

Abstract

Context:

- Study of large kernel matrices for concentrated data.

Motivation:

- GAN data are close to real data [1].
- GAN data are concentrated data by design.

Results:

- Universality of spectral clustering w.r.t. the data distribution.
- Real data behave similar to concentrated vectors.
- RMT allows for the theoretical understanding of ML methods for real data.

Concentrated Vectors

Definition 1. Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $X \in E$ is q -exponentially concentrated if for any 1-Lipschitz real function \mathcal{F} , there exists $C, c > 0$ s.t.

$$\forall t > 0, \mathbb{P}\{|\mathcal{F}(X) - \mathbb{E}\mathcal{F}(X)| \geq t\} \leq C e^{-c t^q} \text{ denoted } X \in \mathcal{O}(e^{-q}) \text{ in } (E, \|\cdot\|_E)$$

(P1) $X \sim \mathcal{N}(0, I_p)$ is 2-exponentially concentrated [2].

(P2) If $X \in \mathcal{O}(e^{-q})$ and \mathcal{G} is ℓ -Lipschitz, then $\mathcal{G}(X) \in \mathcal{O}(e^{-(\cdot/\ell)^q})$.

Model & Assumptions

Data matrix (distributed in k classes):

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1, \dots, \mathbf{x}_{n_1}, \mathbf{x}_{n_1+1}, \dots, \mathbf{x}_{n_2}, \dots, \mathbf{x}_{n-k+1}, \dots, \mathbf{x}_n \\ \in \mathcal{O}(e^{-q_1}) \quad \in \mathcal{O}(e^{-q_2}) \quad \dots \quad \in \mathcal{O}(e^{-q_k}) \end{bmatrix}$$

Model statistics:

$$\text{(Means)} \quad \mathbf{m} = \sum_{\ell=1}^k \frac{n_\ell}{n} \mathbf{m}_\ell, \quad \bar{\mathbf{m}}_\ell = \mathbf{m} - \mathbf{m}_\ell$$

$$\text{(Covariances)} \quad \mathbf{C} = \sum_{\ell=1}^k \frac{n_\ell}{n} \mathbf{C}_\ell, \quad \bar{\mathbf{C}}_\ell = \mathbf{C} - \mathbf{C}_\ell$$

(A1) Growth rate assumptions:

As $p \rightarrow \infty$,

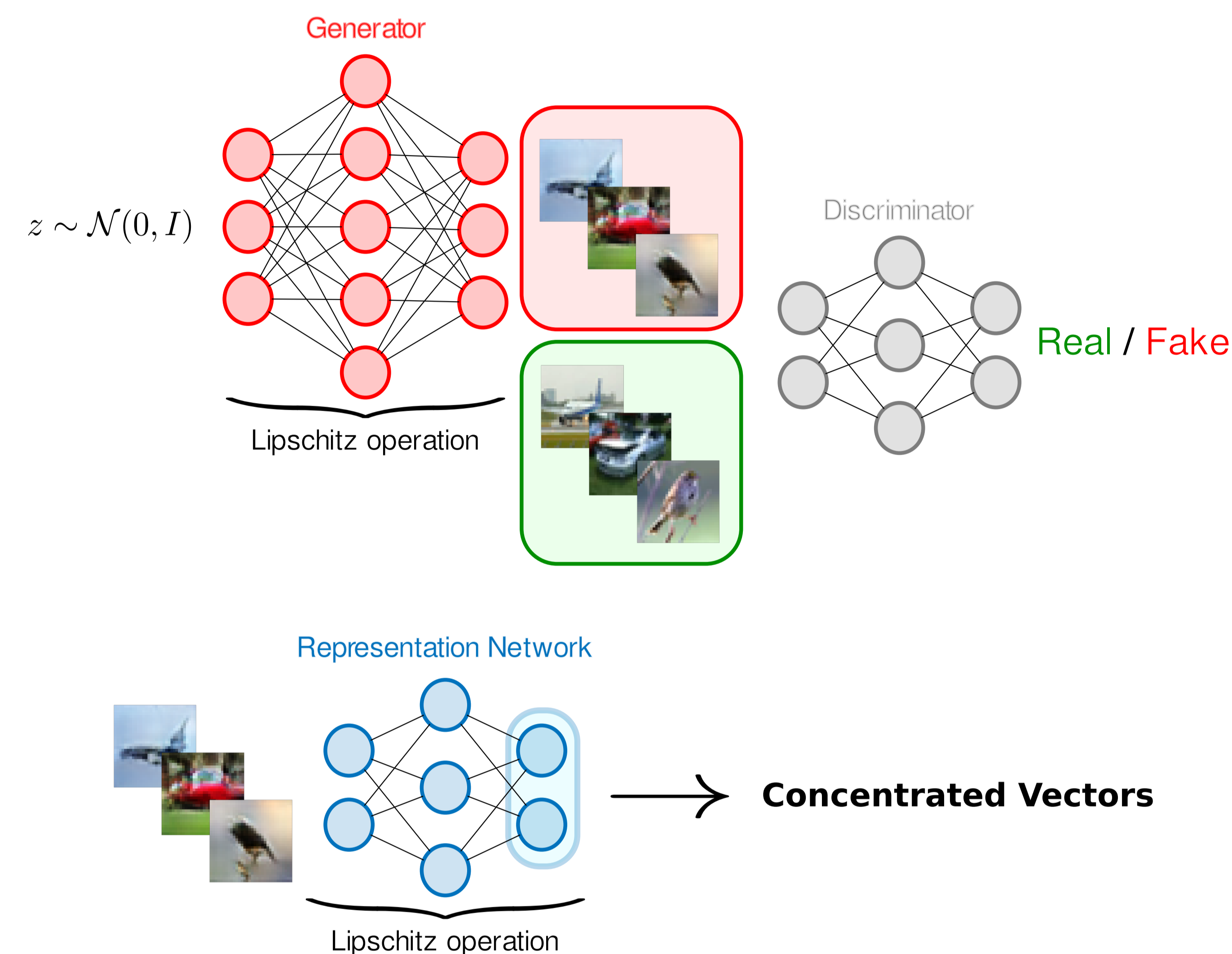
- Data: $\frac{n}{n} \rightarrow c_0 \in (0, \infty)$, $\frac{n_\ell}{n} \rightarrow c_\ell \in (0, 1)$
- Means: $\|\bar{\mathbf{m}}_\ell\| = \mathcal{O}(1)$, $\mathbb{E}\|\mathbf{x}_i\| = \mathcal{O}(\sqrt{p})$
- Covariances: $\|\bar{\mathbf{C}}_\ell\| = \mathcal{O}(1)$, $\text{tr} \bar{\mathbf{C}}_\ell = \mathcal{O}(\sqrt{p})$, $\text{tr} \bar{\mathbf{C}}_a \bar{\mathbf{C}}_b = \mathcal{O}(\sqrt{p})$

(A2) Kernel function: Let $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ three-times continuously differentiable function in $\tau \equiv \frac{2}{p} \text{tr} \mathbf{C}$.

Kernel matrix:

$$\mathbf{K} \equiv \left\{ f \left(\frac{1}{p} \|\mathbf{x}_i - \mathbf{x}_j\|^2 \right) \right\}_{i,j=1}^n$$

Why Concentrated Vectors?



Between and Within Class Vectors are "equidistant" in High-dimension

Proposition 1. Denote $\tau \equiv \frac{2}{p} \text{tr} \mathbf{C}$. Under (A1), with probability $1 - \delta$

$$\max_{1 \leq i \neq j \leq n} \left\{ \left| \frac{1}{p} \|\mathbf{x}_i - \mathbf{x}_j\|^2 - \tau \right| \right\} = \mathcal{O} \left(\frac{\log(\frac{n}{\sqrt{\delta}})^{1/q}}{\sqrt{n}} \right)$$

Random Matrix Equivalent for \mathbf{K}

Proposition 2. Under (A1) and (A2), Taylor expanding \mathbf{K} entry-wise leads to

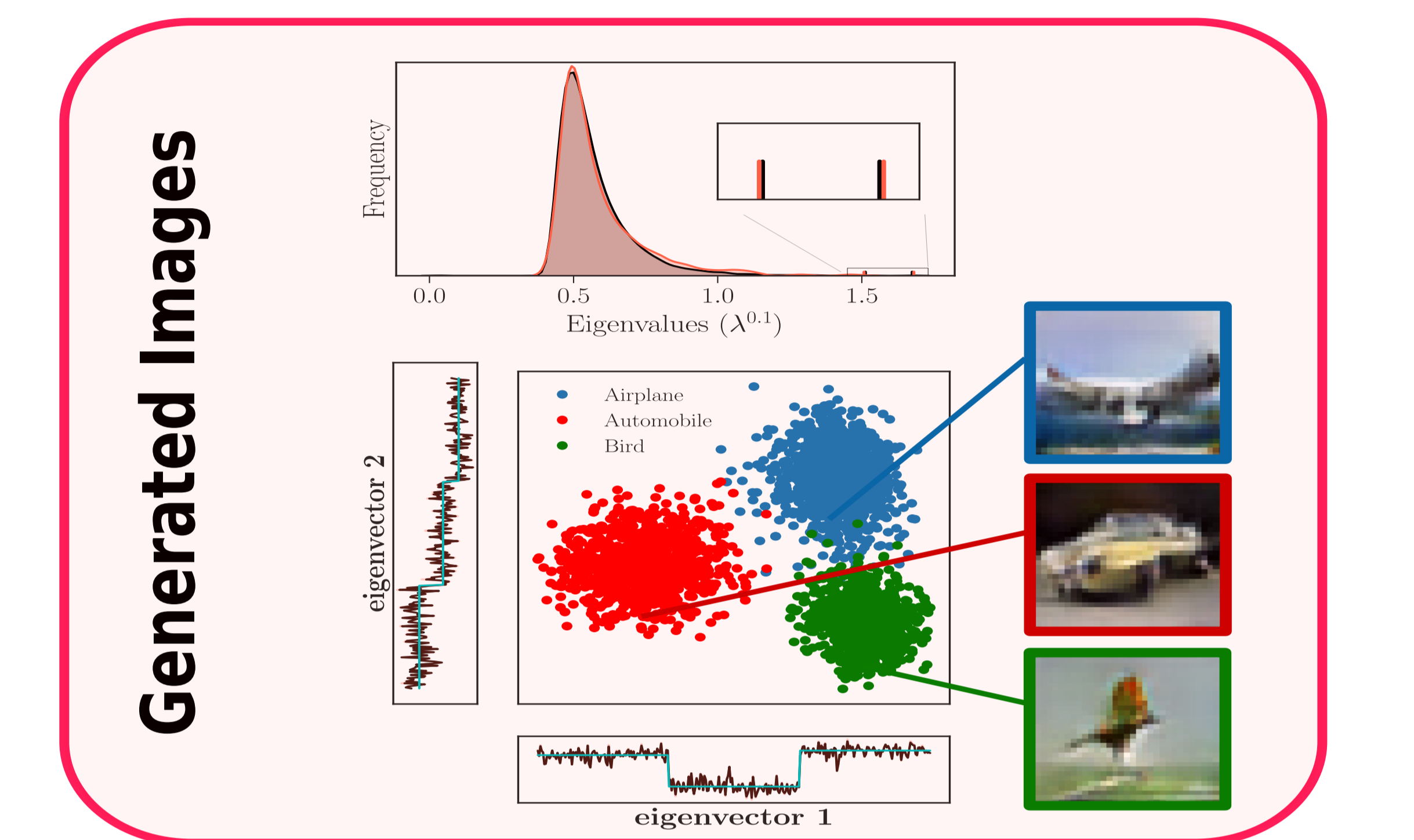
$$\mathbf{K} \propto \underbrace{\mathbf{J} \mathbf{A} \mathbf{J}^T}_{\text{Information}} + \underbrace{f'(\tau) \mathbf{Z}^T \mathbf{Z}}_{\text{Noise}} + *, \quad \mathbf{Z} = (\mathbf{X} - \mathbf{M} \mathbf{J}^T) / \sqrt{p}$$

- R1 \mathbf{K} behaves as a spiked RMT model.
- R2 The classification performance depends on $f'(\tau)$, $f''(\tau)$, \mathbf{M} , \mathbf{t} and \mathbf{T} .
- R3 No other informative statistics \Rightarrow universality of spectral clustering.

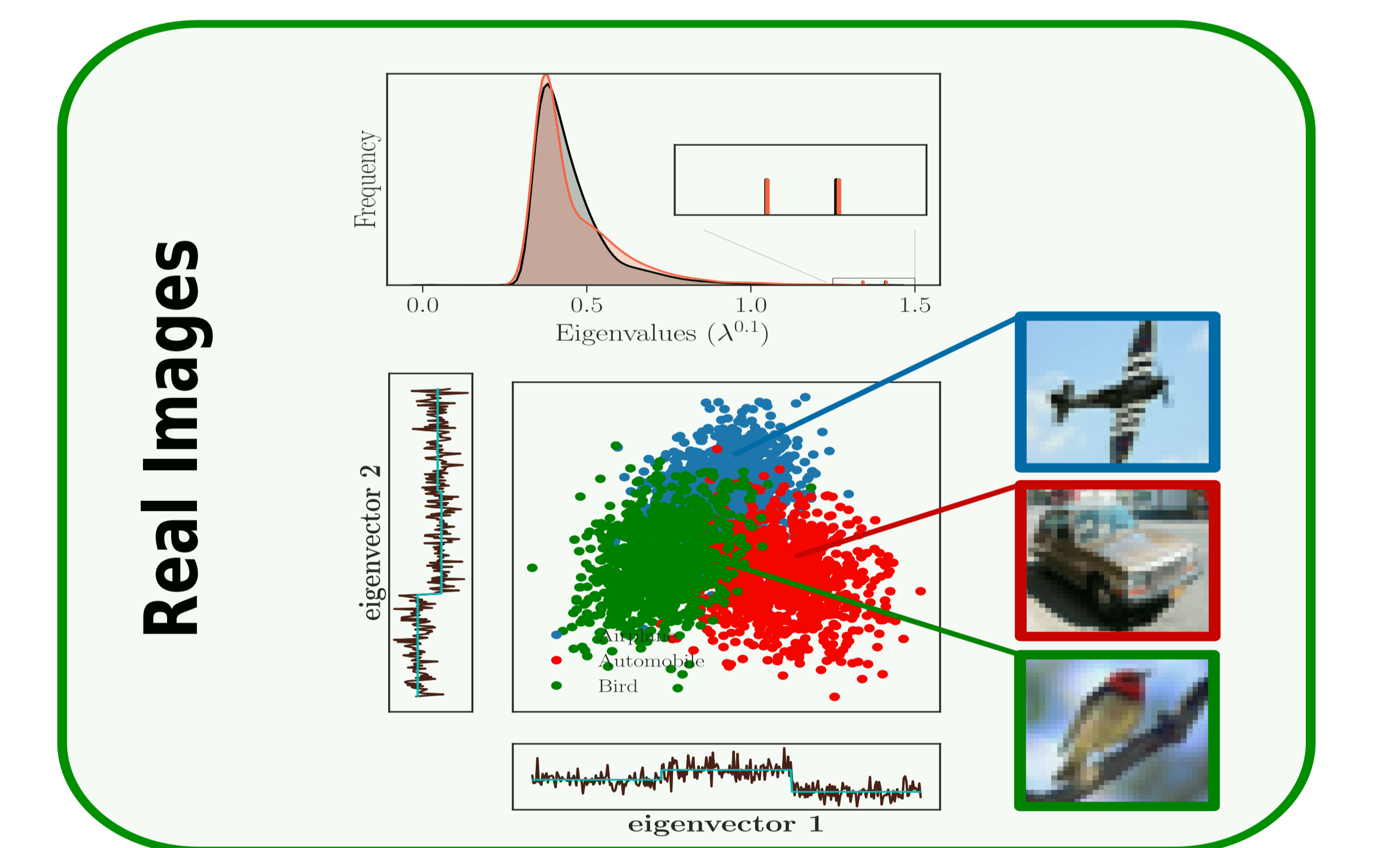
\mathbf{A} is a low-rank matrix depending only on $f'(\tau)$, $f''(\tau)$, \mathbf{M} , \mathbf{t} and \mathbf{T} , where

$$\mathbf{J} = [\mathbf{j}_1, \dots, \mathbf{j}_k], \quad \mathbf{M} = [\bar{\mathbf{m}}_1, \dots, \bar{\mathbf{m}}_k], \quad \mathbf{t} = \left\{ \frac{\text{tr} \bar{\mathbf{C}}_\ell}{\sqrt{p}} \right\}_{\ell=1}^k, \quad \mathbf{T} = \left\{ \frac{\text{tr} \bar{\mathbf{C}}_a \bar{\mathbf{C}}_b}{p} \right\}_{a,b=1}^k$$

Application to GAN-Generated Images



— Spectrum and eigenvectors of \mathbf{K} — Spectrum and eigenvectors of $\hat{\mathbf{K}}$ — Theoretical class-wise means



Perspectives

- Prove a CLT under the concentration assumption.
- Generalize to other ML tasks (Classification, Regression)
- Apply to the dynamics of neural networks and GANs.

References

- [1] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio, "Generative adversarial nets," in Advances in neural information processing systems, 2014.
- [2] Terence Tao. Topics in random matrix theory, volume 132. American Mathematical Society Providence, RI, 2012.