Optimal detection of principal components in high-dimensional data

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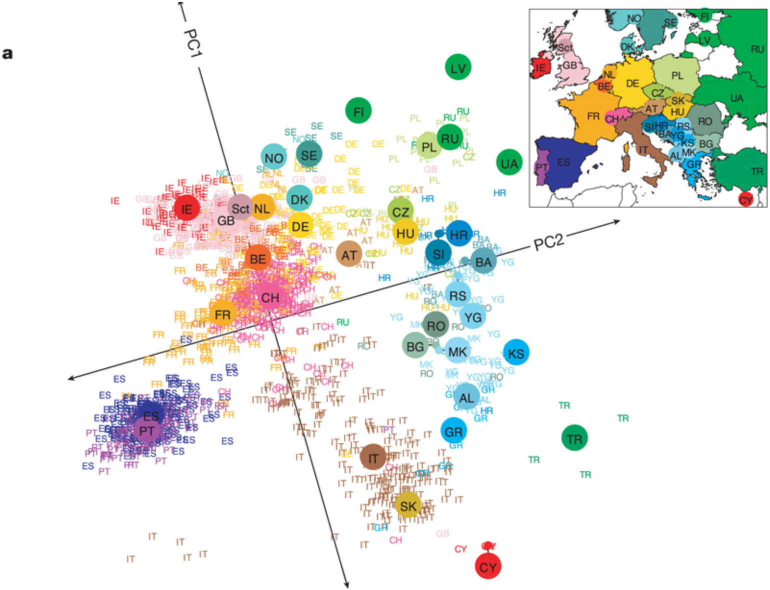
Outline

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)



PCA in practice

- How to choose number of components?
- Scree plot: eigenvalues in decreasing order
- Look for the elbow - gap between eigenvalues
- In high-dimension, this may miss "weak" PCs
- In this talk: such PCs can be still be detected

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: $\mathrm{Cov}\left[x_i, x_i\right] = \Sigma$
- 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 $\widehat{\Sigma} = n^{-1} X^\top X$ inconsistent estimates: $\lambda_i \nrightarrow l_i$
- "Bulk" distribution of λ_i converges to Marchenko-Pastur map $F_{\gamma,H}$

PCA Review: MP map

- MP map (Marchenko and Pastur, 1967) describes the deformation of bulk distribution of eigenvalues due to limited number of samples
- 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 $\Sigma = I_p$

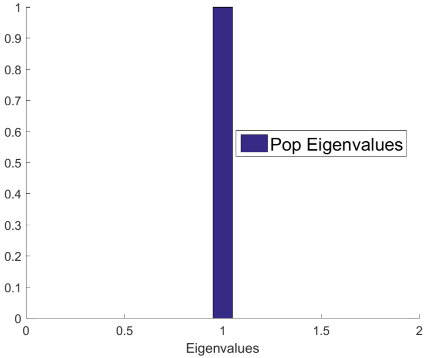


Figure: Eigenvalues $H = \delta_1$ of an identity covariance matrix $\Sigma = I_p$.

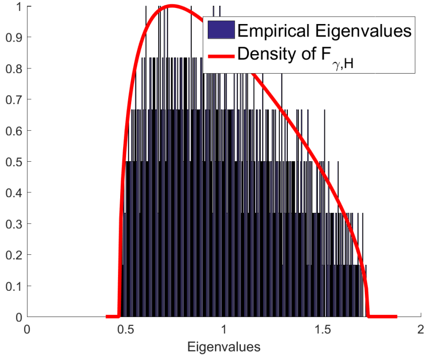


Figure: Marchenko-Pastur density: $g(x) = \sqrt{(\gamma_+ - x)(x - \gamma_-)}/\ (2\pi\gamma x)$, $x \in [\gamma_-, \gamma_+]$, $\gamma_\pm = (1 \pm \sqrt{\gamma})^2$, $\gamma = 1/10$.

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

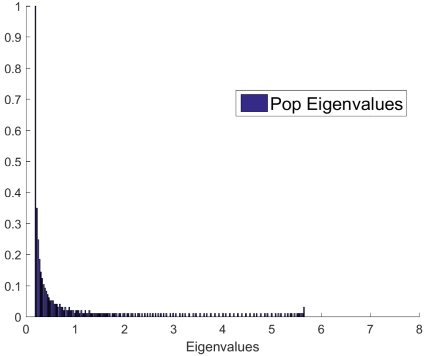


Figure: Eigenvalues H of an AR-1 covariance matrix Σ with $\Sigma_{ij} = \rho^{|i-j|}$ ($p = 400$; $\rho = 0.7$).

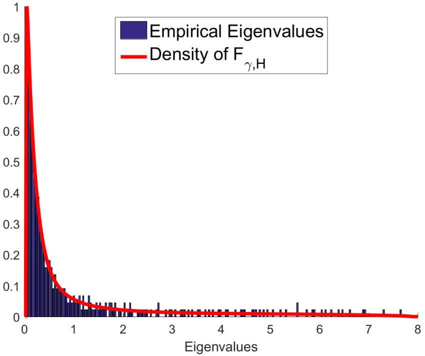


Figure: Eigenvalues of a sample covariance matrix $\widehat{\Sigma}$ with $n = 800$ samples.

PCA Review: spiked covariance model

- (Signal) spike $t = l_1$ fixed
- (Noise) distribution of $l_2, ..., l_p$ converges to H in Restricted KS sense
  - $H_p \Rightarrow_{RKS} H$, 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 phase transition (PT): if l_1 large, λ_1 separates from MP map "bulk"
  - Below 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

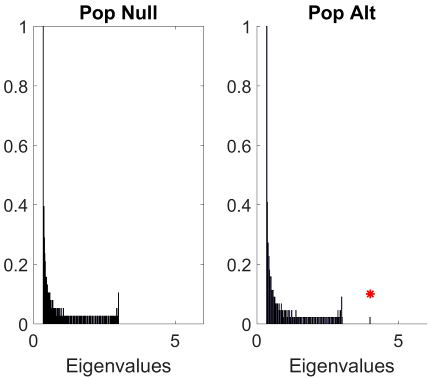


Figure: Eigenvalues of Σ. Null: $t = 1$. Alternative: $t = 4$.

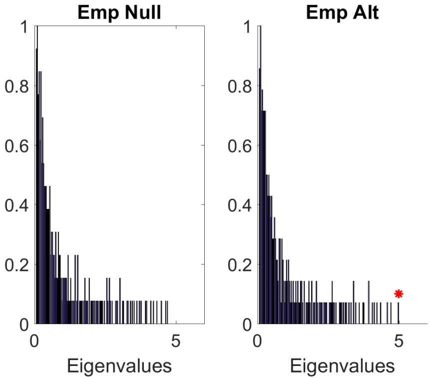


Figure: Eigenvalues of $\widehat{\Sigma}$. Null and alternative.

AR-1 Example - Below PT

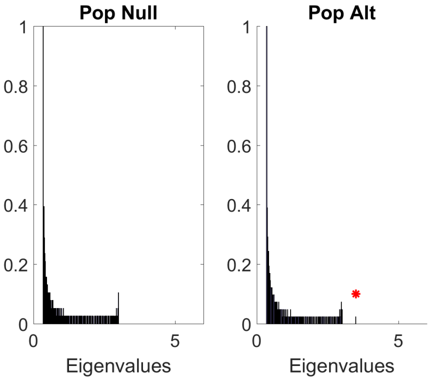


Figure: Eigenvalues of Σ. Null: $t = 1$. Alternative: $t = 3.5$.

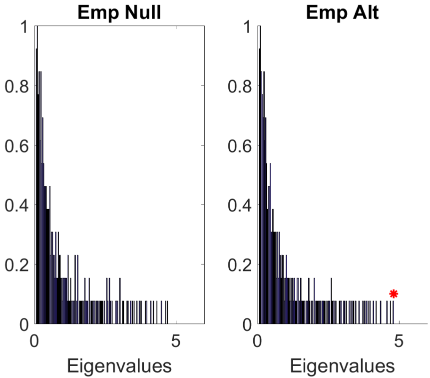


Figure: Eigenvalues of $\widehat{\Sigma}$. Null and alternative.

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? If so, how?
- Onatski et al. (2013, 2014) (OMH) the 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]

University of Cambridge, FGV/EPGE, and Université libre de Bruxelles and Princeton University

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

BY ALEXEI ONATSKI[1], MARCELO J. MOREIRA[2] AND MARC HALLIN[3]

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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.

Results of OMH

- Log-likelihood ratio test (LRT):

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

- LRT for $H_0 : l_1 = 1$ vs $H_1 : l_1 = t$ is equivalent to a linear spectral statistic (LSS)

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

- Using CLT for LSS, find optimal detection power

Onatski, Moreira, Hallin (2013)

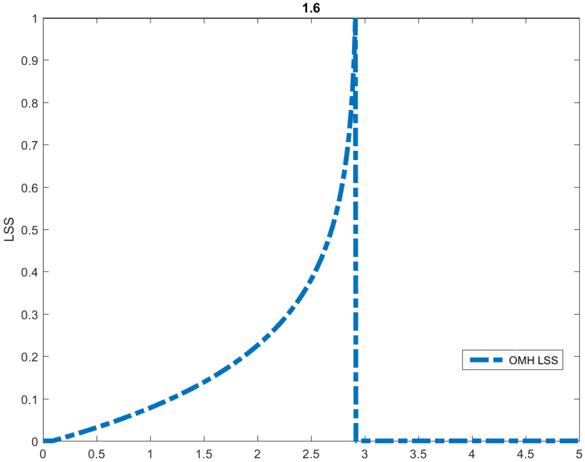

Figure: The OMH LSS $\varphi(x) = -\log[\psi(t) - x]$ with $\gamma = 1/2$ and $t = 1.60$, restricted to the support of the MP distribution

Our results

- OMH is one 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 plus much else

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:

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

- h is number of spikes (fixed)
- 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 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 $\Delta \in \mathrm{Im}(K)$, the optimal linear spectral statistics φ are given by a Fredholm integral equation:*

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

   where $\eta > 0$ is any constant.

2. *On the other hand, if $\Delta \notin \mathrm{Im}(K)$, then the maximal efficacy is $+\infty$.*

Recovering the OMH LSS

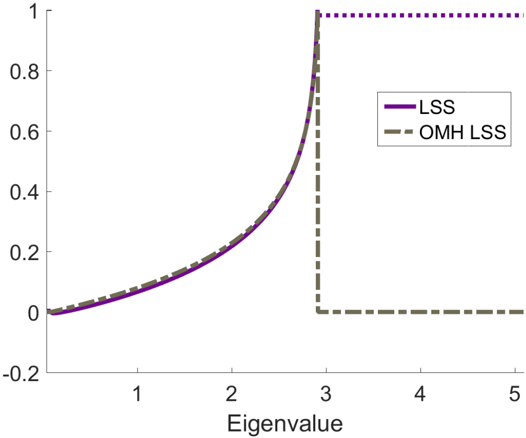

Figure: The optimal LSS and the OMH LSS in the standard spiked model.
$H = G_0 = \delta_1$, $G_1 = \delta_t$. $t = 1.6$ and $\gamma = 1/2$.

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

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

Optimal LSS example: AR-1

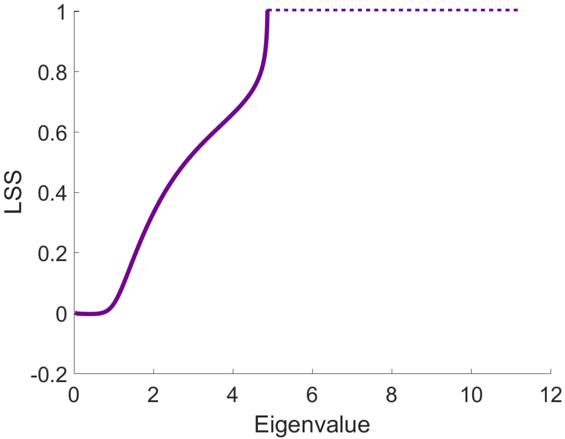

Figure: New optimal LSS $\varphi(x)$ in AR-1 model: $\gamma = 0.5, \rho = 0.5,\ t = 3.5$ below PT.

Example: detection power in AR-1

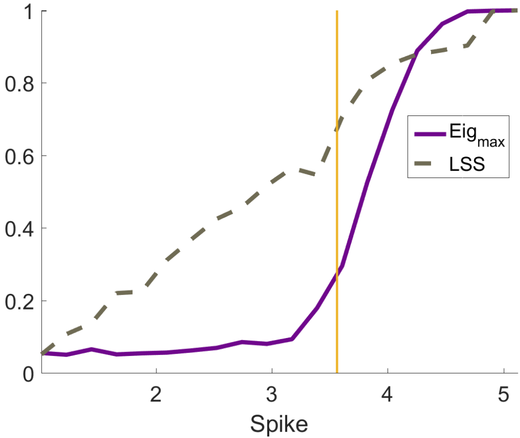

Figure: Detection power of LSS and top-eigenvalue test as a function of spike t. Vertical line: Location of PT. $\gamma = 0.5, \rho = 0.5, n = 500$

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 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

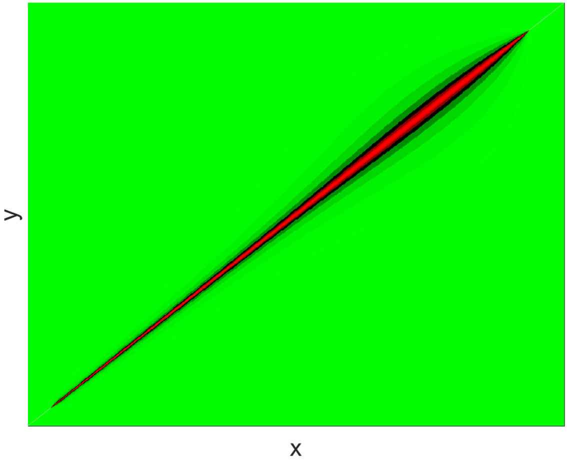

Figure: Heatmap of covariance kernel $k(x, y)$ in AR-1 example $H = spec(\Sigma)$. Within support of $F_{\gamma,H}$.

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 $(1-\gamma)F_{\gamma,H} + \gamma\delta_0$
- Larger problem: How to compute the Marchenko-Pastur forward map?
- Previous proposals.
  - "Successive approximation" (Marchenko and Pastur, 1967)
  - Fixed-pont algorithm (Couillet et al., 2011)
- Dobriban (2015) developed a carefully motivated new approach which is
  1. a new algorithmic idea
  2. with proven properties
  3. empirically much faster than previous proposals

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

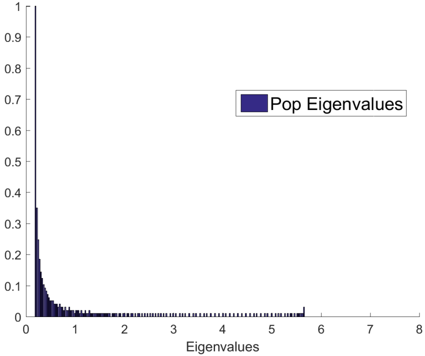

Figure: Eigenvalues H of an AR-1 covariance matrix Σ with $\Sigma_{ij} = \rho^{|i-j|}$ ($p = 400$; $\rho = 0.7$).

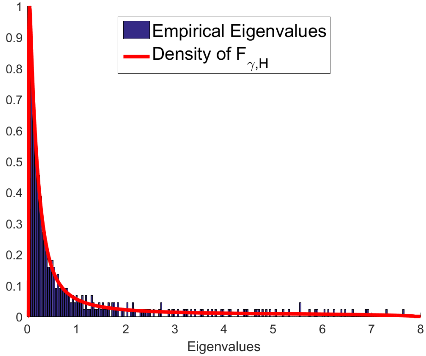

Figure: Eigenvalues of a sample covariance matrix $\widehat{\Sigma}$ with $n = 800$ samples. Density computed with SPECTRODE

Spectrode: "Comb" model

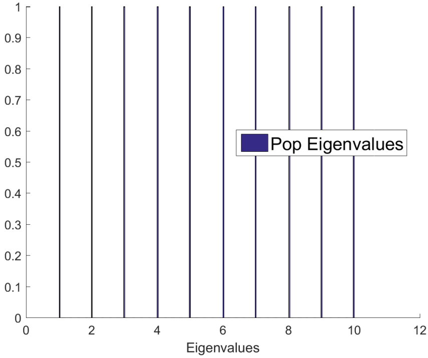

Figure: "Comb" model
$H = 10^{-1} \sum_{i=1}^{10} \delta_{l_i}$, with $l_i = i$.

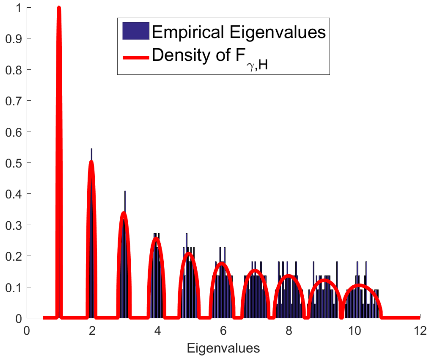

Figure: Eigenvalues of $\widehat{\Sigma}$ with $n = 800$ samples, and density. Density computed with Spectrode

SPECTRODE is fast and accurate

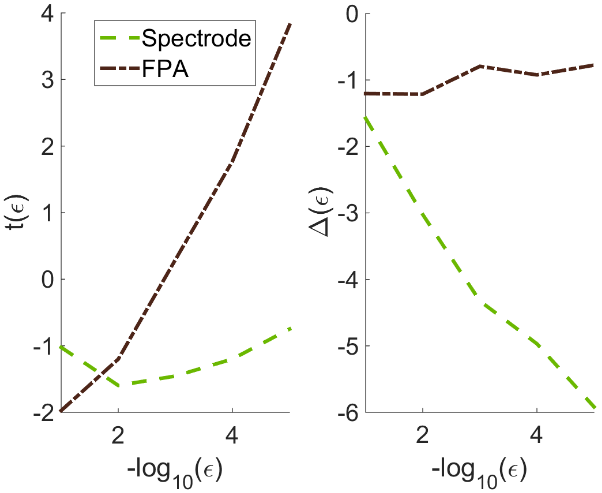

Figure: Running time (left), and average accuracy (right) as a function of the number of correct significant digits k: $\varepsilon = 10^{-k}$. SPECTRODE and fixed-point-algorithm (FPA).

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 MP distribution
- Matlab and R software at github.com/dobriban
  - With documentation and examples

SPECTRODE: HGDP example

- Human Genome Diversity Project (HGDP) data:
  - $n = 1043$ samples, $p = 9730$ SNPs on chr 22
- Processing
  - Standardize SNPs
  - Remove top 15 eigenvalues
  - Scale them to have mean 1
- Fitting
  - For candidate spectrum H, objective is Quantile Mean Deviation (MAD):

    $$QMD(H) = \frac{1}{p}\sum_{i=1}^{p} |\lambda_i - q(i/p; F_{\gamma,H})|,$$

    where $q(x, F)$ is x-th quantile of F (computed by Spectrode)
  - Grid search over γ and $H = \sum_{i=1}^{3} t_i \delta_{w_i}$
- Improve fit: reduce QMD by 50%, compared to optimal γ

SPECTRODE: HGDP example

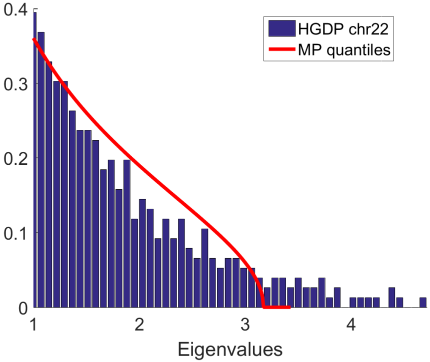

Figure: Standard MP fit: $\hat{\gamma} = 0.61$, $QMD = 0.101$

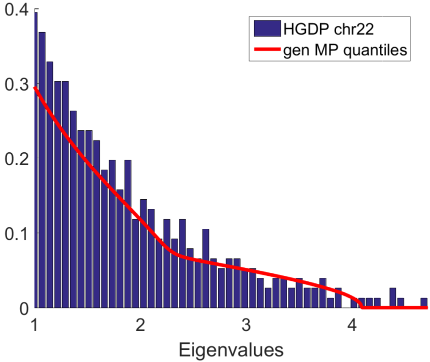

Figure: General MP fit by SPECTRODE: $\hat{\gamma} = 0.61$, $\hat{t} = [1, 0.7, 2.2]$, $\hat{w} = [0.5, 0.4, 0.1]$; $QMD = 0.049$

Spectrode: HGDP example

- Standard spiked model not a good fit to empirical eigenvalue dist
- Can use Spectrode to get better fit
- Consistent with
  - Many sources of common variation
  - Nontrivial correlation structure (linkage disequilibrium)
  - Cryptic relatedness

Summary

- Optimal testing for principal components in high dimensions
  - Detect below the phase transition in a local alternatives model, using LSS
- Enabled by new computational tool SPECTRODE

- Slides at github.com/dobriban/talks
- Dobriban (2016). Sharp detection in PCA under correlations. arxiv:1602.06896
- Thanks
  - Support: NSF, HHMI
  - Discussion: David Donoho, Iain Johnstone

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:

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

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

- 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

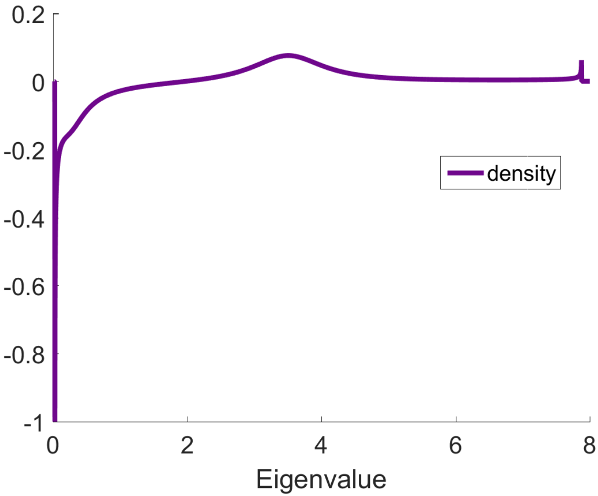

Figure: Density of weak derivative $\delta\mathcal{F}_\gamma(H, G)$ in AR-1 example $H = spec(\Sigma)$, $G = \delta_{3.5}$ below PT;

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