SELF-SUPERVISED LEARNING OF MAXIMUM MANIFOLD CAPACITY REPRESENTATIONS

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ABSTRACT

Self-supervised Learning (SSL) has recently emerged as a successful strategy for learning useful representations of images without relying on hand-assigned labels. Many such methods aim to learn a function that maps distinct views of the same scene or object to nearby points in the representation space. These methods are often justified by showing that they optimize an objective that is an approximation of (or correlated with) the mutual information between representations of different views. Here, we recast the problem from the perspective of *manifold capacity*, a measure for evaluating the classification capabilities of a representation. Specifically, we develop a contrastive learning framework that aims to maximize the number of linearly separable object manifolds, yielding a Maximum Manifold Capacity Representation (MMCR). We apply this method to unlabeled images, each augmented by a set of basic transformations, and find that it learns meaningful features using the standard linear evaluation protocol. Specifically, we find that MMCRs support performance on object recognition comparable to recently developed SSL frameworks, while providing more robustness to adversarial attacks. Finally, empirical analysis reveals the means by which compression of object manifolds gives rise to class separability.

1 INTRODUCTION

Natural images lie, at least locally, within manifolds whose intrinsic dimensionality is low relative to that of their embedding space (the set of pixel intensities). Nevertheless, these manifolds are enormously complex, as evidenced by the variety of natural scenes. A fundamental goal of machine learning is to extract these structures from observations, and use them to perform inference tasks. In the context of recognition, consider the *object submanifold*, $\mathcal{M}_j$, which consists of all images of object j (for example, those taken from different camera locations, or under different lighting conditions). Object recognition networks act to map images within a submanifold to nearby representations, relative to images from other submanifolds, and this concept has been effictively exploited in recent self-supervised learning (SSL) methods (Zbontar et al., 2021; Chen et al., 2020; Caron et al., 2020; Bachman et al., 2019; Wang & Isola, 2020; Wang et al., 2022). Most of these operate by minimizing pairwise distances between images within submanifolds, while contrastively maximizing pairwise distances between images in different submanifolds.

Meanwhile, in computational neuroscience, characterizing manifolds in neural representations has emerged as a promising approach to understanding computation in neural circuits (Kriegeskorte & Kievit, 2013; Chung & Abbott, 2021). Many studies have found interesting geometric structures in neural data underlying task representations across various modalities (Bernardi et al., 2020; DiCarlo & Cox, 2007; Hénaff et al., 2021; Gallego et al., 2017; Nieh et al., 2021), and explored a rich set of metrics for quantifying these representation geometries.

Here, we make use of a recently developed measure of the extent of a submanifold representation known as the manifold capacity (Chung et al., 2018), a geometrical quantity that expresses how many manifolds can be linearly separated in a given space. We incorporate this measure into a novel contrastive objective, that maximizes the extent of the global image manifold while minimizing that of constituent object manifolds. We apply this to an unlabeled set of images, each augmented to form a small set of samples from their corresponding manifold. We show that the learned representations

- support high-quality object recognition, when evaluated using the standard linear evaluation (Chen et al., 2020) paradigm (i.e., training a linear classifer to operate on the output of the unsupervised network). In particular, performance is approximately matched to that of other recently proposed SSL methods.
- extract semantically relevant features from the data, that can be revealed by examining the learning signal derived from the unsupervised task
- have interpretable geometric properties
- are more robust to adversarial attack than those of other recently proposed SSL methods.

1.1 Related Work

Our methodology is closely related to and inspired by recent advances in contrastive self supervised representation learning (SSL) but has a distinct motivation. For example, many recent frameworks craft objectives that are designed to maximize the mutual information between representations of different views of the same object (Oord et al., 2018; Chen et al., 2020; Oord et al., 2018; Tian et al., 2020; Bachman et al., 2019)). However, estimating mutual information in high dimensional feature spaces (which is the regime of modern deep learning models models) has been difficult to compute historically (Belghazi et al., 2018), and furthermore it is not clear that more closely approximating mutual information in the objective produces improved representations (Wang & Isola, 2020). [1] By contrast, capacity estimation theories rooted in statistical physics operate in the regime of large ambient dimension as they are derived in the "large N (thermodynamic) limit" (Chung et al., 2018; Bahri et al., 2020). Therefore we test whether one such measure, which till now had mainly been used to evaluate the quality of representations, might be useful as objective function in SSL.

Operationally, many existing methods are optimized to minimize some notion of distance between the representations of different augmented views of the same image, while maximizing the distance between representations of (augmented views of) distinct images (these are thought of as encouraging alignment and uniformity in the framework of Wang & Isola (2020)). When taking the view that different views of an image form a continuous manifold that we aim to compress, the distance between two randomly sampled points from said manifold seems a strange choice for the size metric to optimize for. Perhaps unsurprisingly it has been demonstrated on multiple occasions, notably by the success of the "multi-crop," strategy implemented SwAV (Caron et al., 2020) and earlier in the contrastive multiview coding work by Tian et al. (2020)). However most commonly the use of multiple views is such that the objective effectively becomes a Monte Carlo estimate with more than one sample of the same pairwise distance function.

Rather than using the mean distance or cosine similarity between pairs of points, we use a nuclear norm as a combined measure of size and dimensionality of groups of points, an idea that is strongly motivated by learning theory. The nuclear norm has been previously used to induce or infer low rank structure in the representation of data, for example, in Hénaff et al. (2015); Wang et al. (2022); Lezama et al. (2018). Note that in the first of these the matrix norm is supplemented with a reconstruction regularizer, and in the latter two the matrix norm is employed in tandem with another loss (InfoNCE, and supervised cross entropy, respectively). Here we demonstrate that nuclear norm *alone* is sufficient to support representation learning.

2 Maximum manifold capacity representations

2.1 Manifold Capacity Theory

A central goal of classical learning theory is to calculate the number of patterns of points that can be linearly separated in a given space (Cover, 1965; Gardner, 1988). However in light of the above observation the more relevant quantity for object recognition is how many *submanifolds* can be embedded in a space while maintaining linear separability. Recent work (Chung et al., 2018) has developed a generalization of classical theory to incorporate a measure of manifold capacity – the

[1] Barlow Twins (Zbontar et al., 2021) notably avoids the curse of dimensionality because their objective effectively estimates information under a Gaussian parameterization rather than doing so non-parametrically as in the InfoNCE loss. Our method also makes use of Guasian/second order parameterizations, as detailed below.

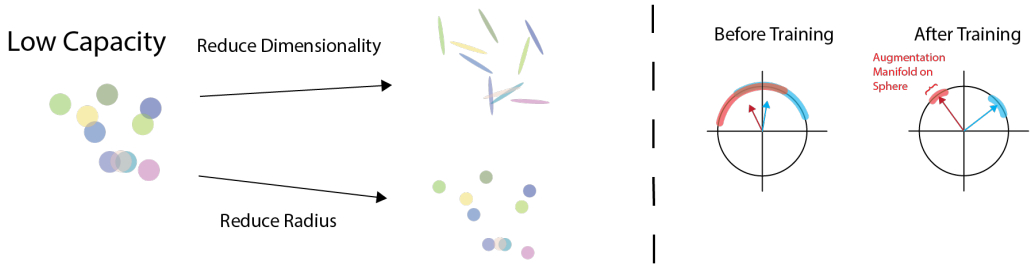

Figure 1: Two dimensional illustrations of high and low capacity representations. Left: the capacity (linear separability) of a random set of elliptical regions can be improved, either by reducing their sizes (while maintaining their dimensionalities), or by reducing their dimensionalities (while maintaining their sizes). Right: the objective proposed in this paper aims to minimize the nuclear norm (product of size and sqrt dimensionality) of normalized data vectors (ie., lying on the unit sphere). Before training the manifolds have a large extent and thus the matrix of their corresponding centroid vectors has low nuclear norm. After training the capacity is increased. The manifolds are compressed and repelled from each other, resulting in centroid matrix with larger nuclear norm and lower similarity.

number of manifolds that can be linearly separated when embedded in an N dimensional space in terms of two geometrical properties of the constituent manifolds. Specifically the capacity can be written $\alpha_C = \phi(R_M\sqrt{D_M})$, where R_M is the effective manifold radius, D_M is the effective manifold dimensionality, and $\phi(\cdot)$ is a monotonically decreasing function. This definition combines two intuitive notions of size – total variance and dimensionality – in a single and natural quantity that expresses how difficult it is to linearly separate the submanifolds.

For manifolds of arbitrary geometry estimating R_M and D_M from data requires a computationally intensive iterative procedure (Cohen et al., 2020). However, if the submanifolds are assumed to be elliptical in shape there is an analytical expression for each of these,

$$R_M = \sqrt{\sum_i \lambda_i^2}, \qquad D_M = \frac{(\sum_i \lambda_i)^2}{\sum_i \lambda_i^2}, \tag{1}$$

where the λ_i^2 are the eigenvalues of the covariance matrix of points on the manifold. Note that when computed on matrices containing images sampled from a submanifold, R_M is simply the total standard deviation, and D_M is a generalized version of the *participation ratio* (Chung et al., 2018; Rajan et al., 2010; Litwin-Kumar et al., 2017). Figure 1 illustrates how the two aspects of manifold size, the radius and dimensionality, can distinctly impact separability.

Alternatively, we may combine the two components to express the manifold capacity as $\alpha_C = \phi(\sum_i \sigma_i)$ where σ_i are the *singular values* of a matrix containing points on the manifold (which are the square roots of the eigenvalues of the covariance matrix). In this form, the sum is the L_1 norm of the singular values, known as the *Nuclear Norm* of the matrix. When used as an objective function, this measure will prefer sparse solutions (i.e., a small number of non-zero singular values) corresponding to low dimensionality. It is worth comparing this objective to another natural candidate for quantifying size: the determinant of the covariance matrix. The determinant is equal to the product of the eigenvalues (which captures the squared volume of the corresponding ellipse), but lacks the preference for lower dimensionality that comes with the Nuclear Norm. Specifically, since the determinant is zero whenever one (or more) eigenvalue is zero, it cannot distinguish zero-volume manifolds of different dimensionality. In Yu et al. (2020), lossy coding rate (entropy) is used as a measure of compactness, which simplifies to the log determinant under a Gaussian model Ma et al. (2007). In that work, the identity matrix is added to a multiple of the feature covariance matrix before evaluating the determinant, which solves the dimensionality issue described above.

2.2 Optimizing Manifold Capacity

Manifold Capacity has been previously used to evaluate and compare network representations (Chung et al., 2018; Cohen et al., 2020). Here, we explore its use as an objective function for

self-supervised learning. For each input image (notated as a vector $\mathbf{x}_b \in \mathbb{R}^{\mathbb{D}}$) we generate K samples from the corresponding manifold by applying a set of random augmentations (each drawn from the same distribution), yielding a manifold sample matrix $\tilde{\boldsymbol{X}}_b \in \mathbb{R}^{D \times K}$. Each augmented image is transformed by a Deep Neural Network, which computes nonlinear function $f(\mathbf{x}_b; \theta)$ parameterized by θ, and the d-dimensional responses are projected onto the unit sphere yielding manifold response matrix $\boldsymbol{Z}_b \in \mathbb{R}^{d \times K}$. The centroid $\boldsymbol{c}_b$ is approximated by averaging across the columns. For a set of images $\{\mathbf{x}_1, ..., \mathbf{x}_B\}$ we compute normalized response matrices $\{\boldsymbol{Z}_1, ..., \boldsymbol{Z}_B\}$ and assemble their corresponding centroids into matrix $\boldsymbol{C} \in \mathbb{R}^{d \times B}$.

Given the responses and their centroids, the loss function is expressed as:

$$\mathcal{L} = -||\boldsymbol{C}||_* + \lambda \mathbb{E}_b[||\boldsymbol{Z}_b||_*] \tag{2}$$

where $|| \cdot ||_*$ indicates the nuclear norm and λ is a tradeoff parameter. The first term maximizes the extent of the "centroid manifold" to encourage separability while the second term encourages object manifold compression .

Compression by Maximizing Centroid Nuclear Norm Alone Interestingly, the first term also has a compressive effect. This is because each centroid vector, as a mean of unit vectors, has norm that is linearly related to the average cosine similarity of vectors of said unit vectors. Specifically,

$$||\boldsymbol{c}_b||^2 = \frac{1}{K} + \frac{2}{K^2} \sum_{k=1}^{K} \sum_{l=1}^{k-1} \boldsymbol{z}_{b,k}^T \boldsymbol{z}_{b,l} \tag{3}$$

Here $\boldsymbol{z}_{b,i}$ denotes the representation of the ith augmentation of $\boldsymbol{x}_b$. Then because the nuclear norm is bounded below by the Frobenius norm (Recht et al., 2010), $||\boldsymbol{C}||_* \geq ||\boldsymbol{C}||_F = \sqrt{\sum_{b=1}^{B} ||\boldsymbol{c}_b||^2}$, maximizing the centroid nuclear norm optimizes an upper bound on the norms of centroid vectors, thus encouraging intra-object manifold similarity. We can gain further insight by considering how the distribution of singular vectors of a matrix depends on the norms and pairwise similarities of the constituent column vectors. While no closed form solution exists for the singular values of an arbitrary matrix, the case where the matrix is composed of two column vectors can provide useful intuition. If $\boldsymbol{C} = [\boldsymbol{c}_1, \boldsymbol{c}_2]$, $\boldsymbol{Z}_1 = [\boldsymbol{z}_{1,1}, \boldsymbol{z}_{1,2}]$, $\boldsymbol{Z}_2 = [\boldsymbol{z}_{2,1}, \boldsymbol{z}_{2,2}]$, the singular values of $\boldsymbol{C}$ and $\boldsymbol{Z}_i$ are:

$$\begin{aligned} \boldsymbol{\sigma}(\boldsymbol{C}) &= \sqrt{\frac{||\boldsymbol{c}_1||^2 + ||\boldsymbol{c}_2||^2 \pm ((||\boldsymbol{c}_1||^2 - ||\boldsymbol{c}_2||^2)^2 + 4(\boldsymbol{c}_1^T \boldsymbol{c}_2)^2)^{1/2}}{2}} \\ \boldsymbol{\sigma}(\boldsymbol{Z}_i) &= \sqrt{1 \pm \boldsymbol{z}_{i,1}^T \boldsymbol{z}_{i,2}} \end{aligned} \tag{4}$$

So, $||\boldsymbol{\sigma}(\boldsymbol{C})||_1 = ||\boldsymbol{C}||_*$ is maximized when the centroid vectors have maximal norms (bounded above by 1, since they are the centroids of unit vectors), and are orthogonal to each other. As we saw above the centroid norms is a linear function of within-manifold similarity. Similarly, $||\boldsymbol{\sigma}(\boldsymbol{Z}_i)||_1 = ||\boldsymbol{Z}_i||_*$ is minimized when the within-manifold similarity is maximal. So, both terms in the objective encourage object manifold compression (in the simple case described above the effect is nearly mathematically equivalent). Surprisingly, this implies the first term alone encapsulates both of the key ingredients of a contrastive learning framework, and we do observe that simply maximizing $||\boldsymbol{C}||_*$ is sufficient to learn a useful representation. This is because the compressive role of "positives" in contrastive learning is carried out by forming the centroid vectors, so the objective is not positive-free even with $\lambda = 0$. For example, if only a single view is used the objective lacks a compressive component and fails to produce a useful representation. We will refer to this version of the objective (with $\lambda = 0$) as "implicit manifold compression."

3 METHODS

We tested our self-supervised contrastive learning method on datasets of different size, including CIFAR-10, STL-10, and CIFAR-100 (Krizhevsky et al., 2009; Coates et al., 2011). We used a standard linear evaluation technique (Chen et al., 2020) to verify that our method extracts semantically relevant features from the data. Additionally we conduct a series of analyses to understand how learning to compress object manifolds gives rise to class manifold separability. Finally we investigate how the geometrical differences between representations trained according to different contrastive SSL methods impact adversarial robustness.

3.1 IMPLEMENTATION DETAILS

Architecture. For all experiments we use ResNet-50 (He et al., 2016) as a backbone architecture (for variants trained on CIFAR we removed max pooling layers). Following Chen et al. (2020), we append a small one perceptron with one hidden layer to the output of the average pooling layer of the ResNet so that $z_i = g(h(x_i))$, where h is the ResNet and g is the MLP. The hidden dimensionality of the MLP was fixed to be 512 and the output dimensionality was 128. During pretraining the loss is definied on z but we subsequently drop the MLP and consider h to define the learned representation.

Optimization We employ a standard set of augmentations: a composition of random cropping (at random aspect ratio), color jitter, horizontal flipping, and conversion to grayscale. We take the parameters of each augmentation directly from Zbontar et al. (2021) (though we omit the Gaussian blurring and solarization augmentations employed in that work). All models were trained for 500 epochs using the Adam optimizer (Kingma & Ba, 2014) with a learning rate of $1\mathrm{e}-3$ and weight decay of $1\mathrm{e}-6$. We swept batch size for each method and chose the one that resulted in the highest downstream task performance. For both SimCLR and Barlow Twins we found that a batch size of 128 was optimal (among 32, 64, 128, 256, and 512) for all 3 datasets. For MMCR there is a trade-off between batch size and the number of augmentations used, and the optimal value of that trade-off is highly dataset dependent. For CIFAR-10 and CIFAR-100 we used batch size of 32 and 40 views, and for STL-10 we used a batch of 64 with 20 views

3.2 EVALUATION METHODS

Classification Accuracy. We follow a standard linear evaluation protocol: the parameters of the encoder, h are frozen and a linear function is trained to classify images using the standard supervised cross entropy loss function, see A.4 for details.

Mean Field Theory Manifold Analysis. In manifold capacity theory Chung et al. (2018), the radius and dimensionality of manifolds with arbitrary geometry (i.e., not restricted to elliptical form) are determined by the statistics of particular anchor points within the convex hull of the manifold. The anchor points of each manifold are those that uniquely specify the maximum margin separating hyperplanes between said manifold and other manifolds. This general measure of capacity is not well-suited for direct use as an objective function, because computation of the anchor points requires a computationally expensive iterative procedure. But we use it to analyze the capacity of our self-supervised representation (see Fig. 3).

Subspace Angle. Besides measuring the size and dimensionality of individual object manifolds we also wish to characterize the degree of overlap between pairs of manifolds. For this, we measure the angle between their subspaces (Knyazev & Argentati, 2002), which is a generalization of the notion of angles that applies to subspaces of arbitrary dimension.

Shared Variance. Object manifolds will generally have a lower intrinsic dimensionality then the space they are embedded in. Therefore, the data will have low variance along several of the principal vectors used to calculate the set of subspace angles, and so many of the principal angles will have little meaning. To address this limitation we also compute the shared variance between the linear subspaces that contain object manifolds. We project one object manifold onto the space spanned by the top k principal components of the second, and measure the fraction of the variance that is preserved.

Adversarial Robustness. Once a linear classifier has been trained on top of the representation, the end-to-end system can be subjected to standard adversarial attacks. We evaluate adversarial robustness under ℓ_∞ PGD attacks and AutoAttack (Madry et al., 2018; Croce & Hein, 2020).

3.3 OTHER MODELS

We chose SimCLR (Chen et al., 2020) and Barlow Twins (Zbontar et al., 2021) for primary comparisons with our model. These methods are recent, simple to implement, and achieve performance comparable to state of the art for self-supervised learning on the Imagenet-1k dataset.

Table 1: Top-1 classification accuracies of linear classifiers for representations trained with various datasets and objective functions.

Method	CIFAR-10	CIFAR-100	STL-10
Barlow Twins (our repro.)	90.91	67.91	89.96
SimCLR (our repro.)	92.22	70.04	91.11
Implicit MMCR (ours)	93.53	69.87	90.62
MMCR ($\lambda = 0.01$)	93.39	70.94	90.77

3.4 PERFORMANCE

Figure 2 details the evolution of the representation during the course of training. The centroid nuclear norm (Fig. 2b) increases steadily as the centroids become increasingly orthogonal to each other (Fig. 2c) and grow in norm (Fig. 2d). The compression of individual augmentation manifolds is reflected in Fig. 2a. The downstream classification accuracies are reported in Table 1. Subsequent analyses are carried out on the CIFAR-10 dataset using the implicit MMCR model as it achieved the highest performance.

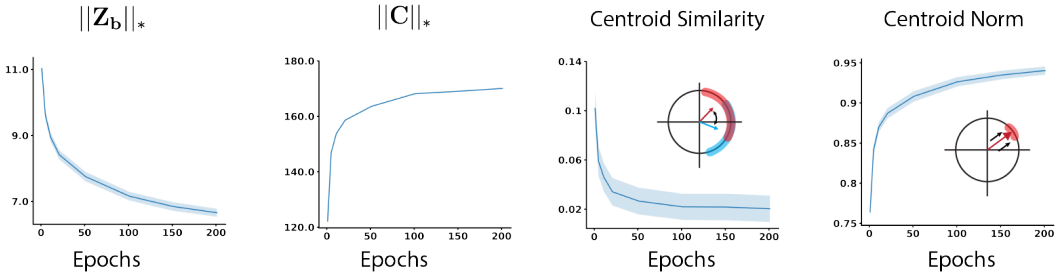

Figure 2: Evolution of various metrics during training. Geometric measures are evaluated on a set of 300 manifolds, each defined by an image drawn from the CIFAR-10 dataset, along with 16 augmentations. Shaded regions indicate a 95% confidence interval around the mean.

3.5 REPRESENTATION GEOMETRIC ANALYSIS

In figure 3 we show that our representation, which is optimized using an objective that assumes elliptical manifold geometry, nevertheless yields representations with high mean field manifold capacity (relative to baseline methods). For completeness we also analyzed the geometries of class manifolds, whose points are the representations of different examples from the same class. This analysis provided further evidence that learning to maximize augmentation manifold capacity compresses and separates class manifolds, leading to a useful representation. Interestingly MMCRs seem to use a different strategy than the baseline methods to increase the capacity, namely MMCRs product class/augmentation manifolds with larger radii, but lower dimensionality (Fig. 3)

3.6 EMERGENCE OF NEURAL MANIFOLDS VIA GRADIENT COHERENCE

We hypothesize the class separability in MMCRs arises because augmentation manifolds corresponding to examples from the same class are optimally compressed by more similar transformations than those stemming from distinct classes. To investigate this empirically, we evaluate the gradient of the objective function for inputs belonging to the same class. We can then check whether gradients obtained from (distinct) batches of the same class are more similar to each other than those obtained from different classes, which would suggest that the strategy for compressing augmentation manifolds from the same class are relatively similar to each other. Figure 4 demonstrates that this is the case: within class gradient coherence, as measured by cosine similarity, is consistently higher than across class coherence across both training epochs and model hierarchy.

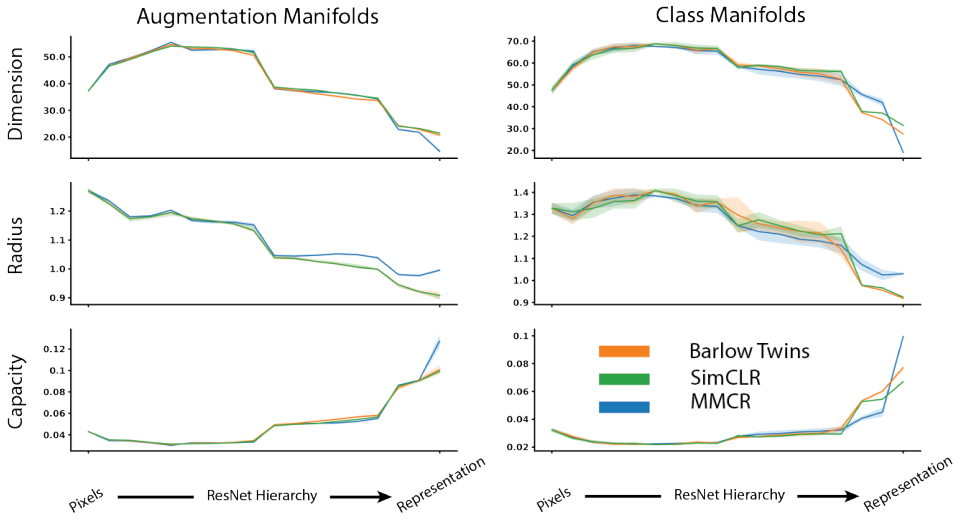

Figure 3: Mean Field Manifold Capacity Analysis. The shared x-axis of all plots is the representational hierarchy, the leftmost entries represent the inputs (pixels) and the rightmost the output of the encoder/learned representation. The top row shows the manifold radius, the middle the dimensionality, and the bottom the resultant capacity. Shaded regions indicate a 95% confidence interval around the mean (analysis was conducted with 5 different random samples from the dataset, see A.3).

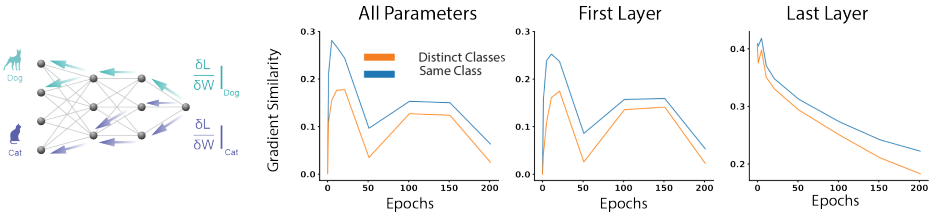

Figure 4: Gradient cosine similarity for pairs of single-class batches. We plot the mean pairwise similarity for pairs of gradients for for different subsets of the model parameters (all parameters, and the first and last linear operators) obtained from single-class-batches coming from the same or distinct classes over the course of training. To the left is a visualization of the fact that single-class gradients flow backward through the model in more similar directions.

3.7 Manifold subspace alignment

Within-class gradient coherence constitutes a plausible mechanistic explanation for the emergence of class separability, but it does not explain why members of the same class share similar compression strategies. To begin answering this question we examine the geometric properties of augmentation manifolds in the pixel domain. Here we observe small but measurable differences between the distributions of within-class similarity and across-class similarity, as demonstrated in the top row of figure 5. The subtle difference in the geometric properties of augmentation manifolds in the pixel domain in turn leads to the increased gradient coherence observed above, which over training leads to a representation that rearranges and reshapes augmentation manifolds from the same class in a similar fashion (bottom row of figure 5), thus allowing for the linear separation of classes. Not only are centroids of same-class-manifolds in more similar regions of the representation space than those coming from distinct classes (Fig 5 third column bottom row) but additionally same-class-manifolds have more similar shapes to each other (Fig 5 bottom row columns 1 and 2).

We next ask how the representation learned according to the MMCR objective differs from those optimized for other self supervised loss functions. While MMCR encourages centroids to be as close to orthogonal to each other, the InfoNCE loss employed in Chen et al. (2020) benefits when negative pairs are as dissimilar as possible, which is achieved when the two points lie in opposite regions of

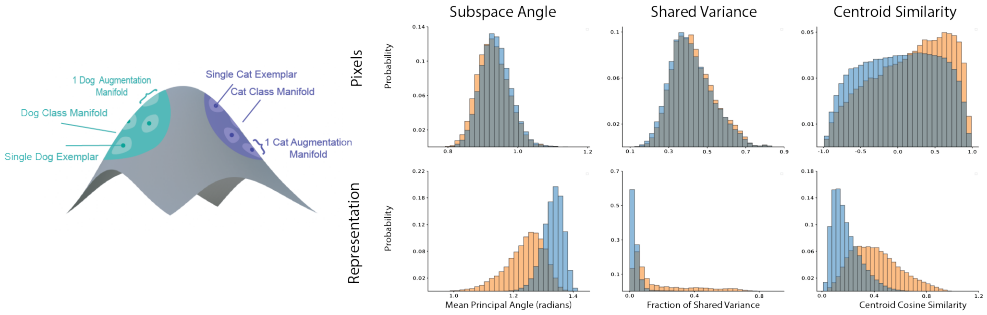

Figure 5: The distributions of various similarity metrics for augmentation manifolds from either the same and distinct classes. In the top row we consider augmentation manifolds in the pixel domain, and in the bottom row we observe how these distributions are transformed by the learned representation. To the left a schematic shows details the exemplar-augmentation manifold-class manifold structure of the learned representation.

the same subspace rather than in distinct subspaces. The Barlow Twins (Zbontar et al., 2021) loss is not an explicit function of feature vector similarities, but instead encourages individual features to be correlated across the batch dimension and distinct features to be uncorrelated. In 6 we demonstrate that these intuitions are borne out empirically: the MMCR representation produces augmentation manifold centroids that are significantly less similar to each other than the two baseline methods.

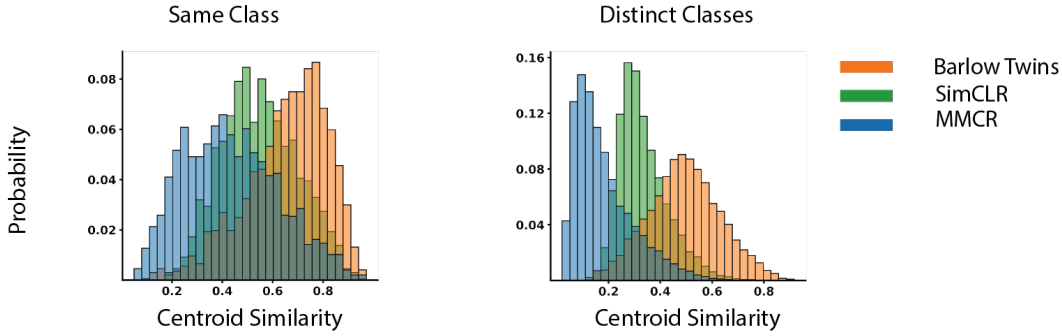

Figure 6: Centroid similarities for models trained according to different SSL objectives. The left panel shows the distribution of centroid cosine similarities for augmentation manifolds for examples of the same class, while the right shows the same distribution for examples from distinct classes.

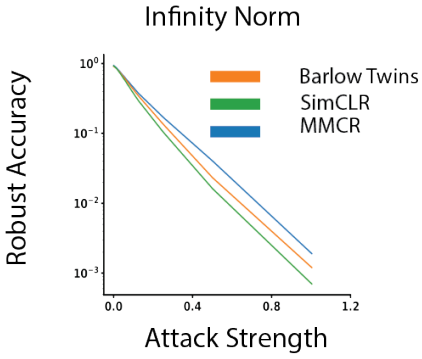

Figure 7: Adversarial Robustness of SSL Models under PGD Attack. For each of the three SSL models with trained classifiers, we apply Projected Gradient Descent (PGD) with ℓ_∞-norm perturbation under 50 attack iterations. Inputs were scaled such that their standard deviation was 1.0, so we report the raw attack strengths on the x-axis. Additional details can be found in A.5

3.8 ADVERSARIAL ROBUSTNESS

Previous works that used similar geometrically motivated loss functions such as the orthogonal low-rank embedding (Lezama et al., 2018) and maximal coding rate reduction Yu et al. (2020) have reported the resulting representations have increased inter-class margins and are more robust to label noise. We therefore tested whether the increased tendency to orthogonalize in MMCR models leads to any benefit in terms of adversarial robustness. In 7 we show that the MMCR model (and attached classifier) is indeed more robust than either Barlow Twins or SimCLR trained models against PGD attacks with a range of strengths (Madry et al., 2018). We found similar results using the stronger AutoAttack protocol (Croce & Hein, 2020), see A.5. Note that Barlow Twins models seem to be more robust than those arising from SimCLR. We speculate that this is a result of the decorrelation (rather than anti-correlation) encouraged by the Barlow Twins objective.

4 DISCUSSION

Previous work has proposed manifold capacity theory as a means of understanding the performance of deep neural networks trained using traditional supervised methods (Cohen et al., 2020). Given that manifold capacity theory is particularly well suited for analyzing high dimensional feature spaces, while many SSL methods are motivated by information criterion, we wondered whether manifold capacity could serve as a useful objective function. By approximating the manifold geometries as elliptical, which significantly reduces the computation required to calculate the geometric properties that dictate capacity, we were able to achieve exactly this. Although representational manifold geometries are generally not elliptical, we have demonstrated that this approximation can nonetheless produce a useful learning signal, and leads to networks with high manifold capacity (Fig. 3).

We demonstrate the utility of our approach by applying the method to three small datasets of unlabeled images and demonstrating that the resulting representations can yield similar downstream task performance to two baselines. Furthermore we conducted a gradient based analysis to begin to understand why the self-supervised learning signal is capable of producing useful representations. Finally, motivated by an empirical exploration of the geometrical differences between the representations produced by the three considered methods, we demonstrate that MMCRs can offer improved robustness to adversarial attacks.

Additionally, we leveraged manifold capacity analysis in its full generality to gain insight into the geometry of the MMCR. Intriguingly, our method produces augmentation and class manifolds with lower dimensionality but larger radius than either Barlow Twins or SimCLR (Fig. 3). Future work will seek to understand why this is the case, but more generally this suggests that capacity analysis can be a fruitful way to understand the different encoding strategies encouraged by various SSL paradigms. Another factor that distinguishs MMCRs from other models is a tendency to orthogonalize augmentation manifold centroids and thus form a representation that is globally high dimensional. Given that the recent observations that the representations in visual cortex and high performing models of visual cortex are surprisingly high dimensional (Stringer et al., 2019; Elmoznino & Bonner, 2022), it may be interesting to test how well MMCRs predict neural activity.

In future work, we aim to apply this approach to recognition in larger datasets. In preliminary experiments applying our method to the ImageNet-1k dataset we observed promising results, but underperformed relative to SOTA methods (specifically, 65% classification accuracy). We also intend to extend maximum capacity representation learning to both fully supervised and fully unsupervised setting. Inspired by Yu et al. (2020), we believe that adjusting (or learning) the partitioning scheme that determines the points belonging to each individual manifold can adapt the method to supervised or unsupervised settings.

In this study, we introduced one specific model of learning using metrics based on a specific theory of representations: self-supervised learning via maximizing neural manifold capacity. More broadly, this work demonstrates the efficacy of a learning objective solely based on representations (rather than relying on classifiers), and motivates new directions of research where representation-level phenomena in neurobiology inform the design choice in neural networks. With recent trends in neuroscience focused on representation geometric observations in neural data, we hope that this work lays foundations for future studies in learning based on representation geometries informed by new discoveries in neuroscience.

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A APPENDIX

A.1 PYTORCH STYLE PSEUDOCODE FOR MMCR

```
# h: encoder
# g: projection head
# B: batch size
# K: number of augmentations
# D: projector output dimensionality
#
# lmbda: trade-off parameter
for x in loader:
    # K randomly augmented views
    x = multi_augment(x) # B x K x H x W

    # push through encoder and projector
    z = g(h(x)) # B x K x D

    # project onto unitsphere
    z = normalize(z, dim=-1)

    # calculate centroids (mean over augmentation axis)
    c = z.mean(dim=1) # B x D

    # calculate singular values
    U_z, S_z, V_z = svd(z) # batch svd
    U_c, S_c, V_c = svd(c)

    # calculate loss
    loss = -1.0 * sum(S_c) + sum(S_z) / B

    # backward pass and optimization step
    loss.backward()
    optim.step()
```

A.2 ADDITIONAL PRE-TRAINING INFORMATION

For Barlow Twins we used $\lambda = \frac{1}{128}$ which normalizes for the number of elements in the on-diagonal and off-diagonal terms in the loss. For SimCLR we used the recommended setting of $\tau = 0.5$. The overall performance of both baseline methods (and likely MMCR as well) could be increased with a more thorough hyperparameter search and by employing methodology that more closely matches the original works. For example, both methods would likely benefit from the combination of larger batch size, the use of the LARS optimizer (which is designed for large batch optimization), a learning rate scheduler consisting of linear warm-up followed by cosine annealing, longer training, and the use of more diverse augmentations (i.e. including solarization and gaussian blur). Additionally Barlow Twins reports that the representation can benefit from using a much larger projector network than we use. Because our goal was primarily to demonstrate that MMCR can produce representations that are comparable to these baselines rather than to produce state-of-the-art results on small scale datasets we opted for simplifications wherever possible (using off the shelf Adam for optimization with a fixed learning rate, and fixing architectural hyperparameters like the projector dimensionality).

A.3 DETAILS OF REPRESENTATIONAL ANALYSES

Manifold Capacity Analysis For each pre-trained model, we extract layer activations across the ResNet hierarchy after a forward pass of a set of images. For class manifold analysis, the set of images contain 10 classes, where each class has 100 examples. Augmentation manifolds instead have 100 exemplars with 100 examples each. Following Cohen et al. (2020), we take activations from all convolutional layers in ResNet-50 after a ReLU non-linearity. The specific extracted layers highlighted in bold fonts are given by Table 2. The final analysis results are averaged over five data samplings with different random seeds and random projections of intermediate features to lower-dimension spaces (default 5000 dimensions).

Table 2: A Total of 18 Extracted ResNet-50 Layers (in **Bold**) for MFTMA Analysis

Layer	Type	Conv2d Size (H × W × C)
pixel	**Input**	None
conv1	$\begin{bmatrix}\text{Conv2d}\\ \text{BatchNorm}\\ \textbf{ReLU}\end{bmatrix} \times 1$	$[7 \times 7 \times 64] \times 1$
conv2_x	$\begin{bmatrix}\begin{bmatrix}\text{Conv2d}\\ \text{BatchNorm}\end{bmatrix} \times 3\\ \textbf{ReLU}\end{bmatrix} \times 3$	$\begin{bmatrix}1 \times 1 \times 64\\ 3 \times 3 \times 64\\ 1 \times 1 \times 256\end{bmatrix} \times 3$
conv3_x	$\begin{bmatrix}\begin{bmatrix}\text{Conv2d}\\ \text{BatchNorm}\end{bmatrix} \times 3\\ \textbf{ReLU}\end{bmatrix} \times 4$	$\begin{bmatrix}1 \times 1 \times 128\\ 3 \times 3 \times 128\\ 1 \times 1 \times 512\end{bmatrix} \times 4$
conv4_x	$\begin{bmatrix}\begin{bmatrix}\text{Conv2d}\\ \text{BatchNorm}\end{bmatrix} \times 3\\ \textbf{ReLU}\end{bmatrix} \times 6$	$\begin{bmatrix}1 \times 1 \times 256\\ 3 \times 3 \times 256\\ 1 \times 1 \times 1024\end{bmatrix} \times 6$
conv5_x	$\begin{bmatrix}\begin{bmatrix}\text{Conv2d}\\ \text{BatchNorm}\end{bmatrix} \times 3\\ \textbf{ReLU}\end{bmatrix} \times 3$	$\begin{bmatrix}1 \times 1 \times 512\\ 3 \times 3 \times 512\\ 1 \times 1 \times 2048\end{bmatrix} \times 3$

Gradient Coherence Analysis In Fig 4, for each of the classes of CIFAR-10, we generate 100 batches of 32 augmentation manifolds of samples from a specific class (with 40 augmentations each). We then measure the gradient of the loss function for each batch during different stages of training, and compute the cosine similarity between every pair of gradients. Across all stages of training the mean cosine similarity between gradients generated from batches of the same class is larger than those from distinct classes (left column). This observation remains true when isolating the gradients of parameters from different stages of in the resnet-50 hierarchy (center and right columns, respectively).

Manifold Subspace Alignment For Fig. 5 we generated 100 samples from the augmentation manfiolds of 500 images in the CIFAR-10 dataset. We then measure the mean subspsace angle (left column), fraction of shared variance (middle column) and centroid cosine similarity between each pair of manifolds. The same procedure was used for generating the data for 6.

A.4 Classification Evaluation Procedure

During pre-training all models were monitored with a k-nearest neighbor classifier (k=200) and checkpointed every 5 epochs. After pre-training, we trained linear classifiers on all checkpoints whose monitor accuracy was within 1% of the highest observed accuracy, and select the model that achieves the highest linear classification accuracy. Linear classifiers were trained using the Adam optimizer with batch size of 1024 and an initial learning rate of 0.1, which decayed according to a cosine scheduler over the course of 50 epochs. For the linear classifier training, at train time we use the same set of augmentations as during unsupervised pretraining, at test time we only use center cropping and random horizontal flipping.

A.5 Additional Details for Adversarial Robustness Analyses

In Figure 7, we choose 50 iterations for the PGD ℓ_∞-norm since it guarantees a robust accuracy value not far away from asymptotically larger PGD attack iterations (Madry et al., 2018; Croce &

Hein, 2020). In our experiment, we have shown that the PGD attack indeed converges in a similar fashion (See Figure 8). However, the robust accuracy for MMCR tends to converge at larger PGD attack iterations.

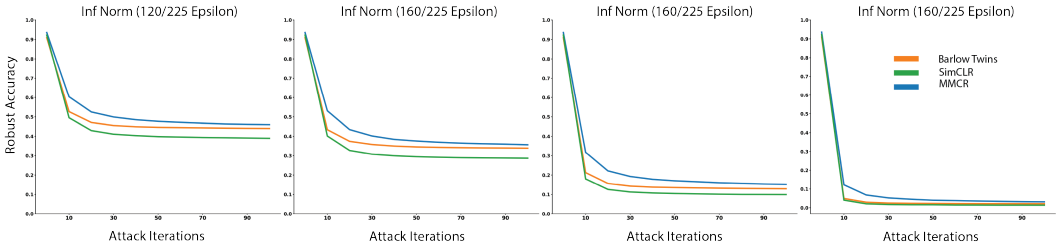

Figure 8: PGD ℓ_∞-norm attack with varying epsilon attack strength.

We therefore also analyzed the robust accuracies for the three SSL methods with varying iterations across all epsilon attack strength. Figure 9 shows MMCR exhibits a significantly higher robust accuracy compared to Barlow-Twins and SimCLR in the low iterations regime.

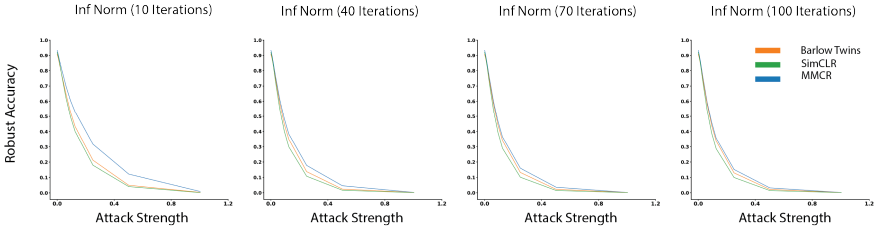

Figure 9: PGD ℓ_∞-norm attack with varying iterations.

Aside from the standard PGD adversarial attack, we also tested three SSL methods under the AutoAttack protocol. The ℓ_∞-norm AutoAttack accuracy is given by Table 3.

Table 3: AutoAttack ℓ_∞-norm Robust Accuracy

Method	Clean Accuracy	Eps = 40/255	Eps = 160/255
Barlow Twins (our repro.)	90.91	74.55	31.53
SimCLR (our repro.)	92.22	72.48	26.37
Implicit MMCR (ours)	93.53	**75.88**	**32.47**