICAL ENERGY

Generally, to handle large datasets, we use large neural networks, which will offer the capacity to fit the data using complex functions. This high degree of representation helps to perform difficult tasks but sometimes results in highly correlated neurons, which can impair generalization ability and incur extra computing costs. To understand the diversity of the features learned by each component of the Resnet architecture, we take motivation from Liu et al. (2018a) to get a quantitative measure.

The Hyperspherical potential energy will provide us the measure of diversity in the feature embeddings (Chen et al., 2021b).

$$E_s(\hat{v}_i | N) = \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} e_s(||\hat{v}_i - \hat{v}_j||) = \left\{ \begin{array}{ll} \sum_{i \neq j} ||\hat{v}_i - \hat{v}_j||^{-s}, & s > 0 \\ \sum_{i \neq j} \log(||\hat{v}_i - \hat{v}_j||^{-1}), & s = 0 \end{array} \right.$$  

In the above equation, $N$ represents the number of examples, $||\cdot||$ represents the Euclidean distance, $f_s(\cdot)$ is a function of decreasing real value. $\hat{v}$ represents the $i^{th}$ neuron weight projection into the unit hypersphere. Also, here $s$ represents the power factor. The lowers $E_s$ (Hyperspherical energy) means the feature vectors are more diverse and scattered onto the unit sphere.

3 EXPERIMENTS

In this section, we describe the experiments performed to analyze the features diversity in models trained using SSL algorithms. These experiments are performed on ImageNet (Deng et al., 2009) where we train models for larger training epochs, different CNN architectures, and SSL algorithms.

We use different versions of ResNet models with the different number of parameters. The models were based on different choices of CNN components: depth (50, 101, 152, 200) and width (1, 2, 4). The implementation of the base ResNet models is based on the VISSL library (Goyal et al., 2021). The choices of hyper-parameters are also based on default configurations used by Goyal et al. (2021).
Once the given model is trained using a SSL algorithm, we randomly sample 500 images from held-out test data and forward-pass to extract the features of the following layers: (i) First convolutional layer (conv1), (ii) Second residual block (res2), (iii) Forth residual block (res4) and (iv) Embedding layer (Head). These extracted features are then used to compute feature diversity using hyperspherical energy $E_s^{(l)}$ (where $l$ denotes the layer) defined in Eq. 2.2. Next, we load the trunk of this trained model and add a linear classification layer at the end. We train this classification layer using labeled data and test the performance on a held-out dataset. We record error ($= 1 - a_1$, where $a_1$ is the top-1 accuracy) obtained on the test data. In our results, we compare test error and diversity ($= -E_s^{(l)}$) for different ResNet architectures and training regimes.

We analyze the characteristics of different layers of the model with Batch-norm and train a ResNet model using SimCLR with varying epochs, depth, and width. By comparing the layer-wise feature diversity, we could infer whether diversity always results in better performance. We also report the results from small-scale experiments on CIFAR100 (Krizhevsky et al., 2009) which are performed with a lower number of training epochs for different shapes of the model in Appendix A.

### 3.1 Epochs

We start by comparing feature diversity with test error for a varying number of epochs by fixing the depth of the model to 50 and training it using SimCLR. The goal of this experiment is to analyze the evolution of feature diversity with increasing epochs and whether early-stopping results in a model with the most diverse features. We also vary the width of the model and plot corresponding results in Figure 1.

We observe that Head layer has the highest feature diversity as compared to other layers. There is also an increasing trend among layers from res2 to Head layer. But the features in conv1 layer still appear to be more diverse than res2. Apart from that, we observe that with increasing width, feature diversity improves in all layers except the first layer i.e., conv1. This could be because, with wider hidden layers, the knowledge learned by the model is more spread out among the hidden layers. On the other hand with width = 1, the first layer learns relatively more diverse features to achieve better performance. In fact, conv1 features diversity in width = 1 model increases even after the model is overfitted (at 1000 epochs). We also observe a correlation between diversity and performance in all layers except Head layer. In particular, the model with width = 1 achieves minimum test error after training for 800 epochs, whereas the feature diversity in the final layer maximum during 100 epochs. A gradual decrease in feature diversity of the final
layer suggests that there could be a trade-off between classification performance and feature diversity of the model in the final layer.

Next, we add early-stopping criteria and plot test error and diversity across different model sizes in Figure 2 trained using SimCLR. For an increasing number of parameters in the model, we observe that test error doesn’t always decrease. We also note that diversity improves with an increasing number of parameters, especially in the wider networks.

![Figure 2: Test error and diversity vs. the number of parameters in the models trained using SimCLR.](image)

### 3.2 Algorithms

Next, we compare test error and feature diversity for models which are trained using different SSL algorithms. We also compare the performances of these SSL algorithms with the supervised setting in Figure 3. We observe that for constant model size, supervised training results in the best feature diversity with minimum test error. We also observe that DeepClusterV2 results in the best test error as compared to other SSL algorithms for the same model size. Rotnet results in best feature diversity but results in high test error.

![Figure 3: Test error vs. feature diversity for models trained using different SSL algorithms.](image)

### 4 Conclusion

We provide a brief survey of different SSL algorithms and the importance of feature diversity in improving feature diversity. When a model is trained using an SSL algorithm, the key idea was to examine how feature diversity for various model layers behaves as compared to the classification error. We performed different experiments on the ImageNet dataset by constructing models with different architectures with varying depth and width. We also vary the number of training epochs to check whether applying early-stopping results in a model with the most diverse features. We found that the final layer remains the most diverse layer throughout the training regime. But although the model’s test error decreases, its diversity also decreases with increasing epochs. We also found that diversity is directly proportional to the width of the model. Overall, understanding the behavior of diversity in final layer features and exploiting layer-wise diversity to improve generalization pose interesting directions for future research.
REFERENCES

Mathilde Caron, Piotr Bojanowski, Armand Joulin, and Matthijs Douze. Deep clustering for unsupervised learning of visual features. *CoRR*, abs/1807.05520, 2018. URL http://arxiv.org/abs/1807.05520.

Mathilde Caron, Ishan Misra, Julien Mairal, Priya Goyal, Piotr Bojanowski, and Armand Joulin. Unsupervised learning of visual features by contrasting cluster assignments. *CoRR*, abs/2006.09882, 2020. URL https://arxiv.org/abs/2006.09882.

Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey E. Hinton. A simple framework for contrastive learning of visual representations. *CoRR*, abs/2002.05709, 2020. URL https://arxiv.org/abs/2002.05709.

Wuyang Chen, Zhiding Yu, Shalini De Mello, Sifei Liu, Jose M Alvarez, Zhangyang Wang, and Anima Anandkumar. Contrastive syn-to-real generalization. *arXiv preprint arXiv:2104.02290*, 2021a.

Wuyang Chen, Zhiding Yu, Shalini De Mello, Sifei Liu, Jose M. Alvarez, Zhangyang Wang, and Anima Anandkumar. Contrastive syn-to-real generalization. *CoRR*, abs/2104.02290, 2021b. URL https://arxiv.org/abs/2104.02290.

J. Deng, W. Dong, R. Socher, L.-J. Li, K. Li, and L. Fei-Fei. ImageNet: A Large-Scale Hierarchical Image Database. In *CVPR09*, 2009.

Spyros Gidaris, Praveer Singh, and Nikos Komodakis. Unsupervised representation learning by predicting image rotations. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=S1v4N2l0-.

Priya Goyal, Dhruv Mahajan, Abhinav Gupta, and Ishan Misra. Scaling and benchmarking self-supervised visual representation learning. *CoRR*, abs/1905.01235, 2019. URL http://arxiv.org/abs/1905.01235.

Priya Goyal, Quentin Duval, Jeremy Reizenstein, Matthew Leavitt, Min Xu, Benjamin Lefaudeux, Mannat Singh, Vinicius Reis, Mathilde Caron, Piotr Bojanowski, Armand Joulin, and Ishan Misra. Vissl. https://github.com/facebookresearch/vissl, 2021.

Priya Goyal, Quentin Duval, Isaac Seessel, Mathilde Caron, Ishan Misra, Levent Sagun, Armand Joulin, and Piotr Bojanowski. Vision models are more robust and fair when pretrained on uncurated images without supervision, 2022.

Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross B. Girshick. Momentum contrast for unsupervised visual representation learning. *CoRR*, abs/1911.05722, 2019. URL http://arxiv.org/abs/1911.05722.

Ashish Jaiswal, Ashwin Ramesh Babu, Mohammad Zaki Zadeh, Debapriya Banerjee, and Fillia Makedon. A survey on contrastive self-supervised learning. *Technologies*, 9(1), 2021. ISSN 2227-7080. doi: 10.3390/technologies9010002. URL https://www.mdpi.com/2227-7080/9/1/2.

Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. https://www.cs.toronto.edu/~kriz/learning-features-2009-TR.pdf, 2009.

Phuc H. Le-Khac, Graham Healy, and Alan F. Smeaton. Contrastive representation learning: A framework and review. *CoRR*, abs/2010.05113, 2020. URL https://arxiv.org/abs/2010.05113.

Weiyang Liu, Rongmei Lin, Zhen Liu, Lixin Liu, Zhiding Yu, Bo Dai, and Le Song. Learning towards minimum hyperspherical energy. *CoRR*, abs/1805.09298, 2018a. URL http://arxiv.org/abs/1805.09298.

Weiyang Liu, Rongmei Lin, Zhen Liu, Lixin Liu, Zhiding Yu, Bo Dai, and Le Song. Learning towards minimum scaling and benchmark energy. *CoRR*, abs/1805.09298, 2018b. URL http://arxiv.org/abs/1805.09298.

Xiao Liu, Fanjin Zhang, Zhenyu Hou, Zhaoyu Wang, Li Mian, Jing Zhang, and Jie Tang. Self-supervised learning: Generative or contrastive. *CoRR*, abs/2006.08218, 2020. URL https://arxiv.org/abs/2006.08218.

Ishan Misra and Laurens van der Maaten. Self-supervised learning of pretext-invariant representations. *CoRR*, abs/1912.01991, 2019. URL http://arxiv.org/abs/1912.01991.
Jovana Mitrovic, Brian McWilliams, Jacob Walker, Lars Buesing, and Charles Blundell. Representation learning via invariant causal mechanisms. *arXiv preprint arXiv:2010.07922*, 2020.

Mehdi Noroozi and Paolo Favaro. Unsupervised learning of visual representations by solving jigsaw puzzles. *CoRR*, abs/1603.09246, 2016. URL http://arxiv.org/abs/1603.09246.

Zhirong Wu, Yuanjun Xiong, Stella X. Yu, and Dahua Lin. Unsupervised feature learning via non-parametric instance discrimination. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2018.

Pengtao Xie, Aarti Singh, and Eric P. Xing. Uncorrelation and evenness: a new diversity-promoting regularizer. In Doina Precup and Yee Whye Teh (eds.), *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pp. 3811–3820. PMLR, 06–11 Aug 2017. URL [https://proceedings.mlr.press/v70/xie17b.html](https://proceedings.mlr.press/v70/xie17b.html).

A APPENDIX

The goal of the CIFAR100 experiment was to analyze the characteristics of different layers of the model during the initial stages of the training process. By comparing the layer-wise feature diversity, we could infer whether diversity always results in better performance.

This experiment was performed on the CIFAR100 dataset ([Krizhevsky et al., 2009](http://papers.nips.cc/paper/3734-cifar10-cifar100-datasets)). We train a ResNet model for 30 epochs with varying depth sizes and choices of norms using *SimCLR* loss function. We plot the results in Figure 4. We observe that *Head* is the most diverse layer as compared to any other layers in the ResNet. Moreover, none of the layers indicate the correlation between diversity and the performance of the model. Second to *Head* layer, it is the *conv1* layer that is most diverse during initial stages of *SimCLR* learning. We can also see a decreasing trend in feature diversity from *conv1* to *res4* layers. Apart from that, a high test error with increasing depth suggests that the deeper model requires more training epochs for better performance. But even with fewer epochs, we observe that deeper models can learn diverse features. We also observe a greater diversity and lower test error when using LayerNorm instead of BatchNorm.
Figure 4: Test error vs feature diversity of different layers of the models (with varying depth and choice of norms) during initial stages of the training process.