Random Matrix Theory Proves that Deep Learning Representations of GAN-data Behave as Gaussian Mixtures

ICML 2020

MEA. Seddik[12], C.Louart[13], M. Tamaazousti[1], R. Couillet[23]

[1]http://melaseddik.github.io/

[1]CEA List, France
[2]CentraleSupélec, L2S, France
[3]GIPSA Lab Grenoble-Alpes University, France

June 8, 2020

Abstract

Context:

- Study of large **Gram** matrices of **concentrated** data.

Motivation:

- **Gram** matrices are at the core of various ML algorithms.
- RMT predicts their performances under **Gaussian** assumptions on the data.
- **BUT Real data** are **unlikely close** to **Gaussian** vectors.

Results:

- **GAN data ($\approx$ Real data)** fall within the class of **Concentrated** vectors.
- **Universality result:**

  Only **first** and **second** order statistics of **Concentrated** data matter to describe the behavior of **Gram** matrices.

Notion of Concentrated Vectors

Definition (Concentrated Vectors)

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\boldsymbol{Z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz**[1] function $\mathcal{F} : E \to \mathbb{R}$, there exists $C, c > 0$ such that

$$\forall t > 0,\ \mathbb{P}\left\{|\mathcal{F}(\boldsymbol{Z}) - \mathbb{E}\mathcal{F}(\boldsymbol{Z})| \geq t\right\} \leq Ce^{-(t/c)^q} \xrightarrow{\text{denoted}} \boxed{\boldsymbol{Z} \in \mathcal{E}_q(c)}$$

If c independent of $\dim(E)$, we denote $\boxed{\boldsymbol{Z} \in \mathcal{E}_q(1)}$

Concentrated vectors enjoy:

(P1) If $\boldsymbol{X} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}_p)$ then $\boldsymbol{X} \in \mathcal{E}_2(1)$

"Gaussian vectors are concentrated vectors"

(P2) If $\boldsymbol{X} \in \mathcal{E}_q(1)$ and $\mathcal{G}$ is a $\lambda_{\mathcal{G}}$-**Lipschitz** map, then $\mathcal{G}(\boldsymbol{X}) \in \mathcal{E}_q(\lambda_{\mathcal{G}})$

"Concentrated vectors are stable through Lipschitz maps"

[1] **Reminder:** $\mathcal{F} : E \to F$ is $\lambda_{\mathcal{F}}$-Lipschitz if $\forall (\boldsymbol{x}, \boldsymbol{y}) \in E^2 : \|\mathcal{F}(\boldsymbol{x}) - \mathcal{F}(\boldsymbol{y})\|_F \leq \lambda_{\mathcal{F}} \|\boldsymbol{x} - \boldsymbol{y}\|_E$.

Why Concentrated Vectors?

Figure: Images artificially generated using the BigGAN model [Brock *et al*, ICLR'19].

$$\textbf{Real Data} \approx \textbf{GAN Data} = \underbrace{\mathcal{F}_L \circ \mathcal{F}_{L-1} \circ \cdots \circ \mathcal{F}_1}_{\mathcal{G}}(\textbf{Gaussian})$$

where the $\mathcal{F}_i$'s correspond to Fully Connected layers, Convolutional layers, Sub-sampling, Pooling and activation functions, residual connections or Batch Normalisation.

$\Rightarrow$ The $\mathcal{F}_i$'s are essentially ***Lipschitz*** operations.

Why Concentrated Vectors?

- **Fully Connected Layers and Convolutional Layers** are affine operations:

$$\mathcal{F}_i(\boldsymbol{x}) = \boldsymbol{W}_i \boldsymbol{x} + \boldsymbol{b}_i,$$

  and $\|\mathcal{F}_i\|_{lip} = \sup_{\boldsymbol{u} \neq \boldsymbol{0}} \frac{\|\boldsymbol{W}_i \boldsymbol{u}\|_p}{\|\boldsymbol{u}\|_p}$, for any p-norm.
- **Pooling Layers and Activation Functions:** Are 1-Lipschitz operations with respect to any p-norm (e.g., ReLU and Max-pooling).
- **Residual Connections:** $\mathcal{F}_i(\boldsymbol{x}) = \boldsymbol{x} + \mathcal{F}_i^{(\ell)} \circ \cdots \circ \mathcal{F}_i^{(1)}(\boldsymbol{x})$
  where the $\mathcal{F}_i^{(j)}$'s are Lipschitz operations, thus $\mathcal{F}_i$ is a Lipschitz operation with Lipschitz constant bounded by $1 + \prod_{j=1}^{\ell} \|\mathcal{F}_i^{(j)}\|_{lip}$.
- ...

By:

(P1) If $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_p)$ then $\boldsymbol{X} \in \mathcal{E}_2(1)$

(P2) If $\boldsymbol{X} \in \mathcal{E}_q(1)$ and $\mathcal{G}$ is a $\lambda_{\mathcal{G}}$-**Lipschitz** map, then $\mathcal{G}(\boldsymbol{X}) \in \mathcal{E}_q(\lambda_{\mathcal{G}})$

$\Rightarrow$ **GAN data** are **concentrated** vectors by design.

Remark: Still we need to control $\lambda_{\mathcal{G}}$.

Control of $\lambda_{\mathcal{G}}$ with Spectral Normalization

Let $\sigma_* > 0$ and $\mathcal{G}$ be a neural network composed of N affine layers, each one of input dimension d_{i-1} and output dimension d_i for $i \in [N]$, with 1-Lipschitz activation functions. Consider the following dynamics with learning rate η:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \boldsymbol{E}, \text{ with } \boldsymbol{E}_{i,j} \sim \mathcal{N}(0,1)$$
$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \max(0, \sigma_1(\boldsymbol{W}) - \sigma_*)\, \boldsymbol{u}_1(\boldsymbol{W}) \boldsymbol{v}_1(\boldsymbol{W})^\intercal.$$

The Lipschitz constant of $\mathcal{G}$ is bounded at convergence with high probability as:

$$\lambda_{\mathcal{G}} \leq \prod_{i=1}^{N} \left(\varepsilon + \sqrt{\sigma_*^2 + \eta^2 d_i d_{i-1}} \right).$$

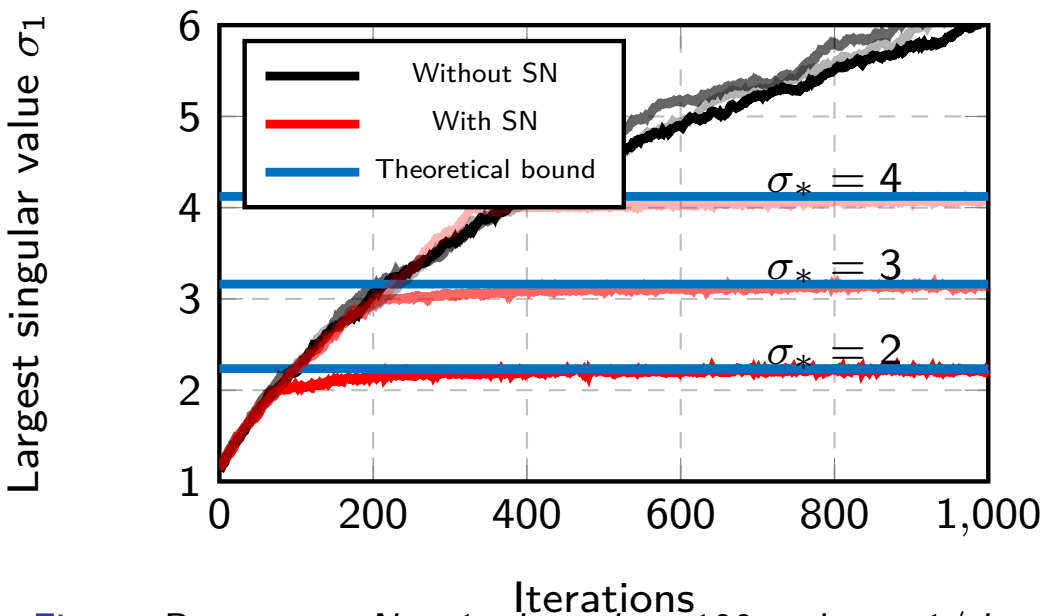


Figure: Parameters $N = 1$, $d_0 = d_1 = 100$ and $\eta = 1/d_0$.

Model & Assumptions

(A1) Data matrix (distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$):

$$\boldsymbol{X} = \left[\underbrace{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{n_1}}_{\in \mathcal{E}_{q_1}(1)}, \underbrace{\boldsymbol{x}_{n_1+1}, \ldots, \boldsymbol{x}_{n_2}}_{\in \mathcal{E}_{q_2}(1)}, \ldots, \underbrace{\boldsymbol{x}_{n-n_k+1}, \ldots, \boldsymbol{x}_n}_{\in \mathcal{E}_{q_k}(1)} \right] \in \mathbb{R}^{p \times n}$$

Model statistics: $\boldsymbol{\mu}_\ell = \mathbb{E}_{\boldsymbol{x}_i \in \mathcal{C}_\ell}[\boldsymbol{x}_i], \quad \boldsymbol{C}_\ell = \mathbb{E}_{\boldsymbol{x}_i \in \mathcal{C}_\ell}[\boldsymbol{x}_i \boldsymbol{x}_i^\mathsf{T}]$

(A2) Growth rate assumptions: As $p \to \infty$,

1. $p/n \to c \in (0, \infty)$.
2. The number of classers k is bounded.
3. For any $\ell \in [k]$, $\|\boldsymbol{\mu}_\ell\| = \mathcal{O}(\sqrt{p})$.

Gram matrix and its resolvent:

$$\boxed{\boldsymbol{G} = \frac{1}{p} \boldsymbol{X}^\mathsf{T} \boldsymbol{X}, \quad \boldsymbol{Q}(z) = (\boldsymbol{G} + z \boldsymbol{I}_n)^{-1}}$$

$$m_L(z) = \frac{1}{n} \mathrm{tr}\,(\boldsymbol{Q}(-z)), \quad \boldsymbol{U}\boldsymbol{U}^\mathsf{T} = \frac{-1}{2\pi i} \oint_\gamma \boldsymbol{Q}(-z) dz$$

Main Result

Theorem

*Under Assumptions **(A1)** and **(A2)**, we have* $\boldsymbol{Q}(z) \in \mathcal{E}_q(p^{-\frac{1}{2}})$. *Furthermore,*

$$\left\|\mathbb{E}[\boldsymbol{Q}(z)] - \tilde{\boldsymbol{Q}}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \text{where} \quad \tilde{\boldsymbol{Q}}(z) = \frac{1}{z}\boldsymbol{\Lambda}(z) + \frac{1}{p\,z}\boldsymbol{J}\Omega(z)\boldsymbol{J}^{\mathsf{T}}$$

with $\boldsymbol{\Lambda}(z) = diag\left\{\frac{\mathbf{1}_{n_\ell}}{1+\delta_\ell(z)}\right\}_{\ell=1}^{k}$ *and* $\Omega(z) = diag\{\boldsymbol{\mu}_\ell^{\mathsf{T}}\tilde{\boldsymbol{R}}(z)\boldsymbol{\mu}_\ell\}_{\ell=1}^{k}$

$$\tilde{\boldsymbol{R}}(z) = \left(\frac{1}{k}\sum_{\ell=1}^{k}\frac{\boldsymbol{C}_\ell}{1+\delta_\ell(z)} + z\boldsymbol{I}_p\right)^{-1}$$

with $\delta(z) = [\delta_1(z), \ldots, \delta_k(z)]$ *is the unique fixed point of the system of equations*

$$\delta_\ell(z) = tr\left(\boldsymbol{C}_\ell\left(\frac{1}{k}\sum_{j=1}^{k}\frac{\boldsymbol{C}_j}{1+\delta_j(z)} + z\boldsymbol{I}_p\right)^{-1}\right) \quad \text{for each} \quad \ell \in [k].$$

Main Result

Theorem

*Under Assumptions **(A1)** and **(A2)**, we have* $\boldsymbol{Q}(z) \in \mathcal{E}_q(p^{-\frac{1}{2}})$. *Furthermore,*

$$\left\| \mathbb{E}[\boldsymbol{Q}(z)] - \tilde{\boldsymbol{Q}}(z) \right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}} \right) \quad \text{where} \quad \tilde{\boldsymbol{Q}}(z) = \frac{1}{z}\boldsymbol{\Lambda}(z) + \frac{1}{p\,z}\boldsymbol{J}\Omega(z)\boldsymbol{J}^{\mathsf{T}}$$

with $\boldsymbol{\Lambda}(z) = \mathrm{diag}\left\{ \frac{\mathbf{1}_{n_\ell}}{1+\delta_\ell(z)} \right\}_{\ell=1}^{k}$ *and* $\Omega(z) = \mathrm{diag}\{\boldsymbol{\mu}_\ell^{\mathsf{T}} \tilde{\boldsymbol{R}}(z) \boldsymbol{\mu}_\ell\}_{\ell=1}^{k}$

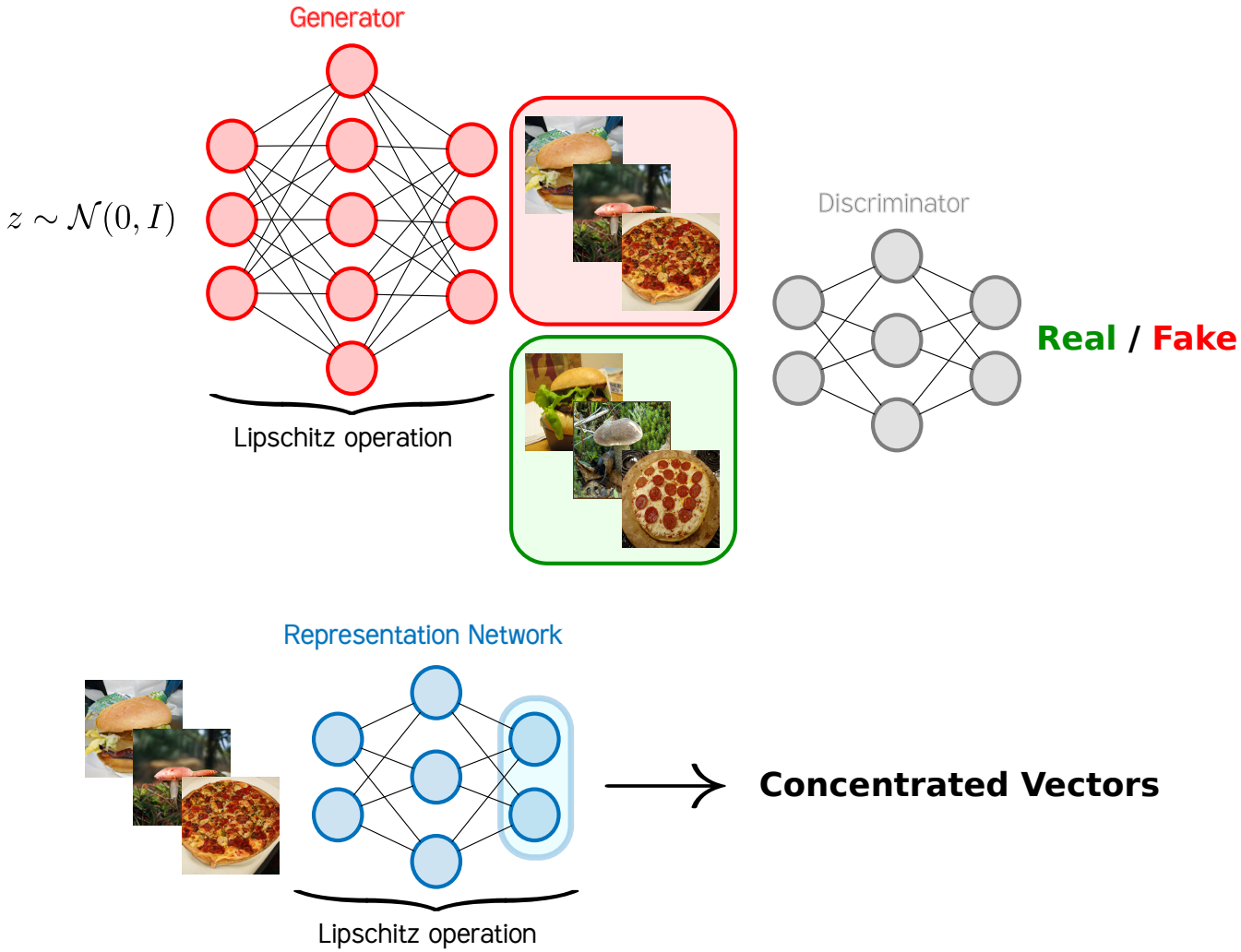
$$\tilde{\boldsymbol{R}}(z) = \left(\frac{1}{k} \sum_{\ell=1}^{k} \frac{\boldsymbol{C}_\ell}{1+\delta_\ell(z)} + z\boldsymbol{I}_p \right)^{-1}$$

with $\delta(z) = [\delta_1(z), \ldots, \delta_k(z)]$ *is the unique fixed point of the system of equations*

$$\delta_\ell(z) = tr\left(\boldsymbol{C}_\ell \left(\frac{1}{k} \sum_{j=1}^{k} \frac{\boldsymbol{C}_j}{1+\delta_j(z)} + z\boldsymbol{I}_p \right)^{-1} \right) \quad \text{for each } \ell \in [k].$$

Key Observation: Only **first** and **second** order statistics matter!

Application to CNN Representations of GAN Images



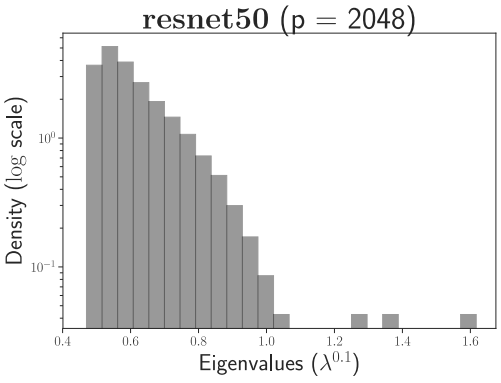
- CNN representations correspond to the **penultimate** layer.
- Popular architectures considered in practice are: **Resnet, VGG, Densenet**.

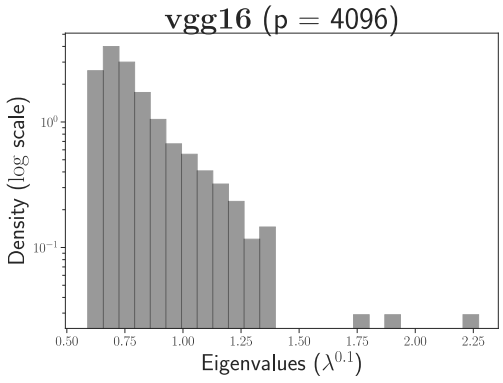
Application to CNN Representations of GAN Images

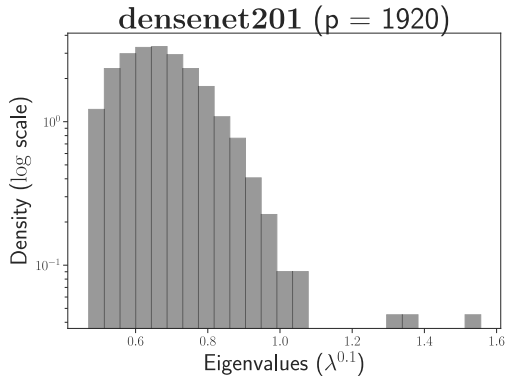
Figure: $k = 3$ classes, $n = 3000$ images.

Application to CNN Representations of GAN Images

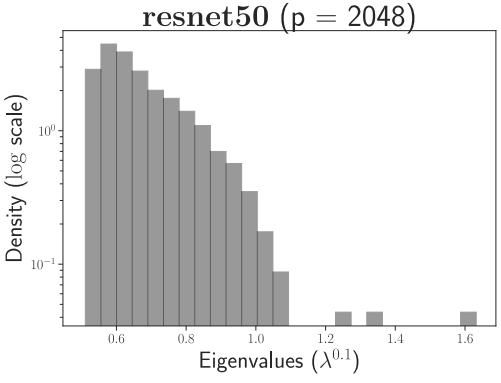
GAN Images

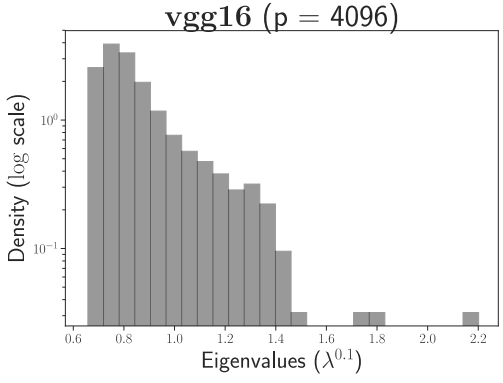


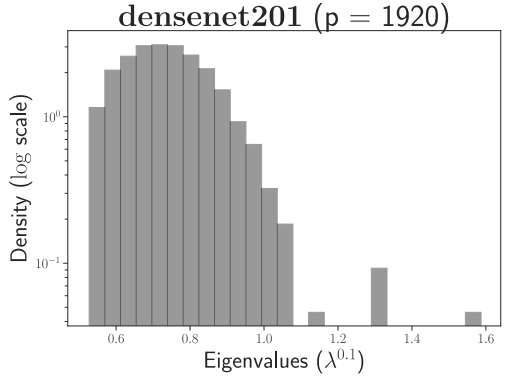




Real Images

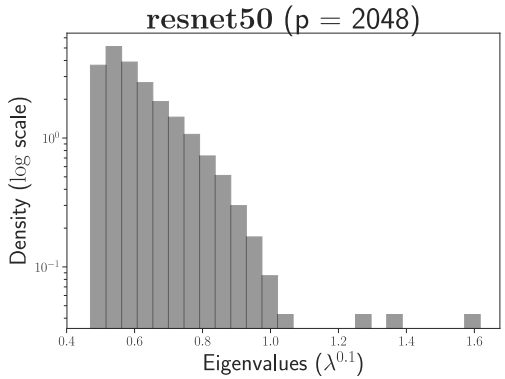


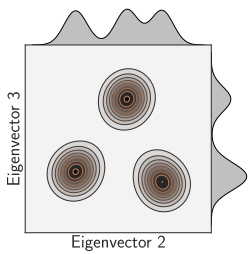


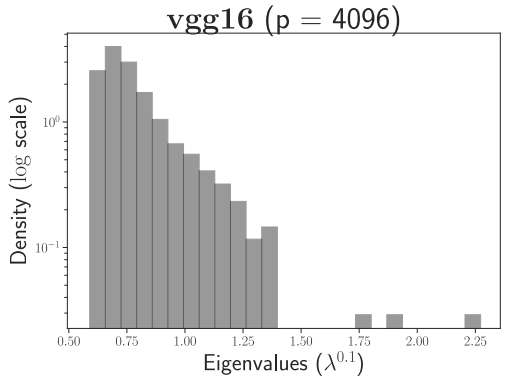


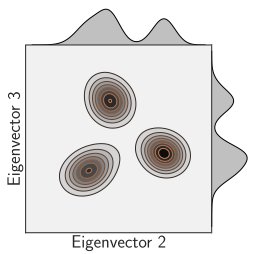
Application to CNN Representations of GAN Images

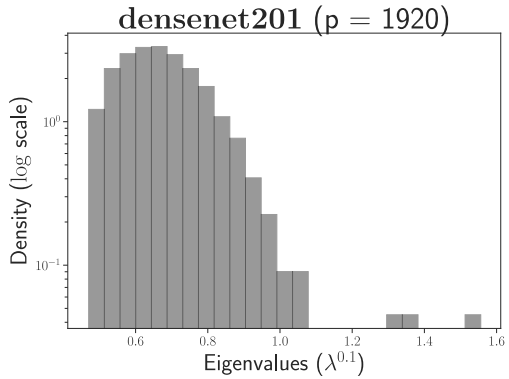
GAN Images

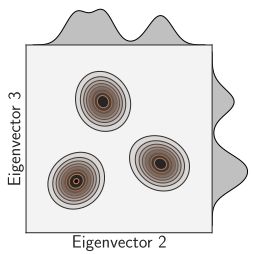




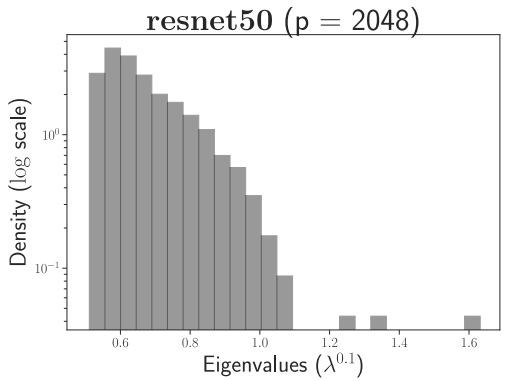


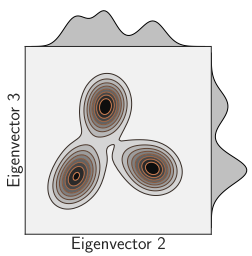


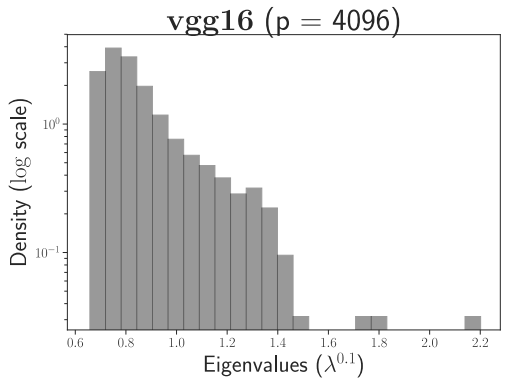


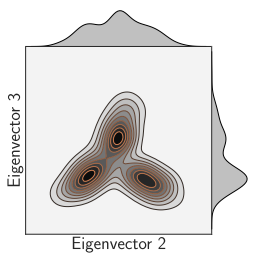


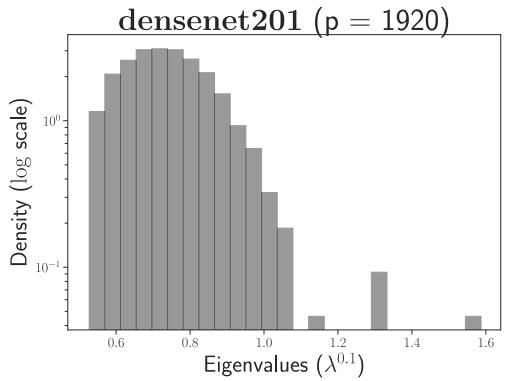
Real Images

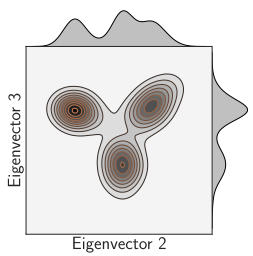




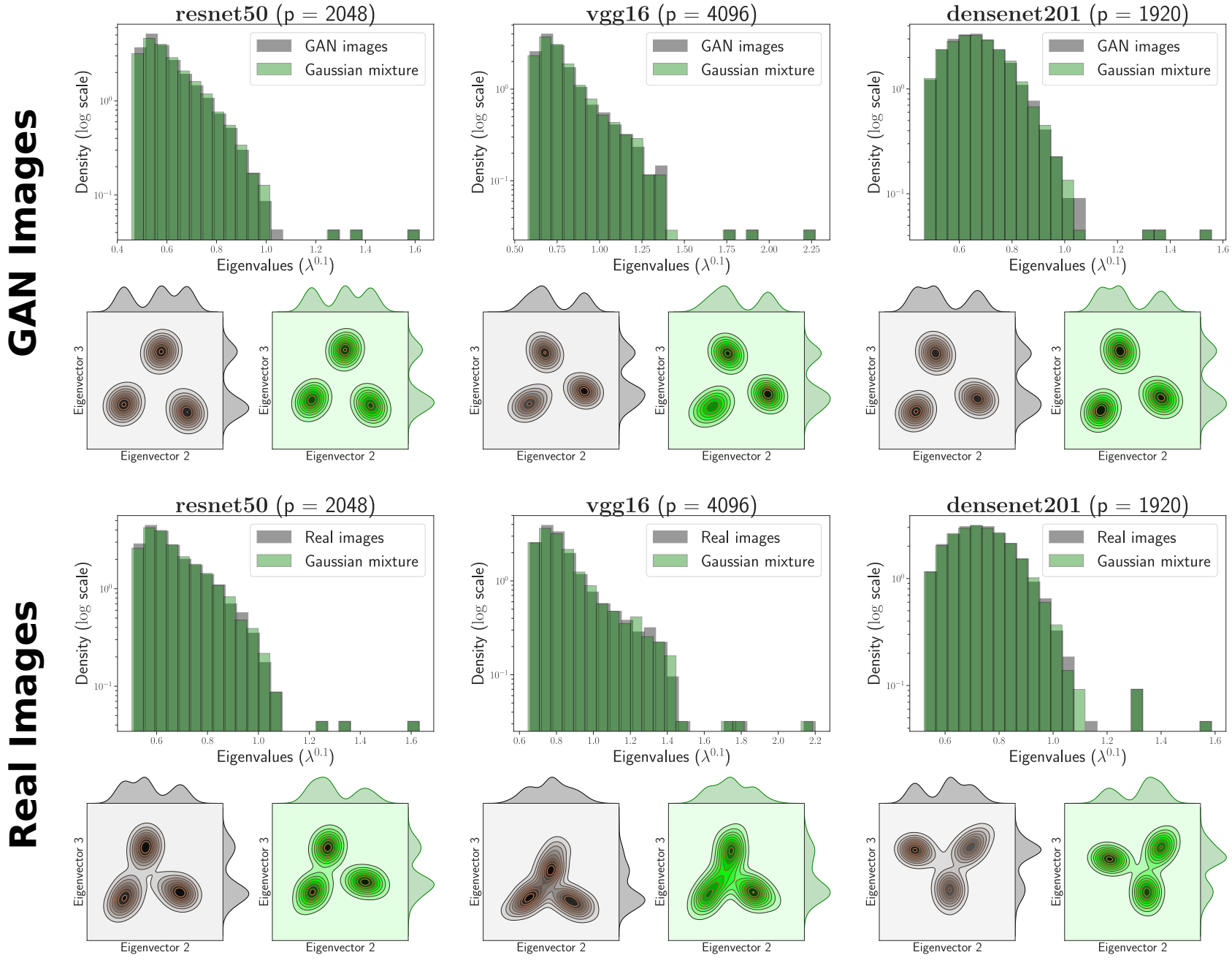




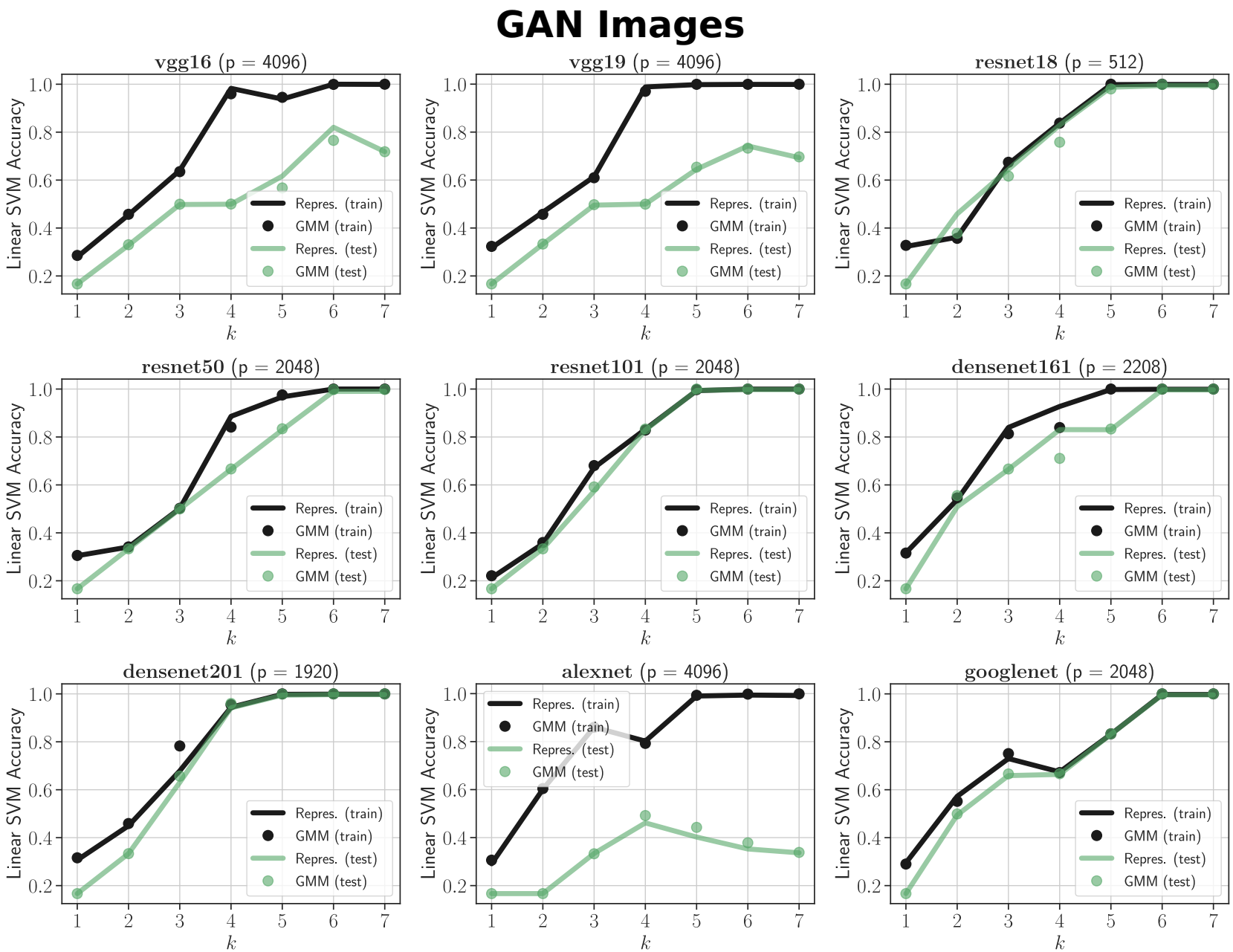




Application to CNN Representations of GAN Images

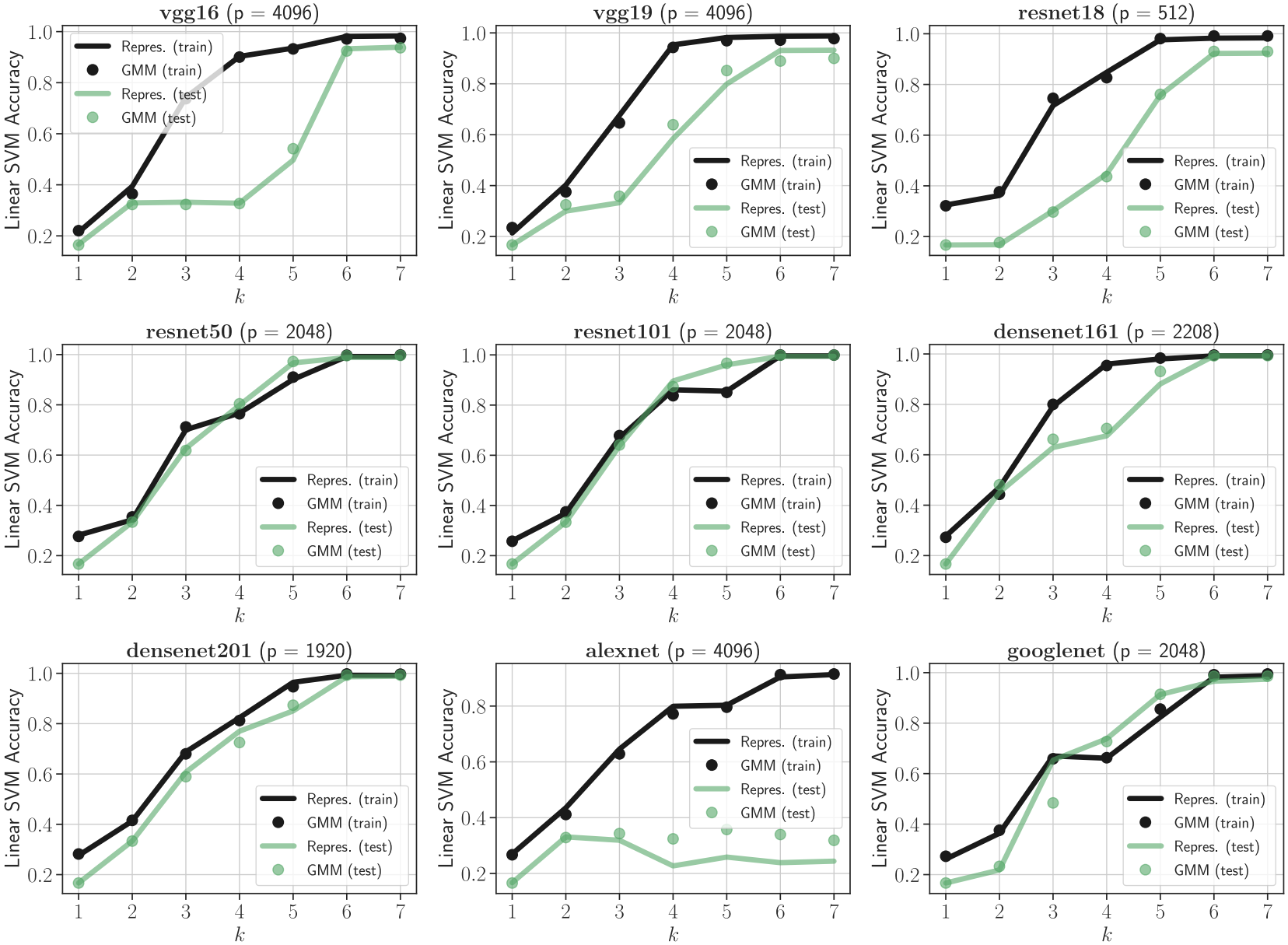


Performance of a linear SVM classifier



Performance of a linear SVM classifier

Real Images



Take away messages

- **Concentrated Vectors** seem appropriate for realistic data modelling.
- ***Universality*** of linear classifiers regardless of the data distribution.
- RMT can ***anticipate*** the performances of standard classifiers for DL representations of GAN images.
- Universality supports the **Gaussianity** assumption on the data representations as considered in the literature, e.g., the FID metric

$$d^2((\boldsymbol{\mu}, \boldsymbol{C}), (\boldsymbol{\mu}_w, \boldsymbol{C}_w)) = \|\boldsymbol{\mu} - \boldsymbol{\mu}_w\|^2 + \mathrm{tr}\left(\boldsymbol{C} + \boldsymbol{C}_w - 2(\boldsymbol{C}\boldsymbol{C}_w)^{\frac{1}{2}}\right).$$