# Random Matrix Advances in Large Dimensional Machine Learning Random Matrices and Complex Data Analysis Workshop

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#### Outline

- Motivation
- Random matrix understanding of large dimensional classification
  - Kernel methods for large dimensional data
  - Properly scaled inner-product kernels
- From theory to practice in large dimensional machine learning
  - From toy to more realistic learning schemes
  - From toy to more realistic data models

## The pitfalls of large dimensional statistics: sample covariances in the large n, p regime

- ▶ For  $\mathbf{x}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$ , estimate population covariance  $\mathbf{C}$  from n data samples  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$ .
- ► Maximum likelihood sample covariance matrix:

$$\hat{\mathbf{C}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_{i} \mathbf{x}_{i}^{\mathsf{T}} = \frac{1}{n} \mathbf{X} \mathbf{X}^{\mathsf{T}} \in \mathbb{R}^{p \times p}$$

of rank at most n: optimal for  $n \gg p$  (or, for p "small").

▶ When  $n \sim p$ , conventional wisdom breaks down: for  $\mathbf{C} = \mathbf{I}_p$  with n < p,  $\hat{\mathbf{C}}$  has  $\geq p - n$  zero eigenvalues.

$$\boxed{\|\hat{\mathbf{C}} - \mathbf{C}\| \not\to 0, \quad n, p \to \infty}$$

⇒ eigenvalue mismatch and not consistent!

## When is one under the random matrix regime? Almost always!

What about n=100p? For  $\mathbf{C}=\mathbf{I}_p$ , as  $n,p\to\infty$  with  $p/n\to c\in(0,\infty)$ : the Marčenko–Pastur law

$$\mu(dx) = (1 - c^{-1})^{+} \delta(x) + \frac{1}{2\pi cx} \sqrt{(x - a)^{+} (b - x)^{+}} dx$$

where  $a = (1 - \sqrt{c})^2$ ,  $b = (1 + \sqrt{c})^2$  and  $(x)^+ \equiv \max(x, 0)$ .

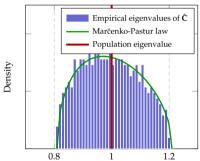


Figure: Eigenvalue distribution of  $\hat{\mathbf{C}}$  versus Marčenko-Pastur law, p=500,  $n=50\,000$ .

- eigenvalues span on  $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$ .
- for n = 100p, on a range of  $\pm 2\sqrt{c} = \pm 0.2$  around population eigenvalue 1.

## Random matrix for large dimensional machine learning

#### Take-away message:

- ightharpoonup Counterintuitive phenomena in the large n, p regime
- ▶ RMT as a tool to assess, understand and improve large dimensional machine learning

#### Challenges:

- entry-wise nonlinearity: kernel function in kernel methods, activation function in neural networks
- (convex or non-convex) optimization-based methods with **implicit** solution
- more realistic data modeling

## "Curse of dimensionality": loss of relevance of Euclidean distance

Binary Gaussian mixture classification:

$$C_1: \mathcal{N}(\mu_1, C_1)$$
 versus  $C_2: \mathcal{N}(\mu_2, C_2)$ 

Neyman-Pearson test: classification possible only when

$$\|\mu_1 - \mu_2\| \ge O(1), \quad \|\mathbf{C}_1 - \mathbf{C}_2\| \ge O(p^{-1/2}), \quad |\operatorname{tr}(\mathbf{C}_1 - \mathbf{C}_2)| \ge O(\sqrt{p}), \quad \|\mathbf{C}_1 - \mathbf{C}_2\|_F^2 \ge O(1).$$

▶ In this non-trivial setting, for  $\mathbf{x}_i \in C_a$  and  $\mathbf{x}_j \in C_b$ ,

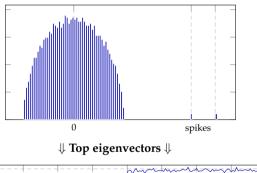
$$\left| \max_{1 \le i \ne j \le n} \left\{ \frac{1}{p} \|\mathbf{x}_i - \mathbf{x}_j\|^2 - \tau \right\} \stackrel{\text{a.s.}}{\longrightarrow} 0$$

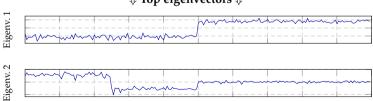
as  $n, p \to \infty$ , regardless of the classes  $C_a, C_b$ !

direct consequence to large dimensional (distance-based) kernel matrices!

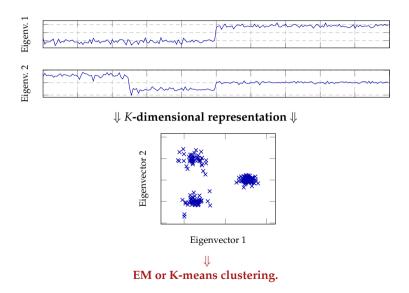
## Reminder on kernel spectral clustering

Two-step classification of n data points based on similarity kernel  $\mathbf{K} \in \mathbb{R}^{n \times n}$ , e.g.,  $\mathbf{K}_{ij} = \exp\left(-\frac{1}{2p}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$ :





## Reminder on kernel spectral clustering



## Kernel matrices of small and large dimensional Gaussian data

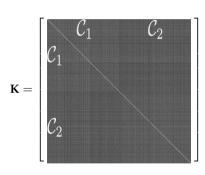
 $\mathbf{K}_{ij} = \exp\left(-\frac{1}{2p}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$  and the second top eigenvectors  $\mathbf{v}_2$  for small and large dimensional Gaussian data.

(a) 
$$p = 5, n = 500$$

$$\mathbf{K}=egin{array}{cccc} \mathcal{C}_1 & \mathcal{C}_2 \ \mathcal{C}_1 & \mathcal{C}_2 \ \mathcal{C}_2 & \mathcal{C}_2 \end{array}$$

$$\mathbf{v}_2 = [\sqrt{|\mathbf{v}_1|^2 + |\mathbf{v}_2|^2 + |\mathbf{v}_3|^2 + |\mathbf{v$$

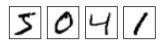
(b) 
$$p = 250, n = 500$$

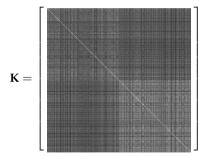


$$\mathbf{v}_2 = [ \frac{\mathbf{v}_1 \mathbf{v}_2 \mathbf{v}_3 \mathbf{v}_4 \mathbf$$

## Kernel matrices of small and large dimensional real-world data

(a) MNIST

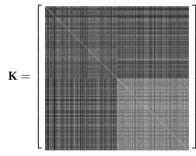




$$\mathbf{v}_2 = [$$
 hyphathytharhynafaribathynishiphathyngalaidithautuidithafa

#### (b) Fashion-MNIST





$$\mathbf{v}_2 = [$$
 which approximately regularly approximately  $]$ 

## A random matrix viewpoint of large kernel matrices

## Asymptotic behavior of K [Couillet and Benaych-Georges'16]

For non-trivial classification of *K*-class Gaussian mixture  $\mathcal{N}(\mu_a, \mathbf{C}_a)$ ,  $a \in \{1, \dots, K\}$ ,  $\mathbf{K}_{ij} = f(\|\mathbf{x}_i - \mathbf{x}_j\|^2/p)$  with f three-times differentiable around  $\tau$ , we have, as  $n, p \to \infty$  with  $p/n \to c \in (0, \infty)$ 

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \xrightarrow{\text{a.s.}} 0, \quad \tilde{\mathbf{K}} \simeq f(\tau) \mathbf{1}_n \mathbf{1}_n^{\mathsf{T}} + \mathbf{N} + \frac{1}{p} \mathbf{J} \mathbf{A} \mathbf{J}^{\mathsf{T}} + *$$

with  $\mathbf{J} = [\mathbf{j}_1, \dots, \mathbf{j}_K] \in \mathbb{R}^{n \times K}$ ,  $\mathbf{j}_a = [\mathbf{0}, \mathbf{1}_{n_a}, \mathbf{0}]^\mathsf{T}$  (class-info vector!),  $\mathbf{N}$  random noise and  $\mathbf{A}$  function of

- $\blacktriangleright f(\tau), f'(\tau) \text{ and } f''(\tau)$
- ▶ statistical information  $\|\mu_a \mu_b\|^2$ , tr( $\mathbf{C}_a \mathbf{C}_b$ ) and  $\|\mathbf{C}_a \mathbf{C}_b\|_F^2$ , for  $a, b \in \{1, ..., K\}$
- our low-dimensional machine learning intuitions collapse
- ightharpoonup "curse of dimensionality"  $\Rightarrow$  Taylor expansion and local linearization of f
- ▶ RMT provides a fully accessible spiked-model description of nonlinear **K**

## Intuition: from small to large dimensional kernels

Accumulated effect of small but structural "hidden" statistical information.

► <u>entry-wise</u>: for  $\mathbf{K}_{ij} = \exp\left(-\frac{1}{2p}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$  with  $\mathbf{x}_i = (-1)^a \mu + \mathbf{z}_i$ ,  $\mathbf{x}_j = (-1)^b \mu + \mathbf{z}_j$ ,  $\mathbf{z}_i$ ,  $\mathbf{z}_j \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ 

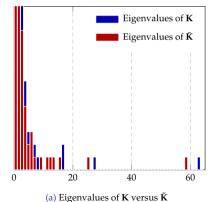
$$\mathbf{K}_{ij} \simeq \exp(-1)\left(1 + \underbrace{\frac{1}{p}\mathbf{z}_{i}^{\mathsf{T}}\mathbf{z}_{j}}_{O(p^{-1/2})}\right) \pm \underbrace{\frac{1}{p}\|\boldsymbol{\mu}\|^{2}(-1)^{a+b}}_{O(p^{-1})} + *$$

so that  $\frac{1}{p} \|\boldsymbol{\mu}\|^2 \ll \frac{1}{p} \mathbf{z}_i^\mathsf{T} \mathbf{z}_j$ ;

- **spectrum-wise**:  $\|\frac{1}{p}\mathbf{Z}^{\mathsf{T}}\mathbf{Z}\| = O(1)$  and  $\|\mu\|^2 \|\frac{1}{p}\mathbf{j}\mathbf{j}^{\mathsf{T}}\| = O(1)$  as well!
- we understand how kernel spectral clustering works for large dimensional data!

## Experiments on real-world data: MNIST



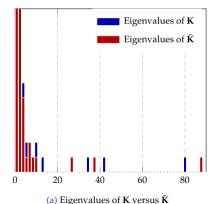


Top eigenvectors of **K** Top eigenvectors of  $\tilde{\mathbf{K}}$ 50 100 150 200

(b) Isolated eigenvectors of K and  $\tilde{K}$ 

## Experiments on real-world data: Fashion-MNIST





Top eigenvectors of **K** - Top eigenvectors of  $\tilde{\mathbf{K}}$ 50 100 150 200

(b) Isolated eigenvectors of K and  $\tilde{K}$ 

## How to better exploit the nonlinear *f*?

Due to "curse of dimensionality",  $\frac{1}{p} ||\mathbf{x}_i - \mathbf{x}_j||^2 \to \tau$ .

- ► Taylor-expand  $\mathbf{K}_{ij} = f(\|\mathbf{x}_i \mathbf{x}_j\|^2/p)$  around  $f(\tau)$
- ▶ **K** depends only on <u>local</u> behavior of smooth *f*
- ightharpoonup use a single point of nonlinear f

To exploit global information of  $f \Rightarrow$  properly scaled kernel

$$f\left(\sqrt{p}\left(\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 - \tau\right)\right)$$
 or  $f(\mathbf{x}_i^\mathsf{T}\mathbf{x}_j/\sqrt{p})$ 

- $\mathbf{x}_{i}^{\mathsf{T}}\mathbf{x}_{i}/\sqrt{p} \to \mathcal{N}(0,1)$ , use **whole** domain of f
- ▶ however, no "concentration" ⇒ CLT expansion with orthogonal polynomials

## Key object

$$\mathbf{K} \equiv \{\delta_{i \neq j} \mathbf{f}(\mathbf{x}_i^\mathsf{T} \mathbf{x}_j / \sqrt{p}) / \sqrt{p}\}_{i,j=1}^n$$

**Question**: How *f* impacts the performance of kernel spectral clustering?

## Orthogonal polynomials and inner-product kernels

$$\sqrt{p}\mathbf{K}_{ij} = f(\mathbf{x}_i^\mathsf{T}\mathbf{x}_j/\sqrt{p})$$
: since  $\mathbf{x}_i^\mathsf{T}\mathbf{x}_j/\sqrt{p} \to \mathcal{N}(0,1)$ , essentially evaluate  $f(\mathcal{N}(0,1))$ .

## Orthogonal polynomial decomposition

Any  $f \in L^2(\mu_N)$  admits formal expansion (with Hermite polynomial)

$$f(x) \sim \sum_{l=0}^{\infty} a_l P_l(x), \quad \int P_{l_1}(x) P_{l_2}(x) \mu_{\mathcal{N}}(dx) = \delta_{l_1 - l_2}, \quad a_l = \int f(x) P_l(x) \mu_{\mathcal{N}}(dx)$$

with 
$$a_0 = \mathbb{E}_{\xi \sim \mathcal{N}(0,1)} f(\xi) = 0$$
, and generalized moments  $a_1 = \mathbb{E}[\xi f(\xi)], \sqrt{2}a_2 = \mathbb{E}[\xi^2 f(x)], \nu = \mathbb{E}[f^2(x)]$ .

#### Asymptotic behavior of inner-product K [Liao and Couillet'19]

Under non-trivial classification condition and  $\mathbf{C}_a = \mathbf{I}_p + \mathbf{E}_a$ , for  $f \in L^2(\mu_N)$ ,  $n, p \to \infty$  with  $p/n \to c \in (0, \infty)$ 

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \xrightarrow{\text{a.s.}} 0, \quad \tilde{\mathbf{K}} \simeq \mathbf{N} + \frac{1}{p} \mathbf{J} \mathbf{A} \mathbf{J}^{\mathsf{T}} + *$$

with J class-info vectors, N random noise and A function of f and statistical information

$$\mathbf{A} = \mathbf{a_1} \cdot \{ \| \boldsymbol{\mu}_a - \boldsymbol{\mu}_b \|^2 \}_{a,b=1}^K + \mathbf{a_2} \cdot g(\text{tr}(\mathbf{C}_a - \mathbf{C}_b), \|\mathbf{C}_a - \mathbf{C}_b\|_F^2)_{a,b=1}^K.$$

## Consequences

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \xrightarrow{\text{a.s.}} 0, \quad \tilde{\mathbf{K}} \simeq \frac{1}{p} \mathbf{J} \mathbf{A} \mathbf{J}^{\mathsf{T}} + \mathbf{N} + *, \quad \mathbf{A} = \frac{\mathbf{a_1} \cdot \{\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2\}_{a,b=1}^K + \frac{\mathbf{a_2} \cdot g(\text{tr}(\mathbf{C}_a - \mathbf{C}_b), \|\mathbf{C}_a - \mathbf{C}_b\|_F^2)_{a,b=1}^K}{\mathbf{A} - \mathbf{A} -$$

▶ **JAJ**<sup>T</sup> of low rank, limiting spectrum measure  $\mu_K$  same as  $\mu_N$ , characterized by unique  $m(z) \in \mathbb{C}^+$  [Cheng and Signer'13]

$$-\frac{1}{m(z)} = z + \frac{a_1^2 m(z)}{c + a_1 m(z)} + \frac{\nu - a_1^2}{c} m(z) \tag{1}$$

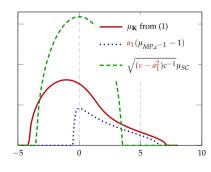
with  $a_1 = \mathbb{E}[\xi f(\xi)]$ ,  $\sqrt{2}a_2 = \mathbb{E}[\xi^2 f(x)]$  and  $\nu = \mathbb{E}[f^2(x)]$ .

 $\mu_{\mathbf{K}}$ : "mix" of Marčenko-Pastur law  $\mu_{MP}$  and semicircle law  $\mu_{SC}$ 

$$\mu_{\mathbf{K}} = \mathbf{a_1}(\mu_{MP,c^{-1}} - 1) \boxtimes \sqrt{(\nu - \mathbf{a_1^2})c^{-1}}\mu_{SC}$$

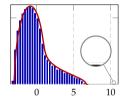
with 
$$\mathbf{K}_{ij} = f(\mathbf{x}_i^\mathsf{T} \mathbf{x}_j / \sqrt{p}) / \sqrt{p}$$
 and  $f(x) = a_1 x + \sqrt{\nu - a_1^2} \tilde{f}(x)$ 

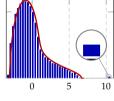
•  $(a_1, v)$  determines "noisy" <u>bulk</u>;  $(a_1, a_2)$  informative **spike**.

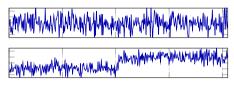


## Practical consequences

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \xrightarrow{a.s.} 0, \quad \tilde{\mathbf{K}} \simeq \frac{1}{p} \mathbf{J} \mathbf{A} \mathbf{J}^{\mathsf{T}} + \mathbf{N} + *, \quad \boxed{\mathbf{A} = \mathbf{a_1} \cdot \{\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2\}_{a,b=1}^K + \mathbf{a_2} \cdot g(\operatorname{tr}(\mathbf{C}_a - \mathbf{C}_b), \|\mathbf{C}_a - \mathbf{C}_b\|_F^2)_{a,b=1}^K}$$



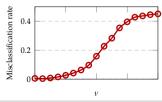




(a) Eigenvalues of N (b) Eigenvalues of K

(c) Top eigenvectors of N (top) and K (bottom)

- ► **K** depend on f only via  $(a_1, a_2, \nu)$ :  $(a_1, a_2)$  impacts info and  $(a_1, \nu)$  impacts noise
- ightharpoonup minimize  $\nu$  for larger eigengap and better performance!
- $ightharpoonup 
  u_{\min} = a_1^2 + a_2^2$ , **quadratic** f is optimal among  $L^2(\mu_N)$



## Practical consequences

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \xrightarrow{\text{a.s.}} 0, \quad \tilde{\mathbf{K}} \simeq \frac{1}{p} \mathbf{J} \mathbf{A} \mathbf{J}^{\mathsf{T}} + \mathbf{N} + *, \quad \boxed{\mathbf{A} = \mathbf{a_1} \cdot \{\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2\}_{a,b=1}^K + \mathbf{a_2} \cdot g(\text{tr}(\mathbf{C}_a - \mathbf{C}_b), \|\mathbf{C}_a - \mathbf{C}_b\|_F^2)_{a,b=1}^K}$$

▶  $a_1$  control info in means and  $a_2$  info in covariances  $\Rightarrow$  tuning  $a_1/a_2$  with data!

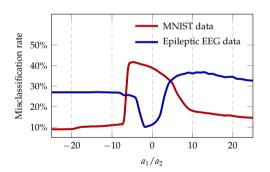


Table: Empirical estimation of differences in means and covariances of MNIST and EEG data

	$\ \hat{\pmb{\mu}}_1 - \hat{\pmb{\mu}}_2\ ^2$	$\ \hat{\textbf{C}}_1 - \hat{\textbf{C}}_2\ $
MNIST	464.17	166.35
EEG	2.41	14.90

<sup>1</sup>http://www.meb.unibonn.de/epileptologie/science/physik/eegdata.html.

#### Conclusion and limitations

#### <u>Conclusion</u> on large dimensional kernel methods:

- "curse of dimensionality"  $\Rightarrow \mathbf{K}_{ij} = f(\|\mathbf{x}_i \mathbf{x}_j\|^2/p)$  depends on f in a local manner
  - proof based on Taylor expansion, holds only for **smooth** *f*
  - ▶ no interpretation for key parameters  $f(\tau)$ ,  $f'(\tau)$ ,  $f''(\tau)$
  - close match between theory and real-world data experiments
- exploit **global** information with properly scaled kernel  $\mathbf{K}_{ij} = f(\mathbf{x}_i^\mathsf{T} \mathbf{x}_i / \sqrt{p}) / \sqrt{p}$ 
  - roof based on orthogonal polynomials, holds for any  $f \in L^2(\mu_N)$
  - better interpretation for key parameters  $(a_1, a_2, v)$
  - only tunning  $a_1/a_2$  in real-world data experiments
- ▶ allow for "plug-and-play" analyses of most kernel-based methods: e.g., kernel ridge regression, support vector machines, graph-based semi-supervised methods, as well as random neural networks etc.

#### Limitations:

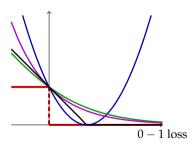
- ? optimization-based problems with implicit solution
- ? limited to Gaussian data

## Large dimensional optimization-based learning problems

**Empirical risk minimization**: for  $\{(\mathbf{x}_i, y_i)\}_{i=1}^n, \mathbf{x}_i \in \mathbb{R}^p, y_i \in \{-1, +1\}$ , find classifier  $\boldsymbol{\beta} \in \mathbb{R}^p$  that minimizes

$$\frac{1}{n}\sum_{i=1}^{n}\ell(y_{i}\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}_{i})+\frac{\lambda}{2}\|\boldsymbol{\beta}\|^{2}$$

for some nonnegative (possibly non-smooth) convex loss  $\ell$  and regularization  $\lambda \geq 0$ .



- logistic regression:  $\ell(t) = \ln(1 + e^{-t})$
- least squares:  $\ell(t) = (t-1)^2$
- **b** boosting algorithm:  $\ell(t) = e^{-t}$
- ► SVM:  $\ell(t) = \max(1 t, 0)$

- **existence**: for different  $\ell$  and x, when such  $\beta$  exists? (function of  $\lambda$ ,  $\lim p/n$ )
- **optimality**: how to choose loss function  $\ell$  with respect to distribution of  $x_i$ ?
- ▶ **difficulty**: no **closed-form** solution: depend on all  $\{(x_i, y_i)\}_{i=1}^n$  in a more involved manner.

## Some related works on optimization-based learning problems

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\arg\min} \frac{1}{n} \sum_{i=1}^n \ell(y_i \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i) + \frac{\lambda}{2} \|\boldsymbol{\beta}\|^2 \quad \text{or} \quad \hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\arg\min} \frac{1}{n} \sum_{i=1}^n \ell(y_i - \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i) + \lambda R(\boldsymbol{\beta})$$

#### Different approaches:

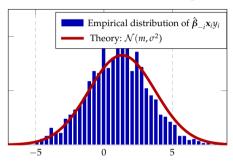
- ▶ approximate message passing and state-evolution analysis [Donoho and Montanari′16]
- convex Gaussian min-max theorem [Taheri, Pedarsani and Thrampoulidis'19]
- ▶ double "leave-one-out" approach [El Karoui et al.'13]: not suitable for data with pattern!

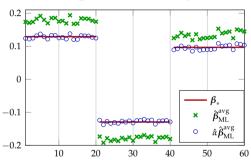
#### Intuition of improved "leave-one-out" approach [Mai and Liao'19]: single "leave-one-out" + RMT

- ▶ binary classification of  $\mathbf{x}_i \sim \mathcal{N}(\pm \mu, \mathbf{C})$
- $lackbox{lack}$  denote  $\hat{eta}_{-i} = \arg\min_{m{eta} \in \mathbb{R}^p} rac{1}{n} \sum_{j \neq i} \ell(y_j m{eta}^\mathsf{T} \mathbf{x}_j) + rac{\lambda}{2} \|m{eta}\|^2$ :  $\hat{m{eta}}_{-i}$  independent of  $(\mathbf{x}_i, y_i)$  and  $\hat{m{eta}}_{-i} \simeq \hat{m{eta}}$
- ▶ but  $\hat{\boldsymbol{\beta}}_{-i}^{\mathsf{T}} \mathbf{x}_i y_i \not\simeq \hat{\boldsymbol{\beta}}^{\mathsf{T}} \mathbf{x}_i y_i \Rightarrow \text{characterize } (\hat{\boldsymbol{\beta}} \hat{\boldsymbol{\beta}}_{-i})^{\mathsf{T}} \mathbf{x}_i y_i \text{: e.g., } (\hat{\boldsymbol{\beta}} \hat{\boldsymbol{\beta}}_{-i})^{\mathsf{T}} \mathbf{x}_i y_i \xrightarrow{\text{a.s.}} \kappa \text{ as } n, p \to \infty$
- ▶ since  $\hat{\beta}_{-i}^T \mathbf{x}_i y_i \to \mathcal{N}(m, \sigma^2)$  by CLT  $\Rightarrow$  form a system of (fixed-point) equations for  $(m, \sigma^2, \kappa)$
- ▶ understand limiting performance for any three-times differentiable and convex  $\ell(\cdot)$ , as a function of p/n, and data statistics ( $\mu$ ,  $\mathbf{C}$ )

#### Some simulations

**Setting**: binary classification  $\mathbf{x}_i \sim \mathcal{N}(\pm \mu, \mathbf{C})$  with  $y_i = \pm 1$ , logistic regression  $\ell(t) = \ln(1 + e^{-t})$  known to be the maximum likelihood solution, with optimal Bayes solution (i.e., "true" parameter vector)  $\boldsymbol{\beta}_* = 2\mathbf{C}^{-1}\boldsymbol{\mu}$ .





#### Remarks:

- ► can we get  $\beta_*$  in the large n, p limit? Not true even in expectation!  $\hat{\beta} \simeq \alpha^{-1} \beta_* + \text{Gaussian noise}$
- $\blacktriangleright$  maximum likelihood not optimal in high dimension: least-squares  $\ell(t)=(t-1)^2$  always better!

#### **Limitations**:

- ✓ optimization-based problems with implicit solution: yes if convex!
  - ? limited to Gaussian data

## From theory to practice: concentrated random vectors

RMT often assumes **x** are affine maps  $A\mathbf{z} + \mathbf{b}$  of  $\mathbf{z} \in \mathbb{R}^p$  with i.i.d. entries.

#### Concentrated random vectors [Ledoux'05]

For Lipschitz function  $f : \mathbb{R}^p \mapsto \mathbb{R}$ , there exists deterministic  $m_f \in \mathbb{R}$ 

$$P(|f(\mathbf{x}) - m_f| > \epsilon) \le e^{-g(\epsilon)}$$
, for some strictly increasing function  $g$ .

## Asymptotic behavior of K for concentrated data [Seddik, Tamaazousti, Couillet'19]

For non-trivial classification of *K*-class (universal) concentrated random mixture of mean  $\mu_a$  and covariance  $\mathbf{C}_a$ ,  $a \in \{1, ..., K\}$ ,  $\mathbf{K}_{ij} = f(\|\mathbf{x}_i - \mathbf{x}_i\|^2/p)$  with f three-times differentiable around  $\tau$ ,

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \stackrel{\mathrm{a.s.}}{\longrightarrow} 0, \quad \tilde{\mathbf{K}} \simeq f(\tau) \mathbf{1}_n \mathbf{1}_n^\mathsf{T} + \mathbf{N} + \frac{1}{v} \mathbf{J} \mathbf{A} \mathbf{J}^\mathsf{T} + *$$

with **J** class-info vectors, **N** random noise and **A** function of  $f(\tau)$ ,  $f'(\tau)$ ,  $f''(\tau)$  and statistical information.

⇒Theory remains valid for concentrated vectors and almost real images!

#### From concentrated random vectors to GANs

# Generator $\mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ Generated examples Concenvectors! Real examples

Figure: Illustration of a generative adversarial network (GAN).



Figure: Images samples generated by BigGAN [Brock et al.'18].

#### Some clues ... and much more can be done!

# RMT as a tool to **analyze**, **understand** and **improve** large dimensional machine learning methods.

- powerful and flexible tool to assess matrix-based machine learning systems;
- ▶ study (convex) optimization-based learning methods, e.g., logistic regression;
- understand impact of optimization methods, the dynamics of gradient descent;
- ▶ non-convex problems (e.g., deep neural nets) are more difficult, but accessible in some cases, e.g., low rank matrix recovery, phase retrieval, etc;
- more to be done: transfer learning, generative models, graph-based methods, robust statistics, etc.

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## Thank you!

## Thank you!

 $More\ info: https://romaincouillet.hebfree.org\ and\ https://zhenyu-liao.github.io!$