An Information-Theoretic Understanding of Maximum Manifold Capacity Representations

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Abstract

Maximum Manifold Capacity Representations (MMCR) is a recent multi-view self-supervised learning (MVSSL) method that matches or surpasses other leading MVSSL methods. MMCR is interesting for at least two reasons. Firstly, MMCR is an oddity in the zoo of MVSSL methods: it is not (explicitly) contrastive, applies no masking, performs no clustering, leverages no distillation, and does not (explicitly) reduce redundancy. Secondly, while many self-supervised learning (SSL) methods originate in information theory, MMCR distinguishes itself by claiming a different origin: a statistical mechanical characterization of the geometry of linear separability of data manifolds. However, given the rich connections between statistical mechanics and information theory, and given recent work showing how many SSL methods can be understood from an information-theoretic perspective, we conjecture that MMCR can be similarly understood from an information-theoretic perspective. In this paper, we leverage tools from high dimensional probability and information theory to demonstrate that an optimal solution to MMCR's nuclear norm-based objective function is the same optimal solution that maximizes a well-known lower bound on mutual information between views.

Keywords: Self-supervised learning, multi-view self-supervised learning, joint embedding self-supervised learning, high dimensional probability, information theory

1. Introduction

Multi-view self-supervised learning (MVSSL; also known as Joint Embedding SSL) is a powerful approach to unsupervised learning. The core idea is to create multiple transformations, or "views", of unsupervised data, then use these transformed data in a supervised-like manner to learn generally useful representations. MVSSL methods are diverse but can be loosely grouped into a number of different families: (1) contrastive, such as CPC (Oord et al., 2018), MoCo 1 (He et al., 2020), SimCLR (Chen et al., 2020a), MoCo 2 (Chen et al., 2020b), CMC (Tian et al., 2020), RPC (Tsai et al., 2021) and TiCo (Zhu et al., 2022); (2) clustering such as Noise-as-Targets (Bojanowski and Joulin, 2017), DeepCluster (Caron

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et al., 2018), Self-Labeling (Asano et al., 2019), Local Aggregation (Zhuang et al., 2019), SwAV (Caron et al., 2020); (3) distillation/momentum such as BYOL (Grill et al., 2020), DINO (Caron et al., 2021), SimSiam (Chen and He, 2021), TiCo (Zhu et al., 2022); (4) redundancy reduction such as Barlow Twins (Zbontar et al., 2021), VICReg (Bardes et al., 2022), TiCo (Zhu et al., 2022). Many MVSSL methods either explicitly originate from information theory (Oord et al., 2018; Bachman et al., 2019) or can be understood from an information-theoretic perspective (Wang and Isola, 2020; Wu et al., 2020; Shwartz-Ziv et al., 2023; Gálvez et al., 2023).

Recently, Yerxa et al. (2023) proposed a new MVSLL method named Maximum Manifold Capacity Representations (MMCR) that achieves similar (if not superior) performance to leading MVSSL methods. MMCR is interesting for at least two reasons. Firstly, MMCR does not fit neatly into any of the MVSSL families: it is not (explicitly) contrastive, it applies no masking, it performs no clustering, it leverages no distillation, and it does not (explicitly) reduce redundancy. Secondly, unlike many MVSSL methods that originate in information theory, MMCR distances itself, writing that estimating mutual information in high dimensions has proven difficult and that more closely approximating mutual information may not improve representations; MMCR instead claims an origin in the statistical mechanical characterization of the geometry of linear separability of data manifolds.

In this work, we seek to better understand what solutions the MMCR loss function incentivizes and how it relates to other well-known MVSSL methods. Our contributions are specifically as follows:

1. We derive a distribution of embeddings that provably minimizes the MMCR loss with high probability by leveraging tools from high dimensional probability.

2. We connect this distribution to information theory by showing it maximizes a well-known variational lower bound on the mutual information between multiple views' embeddings.

2. Background

Multi-View Self-Supervised Learning (MVSSL) Let $f_\theta : \mathcal{X} \to \mathcal{Z}$ denote our neural network with parameters θ. Suppose we have a dataset $\{\boldsymbol{x}_n\}_{n=1}^N$ and a set of transformations (sometimes called augmentations, or "views") $\mathcal{T}$ such as color jittering, Gaussian blur, solarization, etc. For each datum $\boldsymbol{x}_n$ in a batch of inputs, we sample K transformations $t^{(1)}, t^{(2)}, ..., t^{(K)} \sim \mathcal{T}$, then transform the datum: $t^{(1)}(\boldsymbol{x}_n), ..., t^{(K)}(\boldsymbol{x}_n)$. We feed these transformed data into the network and obtain *embeddings* or *representations*:

$$\boldsymbol{z}_n^{(k)} \stackrel{\text{def}}{=} f_\theta(t^{(k)}(\boldsymbol{x}_n)) \in \mathcal{Z}. \tag{1}$$

In practice, $\mathcal{Z}$ is commonly $\mathbb{R}^D$ or the D-dimensional hypersphere $\mathbb{S}^{D-1} \stackrel{\text{def}}{=} \{\boldsymbol{z} \in \mathbb{R}^D : \boldsymbol{z}^T\boldsymbol{z} = 1\}$. Given that this work will later touch on information theory, we need notation to refer to the random variables; we use $Z_n^{(k)}$ to denote the random variable for the embedding whose realization is $\boldsymbol{z}_n^{(k)}$, and $X_n^{(k)}$ to denote the random variable for the transformed datum whose realization is $t^{(k)}(\boldsymbol{x}_n)$.

Maximum Manifold Capacity Representations (MMCR) MMCR (Yerxa et al., 2023) originates from classical results regarding performance of linear binary classifiers (Cover, 1965; Gardner, 1987, 1988). Consider N points in dimension D, with arbitrarily assigned binary class labels; *what is the probability that a linear binary classifier will be able to successfully classify the points?* Statistical mechanical calculations reveal that in the *thermodynamic* limit ($N, D \to \infty$; $N/D \to \alpha \in (0, \infty)$), a phase transition occurs at capacity $\alpha_c = 2$. More precisely, if $\alpha < \alpha_c$, the linear binary classifier will succeed with probability 1; but if $\alpha > \alpha_c$, the classifier will succeed with probability 0. MMCR is based on an extension of this result from points to manifolds (Chung et al., 2018). MMCR proceeds in the following manner: MMCR takes the embeddings output by the network and normalizes them to lie on the hypersphere: $\boldsymbol{z}_n^{(1)}, ..., \boldsymbol{z}_n^{(K)} \in \mathbb{S}^{D-1}$. Then, MMCR compute the average embedding per datum:

$$\boldsymbol{\mu}_n \overset{\text{def}}{=} \frac{1}{K} \sum_k \boldsymbol{z}_n^{(k)}. \tag{2}$$

Next, MMCR forms a $N \times D$ matrix M where the n-th row of M is $\boldsymbol{\mu}_n$ and defines the loss:

$$\mathcal{L}_{MMCR} \overset{\text{def}}{=} -\|M\|_* \overset{\text{def}}{=} -\sum_{r=1}^{rank(M)} \sigma_r(M), \tag{3}$$

where $\sigma_r(M)$ is the r-th singular value of M and $\|\cdot\|_*$ is the nuclear norm (trace norm, Schatten 1-norm). Minimizing the MMCR loss means maximizing the nuclear norm of the mean matrix M. The authors of MMCR note that no closed form solution exists for singular values of an arbitrary matrix, but when $N = 2, D = 2$, a closed form solution exists that offers intuition: $\|M\|_*$ will be maximized when (i) the norm of each mean is maximized i.e., $\|\boldsymbol{\mu}_n\|_2 = 1$ (recalling that $0 \leq \|\boldsymbol{\mu}_n\| < 1$ since the representations live on the hypersphere), and (ii) the means $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$ are orthogonal to one another. While we commend the authors for working to offer intuition, it is unclear to what extent the $N = 2, D = 2$ setting sheds light on MMCR in general, as MMCR was theoretically derived and numerically implemented in the large data and high dimensionality regime.

3. An Information Theoretic Understanding of MMCR

In this section, we prove and intuitively explain two properties of MMCR that shed light on it as well as relate it to other MVSSL methods. We specifically consider MMCR's regime of large dataset size N and high embedding dimension D. We contribute two results:

1. The MMCR loss $\mathcal{L}_{MMCR}$ is minimized by (a) making each mean $\boldsymbol{\mu}_n = \frac{1}{K} \sum_k \boldsymbol{z}_n^{(k)}$ lie on the surface of the hypersphere, and (b) making the distribution of means as close to uniform on the hypersphere as possible.

2. This configuration of means maximizes a well-known variational lower bound on the mutual information between embeddings (Gallager, 1968) that was recently used to study and unify several multi-view SSL (MVSSL) families (Gálvez et al., 2023).

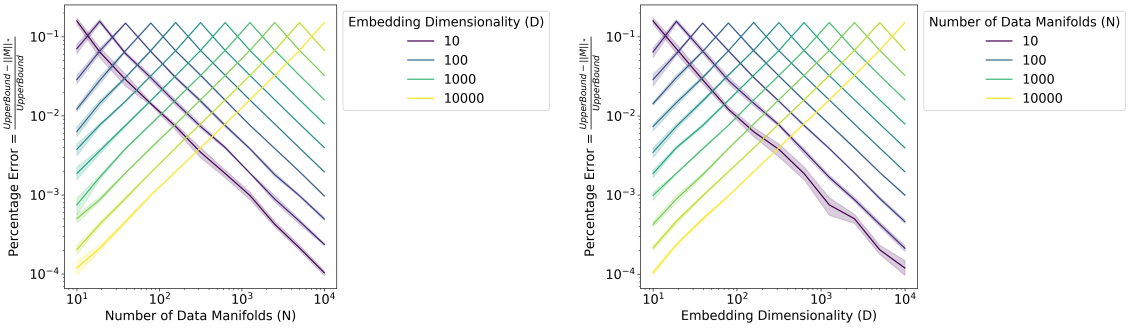

Figure 1: **Numerical simulations confirm that a network achieving perfect reconstruction and perfect uniformity achieves the lowest possible MMCR loss.** Away from the $N = D$ threshold, uniform random vectors achieve the theoretically derived upper bound on the nuclear norm (i.e. lower bound on $\mathcal{L}_{MMCR}$).

More formally, we begin by adapting two useful definitions from relevant prior works (Wang and Isola, 2020; Gálvez et al., 2023):

Definition 1 (Perfect Reconstruction)
We say a network f_θ achieves perfect reconstruction if $\forall \boldsymbol{x} \in \mathcal{X}, \forall\, t^{(1)}, t^{(2)} \in \mathcal{T}$, $\boldsymbol{z}^{(1)} = f_\theta(t^{(1)}(\boldsymbol{x})) = f_\theta(t^{(2)}(\boldsymbol{x})) = \boldsymbol{z}^{(2)}$.

Definition 2 (Perfect Uniformity) *Let $p(Z)$ be the distribution over the network representations induced by the data sampling and transformation sampling distributions. We say a network f_θ achieves perfect uniformity if the distribution $p(Z)$ is the uniform distribution on the hypersphere.*

We will show that a network that achieves both perfect reconstruction and perfect uniformity obtains the lowest possible MMCR loss by first showing that $\mathcal{L}_{MMCR}$ has a lower bound and then showing that such a network achieves this bound.

Proposition 3 *Suppose that* $\forall n \in [N], \boldsymbol{\mu}_n^T \boldsymbol{\mu}_n \leq 1$. *Then,* $0 \leq ||M||_* \leq \begin{cases} N & \text{if } N \leq D \\ \sqrt{ND} & \text{if } N \geq D \end{cases}$.

Proof Let $\sigma_1, \ldots, \sigma_{\min(N,D)}$ denote the singular values of M, so that $\|M\|_* = \sum_{i=1}^{\min(N,D)} \sigma_i$. The lower bound follows by the fact that singular values are nonnegative. For the upper bound, we have

$$\sum_{i=1}^{\min(N,D)} \sigma_i^2 = \mathrm{Tr}\big[MM^T\big] = \sum_{n=1}^{N} \boldsymbol{\mu}_n^T \boldsymbol{\mu}_n \leq N.$$

Then, by Cauchy-Schwarz on the sequences $(1, \ldots, 1)$ and $\left(\sigma_1, \ldots, \sigma_{\min(N,D)}\right)$, we get

$$\sum_{i=1}^{\min(N,D)} \sigma_i \leq \sqrt{\left(\sum_{i=1}^{\min(N,D)} 1\right)\left(\sum_{i=1}^{\min(N,D)} \sigma_i^2\right)} \leq \sqrt{\min(N,D)N} = \begin{cases} N & \text{if } N \leq D \\ \sqrt{ND} & \text{if } N \geq D \end{cases}.$$

■

Proposition 4 *Let f_θ achieve perfect reconstruction. Then, $\|\boldsymbol{\mu}_n\|_2 = 1 \ \forall n$.*

Proof Because f_θ achieves perfect reconstruction, $\forall n, \forall t^{(1)}, t^{(2)}$, $\boldsymbol{z}_n^{(1)} = \boldsymbol{z}_n^{(2)}$. Thus $\boldsymbol{\mu}_n = (1/K)\sum_k \boldsymbol{z}_n^{(k)} = (1/K)\sum_k \boldsymbol{z}_n^{(1)} = \boldsymbol{z}_n^{(1)}$, and since $\|\boldsymbol{z}_n^{(1)}\|_2 = 1$, we have $\|\boldsymbol{\mu}_n\|_2 = 1$. ■

Theorem 5 *Let $f_\theta : \mathcal{X} \to \mathbb{S}^D$ be a network that achieves perfect reconstruction and perfect uniformity. Then f_θ achieves the lower bound of $\mathcal{L}_{MMCR}$ with high probability. Specifically:*

$$\|M\|_* = \begin{cases} N(1 - O(N/D)) & \text{if } N \leq D \\ \sqrt{ND}(1 - O(D/N)) & \text{if } N \geq D \end{cases}$$

with high probability in $\min(N, D)$.

We defer the proof to Appendix A but offer intuition here. To show the inequality in Proposition 3 is roughly tight, we need to show the singular values σ_i are all roughly equal to each other. When $N \ll D$, since M has few rows $\boldsymbol{\mu}_n$, they are almost perfectly orthogonal to each other, so all N singular values will be $\approx \|\boldsymbol{\mu}_n\| = 1$. When $N \gg D$, since M has many rows, for any $x \in \mathbb{R}^D$ the sum $\|Mx\|_2^2 = \sum_n (\boldsymbol{\mu}_n^T x)^2$ will be concentrated, so M scales all vectors roughly equally, and therefore its D singular values are all roughly equal to each other. We confirm this via numerical simulations (Fig. 1); for code, see Appendix B.

We now turn to addressing why perfect reconstruction and perfect uniformity matter from an information theoretic perspective. The results here for MVSSL are known, e.g., (Wang and Isola, 2020; Gálvez et al., 2023), but we repeat them to make the connection with MMCR. For input datum X, consider the mutual information between the learned embeddings of two different views $Z^{(1)} = t^{(1)}(X)$ and $Z^{(2)} = t^{(2)}(X)$; the mutual information must be at least as great as the sum of two terms: the ability of one embedding to "reconstruct" the other, plus the entropy of the embeddings:

$$I[Z^{(1)}; Z^{(2)}] \quad \geq \quad \underbrace{\mathbb{E}_{p(Z^{(1)}, Z^{(2)})}[\log q(Z^{(1)}|Z^{(2)})]}_{\text{Reconstruction}} \quad + \quad \underbrace{H[Z^{(1)}]}_{\text{Entropy}}, \tag{4}$$

where $q(Z^{(1)}|Z^{(2)})$ is a variational distribution because the true distribution $p(Z^{(1)}|Z^{(2)})$ is unknown.

Theorem 6 *Let $f_\theta : \mathcal{X} \to \mathbb{S}^D$ be a network, the number of views per datum be constant, and $\mathcal{Q}$ be the variational family of distributions on the hypersphere. Then f_θ maximizes the mutual information lower bound Eqn. 3 if and only if f_θ achieves perfect reconstruction and perfect uniformity.*

Proof Perfect reconstruction maximizes reconstruction term. Perfect uniformity maximizes entropy since the maximum entropy is achieved with the uniform distribution over the support (Cover and Thomas, 2006). ■

Theorem 7 *Let f_{θ^*} be a network that achieves perfect reconstruction and perfect uniformity, let the number of views per datum K be a constant, and let $\mathcal{Q}$ be the variational family of distributions on the hypersphere. Then f_{θ^*} is both a minimizer of $\mathcal{L}_{MMCR}$ and a maximizer of the variational lower bound of mutual information Eqn. 3.*

Proof The proof follows by Theorem 5 and Theorem 6. ■

4. Discussion

In this work, we leveraged tools from high dimensional probability to prove that in the large data and high dimensional regime, the MMCR loss is minimized with high probability by a network achieving perfect reconstruction and perfect uniformity. These two properties together are known to maximize a well-known variational lower bound on the mutual information between multi-view embeddings.

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Appendix A. Proof of Theorem 5

Recall that $\mathcal{L}_{MMCR} = -\|M\|_*$ is minimized when $\|M\|_*$ is maximized and that $\|M\|_*$ is upper bounded by $\sqrt{ND}$ if $N > D$ and N if $N < D$ (Proposition 3). We want to show a network that achieves perfect reconstruction and perfect uniformity achieves this upper bound on the nuclear norm (equivalently, lower bound on the MMCR loss).

Following the proof of Proposition 3, let $\sigma_1, \ldots, \sigma_{\min(N,D)}$ denote the singular values of M, so that $\|M\|_* = \sum_i \sigma_i$. By Proposition 4, we have

$$\sum_i \sigma_i^2 = \mathrm{Tr}\big[MM^T\big] = \sum_{n=1}^{N} \boldsymbol{\mu}_n^T \boldsymbol{\mu}_n = N.$$

Now, by the equality version of Cauchy–Schwarz on the sequences $(1, \ldots, 1)$ and $\big(\sigma_1, \ldots, \sigma_{\min(N,D)}\big)$, we have

$$\sum_i \sigma_i = \sqrt{\min(N,D)\left(\sum_i \sigma_i^2 - \sum_i \left(\sigma_i - \frac{\sum_j \sigma_j}{\min(N,D)}\right)^2\right)}. \tag{5}$$

So if we can bound this "variance" of the singular values $\sum_i \left(\sigma_i - \frac{\sum_j \sigma_j}{\min(N,D)}\right)^2$, we can show that $\|M\|_*$ closely matches the upper bound obtained in Proposition 3.

To do this, let us consider matrix $\sqrt{D}M$. The vectors $\boldsymbol{\mu}_n$ are uniform over the D-dimensional hypersphere $\mathbb{S}^D$, so its rows $\sqrt{D}\boldsymbol{\mu}_n$ have mean zero, are isotropic, and (by Example 5.25 in Vershynin et al. (2012)) are sub-gaussian with parameter $\|\sqrt{D}\boldsymbol{\mu}_n\|_{\psi_2} = O(1)$.[1] Therefore,

- **If $\mathbf{N \le D}$**, then (using the fact that $\|\boldsymbol{\mu}_n\|_2 = 1$ for all $n \in [N]$) we can to apply Theorem 5.58 in Vershynin et al. (2012) on the transpose of $\sqrt{D}M$, obtaining that for any $t \ge 0$, the singular values of $\sqrt{D}M$ are within $\sqrt{D} \pm O(\sqrt{N}) + t$ with probability at least $1 - 2\exp(-\Omega(t^2))$. Setting t to a large enough multiple of $\sqrt{N}$, they are all within $\sqrt{D} \pm O(\sqrt{N})$ with probability at least $1 - 2\exp(-N)$. Consequently, with the same probability, the singular values of M are all within $\pm O(\sqrt{N/D})$ of each other, and we get $\sum_i \left(\sigma_i - \frac{\sum_j \sigma_j}{\min(N,D)}\right)^2 \le N \cdot O\left(\sqrt{N/D}\right)^2 = O(N^2/D)$. Plugging this into Eqn. 5, we get $\|M\|_* \le \sqrt{N(N - O(N^2/D))} = \sqrt{N}(1 - O(N/D))$.
- **If $\mathbf{N \ge D}$**, then we can apply Theorem 5.39 in Vershynin et al. (2012) on $\sqrt{D}M$, obtaining that for any $t \ge 0$, the singular values of $\sqrt{D}M$ are within $\sqrt{N} \pm O(\sqrt{D}) + t$ with probability at least $1 - 2\exp(-\Omega(t^2))$. Setting t to a large enough multiple of $\sqrt{D}$, they are all within $\sqrt{N} \pm O(\sqrt{D})$ with probability at least $1 - 2\exp(-D)$. Consequently, with the same probability, the singular values of M are all within $\pm O(1)$ of each other, and we get $\sum_i \left(\sigma_i - \frac{\sum_j \sigma_j}{\min(N,D)}\right)^2 \le D \cdot O(1)^2 = O(D)$. Plugging this into Eqn. 5, we get $\|M\|_* \le \sqrt{D(N - O(D))} = \sqrt{ND}(1 - O(D/N))$.

1. Here, $\|\cdot\|_{\psi_2}$ denotes the sub-gaussian norm (intuitively, the "effective standard deviation" of a sub-gaussian random variable). For a scalar random variable X, it is defined as $\|X\|_{\psi_2} \sup_{p \ge 1} p^{-1/2}(\mathbb{E}[|X|^p])^{1/p}$ (Definition 5.7 in Vershynin et al. (2012)), and for a random vector $\boldsymbol{u} \in \mathbb{R}^D$, it is defined as $\|\boldsymbol{u}\|_{\psi_2} \sup_{\boldsymbol{v} \in \mathbb{S}^D} \|\boldsymbol{u}^T \boldsymbol{v}\|_{\psi_2}$ (Definition 5.22 in Vershynin et al. (2012)).

Appendix B. Python Code for Perfect Reconstruction and Perfect Uniformity Embeddings

To test our claim that networks which achieve perfect reconstruction and perfect uniformity achieve the nuclear norm upper bound, we sample a uniform distribution of embeddings and measure the nuclear norm relative to our claimed upper bound. Python code for our simulations is included below:

```
import pandas as pd
import numpy as np


N_list = np.logspace(start=1, stop=4, num=11).astype(int)
D_list = np.logspace(start=1, stop=4, num=11).astype(int)
repeats = np.arange(5).astype(int)
uniform_distribution_nuclear_norm_data_list = []

for N in N_list:
    for D in D_list:
        print(f"N: {N}\tD: {D}")
        for repeat in repeats:
            embeddings = np.random.normal(loc=0, scale=10.0, size=(N, D))
            embeddings /= np.linalg.norm(embeddings, axis=1, keepdims=True)
            row = {
                "Spectrum": "uniform",
                "Number of Data Manifolds (N)": N,
                "Embedding Dimensionality (D)": D,
                "Repeat": repeat,
                "Nuclear Norm": np.linalg.norm(embeddings, ord="nuc"),
            }
            uniform_distribution_nuclear_norm_data_list.append(row)

uniform_distribution_nuclear_norm_df = pd.DataFrame(
    uniform_distribution_nuclear_norm_data_list
)
```