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Topic 18: Eigenvalue and Spike Models

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Key points: .

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18.1 Motivation

Consider n independent observations $\mathbf{X}_i \in \mathbb{R}^p$ drawn from a $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$, then the covariance can be decomposed into 2 parts, white noise and low rank

$$\Sigma = \text{Cov}(\mathbf{X}_i) = \mathbf{I} + \sum_{k=1}^{M} \theta_k \nu_k \nu_k' = \Sigma_0 + \mathbf{\Phi}$$

where M denotes the **number of spikes** in the distribution of eigenvalues. The idea is: spikes deviate from a reference model along a <u>small fixed number</u> of unknown directions. If $\Phi = 0$, then none of the sample eigenvalues is separated from the bulk.

Why a spike model is interesting? A spike model can help determine the latent dimension of the data, some examples being

- Principal component analysis (PCA): spikes are related to the directions of the most variations of the data, i.e., the principal components
- Clustering model: M spikes is equivalent to M+1 clusters
- Economic significance: *M* is related to the number of factor loadings

Then the question is threefold:

- How to determine *M*
- How to estimate v_k
- How to test θ_k

Under rank one alternative, we would like to test the hypothesis

$$H_1: \mathbf{\Sigma} = \mathbf{I}_p + \theta \mathbf{\nu} \mathbf{\nu}', \theta > 0$$

against the null

$$H_0: \mathbf{\Sigma} = \mathbf{I}_p$$

with the key assumptions:

A1 Gaussian error

A2 large p: $p \le n$ but allows $p/n \to \gamma \in (0,1)$

Under these assumptions, for the $n \times p$ data matrix $\mathbf{X} = (\mathbf{X}'_1 \cdots \mathbf{X}'_n)'$, $\mathbf{X}'\mathbf{X}$ has a p-dimensional **Wishart** distribution $W_p(n, \Sigma)$ with the degree of freedom n and covariance matrix Σ , which is a *random matrix*.

If $\mathbf{Y} = \mathbf{M} + \mathbf{X}$, that is, the sum of the *random matrix* \mathbf{X} and a *deterministic matrix* \mathbf{M} (also $n \times p$), then $\mathbf{Y}'\mathbf{Y}$ has a p-dimensional Wishart distribution $W_p(n, \Sigma, \Psi)$ with n degrees of freedom, covariance matrix Σ and non-centrality matrix $\mathbf{\Psi} = \Sigma^{-1}\mathbf{M}'\mathbf{M}$.

Definition 18.1.1: Density of Wishart Distribution

The PDF of Wishart distribution is defined as

$$f(\mathbf{X}) = \frac{1}{2^{np/2} \Gamma_p\left(\frac{n}{2}\right) |\mathbf{\Sigma}|^{n/2}} |\mathbf{X}|^{(n-p-1)/2} \exp\left(-\frac{1}{2} \operatorname{tr}\left(\mathbf{\Sigma}^{-1} \mathbf{X}\right)\right)$$

where **X** is a symmetric positive semidefinite and $\Gamma_p\left(\frac{n}{2}\right)$ is a multivariate gamma function such that

$$\Gamma_p\left(\frac{n}{2}\right) = \pi^{\frac{p(p-1)}{4}} \prod_{j=1}^p \Gamma\left(\frac{n}{2} - \frac{j-1}{2}\right)$$

Notice that the sample covariance matrix $S = \frac{1}{n}X'X$ is just a scaled version of Wishart distribution

$$n\mathbf{S} = \mathbf{X}'\mathbf{X} \sim W_n(n, \mathbf{\Sigma})$$

For $\Sigma = \mathbf{I}_p$, the empirical distribution fo eigenvalues converges to Marcenko-Pastur distribution

$$f^{\text{MP}}(x) = \frac{1}{2\pi\gamma x} \sqrt{(b_+ - x)(x - b_-)}$$

where $b_{\pm} = (1 \pm \sqrt{\gamma})^2$. Then:

• under $H_0: \Sigma = \mathbf{I}_p$, we have

$$n^{2/3} \left(\frac{\lambda_1 - \mu(\gamma)}{\sigma(\gamma)} \right) \stackrel{d}{\to} TW_1$$

where TW₁ is the Tracy-Widom distribution

• under $H_1: \Sigma = \mathbf{I}_p + \theta \nu \nu', \theta > 0$, if θ is strong $(\theta \gg \sqrt{\gamma})$, then

$$n^{1/2}\left(\frac{\lambda_1-\rho(\theta,\gamma)}{\tau(\theta,\gamma)}\right) \xrightarrow{d} \mathcal{N}(0,1)$$

Here, the largest eigenvalue test is the best test. **But** when the signal is weak $(0 \le \theta < \sqrt{\gamma})$, the largest eigenvalue under the alternative converges to the same distribution as null:

$$n^{2/3} \left(\frac{\lambda_1 - \rho(\theta, \gamma)}{\tau(\theta, \gamma)} \right) \xrightarrow{d} TW_1$$

which means that the largest eigenvalue test *fails*. On top of this, **resampling** also fails when p is large. Next, we develop another test to cope with these problems.



Figure 18.1: Failure of Resampling Test (n = p = 100)

18.2 Johnstone and Onatski (2020)

Consider the basic equation of classical multivariate statistics:

$$\det\left(\mathbf{H} - \mathbf{x}\mathbf{E}\right) = 0\tag{18.1}$$

with $p \times p$ matrices

$$n_1\mathbf{H} = \sum_{k=1}^{n_1} \mathbf{x}_k \mathbf{x}'_k$$
 hypothesis SS
$$n_1\mathbf{E} = \sum_{k=1}^{n_1} \mathbf{z}_k \mathbf{z}'_k$$
 error SS

• scalar inputs

$${}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;x) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_p)_k} \frac{x^k}{k!}$$

where $(a_i)_k$ are generalized Pochhammer symbols

- single matrix inputs, where \boldsymbol{S} is symmetric and usually diagonal

$${}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{S}) = \sum_{k=0}^{\infty} \sum_{\kappa} \frac{(a_1)_{\kappa} \cdots (a_p)_{\kappa}}{(b_1)_{\kappa} \cdots (b_p)_{\kappa}} \frac{C_{\kappa}(\mathbf{S})}{k!}$$

where C_k are the zonal polynomials. Easily, $_0\mathcal{F}_0(\mathbf{S}) = e^{\operatorname{tr}(\mathbf{S})}, _1\mathcal{F}_0(a,\mathbf{S}) = |\mathbf{I} - \mathbf{S}|^{-a}$

- two matrix inputs, where $\boldsymbol{S},\boldsymbol{T}$ are both symmetric

$$_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{S},\mathbf{T}) = \int_{O(p)} {}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{SUTU'})(d)\mathbf{U}$$

¹Hypergeometric functions are:

		Statistical method	$n_1\mathbf{H}$	$n_2\mathbf{E}$	Univariate Analog
$_0\mathcal{F}_0$	PCA	Principal components analysis	$W_p(n_1, \Sigma + \Phi)$	$n_2\Sigma$	χ^2
$_1\mathcal{F}_0$	SigD	Signal detection	$W_p(n_1, \Sigma + \Phi)$	$W_p(n_2, \Sigma)$	non-central χ^2
$_0\mathcal{F}_1$	REG_0	Multivariate regression, with known error	$W_p(n_1, \Sigma, n_1\mathbf{\Phi})$	$n_2\Sigma$	F
$_1\mathcal{F}_1$	REG	Multivariate regression, with unknown error	$W_p(n_1, \mathbf{\Sigma}, n_1\mathbf{\Phi})$	$W_p(n_2, \Sigma)$	non-central F
$_2\mathcal{F}_1$	CCA	Canonical correlation analysis	$W_p(n_1, \mathbf{\Sigma}, \mathbf{\Phi}(\mathbf{Y}))$	$W_p(n_2, \Sigma)$	$\frac{r^2}{1-r^2}$

Table 18.1: 5 Statistical Methods

For $_0\mathcal{F}_0$ and $_0\mathcal{F}_1$, **E** is deterministic, Σ is known, n_2 disppears, otherwise **E** is independent of **H**.

18.2.1 Definitions and global assumptions

Let **Z** be an $n \times p$ data matrix with rows (observations) drawn **i.i.d.** from $\mathcal{N}_p(\mathbf{0}, \Sigma)$, and a deterministic matrix **M** of $n \times p$, then for $\mathbf{Y} = \mathbf{M} + \mathbf{Z}$,

- $\mathbf{H} = \mathbf{Y'Y}$ has a p dimensional Wishart distribution $W_p(n, \Sigma, \Psi)$ with n degrees of freedom, covariance matrix Σ and non-centrality matrix $\Psi = \Sigma^{-1}\mathbf{M'M}$
- the corresponding central Wishart distribution with $\mathbf{M} = \mathbf{0}$ is $W_p(n, \Sigma)$

Johnstone and Onatski (2020) assume a relative low dimensionality $p \le \min\{n_1, n_2\}$ where n_1, n_2 are the degrees of freedom as in Table 18.1, where

- $p \le n_2$ ensures almost sure invertibility of matrix **E** in Equation 18.1
- $p \le n_1$ is not essential, but reduces the number of various situations of consideration.

18.2.2 5 classes of problems

With these assumptions, they established a unified statistical problem **symmetric matrix denoising (SMD)** that can be linked to the 5 classes of problems:

PCA n_1 i.i.d. observations drawn from $\mathcal{N}_p(\mathbf{0}, \mathbf{\Omega})$ to test the hull hypothesis that the population covariance $\mathbf{\Omega} = \mathbf{\Sigma}$, with the alternative of interest being

$$\Omega = \Sigma + \Phi$$
, with $\Phi = \theta \phi \phi'$

where $\theta > 0$, ϕ are unknown, and ϕ is normalized s.t. $\|\Sigma^{-1/2}\phi\| = 1$. W.L.O.G., assume $\Sigma = \mathbf{I}_p$, then under the alternative, the first principal component explains a larger portion of the variation than the other principal components. Re-formulate the hypotheses in terms of the spectral *spike* parameter θ , we have

$$H_0: \theta_0 = 0$$
 $H_1: \theta_0 = \theta > 0$ (18.2)

where θ_0 is the true value of the *spike*. A **maximal invariant statistic** consists of the solutions $\lambda_1 \ge \cdots \ge \lambda_p$ of Equation 18.1 with

- *n*₁**H** equal to the sample covariance matrix
- $\mathbf{E} = \mathbf{\Sigma}$

SigD Now consider testing the **equality** of covariance matrices **Ω** and **Σ**, corresponding to 2 independent p-dimensional mean-zero Gaussian samples of size n_1 and n_2 , with the alternative still

$$\Omega = \Sigma + \Phi$$
, with $\Phi = \theta \phi \phi'$

and again, assume $\Sigma = I_p$ (but NOT necessarily known), here, instead of Equation 18.1, consider

$$\det\left(\mathbf{H} - \lambda \left(\mathbf{E} + \frac{n_1}{n_2}\mathbf{H}\right)\right) = 0 \tag{18.3}$$

naturally, SigD reduces to PCA as $n_2 \rightarrow \infty$ while n_1 and p held constant.

REG₀ Next, consider a linear regression with multivariate response

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

with known covariance matrix Σ of the i.i.d. Gaussian rows of the error matrix ϵ . Here, to test linear restrictions on the matrix of coefficients β , we can split the matrix of transformed response variables Y into 3 parts Y_1 , Y_2 , Y_3 , where

• \mathbf{Y}_1 is $n_1 \times p$ where p is the number of response variables, n_1 is the number of linear restrictions (per each of the p columns of matrix $\boldsymbol{\beta}$), under the null H_0 : $\mathbb{E}\mathbf{Y}_1 = 0$, versus the alternative

$$\mathbb{E}\mathbf{Y}_1 = \sqrt{n_1 \theta} \boldsymbol{\psi} \boldsymbol{\phi}' \tag{18.4}$$

where $\theta > 0$, $\left\| \mathbf{\Sigma}^{-1/2} \boldsymbol{\phi} \right\| = 1$ and $\left\| \boldsymbol{\psi} \right\| = 1$

- \mathbf{Y}_2 is $(q n_1) \times p$, where q is the number of regressors
- \mathbf{Y}_3 is $(T q) \times p$, where T is the number of observations

In this case, tests can be based on the solutions $\lambda_1, \dots, \lambda_p$ to

$$\det(\mathbf{H} - \lambda \mathbf{E}) = \mathbf{0}$$

where $\mathbf{H} = \mathbf{Y}_1' \mathbf{Y}_1/n_1$ and $\mathbf{E} = \mathbf{\Sigma}$. The solutions represent a multivaraite analog of the difference between the sum of squared residuals in the restircted and unrestricted regressions. Under the null, $n_1\mathbf{H}$ is distributed as $W_p(n_1, \mathbf{\Sigma})$. Here,

$$n_1 \mathbf{H} \sim W_p(n_1, \mathbf{\Sigma})$$
 under H_0
 $n_1 \mathbf{H} \sim W_p(n_1, \mathbf{\Sigma}, n_1 \mathbf{\Phi})$, where $\mathbf{\Phi} = \theta \mathbf{\Sigma}^{-1} \boldsymbol{\phi} \boldsymbol{\phi}'$ under H_1

Again, W.L.O.G, assume $\Sigma = \mathbf{I}_p$. This **canonical form** of REG₀ is essentially equivalent to the setting of **matrix denoising**

$$Y_1 = M + Z$$

REG Again, consider the linear regression

$$Y = X\beta + \epsilon$$

but NOT knowing the covariance matrix Σ of rows of ϵ . Here, the solutions again solve $\det(H - \lambda E) = 0$ with

$$\mathbf{H} = \mathbf{Y}_{1}' \mathbf{Y}_{1} / n_{1}, \ \mathbf{E} = \mathbf{Y}_{3}' \mathbf{Y}_{3} / n_{2}$$

this represents a multivariate analog of the F ratio: the difference between the sum of squared residuals in the restricted and unrestricted regressions to the sum of squared residuals in the restricted regression. Again, as $n_2 \to \infty$, REG reduces to REG₀.

CCA Consider testing for independence between Gaussian vectors $x_t \in \mathbb{R}^p$ and $y_t \in \mathbb{R}^{n_1}$, given zero-mean observations with $t = 1, \dots, n_1 + n_2$. Partition the population and sample covariance matrices of the observations $(x'_t, y'_t)'$ into

$$\begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix} \qquad \begin{pmatrix} \mathbf{S}_{xx} & \mathbf{S}_{xy} \\ \mathbf{S}_{yx} & \mathbf{S}_{yy} \end{pmatrix}$$

respsectively. Under $H_0: \Sigma_{xy} = \mathbf{0}$, while the alternative is

$$\Sigma_{xy} = \sqrt{\frac{n_1 \theta}{n_1 \theta + n_1 + n_2}} \phi \psi' \tag{18.5}$$

where the nuisance parameters $\phi \in \mathbb{R}^p$ and $\psi \in \mathbb{R}^{n_1}$ are normalized s.t.

$$\left\|\boldsymbol{\Sigma}_{xx}^{-1/2}\boldsymbol{\phi}\right\| = \left\|\boldsymbol{\Sigma}_{yy}^{-1/2}\boldsymbol{\psi}\right\| = 1$$

And the test can be based on the squared sample canonical correlations $\lambda_1, \cdots, \lambda_p$ that solves

$$\det\left(\mathbf{H} - \lambda \mathbf{E}\right) = \mathbf{0}$$

with

$$\mathbf{H} = \mathbf{S}_{xy} \mathbf{S}_{yy}^{-1} \mathbf{S}_{yx}$$

$$\mathbf{E} \mathbf{S}_{xx}$$

18.2.3 SMD

For a $\mathbf{X} = \mathbf{\Phi} + \mathbf{Z}/\sqrt{p}$ where \mathbf{Z} is a noise matrix from the **Gaussian Orthogonal Ensemble** (GOE)² We seek to make inference about a symmetric rank-one *signal* matrix $\mathbf{\Phi} = \theta \phi \phi'$. The null and the alternative is again as in 18.2. The nuisance vector $\boldsymbol{\phi} \in \mathbb{R}^p$ is normalized s.t. $\|\boldsymbol{\phi}\| = 1$.

The problem remains **invariant** under the multiplication of X from the left by an orthogonal matrix, and from the right by its transpose. A maximal invariant statistic consists of the solutions $\lambda_1, \dots, \lambda_p$ to $\det(H - \lambda E) = 0$ with H = X and $E = I_p$.

SMD can be viewed as a degenerate version of the 5 classes of problems, as shown in Figure 18.2:

- SMD, PCA, REG₀: random H and deterministic E
- PCA and SigD are parallel to REG₀
- CCA has a different structure of H and E

18.2.4 The likelihood ratios

The goal is to study the asymptotic behavior of likelihood ratios based on the observed eigenvalues

$$\Lambda = \operatorname{diag}\left\{\lambda_1, \cdots, \lambda_p\right\}$$

$$\mathbf{Z}_{ii} \sim \mathcal{N}(0,2)$$

$$\mathbf{Z}_{ij} \sim \mathcal{N}(0,1)$$
 if $i > j$

²**Z** is from the GOE that it is **symmetric** and

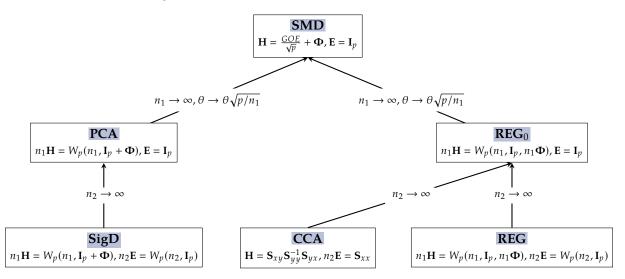


Figure 18.2: SMD and 5 Classes of Statistical Problems

then the likelihood of the alternative versus the null is given by

$$\mathcal{L}(\theta, \Lambda) = \frac{p(\Lambda; \theta)}{p(\Lambda; 0)} = \alpha(\theta)_{p} \mathcal{D}_{q}(\mathbf{a}, \mathbf{b}; \mathbf{\Phi}, \Lambda)$$
(18.6)

where $\Phi = \Phi(\theta)$ is a *p*-dimensional matrix diag $\{\Phi_{11}, 0, \cdots, 0\}$. Consider the hypergeometric functions of 2 matrix arguments Φ, Λ are defined as

$$_{p}\mathcal{F}_{q}(\mathbf{a},\mathbf{b};\mathbf{\Phi},\mathbf{\Lambda}) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\kappa-k} \frac{(a_{1})_{\kappa} \cdots (a_{p})_{\kappa}}{(b_{1})_{\kappa} \cdots (b_{1})_{\kappa}} \frac{C_{\kappa}(\mathbf{\Phi})C_{\kappa}(\mathbf{\Lambda})}{C_{\kappa}(\mathbf{I}_{p})}$$

where $\mathbf{a} = (a_1, \dots, a_p)$ and $\mathbf{b} = (b_1, \dots, b_q)$ are parameters, κ are partitions of the integer k, $(a_j)_{\kappa}$ and $(b_i)_{\kappa}$ are the generalized Pochhammer symbols, C_{κ} are the zonal polynomials. For each of the 6 classes of problems, we have the parameters as in Table where $n = n_1 + n_2$.

Table 18.2: Parameters of the Likelihood Ratios in Eq.18.6

Classes	$_{ m p}\mathcal{F}_{ m q}$	$\alpha(\theta)$	а	b	$\mathbf{\Phi}_{11}$
SMD	$_0\mathcal{F}_0$	$\exp(-p\theta^2/4)$	-	-	$\theta p/2$
PCA	$_0\mathcal{F}_0$	$(1+\theta)^{-n_1/2}$	-	-	$\theta n_1/(2(1+\theta))$
SigD	$_1\mathcal{F}_0$	$(1+\theta)^{-n_1/2}$	-	-	$\theta n_1/(n_2(1+\theta))$
REG_0	$_0\mathcal{F}_1$	$\exp(-n_1\theta/2)$	-	$n_1/2$	$\theta n_1^2/4$
REG	$_1\mathcal{F}_1$	$\exp(-n_1\theta/2)$	n/2	$n_1/2$	$\theta n_1^2/(2n_2)$
CCA	$_2\mathcal{F}_1$	$(1+n_1\theta/n)^{-n/2}$	(n/2, n/2)	$n_1/2$	$\theta n_1^2/(n_2^2 + n_2 n_1(1+\theta))$

Some links in Fig. 18.2 can also be established via asymptotic relations between hypergeometric functions.

Asymptotic behavior of the likelihood ratios consider that as n_1 , n_2 , p go to infinity so that

$$c_1 \equiv \frac{p}{n_1} \to \gamma_1 \in (0, 1)$$
 $c_2 \equiv \frac{p}{n_2} \to \gamma_2 \in (0, 1]$ (18.7)

which can be denoted as \mathbf{n} , $p \to_{\gamma} \infty$ where $\mathbf{n} = \{n_1, n_2\}$ and $\gamma = \{\gamma_1, \gamma_2\}$. Under the null (the true value of the spike $\theta_0 = 0$), $\lambda_1, \dots, \lambda_p$ are the eigenvalues of

- GOE/\sqrt{p} , for **SMD**
- $W_p(n_1, \mathbf{I}_p)/n_1$, for **PCA** and **REG**₀
- a p-dimensional multivariate beta matrix with parameters $n_1/2$ and $n_2/2$ (here scaled by a factor of n_2/n_1), for **SigD**, **REG**, **CCA**

and the empirical distribution of $\lambda_1, \dots, \lambda_p$ follows

$$\hat{F} = \frac{1}{p} \sum_{j=1}^{p} I\left\{\lambda_{j} \leq \lambda\right\} \xrightarrow{a.s.} F_{\gamma} = \begin{cases} F^{SC} & \text{semi-circle distribution, for SMD} \\ F^{MP} & \text{Marchenko-Pastur distribution, for PCA, REG}_{0} \end{cases}$$
 Wachter distribution, for SigD, REG, CCA

A summary of the 3 classes of distributions is shown in Table 18.3. And the cumulative distribution functions $F_{\nu}^{\lim}(\lambda)$ are linked in the sense that

$$F_{\gamma}^{W}(\lambda) \to F_{\gamma_{1}}^{MP}(\lambda) \qquad \qquad \gamma_{2} \to 0$$

$$F_{\gamma_{1}}^{MP}(\sqrt{\gamma_{1}}\lambda + 1) \to F^{SC}(\lambda) \qquad \qquad \gamma_{1} \to 0$$

If φ is a *well-behaved* function, the centered **linear spectral statistic**

$$\sum_{j=1}^{p} \varphi(\lambda_j) - p \int \varphi(\lambda)(d) F_{\mathbf{c}}^{\lim}(\lambda)$$
(18.8)

converges in distribtuion to a Gaussian random variable in each of the semicircle, Marchenko-Pastur and Wachter cases.

Table 18.3: Semi-circle, Marchenko-Pastur, scaled Wachter distributions

Case	$F_{\gamma}^{\mathrm{lim}}$	Density, $\lambda \in [\beta, \beta_+]$	eta_\pm	Threshold $\hat{\theta}$			
SMD	SC	$rac{R(\lambda)}{2\pi} R(\lambda)$	±2	1			
PCA, REG_0	MP	$\frac{R(\lambda)}{2\pi\gamma_1\lambda}$	$(1 \pm \sqrt{\gamma_1})^2$	$\sqrt{\gamma_1}$			
SigD, REG, CCA	W	$\frac{(\gamma_1 + \gamma_2)R(\lambda)}{2\pi\gamma_1\lambda(\gamma_1 - \gamma_2\lambda)}$	$\gamma_1 \left(\frac{\rho \pm 1}{\rho \pm \gamma_2} \right)^2$	$\frac{\rho + \gamma_2}{1 - \gamma_2}$			
where $R(\lambda) = \sqrt{(\beta_+ - \lambda)(\lambda - \beta)}$, $\rho = \sqrt{\gamma_1 + \gamma_2 - \gamma_1 \gamma_2}$							

References

Iain M Johnstone and Alexei Onatski. Testing in high-dimensional spiked models. *The Annals of Statistics*, 48(3), 2020.