Eigenvalues and Variance Components

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On the occasion of the 60th birthday of
Oleg Lepski and Alexandre Tsybakov

Luminy, 19 December, 2017

Joint with Mark Blows & Zhou Fan

Motivating example

- p quantitative phenotypic traits, measured across a population
- Mean $\mu \in \mathbb{R}^p$, covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$

Q: Suppose natural selection acts on one of the traits. What will be the distribution of this trait in the next generation? On the distribution of other traits?

Motivating example

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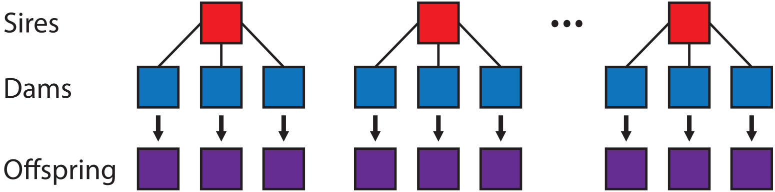
Q: Suppose natural selection acts on one of the traits. What will be the distribution of this trait in the next generation? On the distribution of other traits?

A: Depends on the "additive genetic component" of Σ

Can estimate genetic covariance using variance components models (Fisher 1918)

Half-sib experiment



One-way layout: $n = IJ$ individuals, I groups of size J

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad \in \mathbb{R}^p \qquad \text{(as row vector)}$$

$$\alpha_i \overset{iid}{\sim} \mathcal{N}(0, \Sigma_A), \qquad \text{group effect}$$

$$\varepsilon_{ij} \overset{iid}{\sim} \mathcal{N}(0, \Sigma_E), \qquad \text{residual error}$$

Additive genetic covariance: $G \approx 4\Sigma_A$

[vs. phenotypic covariance: $\mathrm{Cov}(Y) = \Sigma_A + \Sigma_E$]

Understanding G for high-dimensional trait sets

Multivariate breeder's equation (Lande and Arnold 1983):

$$\Delta\mu = G\beta$$

- Leading principal components of G indicate directions of strongest evolutionary response
- Rank of G indicates effective dimensionality of evolution
- Sparsity of G indicates extent of genetic correlations among traits

MANOVA estimator for Σ_A $[\propto G]$

Between-group and within-group "sums of squares": $(p \times p)$

$$SSA = J \sum_i (\bar{Y}_i - \bar{Y})^T (\bar{Y}_i - \bar{Y}) \qquad SSE = \sum_{i,j} (Y_{ij} - \bar{Y}_i)^T (Y_{ij} - \bar{Y}_i)$$

$$= Y^T P_A Y \qquad\qquad = Y^T P_E Y$$

Standard MANOVA estimator:

$$\hat{\Sigma}_A = \frac{1}{J} \left(\frac{1}{I-1} SSA - \frac{1}{n-I} SSE \right) = Y^T B Y,$$

for $B = \tau_A P_A - \tau_E P_E$. NOT positive definite!

Estimation of genetic covariance Σ_A quite different from

'phenotypic covariance' $n^{-1} Y^T Y$ (estimates $\Sigma_A + \Sigma_E$).

Agenda

- Variance component models and quadratic estimators
- Bulk eigenvalue distributions
- Extreme eigenvalue distributions
- Spiked models: effect on $\hat{\Sigma}_A$

Theory is asymptotic ($p, I \to \infty$ proportionally and J fixed), using random matrix theory.

Simulations assess accuracy in finite samples.

Multivariate variance component models

One way design $\quad Y_{ij} = \mu + \alpha_i + \epsilon_{ij} \quad$ is an example of:

$$Y = X\beta + U_1\alpha_1 + \ldots + U_{k-1}\alpha_{k-1} + \epsilon$$

$X\beta$ – fixed effects model

U_r – fixed incidence matrices

α_r – $I_r \times p$ random effects, rows $\sim N(0, \Sigma_r)$

ϵ – $n \times p$ residual errors, rows $\sim N(0, \Sigma_k)$

Covariance components: $\quad \Sigma_1, \ldots, \Sigma_k$

Some designs in quantitative genetics

[Examples, mixed model $Y = X\beta + U_1\alpha_1 + \ldots + U_{k-1}\alpha_{k-1} + \epsilon$]

[e.g. Lynch & Walsh, 1998]

Balanced half-sib	Balanced one way	I, J
Unbalanced half-sib	Unbalanced one way	I, n_i
Full-sib half-sib Monozygotic twin half-sib	Nested two-way	I, J_i, n_{ij}
	Balanced nested multi-way	$I, J, \ldots, n$
Comstock-Robinson	Replicated crossed two-way	I, J, K, L
all cases:		$I \propto p$

Quadratic Estimators of Variance Component Matrices

In the mixed model, consider estimators of Σ_r of form:

$$\hat{\Sigma} = Y^T B Y$$

- (M)ANOVA estimators:

equate Sum of Squares to expectations & solve, e.g. (1-way)

$$B = \tau_A P_A - \tau_E P_E$$

- MINQUE [minimum norm quadratic unbiased estimator]

e.g. unbalanced one way design, with 'prior parameter' $\rho \geq 0$,

$$B = \tau_{\rho A} \Pi_{\rho A} - \tau_{\rho E} P_E$$

Quadratic Estimators - Structure

Insert data

$$Y = U_1\alpha_1 + \cdots + U_k\alpha_k$$

(after setting $X\beta = 0, \epsilon = U_k\alpha_k$)

into estimator

$$\hat{\Sigma}_r = Y^T BY = \sum_{r,s=1}^{k} \alpha_r^T U_r^T BU_s\alpha_s$$

Write $\alpha_s = G_s\Sigma_s^{1/2}$, G_s i.i.d Gaussian matrix; $B_{r,s} = U_r^T BU_s$.

$$\hat{\Sigma}_r = \sum_{r,s} \Sigma_r^{1/2} G_r^T B_{r,s} G_s \Sigma_s^{1/2}$$

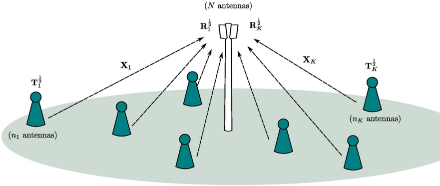
"Doubly correlated", general B.

Models in Wireless Communications

- MIMO-Multiple Access Channels

$$S + \sum_{r=1}^{k} R_r^{1/2} G_r^* T_r G_r R_r^{1/2}$$

$R_r, T_r \succ 0$ — receiver, transmitter covariances.



Couillet-Debbah-Silverstein 2011

- Frequency selective MIMO Moustakas-Simon 2007, Dupuy-Loubaton 2011

$$\sum_{r,s=1}^{k} R_r^{1/2} G_r^* T_r^{1/2} T_s^{1/2} G_s R_s^{1/2}$$

- Variance components: $B = (B_{r,s})$ symmetric, not necess $\succ 0$

$$\sum_{r,s} \Sigma_r^{1/2} G_r^T B_{r,s} G_s \Sigma_s^{1/2}$$

Bulk eigenvalue distribution

Special case: no common random effects

Y has n rows $\overset{\text{iid}}{\sim} N_p(0, \Sigma)$; $\qquad \gamma = p/n \to \gamma_\infty$

$$\hat{\Sigma} = n^{-1} Y^T Y \qquad\qquad (B = n^{-1} I_n)$$

Empirical eigenvalue distribution: $\quad \mu_{\hat{\Sigma}} = p^{-1} \sum_{i=1}^{p} \delta_{\lambda_i(\hat{\Sigma})}$

Theorem [Marčenko-Pastur] There are deterministic measures μ_{0n} s.t.

$$\mu_{\hat{\Sigma}} - \mu_{0n} \to 0 \qquad \text{a.s.}$$

μ_{0n} has Stieltjes transform $m_0(z) = \int (\lambda - z)^{-1} \mu_{0n}(d\lambda)$ given by

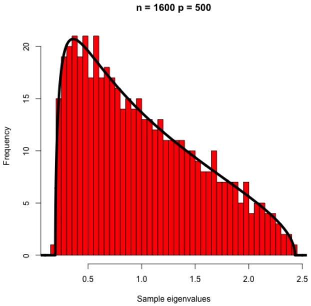
$$m_0(z) = \frac{1}{p} \operatorname{Tr} \left[(1 - \gamma - \gamma z m_0(z)) \Sigma - z \operatorname{Id} \right]^{-1},$$

(with unique solution $m_0(z) \in \mathbb{C}^+$)

Special[2] case: M-P quarter circle law

When $\Sigma = \mathrm{Id}$, $\mu_0 = \mu_{0n}$ has the quarter circle density

$$f(x) = \frac{\sqrt{(E_+ - x)(x - E_-)}}{2\pi x}, \qquad E_\pm = (1 \pm \sqrt{p/n})^2$$



For general Σ, density $f(x)$ can have multiple intervals of support.

General case for $\mu_{\hat{\Sigma}} = p^{-1} \sum_{i=1}^{p} \delta_{\lambda_i(\hat{\Sigma})}$

Assume

- $n, p, l_1, \ldots, l_k \to \infty$ proportionally,
- $\hat{\Sigma} = Y^T B Y$
- $\|\Sigma_r\|, \ \|U_r\| \leq O(1), \quad \|B\| \leq O(1/n).$

General case for $\mu_{\hat{\Sigma}} = p^{-1} \sum_{i=1}^{p} \delta_{\lambda_i(\hat{\Sigma})}$

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Theorem [Fan J 2016] There are deterministic measures μ_{0n} s.t.

$$\mu_{\hat{\Sigma}} - \mu_{0n} \to 0 \qquad \text{a.s.}$$

μ_{0n} has Stieltjes transform $m_0(z) = \int (\lambda - z)^{-1} \mu_{0n}(d\lambda)$ given by

$$m_0(z) = -\frac{1}{p} \operatorname{Tr} \left[\left(z \operatorname{Id} + \sum_{r=1}^{k} b_r(z) \Sigma_r \right]^{-1},$$

for $a_1(z), \ldots, a_k(z), \ b_1(z), \ldots, b_k(z)$ the unique solution to a certain system of $2k$ equations.

Particular cases

Notes:

1. μ_0 depends on $n, p, I_1, \ldots, I_{k-1}, \Sigma_1, \ldots, \Sigma_k$
2. $k = 1$: Recovers Marchenko-Pastur theorem for $\hat{\Sigma} = n^{-1} Y^T Y$

$k = 2$: System of equations for balanced one-way layout, for $\hat{\Sigma}_A$:

$$
\begin{aligned}
a_A(z) &= -(1/I)\,\mathrm{Tr}[(z\,\mathrm{Id} + b_A(z)\Sigma_A + b_E(z)\Sigma_E)^{-1}\Sigma_A] \\
a_E(z) &= -(1/n)\,\mathrm{Tr}[(z\,\mathrm{Id} + b_A(z)\Sigma_A + b_E(z)\Sigma_E)^{-1}\Sigma_E] \\
b_A(z) &= -\frac{1}{1 + a_A(z) + a_E(z)} \\
b_E(z) &= \frac{J-1}{J(J-1-a_E(z))} - \frac{1}{J + Ja_A(z) + Ja_E(z)}
\end{aligned}
$$

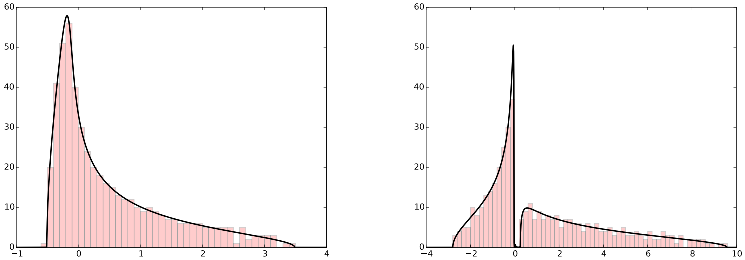
$$
m_0(z) = -(1/p)\,\mathrm{Tr}[(z\,\mathrm{Id} + b_A(z)\Sigma_A + b_E(z)\Sigma_E)^{-1}]
$$

Easily solvable by iteration to compute $\frac{1}{\pi}\Im m_0(z)$ near real-axis.

Computing the deterministic equivalent

Theorem (Fan, J. (cont'd))

To compute $m_0(z)$, the preceding system of equations may be solved by initializing (b_A, b_E) arbitrarily, then iteratively updating (a_A, a_E) and (b_A, b_E) until convergence.



Black curves: $\pi^{-1}\Im m_0(z)$ for $\Im z = 10^{-4}$.

Right: $\Sigma_A = \Sigma_E = \mathrm{Id}$. $I = 200$ groups of size $J = 2$, $p = 500$.

Balanced nested/crossed designs

Lattice subspace structure:

$$S_r = \bigoplus_{r' \preceq r} \mathring{S}_{r'},$$

Mean (Sum of) Squares MS_r for $\mathring{S}_r$

$$\mathbb{E}\, MS_t = \sum_{r \succeq t} c_r \Sigma_r$$

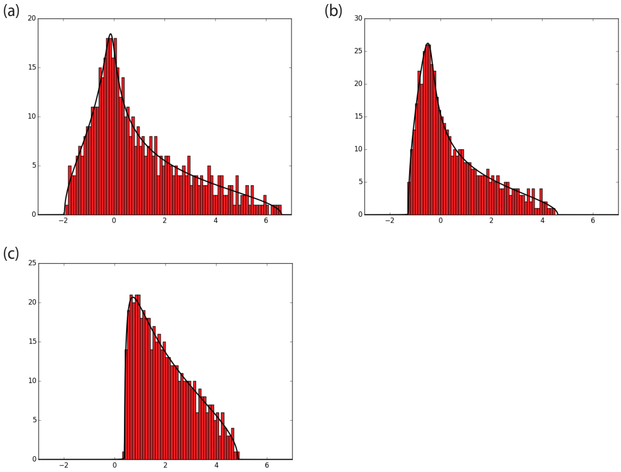
Möbius inversion: $\hat{\Sigma}_t = Y^T B_t Y$

$$\begin{tikzcd}[column sep=small]
S_0 \arrow[d, dash] \\
S_1 \arrow[d, phantom, "\vdots"] \\
S_r \arrow[d, dash] \\
S_{r+1} \arrow[d, phantom, "\vdots"] \\
S_k
\end{tikzcd}
\qquad
\begin{tikzcd}[column sep=small]
 & S_0 \arrow[d, dash] & \\
 & S_1 \arrow[dl, dash] \arrow[dr, dash] & \\
S_2 \arrow[dr, dash] & & S_3 \arrow[dl, dash] \\
 & S_4 \arrow[d, dash] & \\
 & S_5 &
\end{tikzcd}$$

In equation system for $m_0(z)$ for $\hat{\Sigma}_t$,

- compute $b_r(z)$ as rational function of $a_s(z)$
- included in software (forthcoming)

Two-way nested example



$$n = 2400, \quad I_1 = 400, \quad I_2 = 2, \quad I_3 = 3, \quad p = 500$$

$\Sigma_1 = \mathrm{Id}_p, \qquad \Sigma_2 = 0.5\,\mathrm{Id}_p, \qquad \Sigma_3 = 2\,\mathrm{Id}_p,$

(a): $\hat{\Sigma}_1$, $\qquad$ (b): $\hat{\Sigma}_2$, $\qquad$ (c): $\hat{\Sigma}_3$,

About proof of bulk convergence

- Via rectangular free probability
- In classical probability, if scalar variables $W \perp\!\!\!\perp H|B$, then

$$\mathbb{E}[e^{isW}|H, B] = \mathbb{E}[e^{isW}|B]$$

- use operator-valued free probability for eigenvalues of

$$W = Y^T BY = \sum_{r,s=1}^{k} H_r^T G_r^T B_{r,s} G_s H_s, \qquad (H_r = \Sigma_r^{1/2})$$

via block matrix embedding, e.g.

$$\begin{bmatrix} H_A, H_E & G_A^T & G_E^T \\ G_A & B_{AA} & B_{AE} \\ G_E & B_{EA} & B_{EE} \end{bmatrix}$$

Free probability correspondence

All the familiar probability notions have analogues:

(commutative) probability	non-commutative probability
scalar r.v.s X, Y	random matrices A, B
sample space	operator (W^*-)algebra
expectation $\mathbb{E}$	trace τ
moments $\mathbb{E}X^k$	moments $\tau(A^k) = \sum_i \lambda_i^k(A)$
Fourier transform	Stieltjes/Cauchy transform
(asy) independence	(asy) freeness
sub σ-field $\mathcal{H}$	sub (W^*-)algebra $\mathcal{B}$
conditional expectation	$\mathcal{B}$-valued expectation operator
conditional indep. $\lvert\mathcal{H}$	conditional freeness over $\mathcal{B}$
(conditional) Fourier transform	(operator valued) Cauchy transform

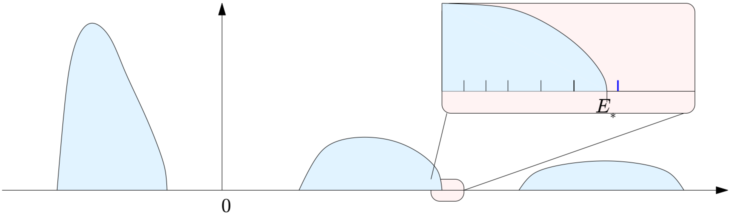
Voiculescu 1991, 1995, Speicher 1998, Nica, Shlyakhtenko and Speicher 2002, Benaych-Georges 2009, Hiai and Petz 2000, Speicher and Vargas 2012, Extreme eigenvalue distribution

Tracy-Widom at each edge

$X = (X_{\alpha i})$ $M \times N$, $\quad X_{\alpha i} \sim (0, N^{-1})$; $\quad T$ symmetric

$\hat{\Sigma} = X^T T X$ $\quad$ (and, if $T \geq 0$, $\tilde{\Sigma} = T^{1/2} X X^T T^{1/2}$)

For $M/N \to d > 0$ and a regular right (or left) edge E_*:



Theorem [Fan, J 17] If $\lambda_{\max}, \lambda_{\min}$ are extreme eigenvalues near E_*,

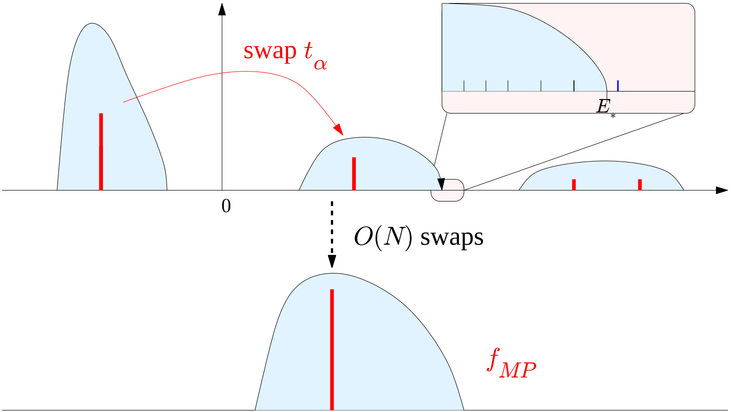
$$(\gamma N)^{2/3}(\lambda_{\max} - E_*) \xrightarrow{L} \mathrm{TW}_1 \qquad \text{(right edge)}$$

$$(\gamma N)^{2/3}(E_* - \lambda_{\min}) \xrightarrow{L} \mathrm{TW}_1 \qquad \text{(left edge)}$$

[Extends Lee – Schnelli, 2016: $T > 0$, largest eigenvalue only]

Lindeberg swapping

Swap eigenvalues (t_α) of T one-at-a-time between bulks:



$O(N)$ swaps with careful scaling doesn't change limit of $\lambda_{\max}$!
Then build on resolvent comparison approach, Lee - Schnelli, 2016.

Largest eigenvalue under "global null hypothesis"

Back to var. components model: $Y = X\beta + U_1\alpha_r + \cdots + U_k\alpha_k$

$$H_0 : \Sigma_r = c_r^2 \,\mathrm{Id}, \quad r = 1, \ldots, k \qquad \text{"sphericity"}$$

$$\hat{\Sigma} = Y^T BY, \qquad [BX = 0]$$

Note: B has $+$ve *and* $-$ve eigenvalues, even in the limit.

Corollary (Fan J 17)

Assume $n, p \to \infty$ proportionally, H_0 holds, $\|B\| \asymp 1/n$, and B satisfies certain regularity conditions. Then

$$(\lambda_{\max}(\hat{\Sigma}) - \mu_{np})/\sigma_{np} \xrightarrow{L} TW_1,$$

where $\mu_{np}, \sigma_{np} = (\kappa p)^{-2/3}$ are functions of $p, \lambda_1(B), \ldots, \lambda_n(B)$.

Formulas for center μ_{np} and scale σ_{np}

Let $t_1, \ldots, t_M$ be eigenvalues of $T = (pc_r c_s U_r^T B U_s)$,
with $M = l_1 + \cdots + l_k$.

$$z(m) = -\frac{1}{m} + \frac{1}{p} \sum_{\alpha=1}^{M} \frac{t_\alpha}{1 + t_\alpha m}$$

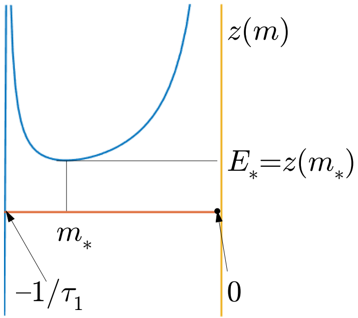
Silverstein-Choi (95)

m_* : solves $z'(m) = 0$

$\mu_{np} = E_+ = z(m_*)$

$\sigma_{np} = [z''(m_*)/(2p^2)]^{1/3}$

El Karoui 2007,
Hachem-Hardy-Najim 2016



Spiked Variance Component models

Spiked models for variance components

Assume [J '01]:

$$\Sigma_A = \sigma_A^2 \, \mathrm{Id} + \text{ finite number of spikes}$$
$$\Sigma_E = \sigma_E^2 \, \mathrm{Id} + \text{ finite number of spikes}$$

Where do corresponding outlier eigenvalues of $\hat{\Sigma}_A$ appear in the spectrum?

Spiked models for variance components

Assume [J '01]:

$$\Sigma_A = \sigma_A^2 \,\mathrm{Id} + \text{ finite number of spikes}$$
$$\Sigma_E = \sigma_E^2 \,\mathrm{Id} + \text{ finite number of spikes}$$

Where do corresponding outlier eigenvalues of $\hat{\Sigma}_A$ appear in the spectrum? i.e. let

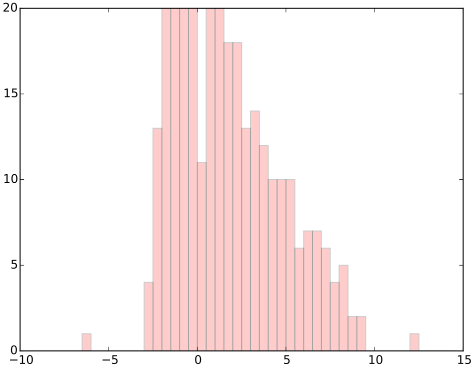
$$\Sigma_A = \sigma_A^2 \,\mathrm{Id} + V_A \Theta_A V_A^T, \qquad \Sigma_E = \sigma_E^2 \,\mathrm{Id} + V_E \Theta_E V_E^T,$$

Θ_A, Θ_E (diagonal) contain spike values, columns of V_A, V_E the corresponding eigenvectors. Set

$$\Theta = \begin{pmatrix} \Theta_A & 0 \\ 0 & \Theta_E \end{pmatrix}, \qquad S = \begin{pmatrix} \mathrm{Id} & V_A^T V_E \\ V_E^T V_A & \mathrm{Id} \end{pmatrix}.$$

S contains eigenvector alignments.

Aliasing from the error covariance

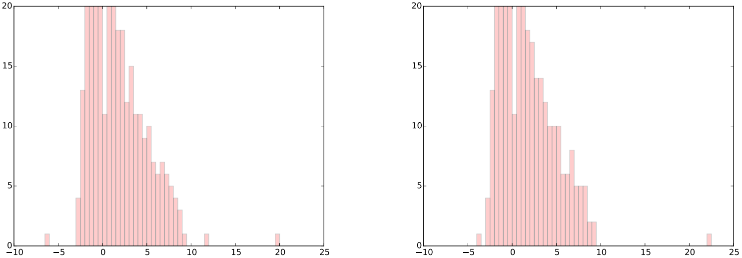


Eigenvalues of $\hat{\Sigma}_A$

$\Sigma_A = \mathrm{Id}$, but $\Sigma_E = \mathrm{Id} +$ spike at 25

$I = 200$ groups of size $J = 2$, $p = 500$ traits.

Dependence on eigenvector alignment



Eigenvalues of $\hat{\Sigma}_A$ Eigenvalues of $\hat{\Sigma}_A$

$\Sigma_A = \mathrm{Id} +$ spike at 15, $\Sigma_E = \mathrm{Id} +$ spike at 25.

Left: Spikes orthogonal. Right: Spikes aligned.

Locations of outliers

Let $\hat{\Sigma} = c_1 \mathrm{MSA} + c_2 \mathrm{MSE}$ w. deterministic equivalent measure μ_0.

$$\Theta = \begin{pmatrix} \Theta_A & 0 \\ 0 & \Theta_E \end{pmatrix}, \quad S = \begin{pmatrix} \mathrm{Id} & V_A^T V_E \\ V_E^T V_A & \mathrm{Id} \end{pmatrix}, \quad T = \begin{pmatrix} t_1(\lambda)\,\mathrm{Id} & 0 \\ 0 & t_2(\lambda)\,\mathrm{Id} \end{pmatrix}$$

Here, t_1 and t_2 are two (explicit) analytic functions of λ, c_1, c_2.

Locations of outliers

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Here, t_1 and t_2 are two (explicit) analytic functions of λ, c_1, c_2.

Theorem (Fan & Yi Sun, informal version)

Suppose $p, I \to \infty$ with $\sigma_A^2, \sigma_E^2, \Theta, S$ fixed. For each root λ of

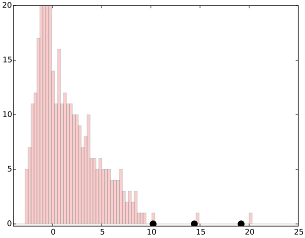
$$\det\left(\mathrm{Id} + S\Theta T(\lambda)\right) = 0$$

outside $\mathrm{supp}(\mu_0)$, *an eigenvalue of $\hat{\Sigma}$ converges to λ.*

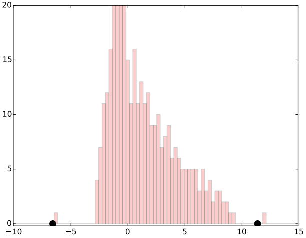
The remaining eigenvalues of $\hat{\Sigma}$ converge to $\mathrm{supp}(\mu_0)$.

$\to$ Algorithm to estimate Θ from loci of outlier eigenvalues of $\hat{\Sigma}(c_1, c_2)$ as (c_1, c_2) vary.

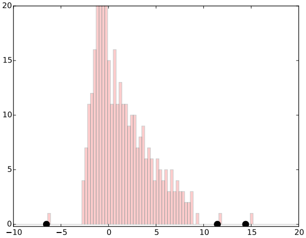
Locations of outliers in $\hat{\Sigma}_A$

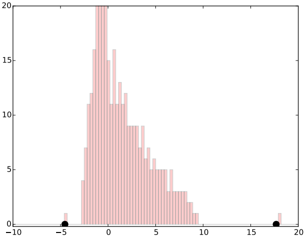


$\Sigma_A = \mathrm{Id} + [2, 5, 10, 15], \Sigma_E = \mathrm{Id},$



$\Sigma_A = \mathrm{Id}, \Sigma_E = \mathrm{Id} + 25$





$\Sigma_A = \mathrm{Id} + 10, \Sigma_E = \mathrm{Id} + 25;$ left: orthogonal, right: aligned

Black dots indicate theoretical predictions for outlier locations.

References

Z Fan, I Johnstone. Eigenvalue distributions of variance components estimators in high-dimensional random effects models. *arXiv:1607.02201*

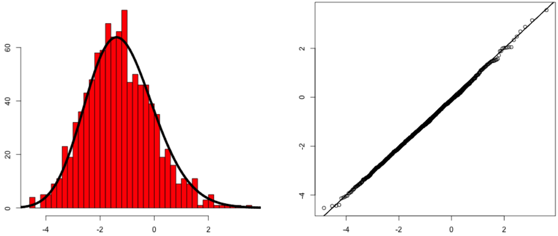
Z Fan, I Johnstone. Tracy-Widom at each edge of real covariance estimators. *arXiv:1707.02352*

M Blows, Z Fan, E Hine, I Johnstone, Y Sun. Spiked covariances and eigenvalue estimation in high-dimensional random effects models. *In preparation.*

THANK YOU!

Largest eigenvalue: balanced one-way example

$$H_0: \ \Sigma_A = 0, \quad \Sigma_E = \mathrm{Id}, \qquad B_A = \tau_A P_A - \tau_E P_E$$



Histogram & QQ-plot of scaled $\lambda_{\max}(\hat{\Sigma}_A)$ $\mu_{np} = 0.91, \sigma_{np} = 0.012$

$I = 400, \quad J = 4, \quad p = 500$

- Conditions ok if $\lambda_{\max}(B) \asymp 1/n$ with multiplicity $\asymp n$
- For c_r unknown, can use $\hat{c}_r^2 = p^{-1}\mathrm{Tr}(\hat{\Sigma}_r)$.

Approximation accuracy in finite samples

	F_1	$n = p$ $J = 2$	$J = 5$	$J = 10$	$n = 4 \times p$ $J = 2$	$J = 5$	$J = 10$
	0.90	0.938	0.944	0.953	0.932	0.937	0.940
$p = 20$	0.95	0.971	0.974	0.978	0.968	0.970	0.972
	0.99	0.995	0.995	0.995	0.993	0.994	0.995
	0.90	0.926	0.934	0.931	0.923	0.919	0.918
$p = 100$	0.95	0.963	0.969	0.968	0.962	0.961	0.961
	0.99	0.992	0.995	0.995	0.993	0.993	0.994
	0.90	0.922	0.917	0.918	0.913	0.909	0.916
$p = 500$	0.95	0.961	0.958	0.959	0.956	0.954	0.959
	0.99	0.992	0.992	0.991	0.993	0.992	0.994

Empirical CDF values at the theoretical 0.90, 0.95, and 0.99 quantiles of the F_1 law. (Standard errors 0.001–0.003.)

The Tracy-Widom test is slightly conservative in practice.