Random Matrix Theory for Modern Machine Learning: New Intuitions, Improved Methods, and Beyond: Part 3

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Outline

1. Linear Machine Learning Models via a Master Theorem
   - A master theorem for affine-transformed model
   - The information-plus-noise spiked model
   - The additive spiked model
2. RMT for Machine Learning: Linear Models
   - Low-rank approximation
   - Classification
   - Linear least squares

Affine-transformed model, a master theorem, and applications to linear ML

Definition (Affine-transformed model)

For $\mathbf{Z} \in \mathbb{R}^{p \times n}$ having i.i.d. sub-gaussian entries of zero mean and unit variance, and let $\mathbf{A} \in \mathbb{R}^{q \times n}$ and $\mathbf{C} \in \mathbb{R}^{q \times p}$ be two deterministic matrices, we say $\mathbf{X}$ is a affine transformed random matrix model

$$\mathbf{X} = \mathbf{A} + \mathbf{C}\mathbf{Z} \in \mathbb{R}^{q \times n}. \tag{1}$$

- this extends SCM, and can be used to derive results for a wide range of **popular ML** methods
- exhibit totally different behaviors and intuitions, on **classical** or **proportional** regime, analogous to SCMs

Table: Roadmap of linear ML models considered.

ML Problem	Classical Regime	Proportional Regime
Low rank approximation $\hat{\mathbf{X}}$ of info-plus-noise matrix $\mathbf{X}$	smooth decay of $\Vert\mathbf{X} - \hat{\mathbf{X}}\Vert_2 / \Vert\mathbf{X}\Vert_2 \simeq (1+\ell)^{-1}$ Proposition 1 Item (i)	sharp transition of $\Vert\mathbf{X} - \hat{\mathbf{X}}\Vert_2 / \Vert\mathbf{X}\Vert_2$ at $\ell = c + \sqrt{c}$ Proposition 1 Item (ii)
Classification of binary Gaussian mixtures of distance in means $\Delta\boldsymbol{\mu}$	pairwise $\simeq$ spectral approach Proposition 2 Item (i)	pairwise $\ll$ spectral approach Proposition 2 Item (ii)
Linear least squares regression risk as $n \uparrow$	bias $= 0$ and variance $\propto n^{-1}$ Proposition 3 Item (i)	monotonic bias and non-monotonic variance Proposition 3 Item (ii)

Affine-transformed model

Definition (Affine-transformed model)

For $\mathbf{Z} \in \mathbb{R}^{p \times n}$ having i.i.d. sub-gaussian entries of zero mean and unit variance, and let $\mathbf{A} \in \mathbb{R}^{q \times n}$ and $\mathbf{C} \in \mathbb{R}^{q \times p}$ be two deterministic matrices, we say $\mathbf{X}$ is a affine transformed random matrix model

$$\mathbf{X} = \mathbf{A} + \mathbf{C}\mathbf{Z} \in \mathbb{R}^{q \times n}. \tag{2}$$

- matrix version of an affine transformation of a vector: for $\mathbf{z} \in \mathbb{R}^p$ having independent entries of zero mean and unit variance, deterministic $\mathbf{a} \in \mathbb{R}^q$ and matrix $\mathbf{C} \in \mathbb{R}^{q \times p}$,
- then

$$\mathbf{x} = \mathbf{a} + \mathbf{C}\mathbf{z} \in \mathbb{R}^q, \tag{3}$$

  is an affine transformation of $\mathbf{z}$ with mean $\mathbb{E}[\mathbf{x}] = \mathbf{a}$ and covariance $\mathrm{Cov}[\mathbf{x}] = \mathbf{C}\mathbf{C}^\mathsf{T} \succeq \mathbf{0}$
- due to the "structure" in the affine-transformed (random matrix) model $\mathbf{X}$, we shall see that:

(i) the (limiting) eigenvalue distribution of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ can significantly diverge from the Marčenko-Pastur law

(ii) depending on the dimension ratio $c = p/n$, a few eigenvalues of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ may isolate from the rest of eigenvalue **bulk**, for which a **phase transition** behavior can be observed

- can be assessed via the **spiked model** analysis of the eigenvalues and eigenvectors to be discussed below

Deterministic Equivalents for resolvent of affine SCM

Theorem (Asymptotic Deterministic Equivalent for resolvent of affine-transformed model)

For random matrix $\mathbf{Z} \in \mathbb{R}^{p \times n}$ having i.i.d. sub-gaussian entries of zero mean and unit variance, let $\mathbf{X} = \mathbf{A} + \mathbf{C}\mathbf{Z}$ be an affine-transformed model, for deterministic $\mathbf{A} \in \mathbb{R}^{q \times n}, \mathbf{C} \in \mathbb{R}^{q \times p}$ such that $\|\mathbf{C}\|_2 \leq C$, $\|\mathbf{A}\|_2 \leq C\sqrt{n}$, and $\|\mathbf{a}_i\| \leq C$ for some universal constant $C > 0$, with $\mathbf{a}_i \in \mathbb{R}^q$ the i^{th} column of $\mathbf{A}$. Then, one has, for $z \in \mathbb{C}$ not an eigenvalue of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ and as $p, q, n \to \infty$ at the same pace, the following asymptotic Deterministic Equivalent,

$$\mathbf{Q}(z) \leftrightarrow \bar{\mathbf{Q}}(z), \quad \bar{\mathbf{Q}}(z) = \left(\frac{\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T}}{1 + \delta(z)} - z\mathbf{I}_q \right)^{-1} \tag{4}$$

for the resolvent $\mathbf{Q}(z) \equiv (\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T} - z\mathbf{I}_q)^{-1}$, with $\delta(z)$ the unique Stieltjes transform solution to the fixed point equation

$$\delta(z) = \frac{1}{n} \operatorname{tr} \mathbf{C}^\mathsf{T} \bar{\mathbf{Q}}(z) \mathbf{C}. \tag{5}$$

- *For the co-resolvent $\tilde{\mathbf{Q}}(z) \equiv (\frac{1}{n}\mathbf{X}^\mathsf{T}\mathbf{X} - z\mathbf{I}_n)^{-1}$, one has instead*

$$\tilde{\mathbf{Q}}(z) \leftrightarrow \bar{\tilde{\mathbf{Q}}}(z), \quad \bar{\tilde{\mathbf{Q}}}(z) = -\frac{\mathbf{I}_n}{z(1 + \delta(z))}. \tag{6}$$

Useful lemmas: recap

Lemma (Resolvent identity)

For invertible matrices $\mathbf{A}$ *and* $\mathbf{B}$*, we have* $\mathbf{A}^{-1} - \mathbf{B}^{-1} = \mathbf{A}^{-1}(\mathbf{B} - \mathbf{A})\mathbf{B}^{-1}$.

Lemma (Woodbury)

For $\mathbf{A} \in \mathbb{R}^{p \times p}$, $\mathbf{U}, \mathbf{V} \in \mathbb{R}^{p \times n}$*, such that both* $\mathbf{A}$ *and* $\mathbf{A} + \mathbf{U}\mathbf{V}^\mathsf{T}$ *are invertible, we have*

$$(\mathbf{A} + \mathbf{U}\mathbf{V}^\mathsf{T})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}(\mathbf{I}_n + \mathbf{V}^\mathsf{T}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}^\mathsf{T}\mathbf{A}^{-1}.$$

In particular, for $n = 1$*, i.e.,* $\mathbf{U}\mathbf{V}^\mathsf{T} = \mathbf{u}\mathbf{v}^\mathsf{T}$ *for* $\mathbf{U} = \mathbf{u} \in \mathbb{R}^p$ *and* $\mathbf{V} = \mathbf{v} \in \mathbb{R}^p$*, the above identity specializes to the following Sherman–Morrison formula,*

$$(\mathbf{A} + \mathbf{u}\mathbf{v}^\mathsf{T})^{-1} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{u}\mathbf{v}^\mathsf{T}\mathbf{A}^{-1}}{1 + \mathbf{v}^\mathsf{T}\mathbf{A}^{-1}\mathbf{u}}, \quad \textit{and } (\mathbf{A} + \mathbf{u}\mathbf{v}^\mathsf{T})^{-1}\mathbf{u} = \frac{\mathbf{A}^{-1}\mathbf{u}}{1 + \mathbf{v}^\mathsf{T}\mathbf{A}^{-1}\mathbf{u}}.$$

And the matrix $\mathbf{A} + \mathbf{u}\mathbf{v}^\mathsf{T} \in \mathbb{R}^{p \times p}$ *is invertible if and only if* $1 + \mathbf{v}^\mathsf{T}\mathbf{A}^{-1}\mathbf{u} \neq 0$.

Heuristic derivation via "leave-one-out"

- we propose $\bar{\mathbf{Q}} = (\mathbf{F} - z\mathbf{I}_q)^{-1}$ for some deterministic $\mathbf{F} \in \mathbb{R}^{q \times q}$ to be determined, and try to "guess" $\mathbf{F}$
- by resolvent identity

$$\mathbb{E}[\mathbf{Q} - \bar{\mathbf{Q}}] = \mathbb{E}\left[\mathbf{Q}\left(\mathbf{F} - \frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}\right)\right]\bar{\mathbf{Q}} = \mathbb{E}[\mathbf{Q}]\mathbf{F}\bar{\mathbf{Q}} - \frac{1}{n}\sum_{i=1}^n \mathbb{E}\left[\mathbf{Q}\mathbf{x}_i\mathbf{x}_i^\mathsf{T}\right]\bar{\mathbf{Q}}$$
$$= \mathbb{E}[\mathbf{Q}]\mathbf{F}\bar{\mathbf{Q}} - \frac{1}{n}\sum_{i=1}^n \mathbb{E}\left[\frac{\mathbf{Q}_{-i}\mathbf{x}_i\mathbf{x}_i^\mathsf{T}}{1 + \frac{1}{n}\mathbf{x}_i^\mathsf{T}\mathbf{Q}_{-i}\mathbf{x}_i}\right]\bar{\mathbf{Q}}$$

  with $\mathbf{x}_i = \mathbf{a}_i + \mathbf{C}\mathbf{z}_i \in \mathbb{R}^q$ the i^{th} column of $\mathbf{X} \in \mathbb{R}^{q \times n}$ for $\mathbf{a}_i \in \mathbb{R}^q$ the i^{th} column of $\mathbf{A} \in \mathbb{R}^{q \times n}$ and $\mathbf{z}_i \in \mathbb{R}^p$ the i^{th} column of $\mathbf{Z}$, $\mathbf{Q}_{-i} = (\frac{1}{n}\sum_{j \neq i}\mathbf{x}_j\mathbf{x}_j^\mathsf{T} - z\mathbf{I}_p)^{-1}$ independent of $\mathbf{x}_i$, and used the Woodbury identity
- in the denominator

$$\frac{1}{n}\mathbf{x}_i^\mathsf{T}\mathbf{Q}_{-i}\mathbf{x}_i = \frac{1}{n}(\mathbf{a}_i + \mathbf{C}\mathbf{z}_i)^\mathsf{T}\mathbf{Q}_{-i}(\mathbf{a}_i + \mathbf{C}\mathbf{z}_i) \simeq \frac{1}{n}\mathbf{a}_i^\mathsf{T}\mathbf{Q}_{-i}\mathbf{a}_i + \frac{1}{n}\mathbf{z}_i^\mathsf{T}\mathbf{C}^\mathsf{T}\mathbf{Q}_{-i}\mathbf{C}\mathbf{z}_i$$
$$\simeq \frac{1}{n}\operatorname{tr}(\mathbf{C}^\mathsf{T}\mathbf{Q}_{-i}\mathbf{C}) \simeq \frac{1}{n}\operatorname{tr}(\mathbf{C}^\mathsf{T}\bar{\mathbf{Q}}\mathbf{C}) \equiv \delta(z),$$

- ignore the cross terms (of the form $2\mathbf{a}_i^\mathsf{T}\mathbf{Q}_{-i}\mathbf{C}\mathbf{z}_i/n$, which, when conditioned on $\mathbf{Q}_{-i}$, is sub-gaussian with zero mean and variance $4\mathbf{a}_i^\mathsf{T}\mathbf{Q}_{-i}\mathbf{C}\mathbf{C}^\mathsf{T}\mathbf{Q}_{-i}\mathbf{a}_i/n^2 \leq 4n^{-2}\|\mathbf{a}_i\|^2 \cdot \|\mathbf{Q}_{-i}\|_2^2 \cdot \|\mathbf{C}\|_2^2 = O(n^{-2})$)
- approximate the term $\frac{1}{n}\mathbf{z}_i^\mathsf{T}\mathbf{C}^\mathsf{T}\mathbf{Q}_{-i}\mathbf{C}\mathbf{z}_i$ by its expectation (e.g., Hanson-Wright) and use Deterministic Equivalent relations $\mathbf{Q}_{-i} \leftrightarrow \mathbf{Q} \leftrightarrow \bar{\mathbf{Q}}$

Heuristic derivation via "leave-one-out": continuation

- the Deterministic Equivalent relations $\mathbf{Q}_{-i} \leftrightarrow \mathbf{Q} \leftrightarrow \bar{\mathbf{Q}}$ holds since

$$0 \preceq \mathbb{E}[\mathbf{Q}_{-i} - \mathbf{Q}] = \mathbb{E}\left[\frac{\mathbf{Q}_{-i} \frac{1}{n} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} \mathbf{Q}_{-i}}{1 + \frac{1}{n} \mathbf{x}_i^\mathsf{T} \mathbf{Q}_{-i} \mathbf{x}_i} \right] \preceq \frac{1}{n} \mathbb{E}[\mathbf{Q}_{-i} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} \mathbf{Q}_{-i}] = \frac{1}{n} \mathbb{E}\left[\mathbf{Q}_{-i} (\mathbf{a}_i \mathbf{a}_i^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T}) \mathbf{Q}_{-i} \right], \tag{7}$$

for $\|\mathbf{a}_i\| = O(1)$ and $\|\mathbf{C}\|_2 = O(1)$.

$$\begin{aligned}
\mathbb{E}[\mathbf{Q} - \bar{\mathbf{Q}}] &= \mathbb{E}[\mathbf{Q}]\mathbf{F}\bar{\mathbf{Q}} - \frac{1}{n} \sum_{i=1}^n \mathbb{E}\left[\mathbf{Q} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} \right] \bar{\mathbf{Q}} \simeq \mathbb{E}[\mathbf{Q}]\mathbf{F}\bar{\mathbf{Q}} - \frac{1}{n} \sum_{i=1}^n \frac{\mathbb{E}\left[\mathbf{Q}_{-i} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} \right]}{1 + \delta(z)} \bar{\mathbf{Q}} \\
&= \mathbb{E}[\mathbf{Q}]\mathbf{F}\bar{\mathbf{Q}} - \frac{1}{n} \sum_{i=1}^n \frac{\mathbb{E}[\mathbf{Q}_{-i}] (\mathbf{a}_i \mathbf{a}_i^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T})}{1 + \delta(z)} \bar{\mathbf{Q}} \\
&\simeq \mathbb{E}[\mathbf{Q}] \left(\mathbf{F} - \frac{\frac{1}{n} \sum_{i=1}^n (\mathbf{a}_i \mathbf{a}_i^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T})}{1 + \delta(z)} \right) \bar{\mathbf{Q}} \\
&= \mathbb{E}[\mathbf{Q}] \left(\mathbf{F} - \frac{\frac{1}{n} \mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T}}{1 + \delta(z)} \right) \bar{\mathbf{Q}}
\end{aligned}$$

- independence between $\mathbf{Q}_{-i}$ and $\mathbf{x}_i$ in the third line
- to have $\mathbb{E}[\mathbf{Q}] \simeq \bar{\mathbf{Q}}$, it thus suffices to take $\mathbf{F}$ such that the middle term vanishes

Remark: on the low-rankness of $\mathbf{A}$

- we consider $\mathbb{E}[\mathbf{X}] = \mathbf{A} \in \mathbb{R}^{q\times n}$ satisfies $\|\mathbf{A}\|_2 \leq C\sqrt{n}$ and $\|\mathbf{a}_i\| \leq C$ for all $i \in \{1,\ldots,n\}$, $\mathbf{a}_i \in \mathbb{R}^q$ the i-th column of $\mathbf{A} \in \mathbb{R}^{q\times n}$, and some constant $C > 0$
- the first is just proper scaling, so that $\|\mathbf{A}\|_2$ and $\|\mathbf{CZ}\|_2$ are of the same order
- the second bound on the Euclidean norm of *all* columns of $\mathbf{A}$ is more subtle: taking $\|\mathbf{A}\|_2 = C_1\sqrt{n}$ and $\|\mathbf{a}_i\| = C_{2,i}$ for $C_1, C_{2,i} > 0$,

$$\sum_{i=1}^{n} \|\mathbf{a}_i\|^2 = \sum_{i=1}^{n} C_{2,i}^2 = \|\mathbf{A}\|_F^2 = \sum_{i=1}^{\operatorname{rank}(\mathbf{A})} \sigma_i^2(\mathbf{A}) = \Theta(n) \tag{8}$$

  with $\sigma_1(\mathbf{A}) \geq \ldots \geq \sigma_{\operatorname{rank}(\mathbf{A})}(\mathbf{A})$ the (nonzero) singular values of $\mathbf{A}$ arranged in a non-increasing order. Since $\sigma_1^2(\mathbf{A}) = \|\mathbf{A}\|_2^2 = \Theta(n)$, the following two typical scenarios:

(i) $\operatorname{rank}(\mathbf{A}) = \Theta(n)$, a majority (of size $\Theta(n)$) of singular values $\sigma_i(\mathbf{A}) = O(1)$, so that the matrix $\mathbf{A}$ has a fast decay in its singular values; or

(ii) $\operatorname{rank}(\mathbf{A}) = \Theta(1)$, a few singular values $\sigma_i(\mathbf{A}) = \Theta(n)$, and $\mathbf{A}$ is exactly of low rank.

- This is in consistent with common ML assumptions, e.g., that the data are drawn from one or a mixture (when in a classification context) of distributions, and the mean $\mathbf{A}$ is of low rank.
- existing RMT results, e.g., on spiked model [BS06; BGN11], mostly focuses on exactly low rank $\mathbf{A}$.
- However, if one further relaxes the assumption $\|\mathbf{a}_i\| = O(1)$ and let $\mathbf{A}$ have a slow singular decay, the result collapses.

Remark: Stieltjes transform can not capture few important eigenvalues

Lemma ([SB95, Lemma 2.6])

For $\mathbf{A}, \mathbf{M} \in \mathbb{R}^{p \times p}$ *symmetric and nonnegative definite,* $\mathbf{u} \in \mathbb{R}^p$, $\tau > 0$ *and* $z < 0$,

$$\left| \operatorname{tr} \mathbf{A}(\mathbf{M} + \tau \mathbf{u}\mathbf{u}^\mathsf{T} - z\mathbf{I}_p)^{-1} - \operatorname{tr} \mathbf{A}(\mathbf{M} - z\mathbf{I}_p)^{-1} \right| \leq \frac{\|\mathbf{A}\|_2}{|z|}.$$

- for low-rank $\mathbf{A}$, $\delta(z)$ is asymptotically independent on $\mathbf{A}$.

$$\delta(z) = \frac{1}{n} \operatorname{tr} \mathbf{C}\mathbf{C}^\mathsf{T} \left(\frac{\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{C}\mathbf{C}^\mathsf{T}}{1+\delta(z)} - z\mathbf{I}_q \right)^{-1} = \frac{1}{n} \operatorname{tr} \mathbf{C}\mathbf{C}^\mathsf{T} \left(\frac{\mathbf{C}\mathbf{C}^\mathsf{T}}{1+\delta(z)} - z\mathbf{I}_q \right)^{-1} + O(n^{-1}). \tag{9}$$

- same holds for $\frac{1}{q} \operatorname{tr} \bar{\mathbf{Q}}(z) = \frac{1}{q} \operatorname{tr} \left(\frac{\mathbf{C}\mathbf{C}^\mathsf{T}}{1+\delta(z)} - z\mathbf{I}_q \right)^{-1} + O(n^{-1})$ for n, p, q large
- while the Deterministic Equivalent $\bar{\mathbf{Q}}(z)$ is itself dependent on $\mathbf{A}$, its normalized trace is NOT
- this independence of $\delta(z)$ and $\frac{1}{q} \operatorname{tr} \bar{\mathbf{Q}}(z)$ on $\mathbf{A}$ is also a limitation of the Stieltjes transform approach, a direct study of which leads to the limiting eigenvalue distribution, but does **not** allow for a characterization of a negligible proportion (of order $o(n)$) of eigenvalues (e.g., due to $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$).
- **contrasts with** Deterministic Equivalents approach: $\mathbf{Q}(z)$ and $\tilde{\mathbf{Q}}(z)$ remain dependent on $\mathbf{A}$, and thus can capture the influence of the low rank $\mathbf{A}$

Remark (DE-SCM as a corollary of the Linear Master Theorem)

The Deterministic Equivalents for resolvents of SCM, can be derived from our Linear Master Theorem above: Taking $q = p$, $c = p/n$, $\mathbf{A} = \mathbf{0}$ *and* $\mathbf{C} = \mathbf{I}_p$, *one obtains from Theorem 3 that*

$$\bar{\mathbf{Q}}(z) = \frac{1}{-z + \frac{1}{1+cm(z)}} \mathbf{I}_p \equiv m(z)\mathbf{I}_p, \tag{10}$$

where we denote $m(z) \equiv \frac{1}{p} \operatorname{tr} \bar{\mathbf{Q}}(z)$ *that satisfies the following quadratic equation*

$$czm^2(z) - (1 - c - z)m(z) + 1 = 0. \tag{11}$$

Table: Overview of upcoming results, illustrating the connection between the Linear Master Theorem different random matrix models, and applications.

$\mathbf{A}$	$\mathbf{C}$	z	RMT results	Related ML applications
$\mathbf{0}$	$\mathbf{I}_p$	complex	Distribution of eigenvalues (Marčenko-Pastur law in **??**)	Previous results on SCM
low rank	$\mathbf{I}_p$	complex	Extreme eigenvalues (Additive spiked eigenvalues in Theorem 12)	Low rank approximation
low rank	$\mathbf{I}_p$	complex	Extreme eigenvectors (Info-plus-noise spiked eigenvectors in Theorem 10)	Classification
$\mathbf{0}$	$\mathbf{I}_p$	real	Resolvent matrix (Deterministic Equivalent in **??**)	Linear least squares

Information-plus-noise spiked model

- $\mathbf{C} = \mathbf{I}_p$, random matrix $\mathbf{Z}$ for homogeneous "**noise**", and $\mathbf{A} \in \mathbb{R}^{p \times n}$ informative "**signal**" matrix, low rank

Definition (Information-plus-noise spiked model)

We say a symmetric random matrix $\mathbf{X} \in \mathbb{R}^{p \times p}$ follows an *information-plus-noise spiked model* if

$$\mathbf{X} = \frac{1}{n}(\mathbf{A} + \mathbf{Z})(\mathbf{A} + \mathbf{Z})^\mathsf{T}, \tag{12}$$

for some *deterministic* matrix $\mathbf{A} \in \mathbb{R}^{p \times n}$ and random matrix $\mathbf{Z} \in \mathbb{R}^{p \times n}$ with $\mathbb{E}[\mathbf{Z}] = \mathbf{0}$.

- determine when the "information in $\mathbf{A}$ can be "found," and when it is "lost" due to the noise in $\mathbf{Z}$
- for $\mathbf{A} \neq \mathbf{0}$, expect a few eigenvalues "jumping" out the Marčenko-Pastur support (due to $\mathbf{A}$, refer to as the spikes) and isolate from the main eigenvalue bulk $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$

$$\frac{1}{n}\mathbb{E}[(\mathbf{A} + \mathbf{Z})(\mathbf{A} + \mathbf{Z})^\mathsf{T}] = \frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \frac{1}{n}\mathbb{E}[\mathbf{Z}\mathbf{Z}^\mathsf{T}] = \frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{I}_p \tag{13}$$

- so for $n \gg p$, the information-plus-noise spiked model $\frac{1}{n}(\mathbf{A} + \mathbf{Z})(\mathbf{A} + \mathbf{Z})^\mathsf{T}$ is close to $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{I}_p$, the largest r eigenvalues are $1 + \lambda_i(\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T})$
- in the case of $n \sim p \gg 1$ both large, expects the top eigenvalues/eigenvectors of $\frac{1}{n}(\mathbf{A} + \mathbf{Z})(\mathbf{A} + \mathbf{Z})^\mathsf{T}$ still somewhat relates to those of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$

Eigenvalue characterization for the information-plus-noise spiked model

- already know that if $\mathbf{Z} \in \mathbb{R}^{p \times n}$ is a random matrix having i.i.d. entries of zero mean and unit variance, then as $n, p \to \infty$, the limiting eigenvalue distribution of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ is the Marčenko-Pastur law
- it does not guarantee that **no eigenvalue** lies outside of the support of the Marčenko-Pastur law (i.e., outside the interval $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$)
- e.g., only states that the averaged number of eigenvalues of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ lying within $[a, b] \subset [(1-\sqrt{c})^2, (1+\sqrt{c})^2]$ converges to $\mu([a,b])$—more precisely, is of the order $p \times \mu([a,b]) + o(p)$
- remains unclear, e.g., **whether there could be a number of order** $o(p)$ **"leaking"** from the limiting Marčenko-Pastur support $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$, even for n, p sufficiently large

Theorem ("No eigenvalue outside the support" in the absence of information, [BS98])

Let $\mathbf{X}_{\mathbf{A}=\mathbf{0}}$ be the information-plus-noise spiked model with $\mathbf{A} = \mathbf{0}$, and random noise matrix $\mathbf{Z} \in \mathbb{R}^{p \times n}$ having independent entries of zero mean, unit variance, and κ-kurtosis, then as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, with probability one, the empirical spectral measure $\mu_{\mathbf{X}_{\mathbf{A}=\mathbf{0}}}$ of $\mathbf{X}_{\mathbf{A}=\mathbf{0}}$, converges weakly to the Marčenko-Pastur law and

(i) *if $\kappa < \infty$, then*

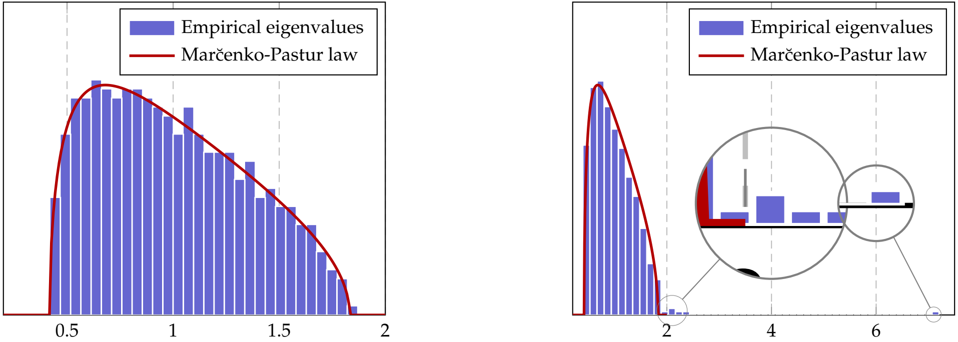
$$\lambda_{\min}\left(\mathbf{X}_{\mathbf{A}=\mathbf{0}}\right) \to (1-\sqrt{c})^2, \quad \lambda_{\max}\left(\mathbf{X}_{\mathbf{A}=\mathbf{0}}\right) \to (1+\sqrt{c})^2 \tag{14}$$

that is, no eigenvalue of $\mathbf{X}_{\mathbf{A}=\mathbf{0}} = \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ appears outside the limiting Marčenko-Pastur support; and

(ii) *if $\kappa = \infty$, then*

$$\lambda_{\max}\left(\mathbf{X}_{\mathbf{A}=\mathbf{0}}\right) \to \infty. \tag{15}$$

Eigenvalue characterization for the information-plus-noise spiked model



(a) Gaussian $\mathbf{Z}$ (b) Student-t $\mathbf{Z}$ with degree of freedom three

Figure: Eigenvalue distribution of sample covariance matrix $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ for Gaussian (**left**) and Student-t (**right**) $\mathbf{Z}$, versus the *same* limiting Marčenko-Pastur law, with $p = 512$ and $n = 8p$.

(i) in the Gaussian case (**left**), no eigenvalue outside the Marčenko-Pastur support; and
(ii) in the Student-t case (**right**), a few eigenvalues are observed to "leak" from the Marčenko-Pastur support, even in the noise -only model with $\mathbf{A} = \mathbf{0}$, in line with the "no eigenvalue outside the support" result

Theorem (Information-plus-noise spiked eigenvalues, [BS06])

Let $\mathbf{Z} \in \mathbb{R}^{p \times n}$ be a random matrix having i.i.d. sub-gaussian entries of zero mean and unit variance, and let $\mathbf{A} \in \mathbb{R}^{p \times n}$ be a deterministic matrix of rank r with $\|\mathbf{A}\| \leq C\sqrt{n}$ for some constants $r, C > 0$. Then, for $\mathbf{X} = \mathbf{A} + \mathbf{Z} \in \mathbb{R}^{p \times n}$ and $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{u}_i^\mathsf{T}$ the spectral decomposition of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$, one has, as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, that

$$\lambda_i \left(\frac{1}{n} \mathbf{X}\mathbf{X}^\mathsf{T} \right) \to \bar{\lambda}_i = \begin{cases} 1 + c + \ell_i + \frac{c}{\ell_i}, & \ell_i > \sqrt{c} \\ (1 + \sqrt{c})^2 \equiv E_+, & \ell_i \leq \sqrt{c}. \end{cases} \tag{16}$$

almost surely, for $\lambda_i(\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T})$ and ℓ_i the i^{th} largest eigenvalue of the information-plus-noise spiked model $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ in Theorem 7 and of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$, respectively.

[1] Jinho Baik and Jack W. Silverstein. "Eigenvalues of large sample covariance matrices of spiked population models". In: *Journal of Multivariate Analysis* 97.6 (2006), pp. 1382–1408

Proof using the Linear Master Theorem

- it follows from Woodbury identity the following Deterministic Equivalent holds

$$\mathbf{Q}(z) \leftrightarrow \bar{\mathbf{Q}}(z), \quad \bar{\mathbf{Q}}(z) = \left(\frac{\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} + \mathbf{I}_p}{1+\delta(z)} - z\mathbf{I}_p \right)^{-1}$$
$$= \frac{1+\delta(z)}{1-z-z\delta(z)} \left(\mathbf{I}_p - \mathbf{U}\left((1-z-z\delta(z))\mathbf{L}^{-1} + \mathbf{I}_r \right)^{-1} \mathbf{U}^\mathsf{T} \right). \tag{17}$$

- here, $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T} = \mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T} = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{u}_i^\mathsf{T}$ is the spectral decomposition of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$, for $\{\ell_i\}_{i=1}^r$ the (non-zero) eigenvalue, $\mathbf{u}_i \in \mathbb{R}^p$ the corresponding eigenvectors, and $\delta(z)$ the unique valid Stieltjes transform solution to the quadratic equation

$$z\delta^2(z) - (1-c-z)\delta(z) + c = 0. \tag{18}$$

- To locate a possibly **isolated** eigenvalue of the information-plus-noise random matrix $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ outside the Marčenko-Pastur support, we are looking for $z \in \mathbb{R}$ such that $\delta(z)$ in Equation (18) is well defined (so that it is "**outside**" the limiting bulk) **but** the Deterministic Equivalent $\bar{\mathbf{Q}}(z)$ in Equation (17) is **undefined** (so that z is an eigenvalue of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$).
- check that $\delta(z) = z^{-1} - 1$ is not a solution to Equation (18), so that the denominator of $\bar{\mathbf{Q}}(z)$ is not zero, and the real z that we are looking for must satisfy

$$z(1+\delta(z)) = 1 + \ell_i. \tag{19}$$

Proof using the Linear Master Theorem

Location of spiked eigenvalues: real z such that

$$\boxed{z(1+\delta(z)) = 1+\ell_i.} \tag{20}$$

- determine the condition under which this equation has a solution: for $z \in \mathbb{R}$ the function $z\delta(z) = \int \frac{z}{t-z}\mu(dt)$ is increasing on its domain of definition and

$$\lim_{z \downarrow (1+\sqrt{c})^2} z(1+\delta(z)) = 1+\sqrt{c}. \tag{21}$$

- admits a solution (that corresponds to an isolated eigenvalue) *if and only if*

$$\ell_i \geq \sqrt{c}. \tag{22}$$

- Plugging back, this leads to the following explicit solution

$$\boxed{z = 1+\ell_i + c + \frac{c}{\ell_i} \geq (1+\sqrt{c})^2}. \tag{23}$$

Phase transition in spiked eigenvalues

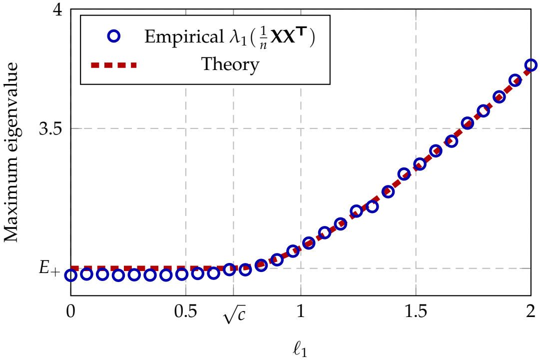


Figure: Phase transition behavior of the largest eigenvalue $\lambda_1(\mathbf{X}\mathbf{X}^\mathsf{T}/n)$ of the information-plus-noise model $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$, as a function of ℓ_1, with $\mathbf{X} = \mathbf{A} + \mathbf{Z}$, $\mathbf{A} = \sqrt{\ell_1} \cdot \mathbf{u}_1 \mathbf{1}_n^\mathsf{T}$ for $\|\mathbf{u}_1\| = 1$, so that $\lambda_1(\mathbf{A}\mathbf{A}^\mathsf{T}/n) = \ell_1$, for $p = 512$ and $n = 1\,024$.

Phase transition: depending on "signal strength" $\ell_1 = \|\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}\|_2$,

- (i) if $\ell_1 \leq \sqrt{c}$: largest eigenvalue of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ asymptotically the same as $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ and independent of ℓ_1
- (ii) if $\ell_1 > \sqrt{c}$: larger than that of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$, and increases as ℓ_1 becomes large

Eigenvector characterization for the information-plus-noise spiked model

Theorem (Information-plus-noise spiked eigenvectors, [Pau07])

In the setting of Theorem 9, assume that the eigenvalues ℓ_i of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$ are all distinct and satisfy $\ell_1 > \ldots > \ell_r > 0$, and let $\hat{\mathbf{u}}_1, \ldots, \hat{\mathbf{u}}_r$ be the eigenvectors associated with the r largest eigenvalues $\lambda_1(\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}) > \ldots > \lambda_r(\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T})$ of the information-plus-noise model $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$. Then, for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^p$ deterministic vectors of unit norm,

$$\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} \to \eta_i = \begin{cases} \frac{1-c\ell_i^{-2}}{1+c\ell_i^{-1}} \cdot \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}, & \ell_i > \sqrt{c}; \\ 0, & \ell_i \leq \sqrt{c}. \end{cases} \tag{24}$$

almost surely as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, for $\mathbf{u}_i$ the eigenvector associated with ℓ_i of $\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}$. In particular, taking $\mathbf{a} = \mathbf{b} = \mathbf{u}_i$ leads to

$$(\hat{\mathbf{u}}_i\mathbf{u}_i^\mathsf{T})^2 \to \eta_i = \begin{cases} \frac{1-c\ell_i^{-2}}{1+c\ell_i^{-1}}, & \ell_i > \sqrt{c}; \\ 0, & \ell_i \leq \sqrt{c}. \end{cases} \tag{25}$$

[1] Debashis Paul. "Asymptotics of Sample Eigenstructure for a Large Dimensional Spiked Covariance Model". In: *Statistica Sinica* 17.4 (2007), pp. 1617–1642

Proof using the Linear Master Theorem

- consider the i^{th} eigenvalue ℓ_i of $\frac{1}{n}\mathbf{A}\mathbf{A}^\top$ that satisfies $\ell_i > \sqrt{c}$ above the phase transition threshold
- by Cauchy's integral formula

$$\mathbf{a}^\top \hat{\mathbf{u}}_i \hat{\mathbf{u}}_i^\top \mathbf{b} = -\frac{1}{2\pi\imath} \oint_{\Gamma_{\lambda_i}} \mathbf{a}^\top \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top - z\mathbf{I}_p \right)^{-1} \mathbf{b}\, dz \tag{26}$$

for Γ_{λ_i} a positively oriented contour enclosing only the i^{th} eigenvalue of $\lambda_i(\frac{1}{n}\mathbf{X}\mathbf{X}^\top)$
- according to Theorem 9, this converges almost surely to $\bar{\lambda}_i = 1 + c + \ell_i + \frac{c}{\ell_i}$ as $n, p \to \infty$
- by our Linear Master Theorem

$$\begin{aligned} \mathbf{a}^\top \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top - z\mathbf{I}_p \right)^{-1} \mathbf{b} &\simeq \frac{1+\delta(z)}{1-z-z\delta(z)} \mathbf{a}^\top \left(\mathbf{I}_p - \mathbf{U} \left((1-z-z\delta(z))\mathbf{L}^{-1} + \mathbf{I}_r \right)^{-1} \mathbf{U}^\top \right) \mathbf{b} \\ &= \frac{1+\delta(z)}{1-z-z\delta(z)} \mathbf{a}^\top \mathbf{b} - \frac{1+\delta(z)}{1-z-z\delta(z)} \sum_{j=1}^r \frac{\mathbf{a}^\top \mathbf{u}_j \mathbf{u}_j^\top \mathbf{b}}{1 + (1-z-z\delta(z))\ell_j^{-1}} \end{aligned}$$

with $\frac{1}{n}\mathbf{A}\mathbf{A}^\top = \mathbf{U}\mathbf{L}\mathbf{U}^\top = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{u}_i^\top$ the spectral decomposition of $\frac{1}{n}\mathbf{A}\mathbf{A}^\top$, and $\delta(z)$ unique solution to

$$z\delta^2(z) - (1-c-z)\delta(z) + c = 0. \tag{27}$$

- $\frac{1+\delta(z)}{1-z-z\delta(z)}\mathbf{a}^\top \mathbf{b}$ has **no pole** outside the Marčenko-Pastur support (i.e., the denominator $1 - z - z\delta(z) \neq 0$).

Proof using the Linear Master Theorem

- we further deduce that

$$\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} \simeq \frac{1}{2\pi\imath}\oint_{\Gamma_{\lambda_i}} \frac{1+\delta(z)}{1-z-z\delta(z)} \frac{\mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}}{1+(1-z-z\delta(z))\ell_i^{-1}} dz, \tag{28}$$

  which has a **pole** satisfying $1+(1-z-z\delta(z))\ell_i^{-1}=0$ and corresponds to spike location $z=\bar{\lambda}_i$ above
- one can evaluate the above expression by residue calculus at $z=\bar{\lambda}_i$ as

$$\begin{aligned}\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} &\simeq \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}\cdot \lim_{z\to\bar{\lambda}_i} \frac{(z-\bar{\lambda}_i)(1+\delta(z))}{(1-z-z\delta(z))+(1-z-z\delta(z))^2\ell_i^{-1}} \\ &= \frac{1+\delta(\bar{\lambda}_i)}{1+\delta(\bar{\lambda}_i)+\bar{\lambda}_i\delta'(\bar{\lambda}_i)}\cdot \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b},\end{aligned}$$

  by L'Hôpital's rule, where we denote $\delta'(z)$ the derivative of $\delta(z)$ with respect to z, given by

$$\delta'(z) = \frac{\delta(z)(1+\delta(z))}{1-c-z-2z\delta(z)}. \tag{29}$$

- This is $\boxed{\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} \to \frac{1-c\ell_i^{-2}}{1+c\ell_i^{-1}}\cdot \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}.}$

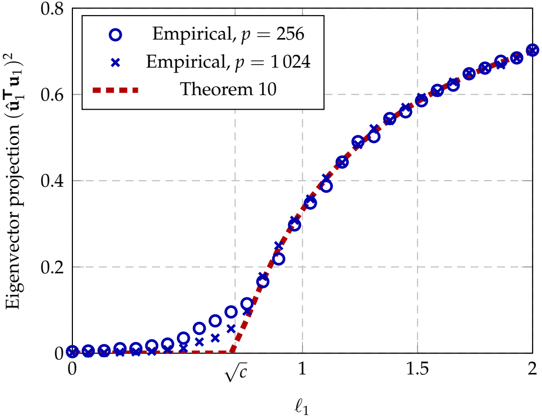


Figure: Phase transition behavior of the eigenvector projection $(\hat{\mathbf{u}}_1^\mathsf{T}\mathbf{u}_1)^2$ of the top eigenvector $\hat{\mathbf{u}}_i$ associated with the largest eigenvalue of the information-plus-noise model $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$, as a function of ℓ_1, with $\mathbf{X} = \mathbf{A} + \mathbf{Z}$, $\mathbf{A} = \sqrt{\ell_1}\mathbf{u}_1\mathbf{1}_n^\mathsf{T}$ for $\|\mathbf{u}_1\| = 1$, so that $\lambda_1(\mathbf{A}\mathbf{A}^\mathsf{T}/n) = \ell_1$, for different values of p, n with $n = 2p$.

(i) empirical transitions for $p = 256, 1\,024$ not sharp, $\mathbf{u}_1^\mathsf{T}\hat{\mathbf{u}}_1 > 0$ even below threshold $\ell_1 \leq \sqrt{c}$;

(ii) become **closer** to the limiting theoretical one as the dimensions n, p grow large

The additive spiked model

Definition (Additive spiked model)

We say a symmetric random matrix $\mathbf{X} \in \mathbb{R}^{p \times p}$ follows an *additive spiked model* if

$$\mathbf{X} = \mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}, \tag{30}$$

for some *deterministic* symmetric matrix $\mathbf{B} \in \mathbb{R}^{p \times p}$ and random matrix $\mathbf{Z} \in \mathbb{R}^{p \times n}$ with $\mathbb{E}[\mathbf{Z}] = \mathbf{0}$.

- useful (and low rank) information $\mathbf{B}$ buried by random symmetric noise matrix $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$
- of interest in low-rank approximation of noise matrices for data science applications of, e.g., recommendation system or LoRA technique in Large Language Models (LLMs) [Hu+21]

[1] Edward J. Hu et al. "LoRA: Low-Rank Adaptation of Large Language Models". In: *International Conference on Learning Representations.* Oct. 2021

Eigenvalue characterization for the information-plus-noise spiked model

- recall from "no eigenvalue outside the support" that in the absence of the additive term $\mathbf{B} = \mathbf{0}$ and sub-gaussian $\mathbf{Z}$, no eigenvalue of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ is outside the Marčenko-Pastur support

Theorem (Additive spiked eigenvalues, [BGN11])

Let $\mathbf{Z} \in \mathbb{R}^{p\times n}$ be a random matrix having i.i.d. sub-gaussian entries of zero mean and unit variance, and let $\mathbf{B} \in \mathbb{R}^{p\times p}$ be a symmetric deterministic matrix of rank r with $\|\mathbf{B}\|_2 \leq C$ for some constants $r, C > 0$. Then, for additive spiked model $\mathbf{X} = \mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} \in \mathbb{R}^{p\times p}$ in Theorem 11 with symmetric $\mathbf{B} = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{u}_i^\mathsf{T}$ the spectral decomposition of $\mathbf{B}$, one has, as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, that

$$\lambda_i(\mathbf{X}) \to \bar{\lambda}_i = \begin{cases} 1 + \ell_i + \frac{c}{\ell_i - c}, & \ell_i > c + \sqrt{c} \\ (1+\sqrt{c})^2, & \ell_i \leq c + \sqrt{c}. \end{cases} \tag{31}$$

almost surely, for $\lambda_i(\mathbf{X})$ and ℓ_i the i^{th} largest eigenvalue of the additive spiked model $\mathbf{X}$ and of $\mathbf{B}$, respectively.

[1] Florent Benaych-Georges and Raj Rao Nadakuditi. "The eigenvalues and eigenvectors of finite, low rank perturbations of large random matrices". In: *Advances in Mathematics* 227.1 (2011), pp. 494–521

Proof using the Linear Master Theorem

- to locate a possibly isolated eigenvalue of $\mathbf{X}$ outside the (limiting) Marčenko-Pastur support (of the eigenvalues of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$), look for $z \in \mathbb{R}$ solution to the following determinant equation

$$0 = \det\left(\mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p\right) = \det\left(\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p\right) \cdot \det\left(\mathbf{I}_p + \mathbf{Q}(z)\mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T}\right). \tag{32}$$

- Here, $\mathbf{Q}(z) = (\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p)^{-1}$ is the resolvent of $\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$, and $\mathbf{B} = \mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T}$ is the spectral decomposition of $\mathbf{B}$, with $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_r] \in \mathbb{R}^{p \times r}$ and $\mathbf{L} = \operatorname{diag}\{\ell_i\}_{i=1}^r$
- looking for $z \in \mathbb{R}$ outside the main bulk, so that $\mathbf{Q}(z)$ is well defined and $\det \mathbf{Q}^{-1}(z) \neq 0$,

$$0 = \det\left(\mathbf{I}_p + \mathbf{Q}(z)\mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T}\right) \Leftrightarrow 0 = \det\left(\mathbf{I}_r + \mathbf{L}\mathbf{U}^\mathsf{T}\mathbf{Q}(z)\mathbf{U}\right), \tag{33}$$

- apply the Linear Master Theorem to approximate

$$\mathbf{U}^\mathsf{T}\mathbf{Q}(z)\mathbf{U} \simeq \mathbf{U}^\mathsf{T}\bar{\mathbf{Q}}(z)\mathbf{U} = m(z)\mathbf{I}_r, \tag{34}$$

with $m(z)$ the unique Stieltjes transform solution to the Marčenko-Pastur equation,

$$0 = \det\left(\mathbf{I}_p + \mathbf{Q}(z)\mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T}\right) \Leftrightarrow 0 = \det(\mathbf{I}_r + m(z)\mathbf{L}) \leftrightarrow \boxed{m(z) = -\ell_i^{-1}}. \tag{35}$$

Proof using the Linear Master Theorem

Spiked eigenvalues $z \in \mathbb{R}$ such that $\boxed{m(z) = -\ell_i^{-1}}$.

- Since $m(z) = \int \frac{\mu(dt)}{t-z}$ is an increasing function of z on its domain of definition and

$$\lim_{z \downarrow (1+\sqrt{c})^2} m(z) = -\frac{1}{c+\sqrt{c}}, \tag{36}$$

the equation $m(z) = -\ell_i^{-1}$ admits a solution *if and only if*

$$\ell_i > c + \sqrt{c}, \tag{37}$$

with explicit solution (and therefore the spike location)

$$\boxed{z = 1 + \ell_i + \frac{c}{\ell_i - c} \geq (1+\sqrt{c})^2.} \tag{38}$$

Comparison of spiked eigenvalues for information-plus-noise versus additive model

- for **information-plus-noise spiked model** $\mathbf{X} = \frac{1}{n}(\mathbf{A}+\mathbf{Z})(\mathbf{A}+\mathbf{Z})^\mathsf{T}$:

$$\lambda_i(\mathbf{X}) \to \bar{\lambda}_i = 1 + c + \ell_i + \frac{c}{\ell_i}, \quad \ell_i > \sqrt{c}, \quad \ell_i = \lambda_i\left(\frac{1}{n}\mathbf{A}\mathbf{A}^\mathsf{T}\right); \tag{39}$$

- for **additive spiked model** $\mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$:

$$\lambda_i(\mathbf{X}) \to \bar{\lambda}_i = 1 + \ell_i + \frac{c}{\ell_i - c}, \quad \ell_i > c + \sqrt{c}, \quad \ell_i = \lambda_i(\mathbf{B}); \tag{40}$$

- connected via the "change-of-variable" $\lambda_i(\mathbf{A}\mathbf{A}^\mathsf{T}/n) + c \sim \lambda_i(\mathbf{B})$ with $c = p/n$, in the sense that:

(i) the phase transition condition is $\lambda_i(\mathbf{A}\mathbf{A}^\mathsf{T}/n) \geq \sqrt{c}$ for the information-plus-noise model and $\lambda_i(\mathbf{B}) \geq c + \sqrt{c}$ for the additive model; and

(ii) above phase transition, the isolated eigenvalues of the information-plus-noise model are given by $1 + c + \lambda_i(\mathbf{A}\mathbf{A}^\mathsf{T}/n) + c/\lambda_i(\mathbf{A}\mathbf{A}^\mathsf{T}/n)$, while those of the additive model are given by $1 + \lambda_i(\mathbf{B}) + c/\left(\lambda_i(\mathbf{B}) - c\right)$.

Eigenvector characterization for the information-plus-noise spiked model

Theorem (Additive spiked eigenvectors, [BGN11])

In the setting of Theorem 12, assume that the eigenvalues ℓ_i of $\mathbf{B}$ are all distinct and satisfy $\ell_1 > \ldots > \ell_r > 0$, and let $\hat{\mathbf{u}}_1, \ldots, \hat{\mathbf{u}}_r$ be the eigenvectors associated with the r largest eigenvalues $\lambda_1(\mathbf{X}) > \ldots > \lambda_r(\mathbf{X})$ of the additive model $\mathbf{X} = \mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$. Then, as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$,

$$(\hat{\mathbf{u}}_i \mathbf{u}_i^\mathsf{T})^2 \to \eta = \begin{cases} 1 - \frac{c}{(\ell_i - c)^2}, & \ell_i > c + \sqrt{c} \\ 0, & \ell_i \leq c + \sqrt{c}. \end{cases} \tag{41}$$

almost surely, for $\mathbf{u}_i$ the eigenvector associated with the eigenvalue ℓ_i of $\mathbf{B}$.

[1] Florent Benaych-Georges and Raj Rao Nadakuditi. "The eigenvalues and eigenvectors of finite, low rank perturbations of large random matrices". In: *Advances in Mathematics* 227.1 (2011), pp. 494–521

Proof using the Linear Master Theorem

- follow the same line of arguments as in the proof of information-plus-noise spiked model
- write, for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^p$ of unit norm,

$$\mathbf{a}^\mathsf{T} \hat{\mathbf{u}}_i \hat{\mathbf{u}}_i^\mathsf{T} \mathbf{b} = -\frac{1}{2\pi\imath} \oint_{\Gamma_{\lambda_i}} \mathbf{a}^\mathsf{T} \left(\mathbf{B} + \frac{1}{n} \mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p \right)^{-1} \mathbf{b} \, dz, \tag{42}$$

  for Γ_{λ_i} a positively oriented contour enclosing only the i^{th} eigenvalue of $\mathbf{X} = \mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T}$ (that admits the almost sure limit $\bar{\lambda}_i = 1 + \ell_i + \frac{c}{\ell_i - c}$)
- let $\mathbf{B} = \mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T} = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{u}_i^\mathsf{T}$ be the spectral decomposition of $\mathbf{B}$, then

$$\mathbf{a}^\mathsf{T} \left(\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p + \mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T} \right)^{-1} \mathbf{b} = \mathbf{a}^\mathsf{T}\mathbf{Q}(z)\mathbf{b} - \mathbf{a}^\mathsf{T}\mathbf{Q}(z)\mathbf{U}(\mathbf{L}^{-1} + \mathbf{U}^\mathsf{T}\mathbf{Q}(z)\mathbf{U})^{-1}\mathbf{U}^\mathsf{T}\mathbf{Q}(z)\mathbf{b},$$

  with $\mathbf{Q}(z) = (\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p)^{-1}$
- applying the Deterministic Equivalent result $\mathbf{Q}(z) \leftrightarrow m(z)\mathbf{I}_p$

$$\mathbf{a}^\mathsf{T} \left(\frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} - z\mathbf{I}_p + \mathbf{U}\mathbf{L}\mathbf{U}^\mathsf{T} \right)^{-1} \mathbf{b} \simeq m(z)\mathbf{a}^\mathsf{T}\mathbf{b} - m^2(z)\mathbf{a}^\mathsf{T}\mathbf{U}\left(m(z)\mathbf{I}_r + \mathbf{L}^{-1} \right)^{-1} \mathbf{U}^\mathsf{T}\mathbf{b},$$

  with $m(z)$ unique solution to

$$zcm^2(z) - (1 - c - z)m(z) + 1 = 0. \tag{43}$$

- the first term $m(z)\mathbf{a}^\mathsf{T}\mathbf{b}$ has no pole outside the Marčenko-Pastur support

Proof using the Linear Master Theorem

- So

$$\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} \simeq \frac{1}{2\pi\imath}\oint_{\Gamma_{\lambda_i}} \frac{m^2(z)\cdot \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}}{m(z)+\ell_i^{-1}}dz. \tag{44}$$

- This has a pole satisfying $m(z) = -\ell_i^{-1}$ and corresponds to spike location at $z = \bar{\lambda}_i = 1 + \ell_i + \frac{c}{\ell_i - c}$ characterized in Theorem 12.
- evaluate this expression by the residue calculus at $z = \bar{\lambda}_i$ as

$$\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}\mathbf{b} \simeq \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}\cdot\frac{m^2(\bar{\lambda}_i)}{m'(\bar{\lambda}_i)} = \mathbf{a}^\mathsf{T}\mathbf{u}_i\mathbf{u}_i^\mathsf{T}\mathbf{b}\left(1-\frac{c}{(\ell_i-c)^2}\right), \tag{45}$$

with $m'(z)$ the derivative of $m(z)$ with respect to z satisfying

$$m'(z) = \frac{m^2(z)}{1-\frac{cm^2(z)}{(1+cm(z))^2}}. \tag{46}$$

- Plugging in we conclude the proof.

Take-away of this section

- a Master Theorem: Deterministic Equivalent for resolvent for affine-transformed SCM model $\mathbf{X} = \mathbf{A} + \mathbf{C}\mathbf{Z}$
- **information-plus-noise spiked model** $\mathbf{X} = \frac{1}{n}(\mathbf{A} + \mathbf{Z})(\mathbf{A} + \mathbf{Z})^{\mathsf{T}}$: phase transition in spiked eigenvalues and eigenvectors
- **additive spiked model** $\mathbf{B} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^{\mathsf{T}}$: phase transition in spiked eigenvalues and eigenvectors

Table: Roadmap of linear ML models considered.

ML Problem	Classical Regime	Proportional Regime
Low rank approximation $\hat{\mathbf{X}}$ of info-plus-noise matrix $\mathbf{X}$	smooth decay of $\Vert\mathbf{X} - \hat{\mathbf{X}}\Vert_2/\Vert\mathbf{X}\Vert_2 \simeq (1+\ell)^{-1}$ Proposition 1 Item (i)	sharp transition of $\Vert\mathbf{X} - \hat{\mathbf{X}}\Vert_2/\Vert\mathbf{X}\Vert_2$ at $\ell = c + \sqrt{c}$ Proposition 1 Item (ii)
Classification of binary Gaussian mixtures of distance in means $\Delta\boldsymbol{\mu}$	pairwise $\simeq$ spectral approach Proposition 2 Item (i)	pairwise $\ll$ spectral approach Proposition 2 Item (ii)
Linear least squares regression risk as $n \uparrow$	bias $= 0$ and variance $\propto n^{-1}$ Proposition 3 Item (i)	monotonic bias and non-monotonic variance Proposition 3 Item (ii)

Low-rank approximation

Definition (Rank-one matrix recovery)

Taking $\mathbf{B} = \ell \mathbf{u}\mathbf{u}^\mathsf{T}$ in Theorem 11 of the additive spiked model, we have

$$\mathbf{X} = \ell \mathbf{u}\mathbf{u}^\mathsf{T} + \frac{1}{n}\mathbf{Z}\mathbf{Z}^\mathsf{T} \in \mathbb{R}^{p\times p}, \tag{47}$$

for $\mathbf{u} \in \mathbb{R}^p$ some deterministic signal of unit norm, i.e., $\|\mathbf{u}\| = 1$, $\ell \geq 0$ the informative "signal strength," and $\mathbf{Z} \in \mathbb{R}^{p\times n}$ a random "noise" matrix having i.i.d. entries of zero mean and unit variance.

- known from **Eckart-Young-Mirsky theorem** that the "best" low-rank approximation of a given matrix $\mathbf{X}$, measured by any unitarily invariant matrix norm (including the Frobenius and the spectral/operator norm) is given by retaining the **top singular/eigenvalue decomposition**
- let $\mathbf{X} = \sum_{i=1}^p \lambda_i(\mathbf{X})\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}$, be the eigenvalue-eigenvector decomposition of a symmetric and nonnegative definite matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, with $\lambda_1(\mathbf{X}) \geq \ldots \geq \lambda_p(\mathbf{X}) \geq 0$ listed in a non-increasing order. Then, for $k \leq \operatorname{rank}(\mathbf{X})$, the solution to

$$\hat{\mathbf{X}}_* = \operatorname*{arg\,min}_{\operatorname{rank}(\hat{\mathbf{X}})=k} \|\mathbf{X} - \hat{\mathbf{X}}\| = \hat{\mathbf{X}}_* = \sum_{i=1}^k \lambda_i(\mathbf{X})\hat{\mathbf{u}}_i\hat{\mathbf{u}}_i^\mathsf{T}, \tag{48}$$

for any unitarily invariant norm $\|\cdot\|$, and is unique *if and only if* $\hat{\ell}_k > \hat{\ell}_{k+1}$

- evaluate the relative spectral norm error $\|\mathbf{X}-\hat{\mathbf{X}}\|_2/\|\mathbf{X}\|_2$ of rank-one approximation under rank-one matrix recovery model, for input $\mathbf{X} \in \mathbb{R}^p$ drawn from additive spiked model, and $\hat{\mathbf{X}} = \lambda_1(\mathbf{X})\hat{\mathbf{u}}_1\hat{\mathbf{u}}_1^\mathsf{T}$ the optimal rank-one approximation of $\mathbf{X}$ given by its top eigenvalue-eigenvector pair $(\lambda_1(\mathbf{X}), \hat{\mathbf{u}}_1)$.

Proposition (Relative spectral error of low-rank approximation)

Let $\mathbf{X} \in \mathbb{R}^{p\times n}$ be an additive spiked random matrix as defined in Equation (47) for $\mathbf{Z}$ having i.i.d. sub-gaussian entries of zero mean and unit variance, and let $\hat{\mathbf{X}} = \lambda_1(\mathbf{X})\hat{\mathbf{u}}_1\hat{\mathbf{u}}_1^\mathsf{T}$ the optimal rank-one approximation of $\mathbf{X}$ given by its top eigenvalue-eigenvector pair $(\lambda_1(\mathbf{X}), \hat{\mathbf{u}}_1)$. Then, one has,

(i) *in the **classical** regime, for p fixed and $n \to \infty$ that*

$$\frac{\|\mathbf{X}-\hat{\mathbf{X}}\|_2}{\|\mathbf{X}\|_2} \to f_{n\gg p}(\ell) \equiv \frac{1}{1+\ell}, \tag{49}$$

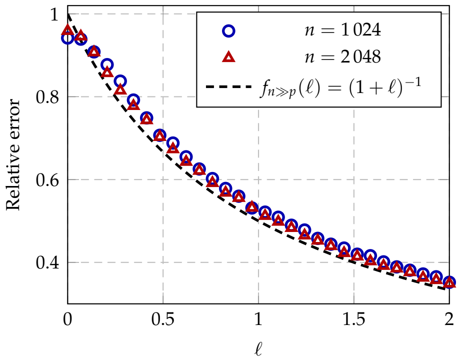
almost surely; and

(ii) *in the **proportional** regime, as $n, p \to \infty$ with $p/n \to c \in (0,\infty)$ that*

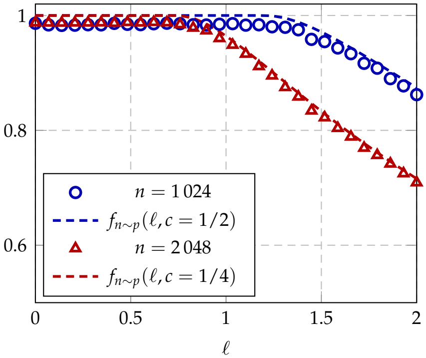
$$\frac{\|\mathbf{X}-\hat{\mathbf{X}}\|_2}{\|\mathbf{X}\|_2} \to f_{n\sim p}(\ell, c) \equiv \begin{cases} \frac{(1+\sqrt{c})^2}{1+\ell+\frac{c}{\ell-c}}, & \ell > c+\sqrt{c} \\ 1, & \ell \leq c+\sqrt{c} \end{cases} \tag{50}$$

almost surely.

Numerical results



(a) $p = 4$



(b) $p = 512$

- sharp phase transition of the relative error as the signal strength ℓ increases
- for p large and fixed, transition thresholds in ℓ are different for different values of n, and they become smaller as the dimension n increases from 1 024 to 2 048

Proof in the classical regime

- evoking the LLN, one has
$$\mathbf{X} \to \mathbb{E}[\mathbf{X}] = \mathbf{I}_p + \ell \mathbf{u}\mathbf{u}^\mathsf{T}, \tag{51}$$
almost surely as $n \to \infty$ for p fixed
- in the classical $n \gg p$ regime, $\mathbf{X}$ is close, in *both* an infinity and a spectral norm sense, to its expectation $\mathbb{E}[\mathbf{X}] = \mathbf{I}_p + \ell \mathbf{u}\mathbf{u}^\mathsf{T}$, and the eigenvalues $\lambda_i(\mathbf{X})$ of $\mathbf{X}$, when arranged in a non-increasing order, are (asymptotically and approximately) given by
$$\|\mathbf{X}\|_2 \approx \lambda_1(\mathbf{X}) = 1 + \ell \geq \lambda_2(\mathbf{X}) = \ldots = \lambda_p(\mathbf{X}) \approx 1. \tag{52}$$
- for $n \gg p$ that
$$\frac{\|\mathbf{X} - \hat{\mathbf{X}}\|_2}{\|\mathbf{X}\|_2} \approx \frac{\lambda_2(\mathbb{E}[\mathbf{X}])}{\lambda_1(\mathbb{E}[\mathbf{X}])} = \frac{1}{1+\ell} \equiv f_{n \gg p}(\ell). \tag{53}$$
The approximation "$\approx$" can be replaced by an almost sure convergence in the limit of $n \to \infty$ for p fixed

Proof in the proportional regime

As a matter of fact, we know precisely what happens in the proportional $n \sim p$ regime:

(i) by **??**, in the absence of the information signal $\ell \mathbf{u}\mathbf{u}^\mathsf{T}$ (i.e., $\ell = 0$), the eigenvalues of $\mathbf{X}$ have a Marčenko-Pastur shape and differ from those of $\mathbb{E}[\mathbf{X}]$ by a relative error of $\pm 20\%$ even with $n = 100p$; and

(ii) by Theorem 12, in the presence of the rank-one informative signal $\ell \mathbf{u}\mathbf{u}^\mathsf{T}$ in Equation (47), that depending the "signal strength" $\|\ell \mathbf{u}\mathbf{u}^\mathsf{T}\|_2 = \ell > 0$, the largest eigenvalue of $\mathbf{X}$ establishes a *phase transition* behavior and is *no longer* a smooth function of ℓ (as opposed to its classical counterpart in Equation (52) and in Item (i) of Proposition 1).

It follows from Theorem 12 that, for additive spiked model of the type Equation (47), one has

$$\|\mathbf{X}\|_2 \to \bar\lambda_1 = \begin{cases} 1 + \ell + \frac{c}{\ell - c}, & \ell > c + \sqrt{c} \\ (1+\sqrt{c})^2, & \ell \leq c + \sqrt{c}. \end{cases} \tag{54}$$

almost surely as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$. Since $\|\mathbf{X} - \hat{\mathbf{X}}\|_2 = \lambda_2(\mathbf{X})$ and $\lambda_2(\mathbf{Z}\mathbf{Z}^\mathsf{T}/n) \leq \lambda_2(\mathbf{X}) \leq \lambda_1(\mathbf{Z}\mathbf{Z}^\mathsf{T}/n)$ (again by Weyl's inequality), one has also

$$\|\mathbf{X} - \hat{\mathbf{X}}\|_2 \to (1+\sqrt{c})^2, \tag{55}$$

almost surely, so that by Slutsky's Theorem, one has $\frac{\|\mathbf{X} - \hat{\mathbf{X}}\|_2}{\|\mathbf{X}\|_2} \to f_{n\sim p}(\ell, c)$.

Gaussian Mixture Model classification

Definition (Gaussian Mixture Model, GMM)

We say $\mathbf{x} \in \mathbb{R}^p$ follows a two-class ($\mathcal{C}_1$ and $\mathcal{C}_2$) Gaussian Mixture Model if it is drawn from one of the two multivariate Gaussian distribution, that is

$$\mathcal{C}_1 : \mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}_1, \mathbf{I}_p), \quad \mathcal{C}_2 : \mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}_2, \mathbf{I}_p); \quad \Delta\boldsymbol{\mu} \equiv \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2, \quad \|\Delta\boldsymbol{\mu}\| = \Theta(1). \tag{56}$$

Proposition (Fundamental limits of GMM classification: pairwise versus spectral approach)

For Gaussian mixture classification between $\mathcal{N}(\boldsymbol{\mu}_1, \mathbf{I}_p)$ and $\mathcal{N}(\boldsymbol{\mu}_2, \mathbf{I}_p)$, with $\Delta\boldsymbol{\mu} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2$, one has, for some constant $C > 0$ independent of p,

(i) *based on a pairwise (Euclidean) distance comparison approach, one is able to separate binary Gaussian mixtures satisfying $\|\Delta\boldsymbol{\mu}\| \geq Cp^{1/4}$; and*

(ii) *based on an eigenspectral approach, one is able to separate a closer distance of $\|\Delta\boldsymbol{\mu}\| \geq C$, which is, up to a constant factor, the minimum distance possible.*

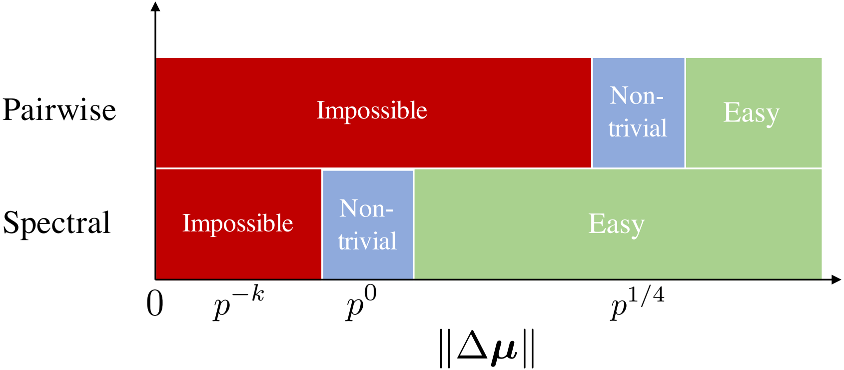


Figure: Illustration of different regimes in separating a binary GMM based on the distance in means $\|\Delta\boldsymbol{\mu}\|$, with $k > 0$, for both pairwise and spectral approaches.

Proof in the classical regime

- classification of the binary Gaussian mixture

$$\mathcal{C}_1 : \mathcal{N}(\boldsymbol{\mu}_1, \mathbf{I}_p) \quad \text{versus} \quad \mathcal{C}_2 : \mathcal{N}(\boldsymbol{\mu}_2, \mathbf{I}_p), \quad \boxed{\Delta\boldsymbol{\mu} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2.} \tag{57}$$

- for two distinct data vectors $\mathbf{x}_i$ and $\mathbf{x}_j$, $i \neq j$, belonging to class $\mathcal{C}_a$ and $\mathcal{C}_b$, $a, b \in \{1, 2\}$, we have $\mathbf{x}_i = \boldsymbol{\mu}_a + \mathbf{z}_i \in \mathcal{C}_a$ and $\mathbf{x}_j = \boldsymbol{\mu}_b + \mathbf{z}_j \in \mathcal{C}_b$, for standard Gaussian $\mathbf{z}_i, \mathbf{z}_j \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$. Then, their (normalized) Euclidean distance is given by

$$\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b + \mathbf{z}_i - \mathbf{z}_j\|^2, \tag{58}$$

which is also the (i, j) entry of the Euclidean distance matrix $\mathbf{E} \equiv \{\|\mathbf{x}_i - \mathbf{x}_j\|^2/p\}_{i,j=1}^n$.

- so

$$\begin{aligned}
\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 &= \frac{1}{p}\|\mathbf{z}_i - \mathbf{z}_j\|^2 + \frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2 + \frac{2}{p}(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^{\mathsf{T}}(\mathbf{z}_i - \mathbf{z}_j) \\
&= \frac{1}{p}\|\mathbf{z}_i\|^2 + \frac{1}{p}\|\mathbf{z}_j\|^2 - \frac{2}{p}\mathbf{z}_i^{\mathsf{T}}\mathbf{z}_j + \frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2 + \frac{2}{p}(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^{\mathsf{T}}(\mathbf{z}_i - \mathbf{z}_j).
\end{aligned} \tag{59}$$

Proof in the classical regime

- in expectation, we have $\frac{1}{p}\mathbb{E}\left[\|\mathbf{x}_i - \mathbf{x}_j\|^2\right] = 2 + \frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2$, for $i \neq j$, where we used the fact that $\mathbb{E}[\mathbf{z}_i^\mathsf{T}\mathbf{z}_i]/p = \operatorname{tr}(\mathbb{E}[\mathbf{z}_i\mathbf{z}_i^\mathsf{T}])/p = 1$;

$$\begin{aligned}
\operatorname{Var}\left[\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right] &= \operatorname{Var}\left[\frac{1}{p}(\Delta\mathbf{z} + 2(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b))^\mathsf{T}\Delta\mathbf{z}\right] \\
&= \frac{4}{p^2}\mathbb{E}\left[(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^\mathsf{T}\Delta\mathbf{z}\Delta\mathbf{z}^\mathsf{T}(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b) + (\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^\mathsf{T}\Delta\mathbf{z}\Delta\mathbf{z}^\mathsf{T}\Delta\mathbf{z}\right] + \frac{1}{p^2}\operatorname{Var}[\|\Delta\mathbf{z}\|^2] \\
&= \frac{8}{p^2}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2 + \frac{8}{p} \leq \frac{16}{p}
\end{aligned}$$

  for $\Delta\mathbf{z} \equiv \mathbf{z}_i - \mathbf{z}_j \sim \mathcal{N}(\mathbf{0}, 2\mathbf{I}_p)$ and $\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\| \leq \sqrt{p}$.
- to ensure that the pairwise approach works, one must have that the distances between data points $\mathbf{x}_i, \mathbf{x}_j$ from the *same* Gaussian (with $a = b$) are, with non-trivial probability, smaller than those from *different* Gaussian (with $a \neq b$). This requires that

$$2 \pm \sqrt{Cp^{-1}} \leq 2 + \|\Delta\boldsymbol{\mu}\|^2/p \pm \sqrt{Cp^{-1}} \tag{60}$$

  and therefore

$$\boxed{\|\Delta\boldsymbol{\mu}\| \geq C' p^{1/4},} \tag{61}$$

  for some $C, C' > 0$ independent of p.

Proof in the proportional regime

- consider the more challenging setting of $\|\Delta\boldsymbol{\mu}\| = \Theta(1)$ in the proportional regime, that classification remains doable via an eigenspectral approach on Euclidean distance matrix $\mathbf{E} = \{\|\mathbf{x}_i - \mathbf{x}_j\|^2/p\}_{i,j=1}^n$
- for $\|\Delta\boldsymbol{\mu}\| = \Theta(1)$ and n, p both large, it follows from the expansion in Equation (59) that

$$\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 = 2 + \underbrace{\psi_i + \psi_j - \frac{2}{p}\mathbf{z}_i^\mathsf{T}\mathbf{z}_j}_{O(p^{-1/2})} + \underbrace{\frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2 + \frac{2}{p}(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^\mathsf{T}(\mathbf{z}_i - \mathbf{z}_j)}_{O(p^{-1})} \tag{62}$$

  where we denote $\psi_i \equiv \|\mathbf{z}_i\|^2/p - 1$ with $\mathbb{E}[\psi_i] = 0$ and $\mathrm{Var}[\psi_i] = 2/p$.
- in matrix form,

$$\mathbf{E} = 2 \cdot \mathbf{1}_n\mathbf{1}_n^\mathsf{T} + \boldsymbol{\psi}\mathbf{1}_n^\mathsf{T} + \mathbf{1}_n\boldsymbol{\psi}^\mathsf{T} - \frac{2}{p}\mathbf{Z}^\mathsf{T}\mathbf{Z} + \frac{1}{p}\mathbf{J}\begin{bmatrix} 0 & \|\Delta\boldsymbol{\mu}\|^2 \\ \|\Delta\boldsymbol{\mu}\|^2 & 0 \end{bmatrix}\mathbf{J}^\mathsf{T} + \boldsymbol{\Theta} - \mathrm{diag}(\cdot) \tag{63}$$

  where we denote $\mathbf{J} = \begin{bmatrix}\mathbf{j}_1 & \mathbf{j}_2\end{bmatrix} \in \mathbb{R}^{n\times 2}$ for $\mathbf{j}_a \in \mathbb{R}^n$ the label vector of class $\mathcal{C}_a$ such that $[\mathbf{j}_a]_i = \delta_{\mathbf{x}_i \in \mathcal{C}_a}$, $\boldsymbol{\psi} \in \mathbb{R}^n$ a random vector containing ψ_i as its i-th entry, $\boldsymbol{\Theta} \equiv \{2(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^\mathsf{T}(\mathbf{z}_i - \mathbf{z}_j)/p\}_{i,j=1}^n$, and we use the notation $\mathbf{X} - \mathrm{diag}(\cdot)$ to remove the diagonal of a given matrix $\mathbf{X}$.

Proof in the proportional regime

$$\mathbf{E} = 2 \cdot \mathbf{1}_n \mathbf{1}_n^\top + \boldsymbol{\psi} \mathbf{1}_n^\top + \mathbf{1}_n \boldsymbol{\psi}^\top - \frac{2}{p} \mathbf{Z}^\top \mathbf{Z} + \frac{1}{p} \mathbf{J} \begin{bmatrix} 0 & \|\Delta \boldsymbol{\mu}\|^2 \\ \|\Delta \boldsymbol{\mu}\|^2 & 0 \end{bmatrix} \mathbf{J}^\top + \boldsymbol{\Theta} - \operatorname{diag}(\cdot) \tag{64}$$

- a low-rank non-informative matrix $2 \cdot \mathbf{1}_n \mathbf{1}_n^\top + \boldsymbol{\psi} \mathbf{1}_n^\top + \mathbf{1}_n \boldsymbol{\psi}^\top$ of spectral norm of order $O(n)$
- a sample covariance-type random matrix $2\mathbf{Z}^\top \mathbf{Z}/p$ for $\mathbf{Z} \in \mathbb{R}^{p \times n}$ having i.i.d. standard Gaussian entries, the spectrum of which follows a Marčenko-Pastur shape (and is of order $O(1)$)
- a low-rank informative matrix $\frac{1}{p} \mathbf{J} \begin{bmatrix} 0 & \|\Delta \boldsymbol{\mu}\|^2 \\ \|\Delta \boldsymbol{\mu}\|^2 & 0 \end{bmatrix} \mathbf{J}^\top + \boldsymbol{\Theta}$ that depends on the label vector $\mathbf{j}_1, \mathbf{j}_2 \in \mathbb{R}^n$ (so of interest for classification) and the statistical difference (in means) $\Delta \boldsymbol{\mu}$, also of spectral norm order $O(1)$

(i) while in the critical regime $\|\Delta \boldsymbol{\mu}\| = \Theta(1)$, data vectors $\mathbf{x}_i, \mathbf{x}_j$ are pairwise indistinguishable based on their Euclidean distance, due to the dominant order of the random $\mathbf{z}_i^\top \mathbf{z}_j/p = O(p^{-1/2})$ over the informative term $\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2/p = \Theta(p^{-1})$ in Equation (62);

(ii) they can still be "clustered" into two classes with a spectral approach based on the global observation of the large Euclidean distance matrix $\mathbf{E}$, since the sample covariance-type random matrix and the low-rank informative matrix are both of spectral norm order $O(1)$, and thus comparable for n, p large.

Numerical results

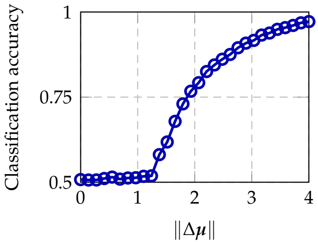


Figure: Phase transition behavior of the classification accuracy using the sign of the second top eigenvector $\mathbf{v}_2$ of the Euclidean distance matrix $\mathbf{E}$, as a function of the statistical difference $\|\Delta\boldsymbol{\mu}\|$ in the non-trivial $\|\Delta\boldsymbol{\mu}\| = \Theta(1)$ regime, for $p = 512$, $n = 4p$, and $\mathbf{C}_1 = \mathbf{C}_2 = \mathbf{I}_p$. Results averaged over 10 independent runs.

"More refined" sharp phase transition, the second dominant eigenvector $\mathbf{v}_2$ of $\mathbf{E}$:

(i) for n, p fixed and large, when $\|\Delta\boldsymbol{\mu}\|$ below threshold, $\mathbf{v}_2$ does not contain data class information, the clustering/classification based on $\operatorname{sign}(\mathbf{v}_2)$ **random guess**

(ii) above the phase transition threshold, the eigenvector $\mathbf{v}_2$ contains data class information $\mathbf{j}_a$, and the classification accuracy increases as $\|\Delta\boldsymbol{\mu}\|$ and/or n/p becomes large.

Noisy linear model

Consider a given set of data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ of size n, composed of the (random) input data $\mathbf{x}_i \in \mathbb{R}^p$ and its corresponding output target $y_i \in \mathbb{R}$, drawn from the following noisy linear model.

Definition (Noisy linear model)

We say a data-target pair $(\mathbf{x}, y) \in \mathbb{R}^p \times \mathbb{R}$ follows a noisy linear model if it satisfies

$$y = \boldsymbol{\beta}_*^\mathsf{T} \mathbf{x} + \epsilon \tag{65}$$

for some deterministic (ground-truth) vector $\boldsymbol{\beta}_* \in \mathbb{R}^p$, and random variable $\epsilon \in \mathbb{R}$ independent of $\mathbf{x} \in \mathbb{R}^p$, with $\mathbb{E}[\epsilon] = 0$ and $\mathrm{Var}[\epsilon] = \sigma^2$.

- aim to find a regressor $\boldsymbol{\beta} \in \mathbb{R}^p$ that best describes the linear relation $y_i \approx \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i$, by minimizing the ridge-regularized mean squared error (MSE)

$$L(\boldsymbol{\beta}) = \frac{1}{n} \sum_{i=1}^n (y_i - \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i)^2 + \gamma \|\boldsymbol{\beta}\|^2 = \frac{1}{n} \|\mathbf{X}^\mathsf{T} \boldsymbol{\beta} - \mathbf{y}\|^2 + \gamma \|\boldsymbol{\beta}\|^2 \tag{66}$$

for $\mathbf{y} = [y_1, \ldots, y_n]^\mathsf{T} \in \mathbb{R}^n$, $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$, and some regularization penalty $\gamma \geq 0$

Out-of-sample prediction risk

- unique solution given by

$$\boldsymbol{\beta}_\gamma = \left(\mathbf{X}\mathbf{X}^\mathsf{T} + n\gamma \mathbf{I}_p\right)^{-1} \mathbf{X}\mathbf{y} = \mathbf{X}\left(\mathbf{X}^\mathsf{T}\mathbf{X} + n\gamma \mathbf{I}_n\right)^{-1} \mathbf{y}, \quad \gamma > 0 \tag{67}$$

- in the $\gamma = 0$ setting, the minimum ℓ_2 norm least squares solution

$$\boldsymbol{\beta}_0 = \left(\mathbf{X}\mathbf{X}^\mathsf{T}\right)^{+} \mathbf{X}\mathbf{y} = \mathbf{X}\left(\mathbf{X}^\mathsf{T}\mathbf{X}\right)^{+} \mathbf{y}, \tag{68}$$

  where $(\mathbf{A})^+$ denotes the Moore–Penrose pseudoinverse, also "ridgeless" least squares solution.
- "quality" of the solution $\boldsymbol{\beta}$, as a function of dimensions n, p, noise level σ^2, and the regularization parameter γ
- evaluating the out-of-sample prediction risk (or simply, risk)

$$R_{\mathbf{X}}(\boldsymbol{\beta}) = \mathbb{E}[(\boldsymbol{\beta}^\mathsf{T}\hat{\mathbf{x}} - \boldsymbol{\beta}_*^\mathsf{T}\hat{\mathbf{x}})^2 \mid \mathbf{X}] = \underbrace{(\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*)^\mathsf{T}\mathbf{C}(\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*)}_{\equiv B_{\mathbf{X}}(\boldsymbol{\beta})} + \underbrace{\operatorname{tr}\left(\operatorname{Cov}[\boldsymbol{\beta} \mid \mathbf{X}]\mathbf{C}\right)}_{\equiv V_{\mathbf{X}}(\boldsymbol{\beta})} \tag{69}$$

  for an *independent* test data point. We denote $\mathbb{E}[\mathbf{x}_i\mathbf{x}_i^\mathsf{T}] = \mathbf{C}$, and $B_{\mathbf{X}}(\boldsymbol{\beta}), V_X(\boldsymbol{\beta})$ the **bias** as well as **variance** of the solution $\boldsymbol{\beta}$.

Proposition (Risk of linear ridge regression)

Let $\mathbf{X} \in \mathbb{R}^{p \times n}$ be a random data matrix having i.i.d. sub-gaussian entries of zero mean and unit variance (so that $\mathbf{C} = \mathbf{I}_p$). Then, under the linear model and for the out-of-sample prediction risk $R_{\mathbf{X}}$ of the linear ridge regressor $\boldsymbol{\beta}_\gamma$ given in Equation (67), one has $R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) + V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma)$ and

(i) *in the **classical** regime, for p fixed and $n \to \infty$ that*

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - \left(\frac{\gamma}{1+\gamma} \right)^2 \|\boldsymbol{\beta}_*\|^2 \to 0, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - \frac{p}{n} \frac{\sigma^2}{(1+\gamma)^2} \to 0, \tag{70}$$

almost surely, so that $R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - R_{n \gg p}(\gamma) \to 0$, with $R_{n \gg p}(\gamma) \equiv \frac{\gamma^2 \|\boldsymbol{\beta}_*\|^2 + \frac{p}{n}\sigma^2}{(1+\gamma)^2}$;

(ii) *in the **proportional** regime, as $n, p \to \infty$ with $p/n \to c \in (0,1) \cup (1, \infty)$ that*

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - \gamma^2 \|\boldsymbol{\beta}_*\|^2 m'(-\gamma) \to 0, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - \sigma^2 c \left(m(-\gamma) - \gamma m'(-\gamma) \right) \to 0, \tag{71}$$

almost surely, with $m'(-\gamma) = \frac{m(-\gamma)(cm(-\gamma)+1)}{2c\gamma m(-\gamma)+1-c+\gamma}$ by differentiating the Marčenko-Pastur equation

$$R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) - R_{n \sim p}(\gamma) \to 0, \quad \text{with} \quad R_{n \sim p}(\gamma) \equiv \sigma^2 c m(-\gamma) + \gamma m'(-\gamma) \left(\sigma^2 c - \gamma \|\boldsymbol{\beta}_*\|^2 \right). \tag{72}$$

Numerical results

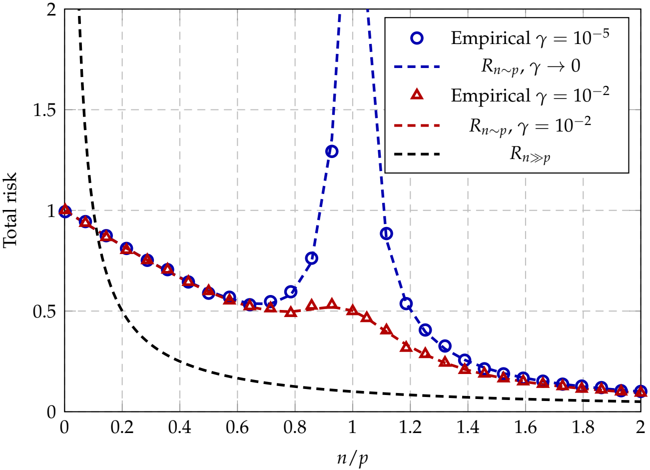


Figure: Out-of-sample risk $R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) + V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma)$ of the ridge regression solution $\boldsymbol{\beta}_\gamma$ defined in Equation (67) as a function of the dimension ratio n/p, for fixed $p = 512$, $\|\boldsymbol{\beta}_*\| = 1$, and different regularization penalty $\gamma = 10^{-2}$ and $\gamma = 10^{-5}$, Gaussian $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2 = 0.1)$.

Remark

for relatively small regularization $\gamma = 10^{-5}$ and as the sample size n increases, that the total risk $R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma)$:

1. first decreases and then increases as n approaches the input dimension p in the under-determined $n < p$ regime; and
2. reaches a singular "peak point" at $n = p$ with a large risk; and
3. decreases again monotonically as n continues to increase, in the over-determined $n > p$ regime.

This phenomenon is largely alleviated, yet still visible, for larger regularization of $\gamma = 10^{-2}$, and is referred to as the "**double descent**" test curve.

Proof in the classical regime

- denote $\mathbf{Q}(-\gamma) \equiv (\hat{\mathbf{C}} + \gamma \mathbf{I}_p)^{-1}$ the **resolvent** of the (un-centered) sample covariance matrix $\hat{\mathbf{C}} = \frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ and $\mathbf{Q}(\gamma = 0) = \lim_{\gamma \downarrow 0} \mathbf{Q}(-\gamma) = \hat{\mathbf{C}}^+$.
- we can write

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \boldsymbol{\beta}_*^\mathsf{T} \left(\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}}\right) \mathbf{C} \left(\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}}\right) \boldsymbol{\beta}_*, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \frac{\sigma^2}{n} \operatorname{tr}\left(\mathbf{Q}(-\gamma)\hat{\mathbf{C}}\mathbf{Q}(-\gamma)\mathbf{C}\right). \tag{73}$$

- for $\gamma > 0$, one has $\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}} = \mathbf{I}_p - \mathbf{Q}(-\gamma)(\hat{\mathbf{C}} + \gamma\mathbf{I}_p - \gamma\mathbf{I}_p) = \gamma\mathbf{Q}(-\gamma)$, so that

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \gamma^2 \boldsymbol{\beta}_*^\mathsf{T} \mathbf{Q}^2(-\gamma)\boldsymbol{\beta}_* = -\gamma^2 \frac{\partial \boldsymbol{\beta}_*^\mathsf{T} \mathbf{Q}(-\gamma)\boldsymbol{\beta}_*}{\partial \gamma}, \tag{74}$$

$$V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \sigma^2 \left(\frac{1}{n}\operatorname{tr}\mathbf{Q}(-\gamma) - \frac{\gamma}{n}\operatorname{tr}\mathbf{Q}^2(-\gamma)\right) = \sigma^2 \left(\frac{1}{n}\operatorname{tr}\mathbf{Q}(-\gamma) + \frac{\gamma}{n}\frac{\partial \operatorname{tr}\mathbf{Q}(-\gamma)}{\partial \gamma}\right), \tag{75}$$

where we used the fact that $\mathbf{C} = \mathbf{I}_p$ and $\partial\mathbf{Q}(-\gamma)/\partial\gamma = -\mathbf{Q}^2(-\gamma)$.

Proof in the classical regime

- by LLN, we have, in the classical regime for fixed p and as $n \to \infty$ that $\hat{\mathbf{C}} \to \mathbf{C} = \mathbf{I}_p$, and therefore

$$\mathbf{Q}(-\gamma) \to (\mathbf{C} + \gamma \mathbf{I}_p)^{-1} = \frac{\mathbf{I}_p}{1+\gamma}. \tag{76}$$

- we have that

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) \to -\gamma^2 \frac{\partial}{\partial \gamma} \frac{\|\boldsymbol{\beta}_*\|^2}{1+\gamma} = \left(\frac{\gamma}{1+\gamma} \right)^2 \|\boldsymbol{\beta}_*\|^2,$$
$$V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) \to \sigma^2 \left(\frac{p}{n} \frac{1}{1+\gamma} + \gamma \cdot \frac{p}{n} \frac{\partial}{\partial \gamma} \frac{1}{1+\gamma} \right) = \frac{p}{n} \frac{\sigma^2}{(1+\gamma)^2}.$$

- in the ridgeless setting with $\gamma = 0$

$$B_{\mathbf{X}}(\boldsymbol{\beta}_0) = 0, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_0) = \frac{\sigma^2}{n} \operatorname{tr} \left(\mathbf{Q}(\gamma = 0) \mathbf{C} \right) \to \sigma^2 \frac{p}{n}, \tag{77}$$

Proof in the proportional regime

- it follows from our Linear Master Theorem that

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) \to -\gamma^2 \|\boldsymbol{\beta}_*\|^2 \frac{\partial m(-\gamma)}{\partial \gamma} = \gamma^2 \|\boldsymbol{\beta}_*\|^2 m'(-\gamma),$$

$$V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) \to \sigma^2 \cdot \frac{p}{n} \left(m(-\gamma) - \gamma m'(-\gamma) \right),$$

with $m'(z) = -\frac{m(z)(cm(z)+1)}{2czm(z)-1+c+z}$ the derivative of the Stieltjes transform $m(z)$

- in the ridgeless setting as $\gamma \to 0$, one has $m(\gamma) = \frac{1}{1-c} > 0$ only if $c < 1$ and $\lim_{\gamma \to 0} m(\gamma)$ undefined otherwise, but satisfying $\lim_{\gamma \to 0} \gamma m(\gamma) = \frac{c-1}{c} > 0$, in the under-determined regime with $n < p$.

$$B_{\mathbf{X}}(\boldsymbol{\beta}_0) \to 0, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_0) \to \sigma^2 \frac{c}{1-c}, \text{ for } c < 1 \tag{78}$$

$$B_{\mathbf{X}}(\boldsymbol{\beta}_0) - \|\boldsymbol{\beta}_*\|^2 \left(1 - \frac{1}{c}\right) \to 0, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_0) \to \sigma^2 \frac{1}{c-1}, \text{ for } c > 1 \tag{79}$$

- **Note**: for $c > 1$, $V_{\mathbf{X}}(\boldsymbol{\beta}_0)$ more involved, as one *cannot* take the limit $\gamma \to 0$. Instead,

$$V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \frac{\sigma^2}{n^2} \operatorname{tr}\left(\tilde{\mathbf{Q}}(-\gamma) \mathbf{X}^\mathsf{T} \mathbf{C} \mathbf{X} \tilde{\mathbf{Q}}(-\gamma) \right), \quad \tilde{\mathbf{Q}}(-\gamma) \equiv \left(\frac{1}{n} \mathbf{X}^\mathsf{T} \mathbf{X} + \gamma \mathbf{I}_n \right)^{-1}. \tag{80}$$

which is more convenient to work with in the $c > 1$ regime.

Take-away messages of this section

Table: Roadmap of linear ML models considered.

ML Problem	Classical Regime	Proportional Regime
Low rank approximation $\hat{\mathbf{X}}$ of info-plus-noise matrix $\mathbf{X}$	smooth decay of $\Vert\mathbf{X}-\hat{\mathbf{X}}\Vert_2/\Vert\mathbf{X}\Vert_2 \simeq (1+\ell)^{-1}$ Proposition 1 Item (i)	sharp transition of $\Vert\mathbf{X}-\hat{\mathbf{X}}\Vert_2/\Vert\mathbf{X}\Vert_2$ at $\ell = c+\sqrt{c}$ Proposition 1 Item (ii)
Classification of binary Gaussian mixtures of distance in means $\Delta\boldsymbol{\mu}$	pairwise $\simeq$ spectral approach Proposition 2 Item (i)	pairwise $\ll$ spectral approach Proposition 2 Item (ii)
Linear least squares regression risk as $n \uparrow$	bias $=0$ and variance $\propto n^{-1}$ Proposition 3 Item (i)	monotonic bias and non-monotonic variance Proposition 3 Item (ii)

Thank you! Q & A?