Optimal detection of principal components in high-dimensional data

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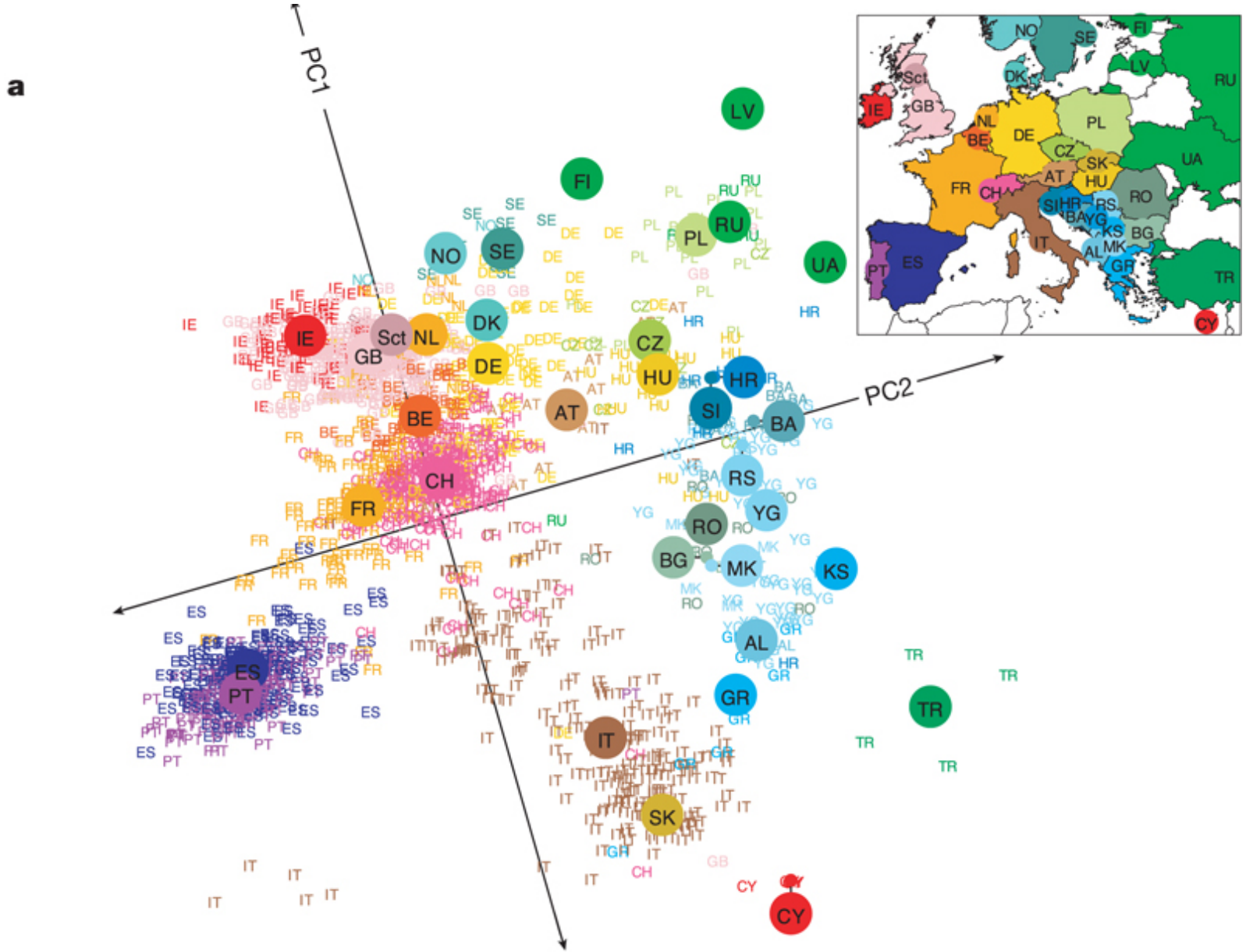
Outline

slides available at github.com/dobriban

PCA

- Principal component analysis (PCA) is a widely used method for dimension reduction
- X an $n \times p$ matrix.
  - n samples from centered p-dimensional population
  - n individuals, p features: genetic markers, phenotypes (age, height...)
- PCs: linear combinations Xu_i of features that explain a lot of variance
- u_i - eigenvectors of sample covariance matrix $\widehat{\Sigma} = n^{-1}X^\top X$
- corresponding eigenvalue λ_i is variance of PC

Genes mirror geography within Europe – Novembre et al. (2008)



Motivating problem: Testing/detection in PCA

- First two eigenvectors "obviously" meaningful
- What about the next ones?
- For objective data analysis, need hypothesis test of the PC variances λ_i

Review: Hypothesis testing (Neyman-Pearson, 1930s)

- observed data X
- depends on unobserved parameter $\Sigma \in S$: $X \sim P_\Sigma$
- partition $S = S_0 \cup S_1$
  - null hypothesis $H_0 : \Sigma \in S_0$
  - alternative hypothesis $H_1 : \Sigma \in S_1$
- Neyman-Pearson: construct test statistic $T(X)$ s.t.
  - under H_0, the level $\mathbb{P}\{T(X) \geq c\} \leq 0.05$
  - under H_1, the power $\mathbb{P}\{T(X) \geq c\}$ is large
- "detect" $\Sigma \in S_1$

Example: Hypothesis testing

- observed data $X \in \mathbb{R}$
- depends on unobserved parameter $\mu \in \mathbb{R}$: $X \sim \mathcal{N}(\mu, 1)$
- partition $\mathbb{R} = (-\infty, 0] \cup (0, \infty)$
  - null hypothesis $H_0 : \mu \leq 0$
  - alternative hypothesis $H_1 : \mu > 0$
- Neyman-Pearson: construct test statistic $T(X)$ s.t.
  - if $\mu \leq 0$, the level $\mathbb{P}\{T(X) \geq c\} \leq 0.05$
  - if $\mu > 0$, the power $\mathbb{P}\{T(X) \geq c\}$ is large
- "detect" $\mu > 0$
- Take $T(X) = X$, c s.t. $\mathbb{P}\{\mathcal{N}(0, 1) \geq c\} = 0.05$

PCA in practice

- "scree plot" : eigenvalues in decreasing order
- look for the elbow - separated eigenvalue
- in high-dimension, this may miss "weak" PCs

PCA Review: bulk eigenvalues

- $X = Z_{n\times p}\Sigma^{1/2}$
  - $Z_{n\times p}$ has iid standardized entries
  - Σ unobserved $p \times p$ covariance matrix: Cov $[x_i, x_i] = \Sigma$
- high dimension: $n, p \to \infty$, $p/n \to \gamma > 0$ (wlog $p/n = \gamma$)
- $l_1 \geq l_2 \geq \ldots \geq l_p$ eigenvalues of Σ. Distribution $H_p = p^{-1}\sum_i \delta_{l_i}$
- $H_p \Rightarrow H$
- sample eigenvalues λ_i of $\widehat{\Sigma} = n^{-1}X_{n\times p}^\top X_{n\times p}$ not consistent estimates of their population counterparts l_i: $\lambda_i \nrightarrow l_i$
- "bulk" distribution of λ_i converges to a different limit: the Marchenko-Pastur map $F_{\gamma,H}$

PCA Review: MP map

- MP map (Marchenko and Pastur, 1967) describes the deformation of the bulk distribution of eigenvalues
- Input:
  - Population spectral distribution $H = \lim p^{-1} \sum_i \delta_{l_i}$ (lim eigenvalues of Σ)
  - Aspect ratio: $\gamma = p/n$
- Output:
  - Limit empirical spectral distribution $F_{\gamma,H}$ (lim eigenvalues of $\widehat{\Sigma}$)

MP map example: white noise $\Sigma = I_p$

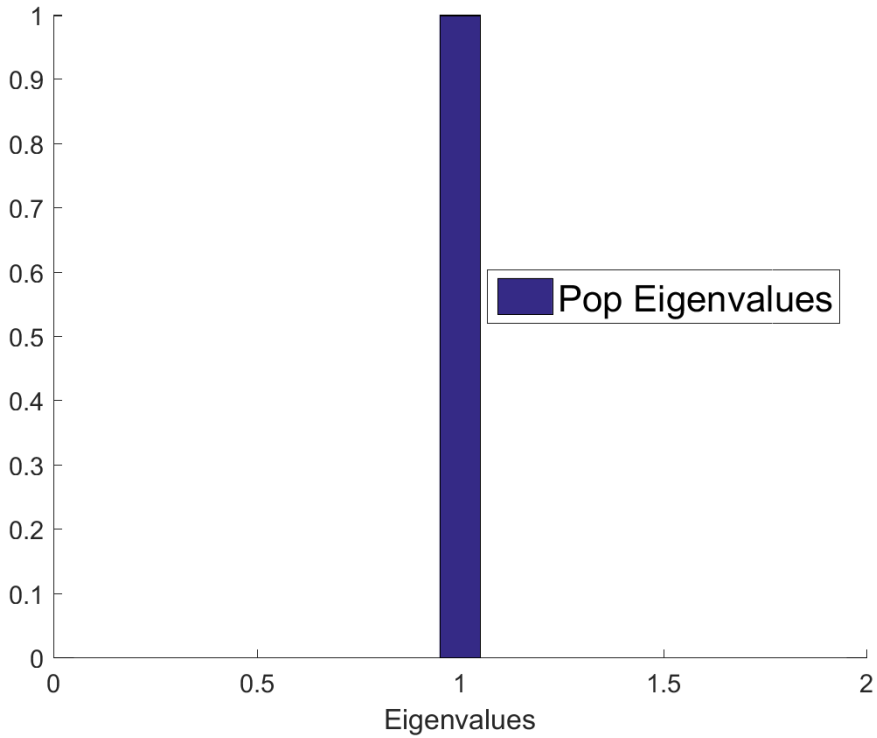


Figure : Eigenvalues $H = \delta_1$ of an identity covariance matrix $\Sigma = I_p$.

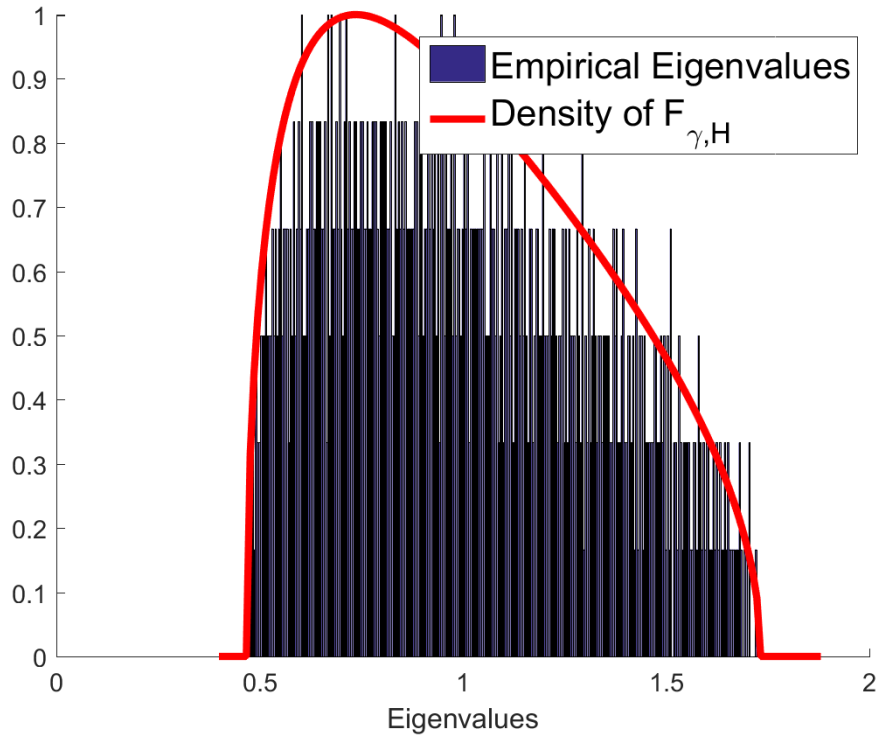


Figure : Marchenko-Pastur density: $g(x) = \sqrt{(\gamma_+ - x)(x - \gamma_-)}/\ (2\pi\gamma x)$, $x \in [\gamma_-, \gamma_+]$, $\gamma_\pm = (1 \pm \sqrt{\gamma})^2$, $\gamma = 1/2$.

MP map example: Autoregressive model, order 1, (AR-1)

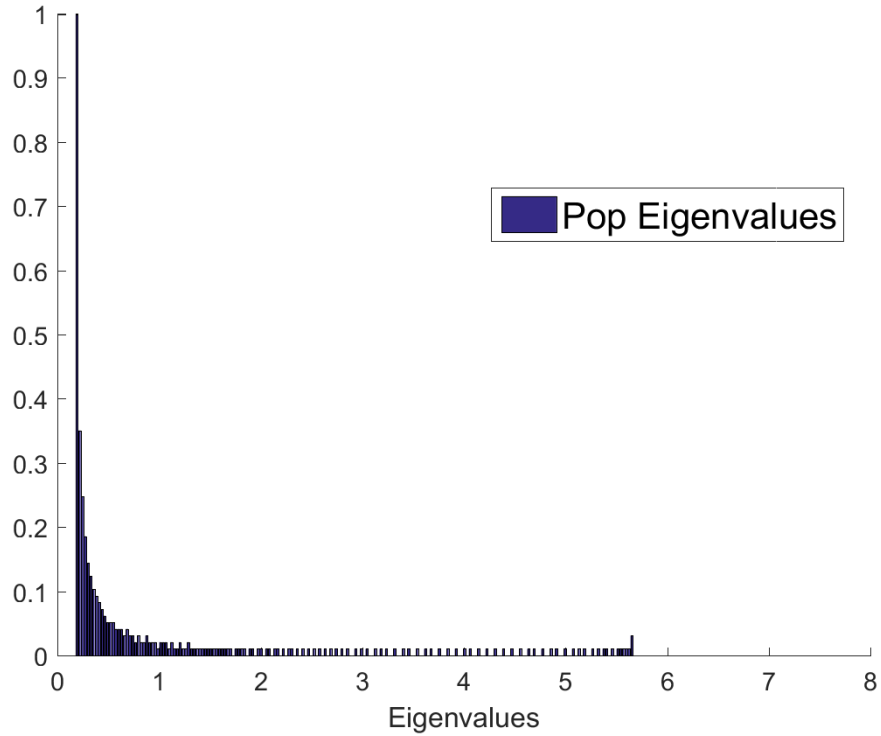


Figure : Eigenvalues H of an AR-1 covariance matrix Σ with $\Sigma_{ij} = \rho^{|i-j|}$ ($p = 400$; $\rho = 0.7$).

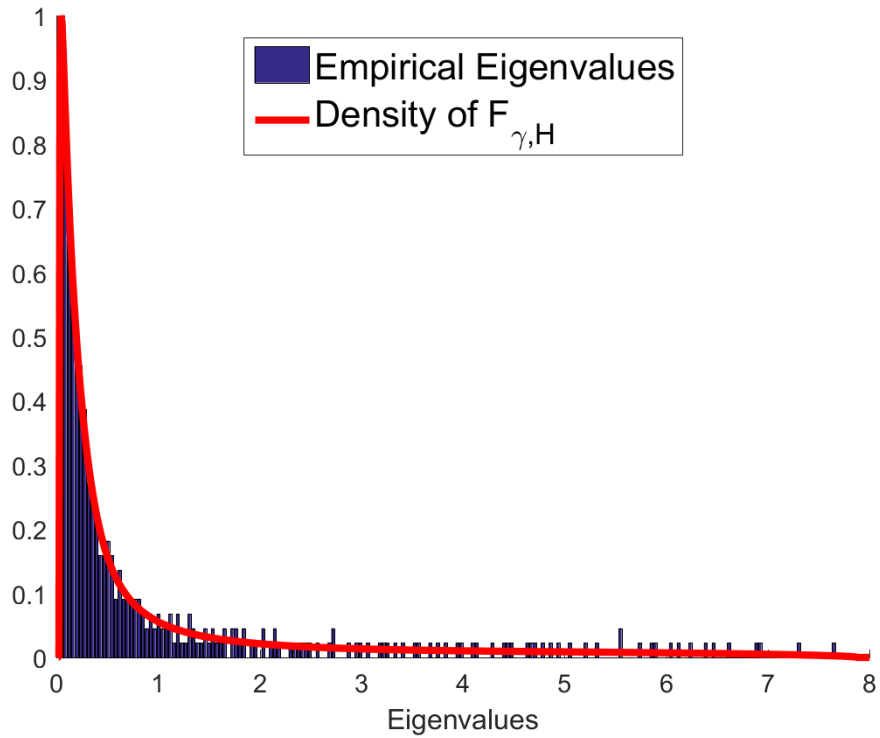


Figure : Eigenvalues of a sample covariance matrix $\widehat{\Sigma}$ with $n = 800$ samples.

PCA Review: spiked covariance model

- Spiked model with a single spike: distribution of $l_2, ..., l_p$ converges in restricted Kolmogorov-Smirnov (RKS) sense to H, and $t = l_1$ stays fixed
  - $H_p \Rightarrow_{RKS} H$, if $H_p \Rightarrow_{KS} H$, and $\max Support(H_p) \to \max Support(H)$
- top sample eigenvalue λ_1 "pushed upward" from l_1
- BBP phase transition (Baik et al., 2005; Benaych-Georges and Nadakuditi, 2011):
  - above the phase transition (PT): if l_1 large enough, λ_1 separates from the MP map "bulk"
  - below the PT: else λ_1 does not separate

Spiked model: AR-1 example

- population covariance matrix

$$\Sigma = \begin{bmatrix} t & 0^\top \\ 0 & M \end{bmatrix}$$

- spike t
- M is a $p \times p$ AR(1) covariance matrix $M_{ij} = \rho^{|i-j|}$. $\rho = 0.5$
- sample $n = 500$ Gaussian variates of $p = 250$ dimensions
- $mean(trace(M)) = 1$
- null: $t = 1$, alternative: larger t

AR-1 Example - Above PT

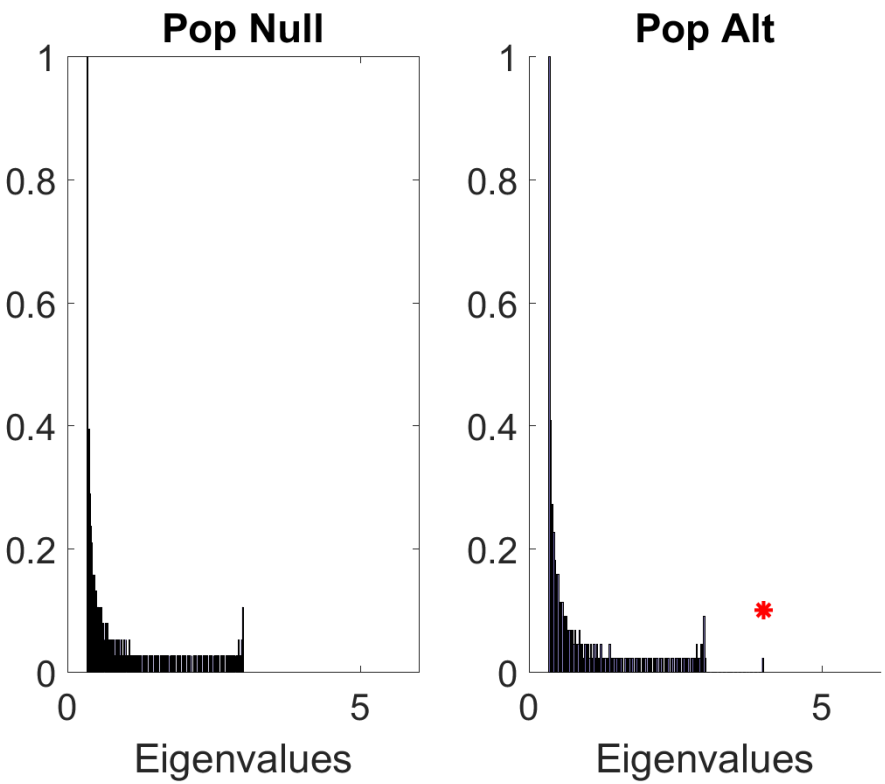


Figure : Eigenvalues of Σ. Null: $t = 1$. Alternative: $t = 4$.

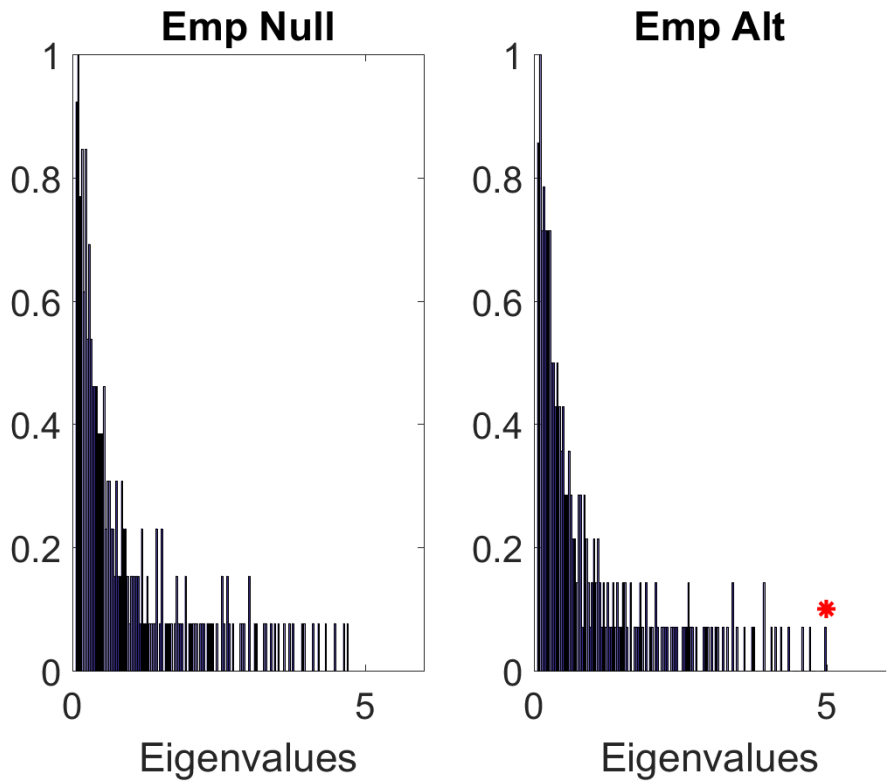


Figure : Eigenvalues of $\widehat{\Sigma}$. Null and alternative.

AR-1 Example - Below PT

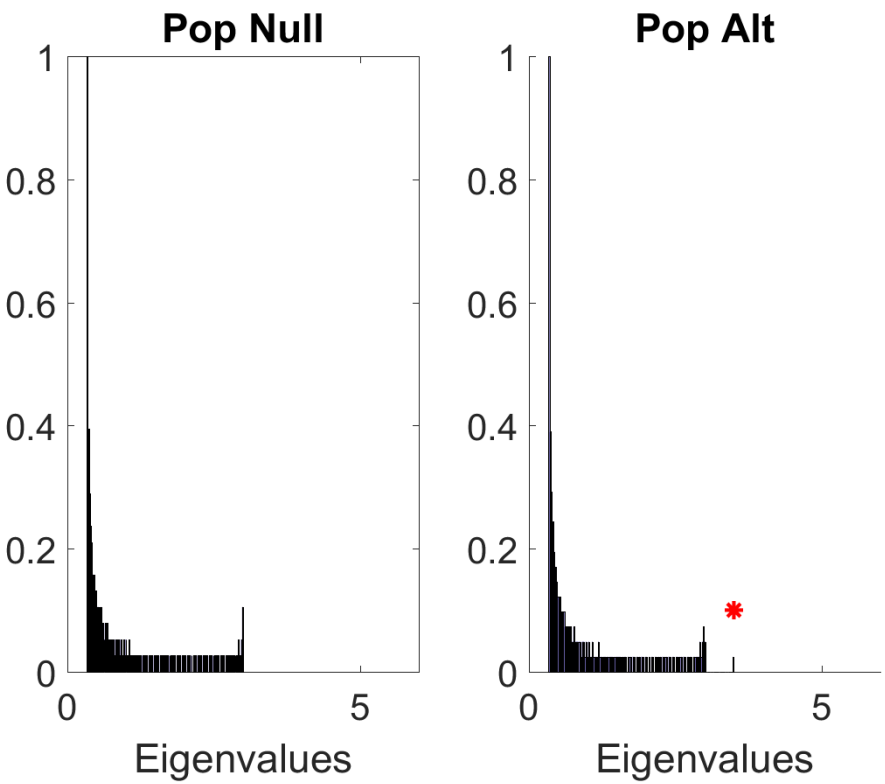


Figure : Eigenvalues of Σ. Null: $t = 1$. Alternative: $t = 3.5$.

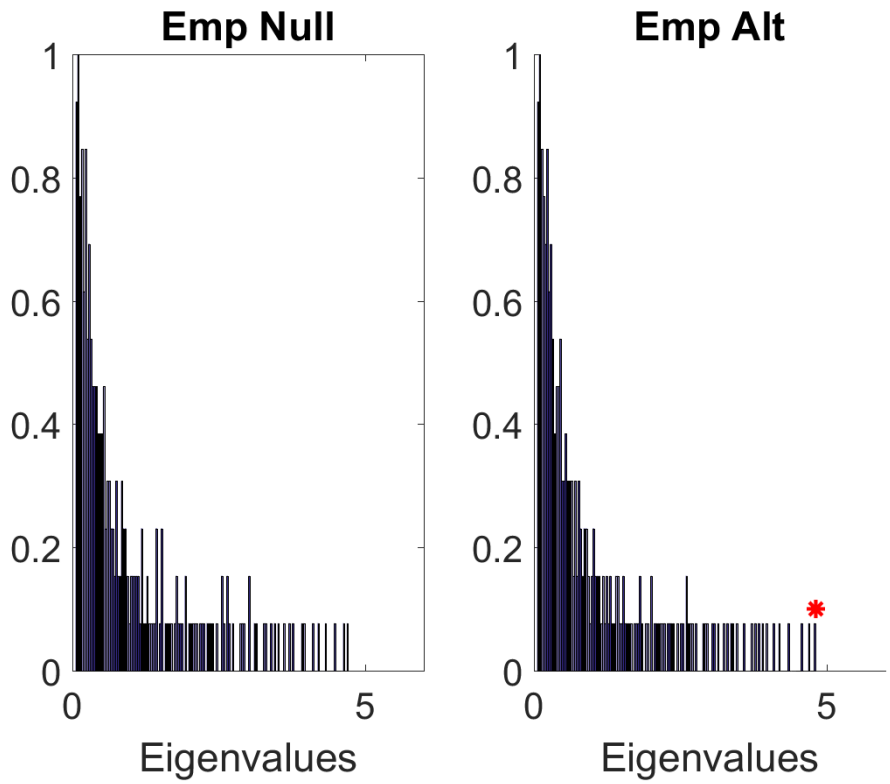


Figure : Eigenvalues of $\widehat{\Sigma}$. Null and alternative.

Statistical implications

- Below PT, top eigenvalue test based on λ_1 has trivial power
- ... despite its near-universal use
- ... despite its asy optimality in low dim, p fixed (Anderson, 1963)
- Can we detect PCs below the phase transition?
- Onatski et al. (2013, 2014) (OMH) consider the real Gaussian standard spiked model of Johnstone (2001)

$$H_0 : \Sigma_p = I_p, \text{ vs}$$

$$H_1 : \Sigma_p = I_p + \sum_{j=1}^{r} (l_j - 1) v_j v_j^\top, \; v_j \text{ unknown orthonormal}$$

Onatski, Moreira, Hallin (2013)

The Annals of Statistics
2013, Vol. 41, No. 3, 1204–1231
DOI: 10.1214/13-AOS1100

ASYMPTOTIC POWER OF SPHERICITY TESTS FOR HIGH-DIMENSIONAL DATA

BY ALEXEI ONATSKI, MARCELO J. MOREIRA[1] AND MARC HALLIN[2]

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This paper studies the asymptotic power of tests of sphericity against perturbations in a single unknown direction as both the dimensionality of the data and the number of observations go to infinity. We establish the convergence, under the null hypothesis and contiguous alternatives, of the log ratio of the joint densities of the sample covariance eigenvalues to a Gaussian process indexed by the norm of the perturbation. When the perturbation norm is larger than the *phase transition threshold* studied in Baik, Ben Arous and Péché [*Ann. Probab.* **33** (2005) 1643–1697] the limiting process is degenerate, and discrimination between the null and the alternative is asymptotically certain. When the norm is below the threshold, the limiting process is nondegenerate, and the joint eigenvalue densities under the null and alternative hypotheses are mutually contiguous. Using the asymptotic theory of statistical experiments, we obtain asymptotic power envelopes and derive the asymptotic power for various sphericity tests in the contiguity region. In particular, we show that the asymptotic power of the Tracy–Widom-type tests is trivial (i.e., equals the asymptotic size), whereas that of the eigenvalue-based likelihood ratio test is strictly larger than the size, and close to the power envelope.

Onatski, Moreira, Hallin (2014)

The Annals of Statistics
2014, Vol. 42, No. 1, 225–254
DOI: 10.1214/13-AOS1181

SIGNAL DETECTION IN HIGH DIMENSION: THE MULTISPIKED CASE

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This paper applies Le Cam's asymptotic theory of statistical experiments to the signal detection problem in high dimension. We consider the problem of testing the null hypothesis of sphericity of a high-dimensional covariance matrix against an alternative of (unspecified) multiple symmetry-breaking directions (*multispiked* alternatives). Simple analytical expressions for the Gaussian asymptotic power envelope and the asymptotic powers of previously proposed tests are derived. Those asymptotic powers remain valid for non-Gaussian data satisfying mild moment restrictions. They appear to lie very substantially below the Gaussian power envelope, at least for small values of the number of symmetry-breaking directions. In contrast, the asymptotic power of Gaussian likelihood ratio tests based on the eigenvalues of the sample covariance matrix are shown to be very close to the envelope. Although based on Gaussian likelihoods, those tests remain valid under non-Gaussian densities satisfying mild moment conditions. The results of this paper extend to the case of multispiked alternatives and possibly non-Gaussian densities, the findings of an earlier study [*Ann. Statist.* **41** (2013) 1204–1231] of the single-spiked case. The methods we are using here, however, are entirely new, as the Laplace approximation methods considered in the single-spiked context do not extend to the multispiked case.

A breakthrough

If the largest population covariance eigenvalue is at or below the threshold, the empirical distribution of the sample covariance eigenvalues still converges to the Marchenko–Pastur distribution, but the largest sample covariance eigenvalue now converges to the upper boundary of its support, both under the null of sphericity and the "spiked" alternative [Silverstein and Bai (1995) and Baik and Silverstein (2006)].

This similarity in the asymptotic behavior of covariance eigenvalues under the null and the alternative prompts Nadakuditi and Edelman (2008) and Nadakuditi and Silverstein (2010) to call the transition threshold "the fundamental asymptotic limit of sample-eigenvalue-based detection." They claim that no reliable signal detection is possible below that limit in the asymptotic sense. This asymptotic impossibility is also pointed out and discussed in several other recent studies, including Patterson, Price and Reich (2006), Hoyle (2008), Nadler (2008), Kritchman and Nadler (2009) and Perry and Wolfe (2010).

In this paper, we analyze the capacity of statistical tests to detect a one-dimensional signal with the corresponding population covariance eigenvalue below the "impossibility threshold," showing that the terminology "impossibility threshold" is overly pessimistic.

Results of OMH

- log-likelihood ratio test (LRT):

$$L_{n,p}(l_1, \ldots, l_r; \lambda_1, \ldots, \lambda_p) = \log \left[\frac{p_{n,p}(\lambda_1, \ldots, \lambda_p; l_1, \ldots, l_r)}{p_{n,p}(\lambda_1, \ldots, \lambda_p; 1, \ldots, 1)} \right]$$

- for $r = 1$, $L_{n,p}$ for $H_0 : l_1 = 1$ vs $H_1 : l_1 = t$ is equivalent to a linear spectral statistic (LSS)

$$L_{n,p}(t; \lambda_1, \ldots, \lambda_p) = \mathrm{tr}(\varphi(\widehat{\Sigma})) + c_p + o_P(1)$$

- explicitly, the score $\varphi(x) = -\log[\psi(t) - x]$, with $\psi(t) = t[1 + \gamma/(t-1)]$ "spike forward map" known by BBP
- using CLT for LSS, find the optimal detection power achievable by any test

Onatski, Moreira, Hallin (2013)

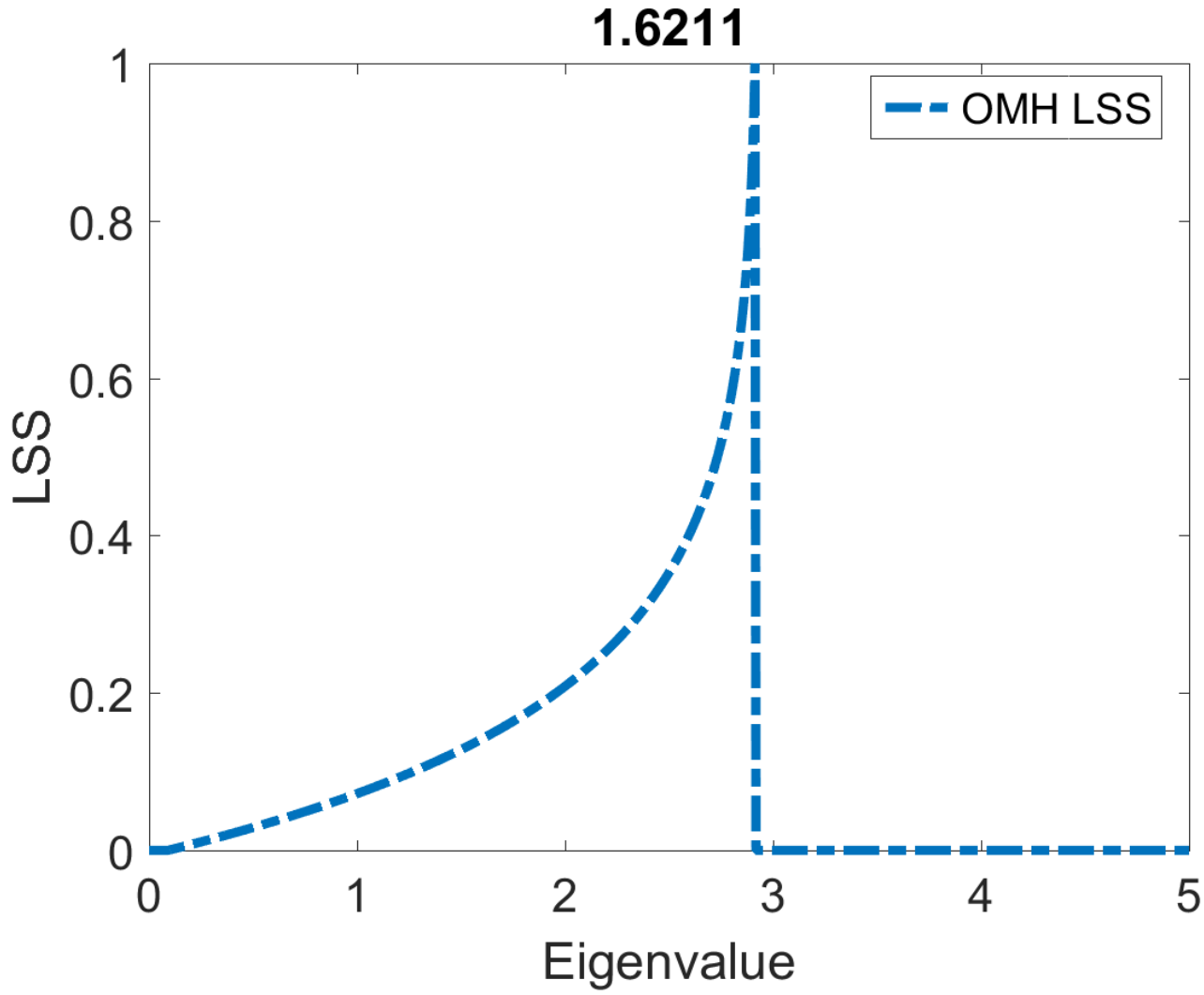

Figure : The OMH LSS $\varphi(x) = -\log[\psi(t) - x]$ with $\gamma = 1/2$ and $t = 1.62$, restricted to the support of the MP distribution

Our results

- OMH is one very specific example where we can calculate optimal tests
- In this talk, we find optimal tests for local alternatives generally
- Our construction is mathematically precise and clean. It can derive OMH results plus much else
- Before this work, we had very little information about optimal tests. Now we have a great deal

Local alternatives model

- Recall $X = Z_{n\times p}\Sigma^{1/2}$ and $H_p = p^{-1}\sum_{i=1}^{p}\delta_{l_i}$ the spectrum of Σ
- model bulk H perturbed by spikes G_0 vs G_1
- Local alternatives model:

$$H_{p,0} : H_p = \left(1 - \frac{h}{p}\right) H + \frac{h}{p} G_0, \text{ vs}$$
$$H_{p,1} : H_p = \left(1 - \frac{h}{p}\right) H + \frac{h}{p} G_1.$$

- e.g., standard spiked model: $H = G_0 = \delta_1$, $G_1 = \delta_t$
- allows correlations, flexible data modelling

Optimal tests in local alternatives model

- Given (H, h, G_0, G_1, γ) we derive a function φ, the score function of a linear spectral statistic $T = \mathrm{tr}\{\varphi(\widehat{\Sigma})\}$.
- Gives the asymptotically best test for $H_{p,0}$ against $H_{p,1}$

Mean-variance problem

- There are mean and variance parameters $\mu_\varphi, \sigma_\varphi^2$ s.t for some constants c_p
  - under $H_{p,0}$, $\mathrm{tr}(\varphi(\widehat{\Sigma})) - c_p \Rightarrow \mathcal{N}(0, \sigma_\varphi^2)$
  - under $H_{p,1}$, $\mathrm{tr}(\varphi(\widehat{\Sigma})) - c_p \Rightarrow \mathcal{N}(\mu_\varphi, \sigma_\varphi^2)$.
- With $\langle f, g \rangle = \int_{\mathcal{I}} f(x)g(x)dx$

$$\mu_\varphi = -h\langle \varphi', \Delta \rangle \quad \text{and}$$
$$\sigma_\varphi^2 = \langle \varphi', K\varphi' \rangle.$$

- Find optimal LSS φ, maximizing the efficacy

$$\max_\varphi \frac{\mu_\varphi}{\sigma_\varphi}$$

Main result: Finding the optimal LSS

Theorem (D.,2016)

Two cases for testing (H, G_0) *vs* (H, G_1) *in the local alternatives model:*

1. *If* $\Delta \in \mathrm{Im}(K)$*, then the optimal linear spectral statistics* φ *are given by a Fredholm integral equation of the first kind:*

$$K(\varphi') = -\eta\Delta,$$

   where $\eta > 0$ *is any constant.*

2. *On the other hand, if* $\Delta \notin \mathrm{Im}(K)$*, then the maximal efficacy is* $+\infty$*. The optimal LSS are all functions* φ *with* $K(\varphi') = 0$ *and* $\langle \varphi', \Delta \rangle < 0$*.*

Recovering the OMH LSS

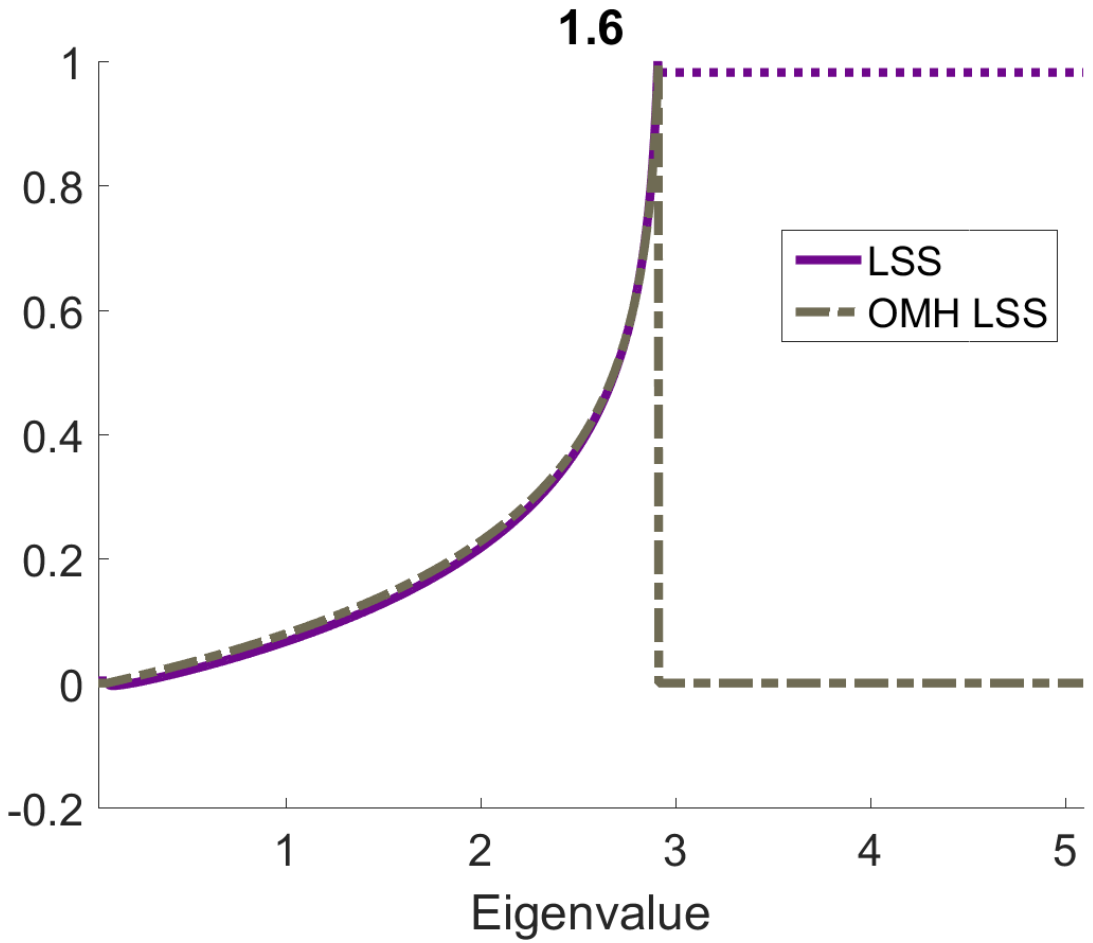

Figure : The optimal LSS and the OMH LSS in the standard spiked model. $H = G_0 = \delta_1$, $G_1 = \delta_t$. $t = 1.6$ and $\gamma = 1/2$.

Optimal LSS example: AR-1

- population covariance matrix

$$\Sigma = \begin{bmatrix} t & 0^\top \\ 0 & M \end{bmatrix}$$

- spike t
- $M_{ij} = \rho^{|i-j|}$
- $H = spec(M)$
- test

$$H_{p,0} : H_p = \left(1 - \frac{1}{p}\right) H + \frac{1}{p}\delta_1, \text{ vs}$$
$$H_{p,1} : H_p = \left(1 - \frac{1}{p}\right) H + \frac{h}{p}\delta_t.$$

Optimal LSS example: AR-1

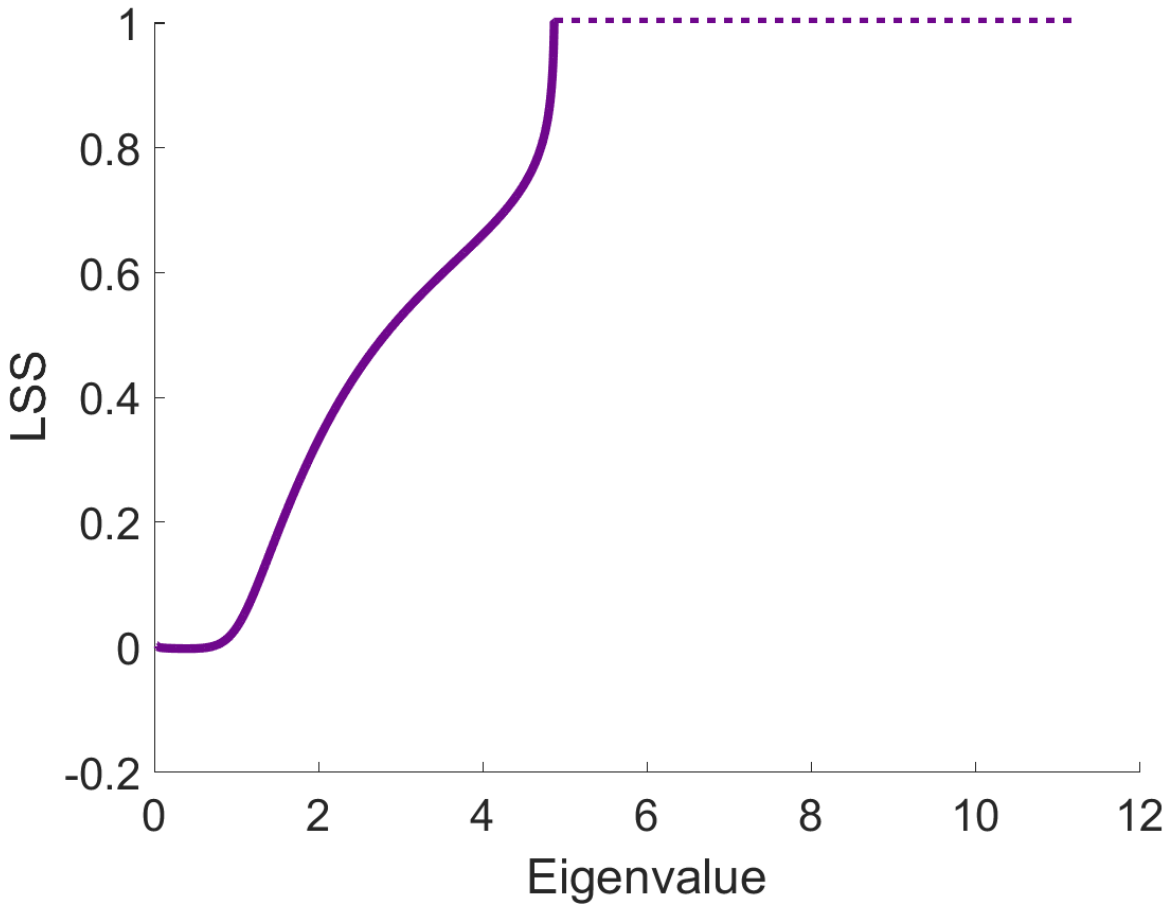

Figure : Our new optimal LSS $\varphi(x)$ in AR-1 example with $\gamma = 0.5, \rho = 0.5,\ t = 3.5$ below PT.

Example: detection power in AR-1

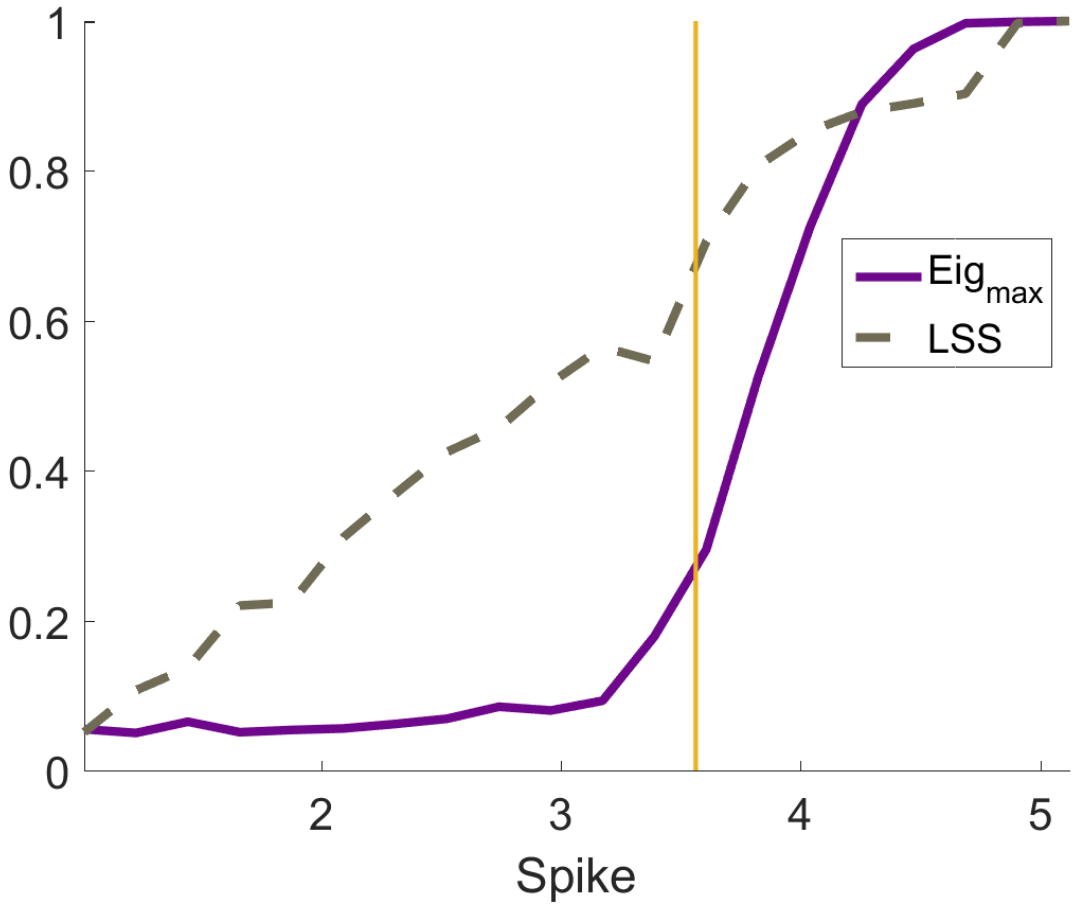

Figure : Detection power of LSS and top-eigenvalue test as a function of spike t. Vertical line: Location of PT. $\gamma = 0.5, \rho = 0.5, n = 500$

Probability background - CLT for LSS

Theorem. [Bai and Silverstein (2004) CLT]: Let $X = Z_{n\times p}\Sigma^{1/2}$ and Z_{ij} iid real standardized with $\mathbb{E}Z_{ij}^4 = 3$. If $H_p \Rightarrow H$, for φ analytic on a compact interval $\mathcal{I}$ including all supports of ESDs, we have

$$\mathrm{tr}(\varphi(\widehat{\Sigma})) - p\int_{\mathcal{I}} \varphi(x) dF_{\gamma,H_p}(x) \Rightarrow \mathcal{N}(m_\varphi, \sigma_\varphi^2)$$

- $\sigma_\varphi^2 = \int_{\mathcal{I}\times\mathcal{I}} \varphi'(x)\varphi'(y)k(x,y)dx\,dy = \langle \varphi', K\varphi'\rangle$, where k is a covariance kernel, and K is the associated operator

Covariance kernel

- the Stieltjes transform s_μ of a (signed) measure μ on $\mathbb{R}$ is, for $z \notin Supp(\mu)$

$$s_\mu(z) = \int \frac{d\mu(t)}{t - z}$$

- $\underline{s}(x)$ is the limit limit Stieltjes transform of $(1-\gamma)F_{\gamma,H} + \gamma\delta_0$ as $z \to x \in \mathbb{R}$

$$k(x,y) = \frac{1}{2\pi^2} \log\left(1 + 4\frac{\Im(\underline{s}(x))\,\Im(\underline{s}(y))}{|\underline{s}(x) - \underline{s}(y)|^2}\right)$$

- k is
  - zero outside of the support of $F_{\gamma,H}$: $\lim_{\varepsilon\to 0} \pi^{-1}\Im\underline{s}(x + i\varepsilon) = f_{\gamma,H}(x)$.
  - singular on the diagonal $x = y$

Covariance kernel—heatmap

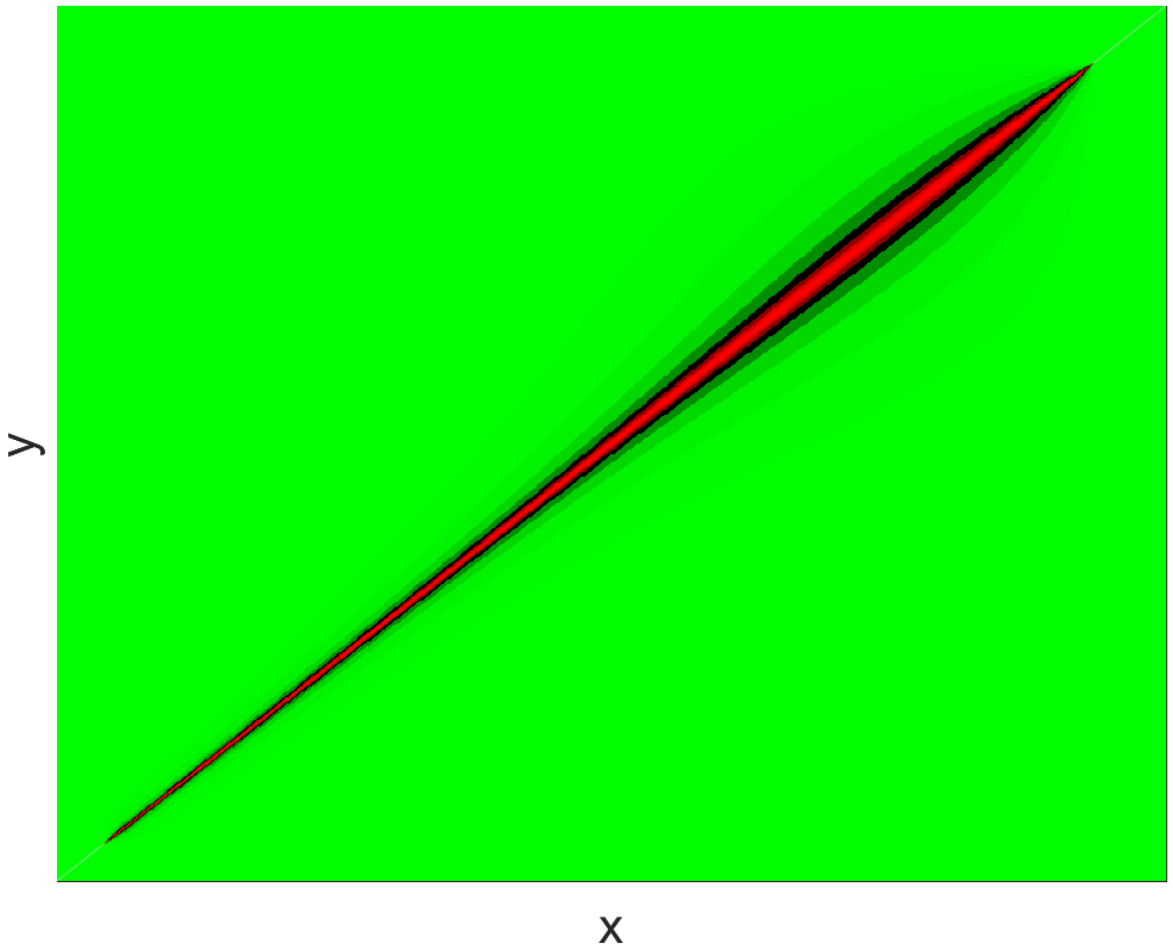

Figure : Heatmap of covariance kernel $k(x, y)$ in AR-1 example $H = spec(\Sigma)$. Within support of $F_{\gamma,H}$.

Computation

- Solve $Kg = -\Delta$, i.e., $\int k(x,y)g(y)dy = -\Delta(x)$,

$$k(x,y) = \frac{1}{2\pi^2} \log\left(1 + 4\frac{\Im(\underline{s}(x))\,\Im(\underline{s}(y))}{|\underline{s}(x) - \underline{s}(y)|^2}\right)$$

  and $\underline{s}(x)$ is Stieltjes transform of $(1-\gamma)F_{\gamma,H} + \gamma\delta_0$
- Bigger problem: How to compute the Marchenko-Pastur forward map?
- surprisingly, not well studied.
  - "successive approximation" (Marchenko and Pastur, 1967)
  - fixed-pont algorithm (Couillet et al., 2011)
- in Dobriban (2015) developed a fast ODE-based method SPECTRODE

SPECTRODE computes of MP map $F_{\gamma,H}$

SPECTRODE: Input and Output
Input: $H \leftarrow$ population spectrum $\gamma \leftarrow$ aspect ratio $\varepsilon \leftarrow$ precision control
Output: $\hat{l}_k, \hat{u}_k \leftarrow$ endpoints of intervals in the support $\hat{f}(x) \leftarrow$ density of MP map $F_{\gamma,H}$ $\hat{s}(x) \leftarrow$ Stieltjes transform of MP map $F_{\gamma,H}$

SPECTRODE: Autoregressive model

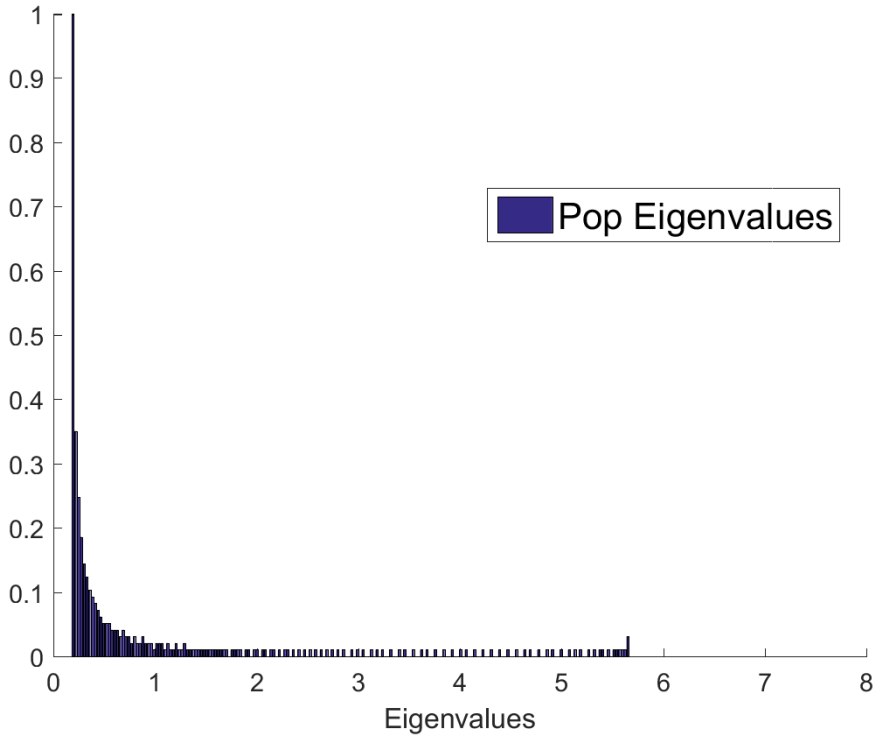

Figure : Eigenvalues H of an AR-1 covariance matrix Σ with $\Sigma_{ij} = \rho^{|i-j|}$ ($p = 400$; $\rho = 0.7$).

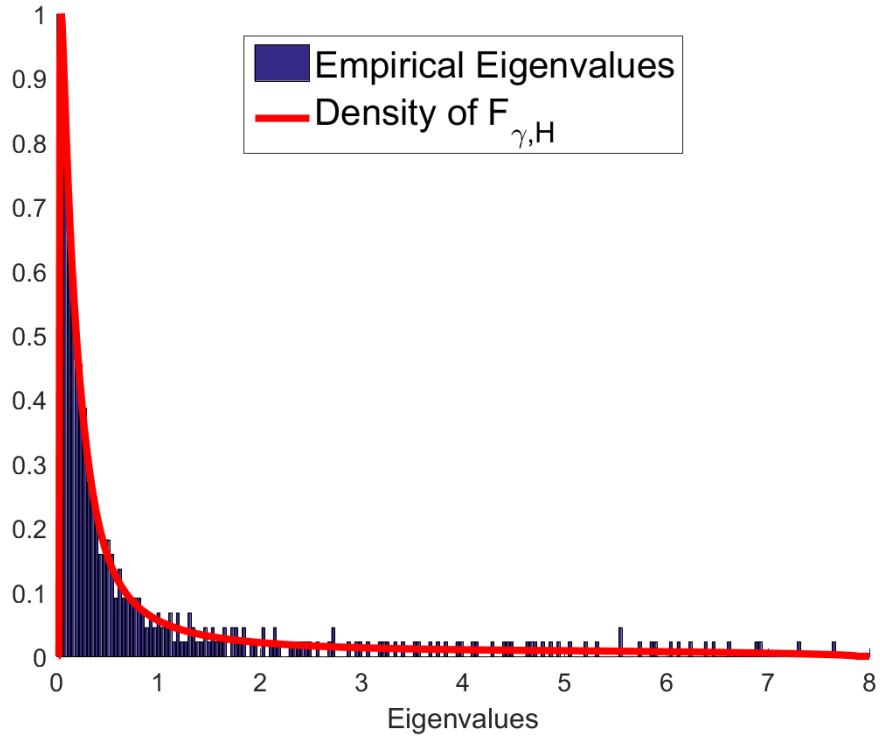

Figure : Eigenvalues of a sample covariance matrix $\widehat{\Sigma}$ with $n = 800$ samples. Density computed with SPECTRODE

SPECTRODE: "Comb" model

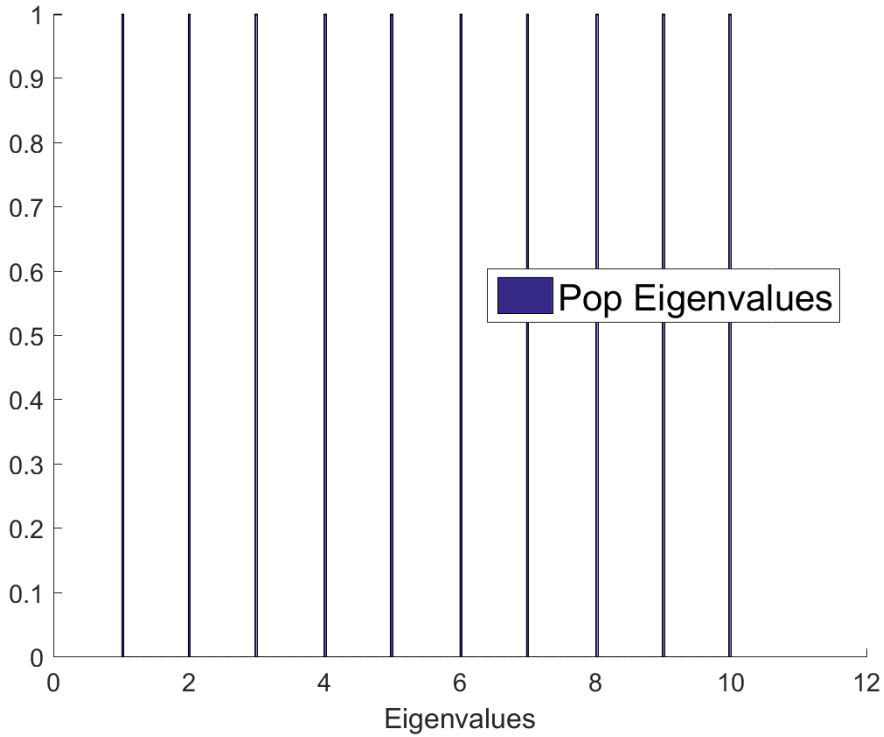

Figure : "Comb" model
$H = 10^{-1} \sum_{i=1}^{10} \delta_{l_i}$, with $l_i = i$.

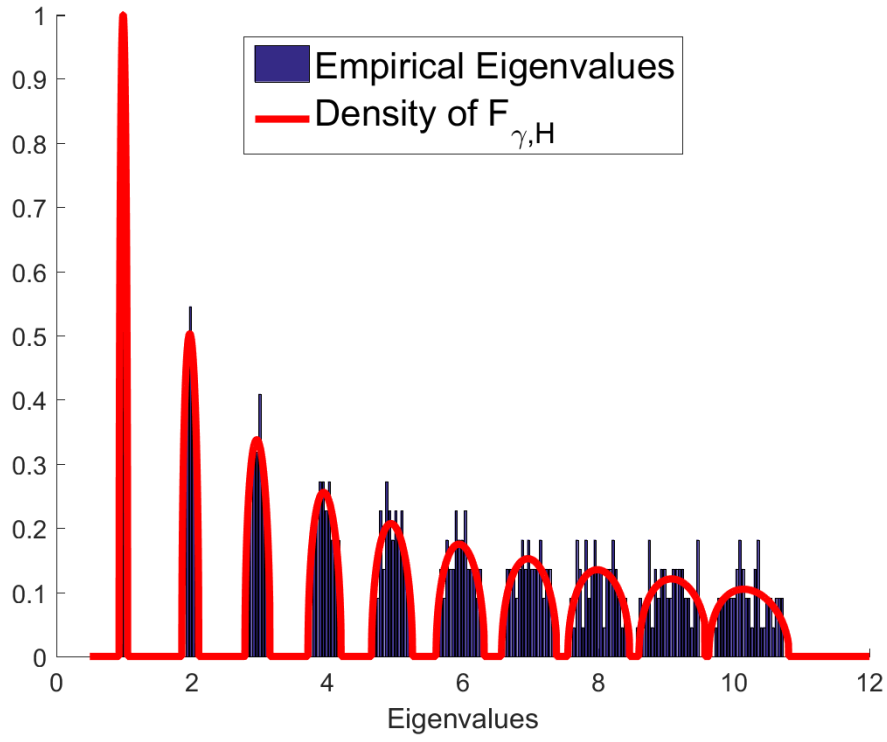

Figure : Eigenvalues of $\widehat{\Sigma}$ with $n = 800$ samples, and density. Density computed with SPECTRODE

SPECTRODE is fast and accurate

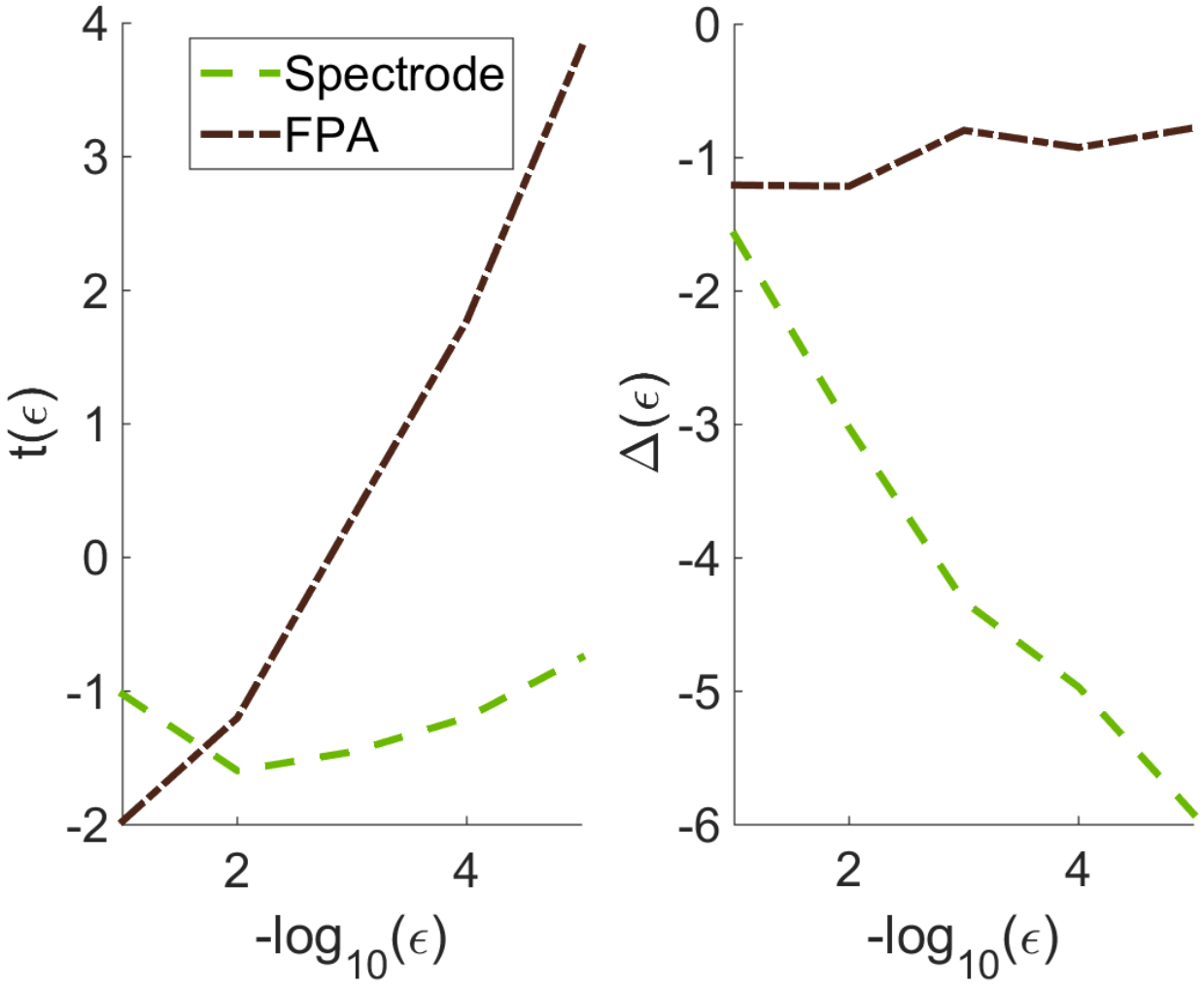

Figure : Running time (left), and average accuracy (right) as a function of the number of correct significant digits k: $\varepsilon = 10^{-k}$. SPECTRODE and fixed-point-algorithm (FPA).

SPECTRODE: a "universal" MP calculator

- Useful for a variety of problems, see Dobriban (2015):
  - examples of limit spectra, teaching
  - principal component analysis (here)
  - covariance matrix estimation
  - bootstrap
  - quantiles, moments and contour integrals of the MP map
- Matlab and R software at github.com/dobriban
  - with documentation and examples

Idea behind SPECTRODE

1. Stieltjes transform $x \to \underline{s}(x) = \mathbb{E}\frac{1}{\lambda - x}$ increasing for $x \in \mathbb{R}$ outside of the support of $F_{\gamma,H}$.
   - ST has increasing inverse there (Silverstein and Choi, 1995)
2. MP/Silverstein equation defines inverse ST, for $z \in \mathbb{C}^+$

$$z = -\frac{1}{\underline{s}(z)} + \gamma \int \frac{t}{1 + t\underline{s}(z)} dH(t).$$

   - Use this for $z = x + i\varepsilon$, small ε, to find the edges of the support
3. Run ODE derived from Silv eq to find smooth density within support
   - Starting point using fixed-pont algoritm

Using the CLT

Goal: get an expression for the mean

- In the local alternatives model:

$$\text{under } H_0 : \operatorname{tr}(\varphi(\widehat{\Sigma})) - p \int_{\mathcal{I}} \varphi(x) dF_{\gamma, H_{p,0}} \Rightarrow \mathcal{N}(m_\varphi, \sigma_\varphi^2), \text{ while}$$

$$\text{under } H_1 : \operatorname{tr}(\varphi(\widehat{\Sigma})) - p \int_{\mathcal{I}} \varphi(x) dF_{\gamma, H_{p,1}} \Rightarrow \mathcal{N}(m_\varphi, \sigma_\varphi^2).$$

- In the limit, test $\mathcal{N}(0, \sigma_\varphi^2)$ vs $\mathcal{N}(\mu_\varphi, \mu_\varphi^2)$, where

$$\mu_\varphi = \lim_{p \to \infty} \int_{\mathcal{I}} \varphi(x) d \left[p(F_{\gamma, H_{p,1}} - F_{\gamma, H_{p,0}}) \right],$$

Key new object: Weak derivative of MP map

- The weak derivative of MP map F_γ is the signed measure

$$\delta\mathcal{F}_\gamma(H, G) = \lim_{\varepsilon \to 0} \frac{F_{\gamma,(1-\varepsilon)H+\varepsilon G} - F_{\gamma,H}}{\varepsilon}.$$

- so $p[F_{\gamma,H_{p,1}} - F_{\gamma,H_{p,0}}] \Rightarrow h \cdot \Delta$, where $\Delta = \delta\mathcal{F}_\gamma(H, G_1) - \delta\mathcal{F}_\gamma(H, G_0)$
- integrate by parts

$$\mu_\varphi = h \cdot \langle \varphi, d\Delta \rangle = -h \cdot \langle \varphi', \Delta \rangle.$$

Key new object: Weak derivative of MP map

- nice properties:
  - has a density within support of F_γ
  - spike is above PT iff isolated point mass in $\delta\mathcal{F}_\gamma$ — a new perspective on phase transitions in spiked models

Weak derivative: Example

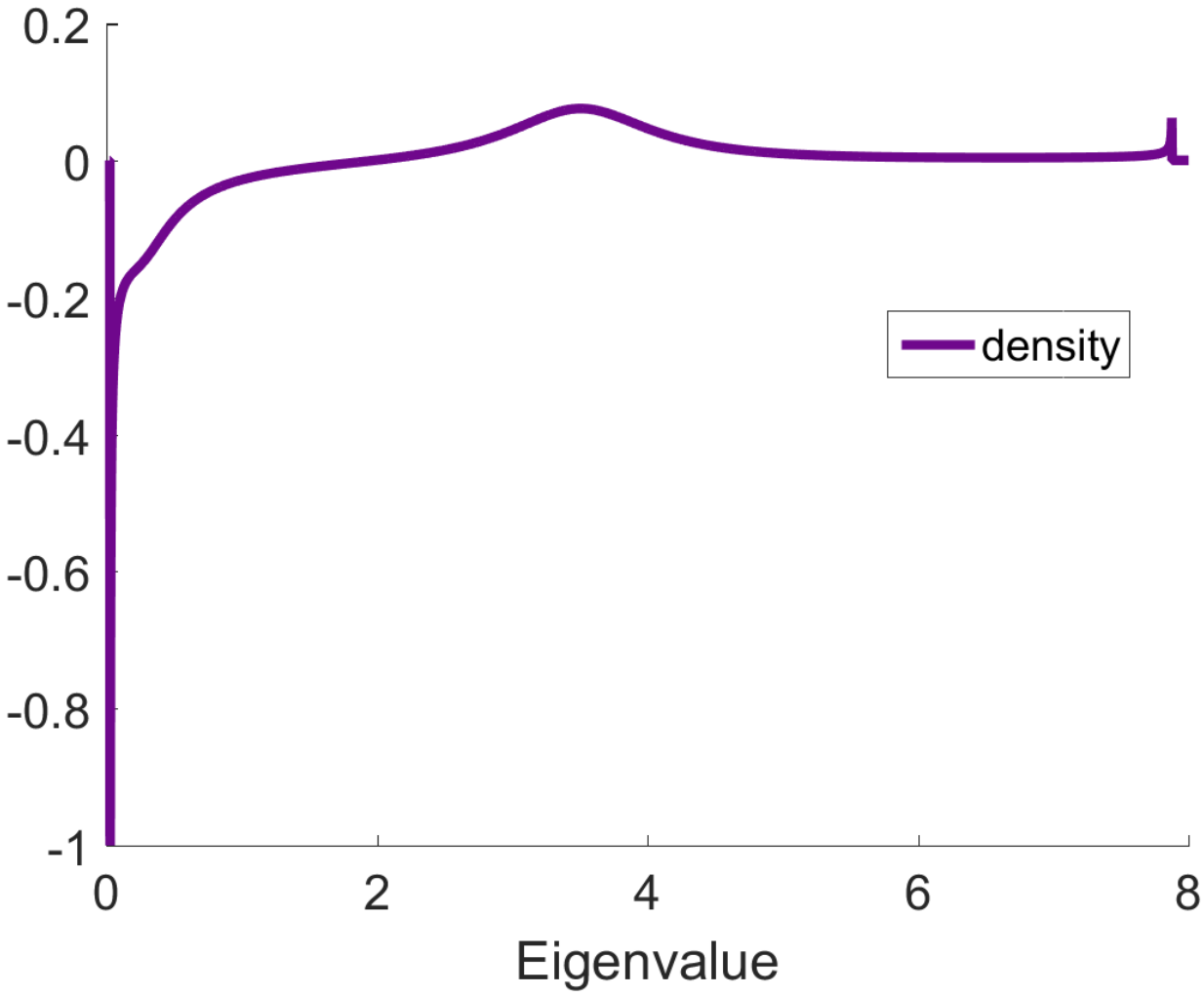

Figure : Density of weak derivative $\delta\mathcal{F}_\gamma(H, G)$ in AR-1 example $H = spec(\Sigma)$, $G = \delta_{3.5}$ below PT;

Summary

- Optimal testing for principal components in high dimensions
  - Detection below the phase transition using linear spectral statistics
- Enabled by SPECTRODE—new general computational tool for RMT

- Thanks
  - Support: NSF, HHMI
  - Discussion: David Donoho, Iain Johnstone

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