# LECTURE 24

Last Class: Covariance estimation problem for $X \in \mathbb{R}^d$, $\mathbb{E}X = 0$.

- (Population) covariance matrix: $\Sigma = \mathbb{E}XX^T$
- Sample covariance matrix: $\Sigma_n = \frac{1}{n}\sum_{i=1}^n X_i X_i^T$, where $X_i$ are iid copies of $X$

$$\Sigma_n \overset{?}{\approx} \Sigma \qquad \text{in the operator norm}$$

- $\|\Sigma_n - \Sigma\| = \max_{v \in S^{d-1}} |v^T (\Sigma_n - \Sigma) v|$ (HW)
- $\exists$ $\varepsilon$-net $\mathcal{N} \subset S^{d-1}$, $|\mathcal{N}| \overset{\text{lec. 23}}{\le} \left(\frac{2}{\varepsilon}+1\right)^d = 9^d$ if we choose $\boxed{\varepsilon = 1/4}$
- $\|\Sigma_n - \Sigma\| \le \frac{1}{1-2\varepsilon} \max_{v \in \mathcal{N}} |v^T(\Sigma_n - \Sigma)v|$ (lec. 23 & HW)

$$= 2 \cdot \max_{v \in \mathcal{N}} \underbrace{\left| \frac{1}{n}\sum_{i=1}^n \langle X_i, v\rangle^2 - \mathbb{E}\langle X, v\rangle^2 \right|}_{= S(v)} \le \; ? \qquad (*)$$

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- For each $v$, $S(v)$ = sum of indep. r.v.'s. Use:

THM (Bernstein's inequality: lec. 14 Oct. 3)

i.e. $\mathbb{P}\{|X_i| \ge t\} \le 2\exp\left(-\frac{t}{M}\right)$ $\forall t$, smallest $M = \|X_i\|_{\psi_1}$

> If $X_i$ are independent subexponential r.v.'s
>
> $$\mathbb{P}\left\{\sum_{i=1}^n (X_i - \mathbb{E}X_i) \ge t\right\} \le 2\exp\left[-c \cdot \min\left(\frac{t^2}{\sigma^2}, \frac{t}{K}\right)\right]$$
>
> where $\sigma^2 = \sum_{i=1}^n \|X_i\|_{\psi_1}^2$, $K = \max_i \|X_i\|_{\psi_1}$

Simplify:

If all $X_i$ are independently distributed $\Rightarrow$ $\sigma^2 = K^2 n$

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^n X_i - \mathbb{E}X\right| \ge \delta\right\} \overset{t=\delta n}{\le} 2\exp\left[-c \cdot \min\left(\frac{\delta^2 n^2}{K^2 n}, \frac{\delta n}{K}\right)\right] = 2\exp\left[-c \cdot \min\left(\frac{\delta^2}{K^2}, \frac{\delta}{K}\right) n\right]$$

$(**)$

ALL TOOLS ARE READY TO PROVE:

$$\boxed{\begin{array}{l}\underline{\text{THM}} \text{ (Covariance Estimation) If } X_i \sim N(0,\Sigma) \text{ and } n \geq Cd \\ \qquad \|\Sigma_n - \Sigma\| \leq 0.1\,\|\Sigma\| \\ \text{with probability at least } 1-2e^{-cn}.\end{array}}$$

Proof W.L.O.G. $\|\Sigma\|=1$.

① Fix any $v \in S^{d-1}$. ← unit sphere of $\mathbb{R}^d$.

$X$ = mean 0 normal r. vector $\Rightarrow \langle X,v\rangle \sim$ mean 0 normal r. vector

$\Rightarrow \langle X,v\rangle \sim N(0,\sigma^2)$.
↖? let's compute it.

$$\sigma^2 = \mathbb{E}\langle X,v\rangle^2 = v^T(\mathbb{E}XX^T)v = v^T\Sigma v \leq \|\Sigma\| = 1.$$

$$\Rightarrow \mathbb{P}\{|\langle X,v\rangle| \geq t\} \underset{\uparrow}{\leq} 2\exp\left(-\frac{t^2}{\sigma^2}\right) \leq 2\exp(-t^2)$$

gaussian tail

$$\Rightarrow \mathbb{P}\{\langle X,v\rangle^2 \geq s\} = \mathbb{P}\{|\langle X,v\rangle| \geq \sqrt{s}\} \leq 2\exp(-s)$$

$\Rightarrow \langle X,v\rangle^2$ is subexponential, $\|\langle X,v\rangle^2\|_{\psi_1} \underset{\uparrow}{\leq} C$.

- Apply Bernstein (**p.1) for $X_i = \langle X_i,v\rangle^2$, $K=C$, $\delta=0.01$ $\Rightarrow$

$$\mathbb{P}\Big\{\underbrace{\Big|\frac{1}{n}\sum_{i=1}^n \langle X_i,v\rangle^2 - \mathbb{E}\langle X,v\rangle^2\Big|}_{=\,S(v)} \geq 0.01\Big\} \leq 2\exp(-c'n)$$

② $$\mathbb{P}\Big\{\max_{v\in\mathcal{N}} |S(v)| \geq 0.01\Big\} \leq \underbrace{|\mathcal{N}|}_{\leq\, 9^d \text{ (p.1)}} \cdot 2\exp(-c'n) \leq 2\exp\left(-\frac{c'n}{2}\right)$$

if $\boxed{d < c''n}$ ☺

③ The complement holds w/prob. $\geq 1-2\exp(-c'n/2)$. When it holds,

$$\|\Sigma_n - \Sigma\| \overset{(*)\,p.1}{\leq} 2\cdot\max_{v\in\mathcal{N}}|S(v)| \leq 2\cdot 0.01 \leq 0.1.$$

QED

# PERTURBATION THEORY

From $\Sigma_n \approx \Sigma$ to $\lambda_i(\Sigma_n) \approx \lambda_i(\Sigma)$, $v_i(\Sigma_n) \approx v_i(\Sigma)$:

**THM** (Weyl's inequality) $\forall$ $d\times d$ symmetric matrices $A, B$:

$$\max_i |\lambda_i(A) - \lambda_i(B)| \leq \|A - B\|$$

Eigenvectors: (a) up to sign
(b) spectral gap needed: if $\lambda_k(A) \approx \lambda_{k+1}(A)$, perturbation can swap the order of eigenvectors.

**THM** (Davis–Kahan inequality)

Let $A, B$ be $d\times d$ symmetric matrices, $1 \leq k \leq d$,

$P_A :=$ orthogonal projection onto $\text{span}\{v_1(A), \dots, v_k(A)\}$ and
$P_B :=$ orthogonal projection onto $\text{span}\{v_1(B), \dots, v_k(B)\}$. Then

$$\|P_A - P_B\| \leq \frac{\|A - B\|}{\lambda_k(A) - \lambda_{k+1}(A)}.$$

[see eg. our BSM paper]

- Combine Cov. Est. Thm (p. 2) with Weyl & Davis-Kahan

$\Downarrow$

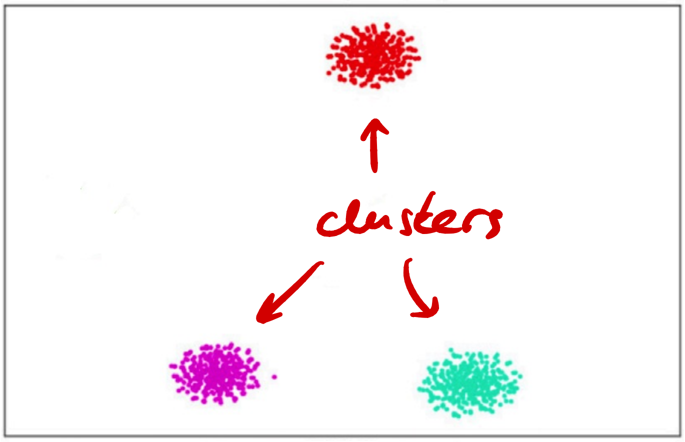
**SUMMARY** $PCA_k(\text{sample}) \approx PCA_k(\text{population})$ as long as:

(a) sample size $n$ is linear in dim $d$ (or larger)

(b) there is an eigengap: the top $k$ eigenvalues of $\Sigma$ are separated from the rest of the spectrum.

HW -state?

Example: single-cell data from [Aparicio et al. 2020]

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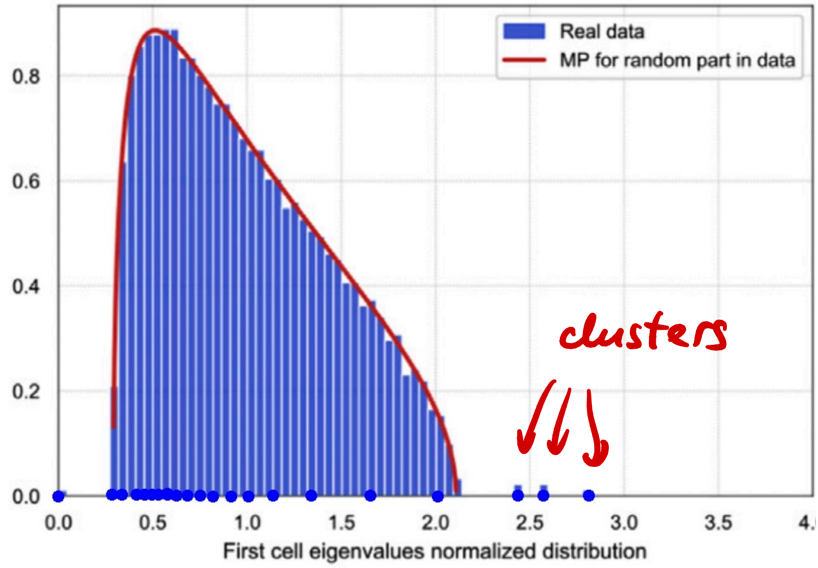



noise
"
bulk

"signal"
"
outliers

$$X \sim N(0, I_n)$$

$$\Sigma = I_n$$

REMARKS: ① Linear sample size $n = O(d)$ is optimal **(HW)**

② Normal distribution $X \sim N(0, \Sigma)$ can be generalized to $\forall$ subgaussian (simple - see book)

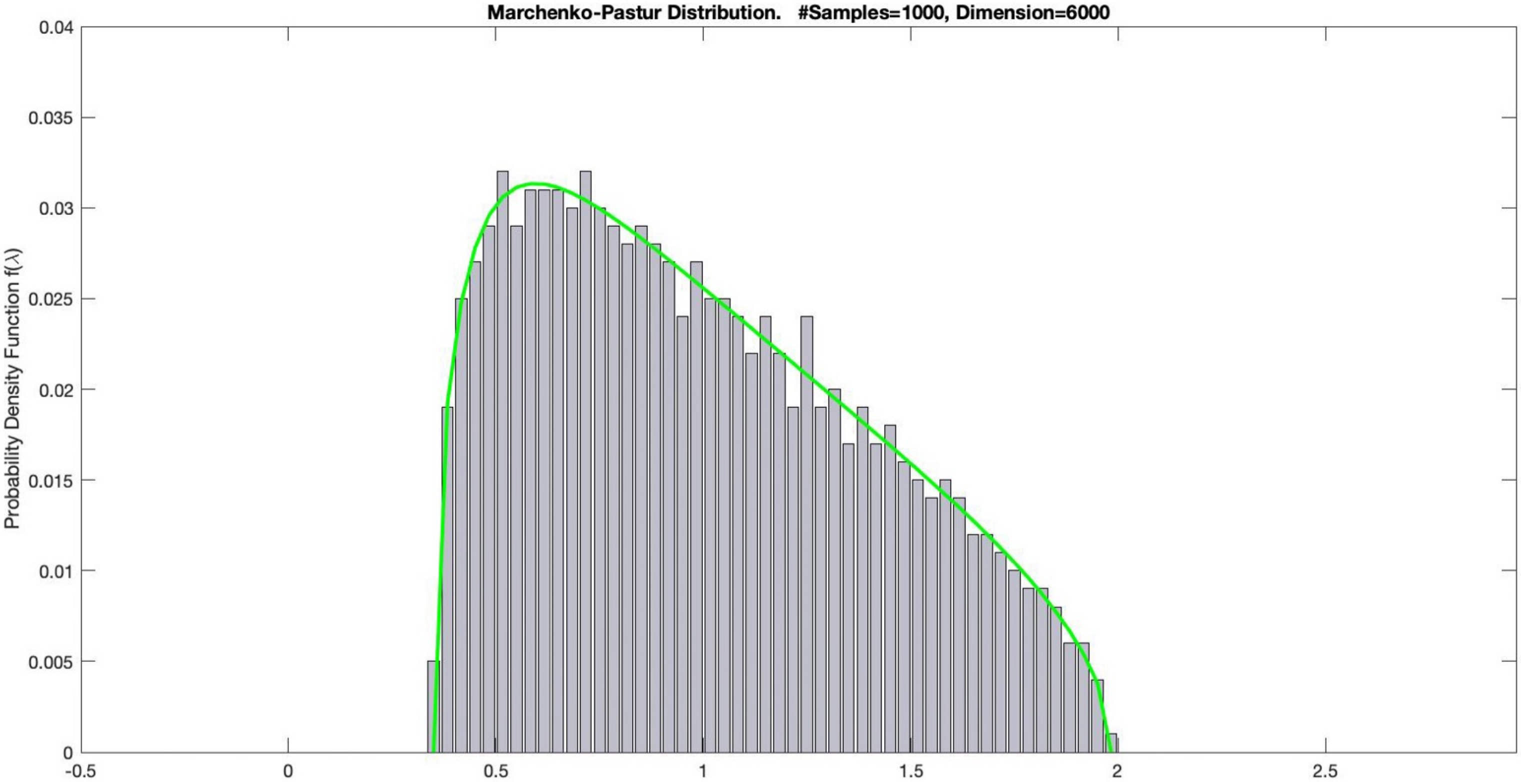
③ Structured data $\Rightarrow$ smaller sample size $n$?

Yes: (a) trivially, if $X = (X_1, X_1, \dots, X_1)$ then represent $X \in \mathbb{R}^1 \Rightarrow n = O(1)$.

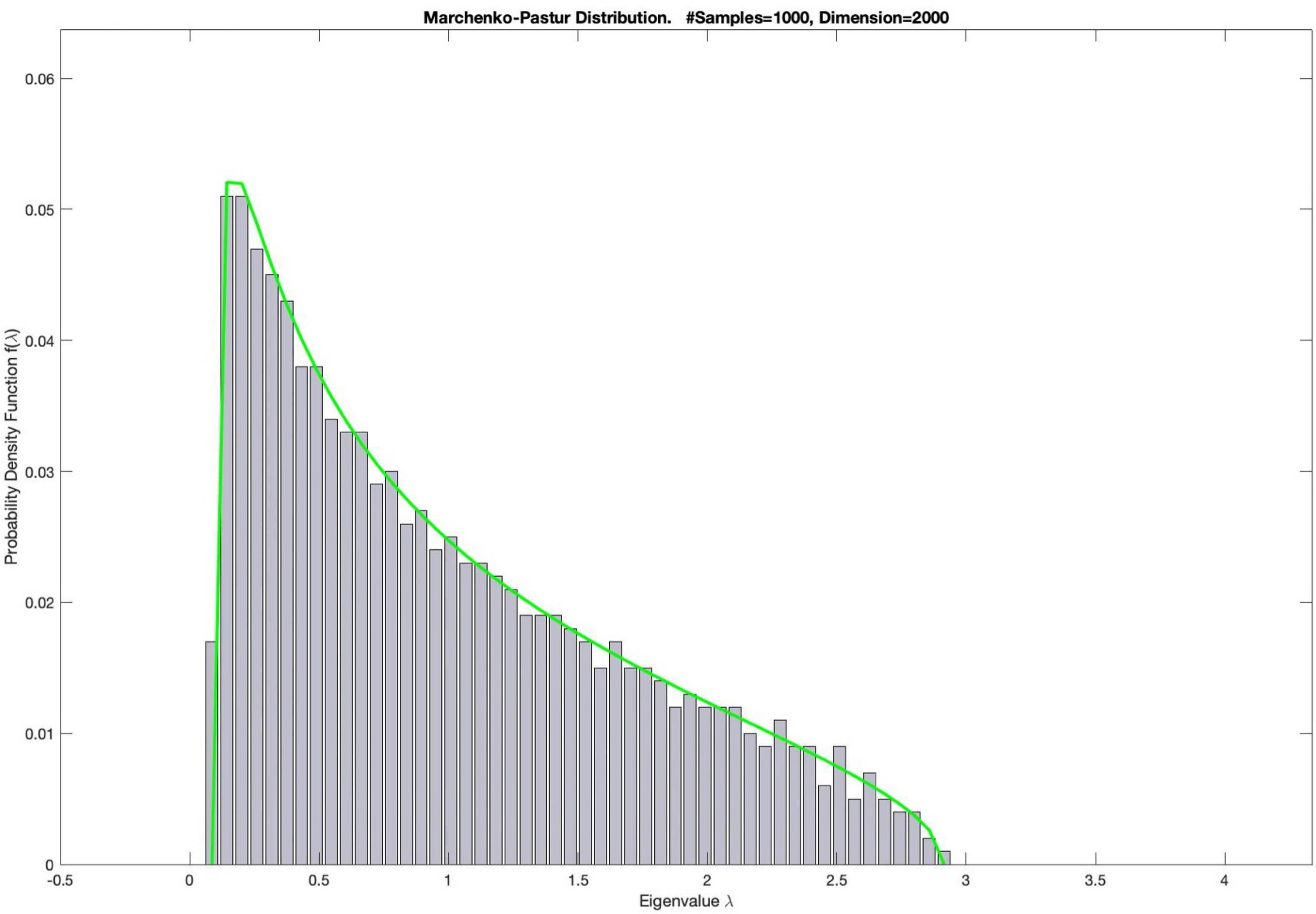
(b) more generally, if data is approximately $k$-dimensional, $k = O(n)$ is enough.

[Koltchinskii-Lounici 2017] = Thm. 9.2.4 in the book

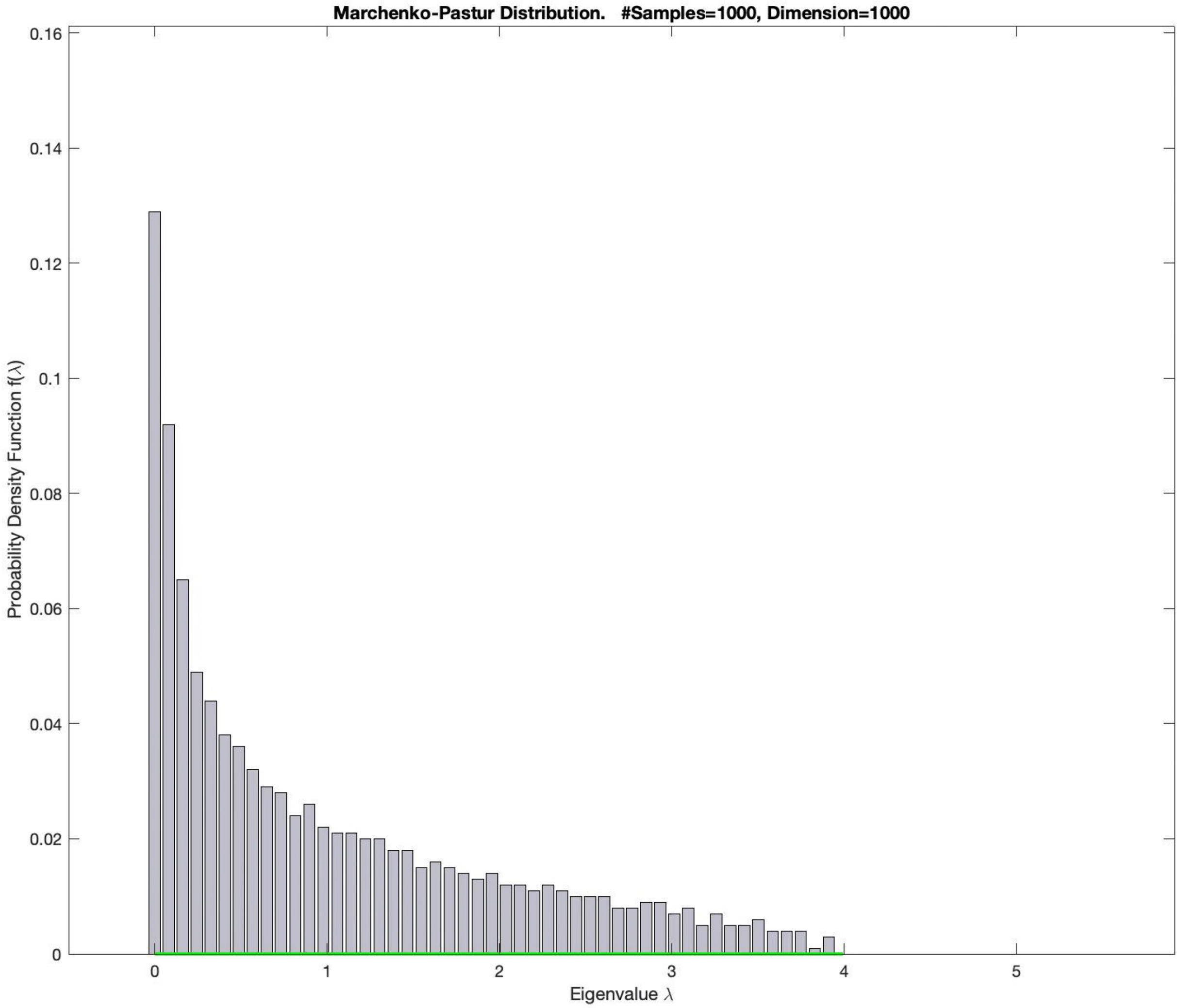
We will prove later (a version).

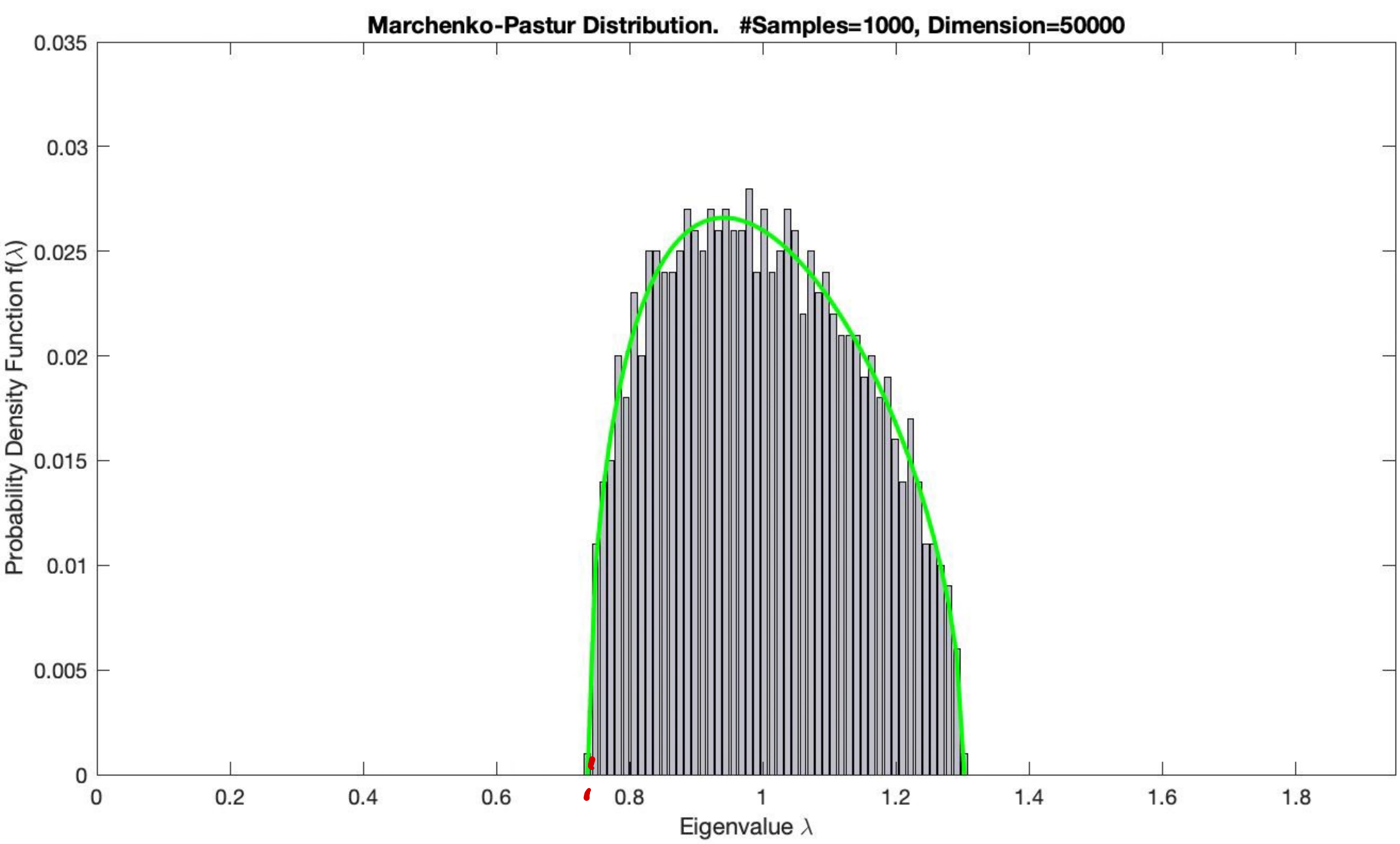


Marchenko-Pastur Distribution. #Samples=1000, Dimension=6000
Probability Density Function f(λ)
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
-0.5
0
0.5
1
1.5
2
2.5

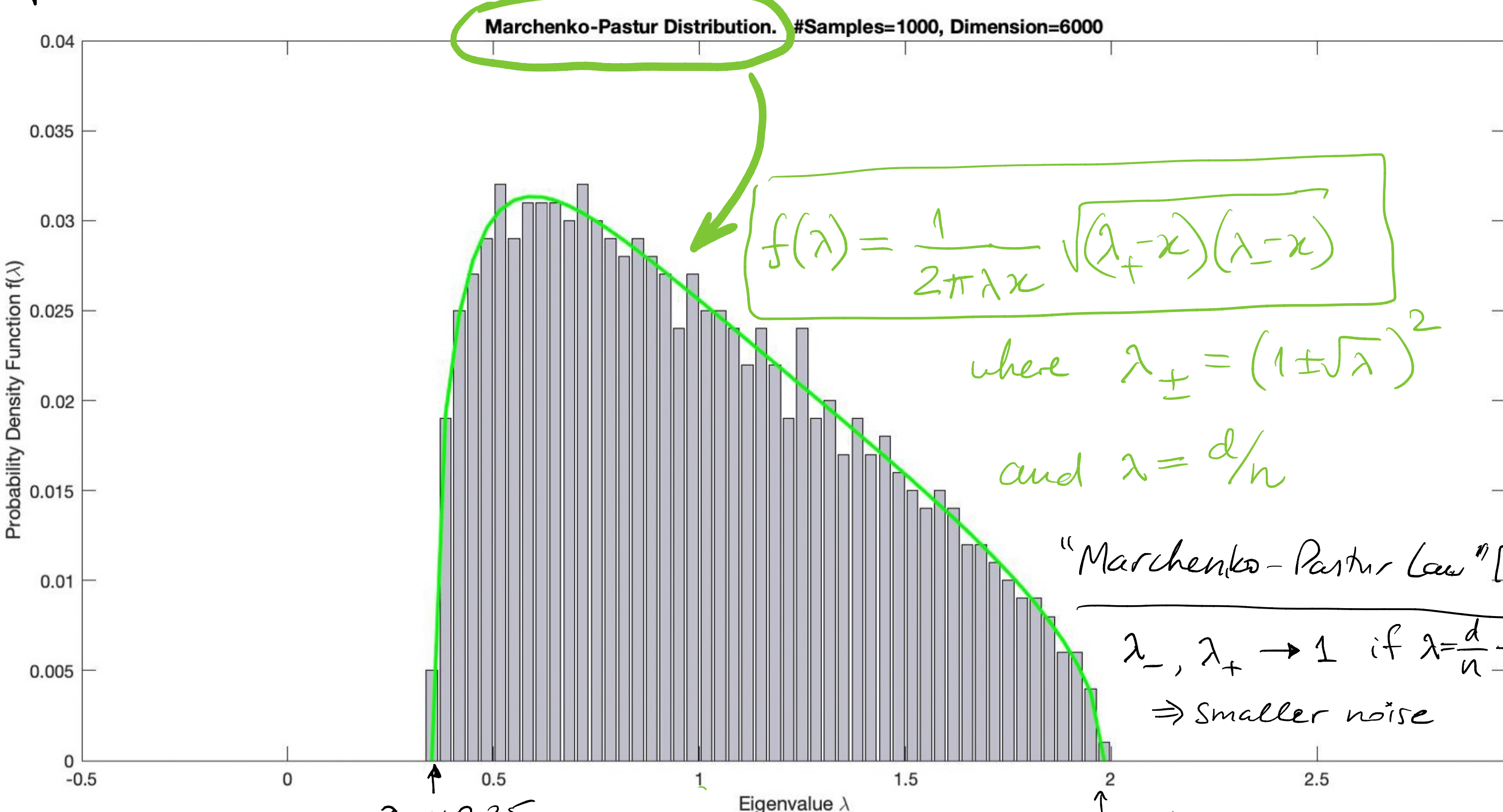
Marchenko-Pastur Distribution. #Samples=1000, Dimension=2000
Probability Density Function f(λ)
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.5
0
0.5
1
1.5
2
2.5
3
3.5
4
Eigenvalue λ


Marchenko-Pastur Distribution. #Samples=1000, Dimension=1000
Probability Density Function f(λ)
Eigenvalue λ


Marchenko-Pastur Distribution. #Samples=1000, Dimension=50000
Probability Density Function f(λ)
Eigenvalue λ

- histogram $\operatorname{eigs}(\Sigma_n)$ seems $\rightarrow$ density as $d, n \rightarrow \infty$, $\boxed{\frac{d}{n} \rightarrow \lambda}$

compactly supported! No outliers (good for PCA)




$$\boxed{f(\lambda) = \frac{1}{2\pi\lambda x}\sqrt{(\lambda_+ - x)(\lambda_- - x)}}$$

where $\lambda_\pm = (1 \pm \sqrt{\lambda})^2$

and $\lambda = d/n$

"Marchenko-Pastur Law" [1967]

$\lambda_-, \lambda_+ \rightarrow 1$ if $\lambda = \frac{d}{n} \rightarrow \infty$

$\Rightarrow$ smaller noise

$\lambda_- \approx 0.35$

$\lambda_+ \approx 1.9$