Exact Largest Eigenvalue Distribution for Doubly Singular Beta Ensemble

Stepan Grinek
Institute for Systems Genetics, NYU Langone Medical Center, New York, NY, USA

Abstract
In [1] beta type I and II doubly singular distributions were introduced and their densities and the joint densities of nonzero eigenvalues were derived. In such matrix variate distributions $p$, the dimension of two singular Wishart distributions defining beta distribution is larger than $m$ and $q$, degrees of freedom of Wishart matrices. We found simple formula to compute exact largest eigenvalue distribution for doubly singular beta ensemble in case of identity scale matrix, $\Sigma = I$. Distribution is presented in terms of existing expression for CDF of Roys statistic:

$$\lambda_{\text{max}} \sim \max \text{eig} \left\{ W_q(m, I) W_q(p - m + q, I)^{-1} \right\},$$

where $W_k(n, I)$ is Wishart distribution with $k$ dimensions, $n$ degrees of freedom and identity scale matrix.

1. Introduction

The presented work is motivated by recent research on the method in the field of multivariate genomics data, Principal Component of Heritability (PCH). PCH is a method to reduce multivariate measurements on multiple samples to one or two vectors representing the relative importance of the measurements. The criterion of the optimisation is the ratio between explained (model) variance and residual variance in the multivariate regression model [3]. We recently achieved exact generalisation of this method to the case when number of measurements, $p$, is higher than number of observations,
PCH optimisation procedure in case \( p > n \) means that both the residual and the model variance components are singular. Thus, the definition of beta ensemble should be extended in this doubly singular settings:

**Definition of beta ensemble (doubly singular):** Let \( A \sim W_p(m, \Sigma) \) and \( B \sim W_p(q, \Sigma) \) be singular Wishart matrices with \( p > \max(m, q) \). There exist \( m \) \( p \)-dimensional vectors constituting \( p \times m \) matrix \( T_1 \) such that \( T_1^T A T_1 = I_m \). Then the matrix \( T_1^T B T_1 \) is called doubly singular beta distributed.

One can show that our definition coincides with the definition of doubly singular beta-ensemble of type II from [1] or, if \( A \) is non-singular, with the Definition 1 of matrix variate beta type II distribution from [2], see former reference for densities and the joint densities of nonzero eigenvalues.

Analytical computation of the extreme latent roots of beta ensemble is a difficult task. We are not aware of any exact analytical results in doubly singular settings. In the next section of the manuscript we present some already known approximations which were found in the literature and develop the intuition needed to derive the main result, the exact distribution of largest eigenvalue for the doubly singular beta ensemble. We give derivation of approximations in section 3 and conclude with the proof of the main theorem in section 4. In Appendix we present graphs demonstrating properties of approximations presented in section 2.

To demonstrate correctness of our result numerically we provide an R script, available at [https://github.com/stepanv1/DoubleWishart](https://github.com/stepanv1/DoubleWishart).

2. Previously known results and main theorem

Our first approximation of the largest root CDF of singular beta random matrix is given in case of fixed (arbitrary) sample size \( (n) \) and fixed number of covariates \( (q) \) expressed using the distribution of the largest root of Wishart matrix. This is essentially a reformulation of results [3, 4]. The result states:

**Theorem 1:** Let \( p, m, q \) and \( \Sigma = I \) define doubly singular beta ensemble and \( p \gg n, p \gg q, n \) and \( q \) are fixed, i.e. \( p/\max(m, q) \to \infty \) (e.g. \( p \) is the number of genetic loci, \( q \) is the number of covariates, \( m = n - q \), where \( n = N - 1 \), \( N \) is the number of samples, if one thinks in terms of MANOVA test). Then the asymptotic distribution of largest root statistics \( \lambda_{\text{max}} \) is given
by:
\[ \lambda_{\text{max}} \sim \max \text{eig}\{ \frac{1}{p} W_q(m, I) \}, \]  
(1)

where \( W_q(m, I) \) is a Wishart ensemble with zero mean, \( m \) degrees of freedom and dimension \( q \) and identity scale matrix \( I \). \( \text{eig} \) \( C \) denotes eigenvalues of matrix \( C \).

Another important observation is that the roots of singular beta matrix are affected by the unknown scale matrix of underlying Wishart distribution, which is different from non-singular case. Apparently, this can be explained by the fact that the sample matrix is not a consistent estimator of the scale matrix of singular Wishart. Here is the formula to correct for that, again, following [4, 5, 6]:

**Theorem 2**: Under condition of Theorem 1 and if \( \Sigma \neq I \) asymptotic distribution of largest root statistics \( \lambda_{\text{max}} \) is given by

\[ \lambda_{\text{max}} \sim \max \text{eig}\{ \frac{1}{pb} W_q(m, I) \}, \]  
(2)

where

\[ b = a_1^2 / a_2, \]

and where \( a_1 \) and \( a_2 \) can be estimated using

**Proposition, [6]**: Let \( A \sim W_p(m, \Sigma) \) is a sample from Wishart distribution, \( a_i = \text{tr} \Sigma / p \), then \( \hat{a}_1, \hat{a}_2 \) are consistent estimators of \( a_1, a_2 \) as \( n, p \to \infty \):

\[ \hat{a}_1 = \text{tr} A / mp, \]
\[ \hat{a}_2 = \frac{1}{(m-1)(m+2)p} \left[ \text{tr}(A^2) - \frac{1}{m} (A)^2 \right]. \]

Proof Theorem 2 is based on the property of the roots of Wishart-distributed matrix, namely that \( \text{eig} W_m(p, \Sigma) \) at \( p >> m \) is approximately proportional to identity matrix. In case of identity scale matrix we can work with exact roots of \( W_m(p, I) \). This leads to the main result of this manuscript, the exact largest eigenvalue distribution of doubly singular beta ensemble:

**Theorem 3**: Let \( A \sim W_p(I, m) \) and \( B \sim W_p(I, q) \) be independent Wishart variates, \( p > \max(m, q) \). The distribution of the largest root statistic \( \lambda_{\text{max}} \) for the corresponding doubly singular beta ensemble is given by

\[ \lambda_{\text{max}} \sim \max \text{eig} \left\{ W_m(q, I) W_m(p, I)^{-1} \right\}, \]  
(3)
In our setting $p > m$, so we use identity $\lambda_{\max}(P, M, N) = \lambda_{\max}(N, M + N - P, P)$, [10], leading to:

$$\lambda_{\max} \sim \max \text{eig}\left\{W_q(m, I)W_q(p - m + q, I)^{-1}\right\}.$$  \hspace{1cm} (4)

Initially doubly singular problem was reduced to non-singular representation in (4). The CDF for the distribution in the form above can be computed nicely using exact algorithm for double Wishart CDF by Chiani, [7]. This is illustrated at Figure [1] Good approximation at the regime $p > m >> q$ is obtained by Johnstone using Tracy–Widom (TW) law [9], see Figure [2] in Appendix. We mention TW approximation here since it is faster to compute, fact of importance for applications. Derivation of exact result in case $\Sigma \neq I$ would be much more complex, but approximation expressed in terms of double Wishart distribution, synthesising results of Theorem 2 and Theorem 3, in our opinion, might exist.

3. Proof of the Theorems 1 and 2

Many applications, such as MANOVA, for arbitrary parameters $p, m$ and $q$ lead to the generalised eigenvalue problem:

$$Be = \lambda Ae \hspace{1cm} (5)$$

We will follow notations of [9]. Let $A \sim W_p(m, \Sigma)$ and $B \sim W_p(q, \Sigma)$ be singular Wishart matrices with $m, q$ degrees of freedom respectively and of the same dimension $p$. In our analysis $p > (m, q)$, so the $A^{-1}$ is not defined. Thus the product $A^{-1}B$ does not exist and we need a trick to solve (5).

The solution is to find the coordinate transformation $T$ such that [11]:

$$T^TB = \Lambda \hspace{1cm} T^TA = I_m,$$  \hspace{1cm} (6)

here $T = T_1T_2$ is a composition of two transformations. $T_1$ transforms $A$ into identity matrix of lower rank, $T_2$ diagonalises $T_1^TB_1T_1$ where $\Lambda$ is a matrix of eigenvalues for the problem [5] and columns of $T$ are the eigenvectors $e$ in [7]. Our goal is to prove the results [1, 2] giving asymptotic distribution for the largest eigenvalue in $\Lambda$.

First, we need to establish a useful fact, that $\text{eig}\{BA^+\} = \Lambda$, where $A^+$ is a Moore-Penrose pseudoinverse of $A$. Now, from the second equation
Figure 1: **Doubly Singular Wishart statistics**: We compare doubly Wishart calculation with empirical CDF at different values of $p$, $m = 100$, $q=6$, scale matrix is set to identity matrix.
Figure 2: TW approximation to the largest root statistics: We compare empirical CDF with TW asymptotics at different values of $p$, $m = 100$, $q=6$, scale matrix is set to identity matrix.
in (6) follows that \( T_1 = HL^{-1/2}, \) where \( H \) are the matrix of eigenvectors \( p \times m \) of the matrix \( A, \) such that \( HTH = I_m \) and \( L \) is \( m \times m \) diagonal matrix of eigenvalues. Thus, the first equation in (6) can be stated as \( \text{eig}(L^{-1/2}HTBHL^{-1/2}) = \Lambda. \) It is easy to see then:

\[
\text{eig}\{L^{-1/2}HTBHL^{-1/2}\} = \text{eig}\{BHL^{-1/2}L^{-1/2}HT\} = \text{eig}\{BHL^{-1}HT\} = \text{eig}\{BA^+\},
\]

where the presentation of Moore-Penrose pseudoinverse of matrix \( A \) as \( A^+ = HL^{-1}H^T \) was used.

Let us calculate the asymptotic distribution of the largest root of \( BA^+ \). We essentially follow derivation developed for MANOVA test in [4, 5]. Since \( B \) is Wishart distributed it can be represented as:

\[ B = ZZ^T, \]

where \( Z = (v_1, v_2, .., v_q) \) and \( v_i \) is multivariate normal \( N_p(0, \Sigma). \) Thus,

\[
\text{eig}\{BA^+\} = \text{eig}\{Z^TA^+Z\} = \text{eig}\{Z^THL^{-1}H^TZ\} = \text{eig}\{Z^THC(CL)^{-1}CH^TZ\},
\]

where \( C = (HT\Sigma H)^{-1/2}. \) Now, it is easy to check using theorem about linear transformation of multivariate normal random vector that the matrix \( V = CH^TZ \) is constituted of \( q \) columns, which are multivariate normal vectors \( N_m(0, I). \) We arrive to:

\[
\text{eig}\{BA^+\} = \text{eig}\{V^T(CL)^{-1}V\}. \tag{7}
\]

In (2.7) from [5] was proven that in probability \( \lim_{p \to \infty} (CL)^{-1} = \frac{1}{pb}I_m, \) where \( b \) is defined in (1.12), [5] and hence:

\[
\lim_{p \to \infty} V^T(CL)^{-1}V = \frac{1}{pb}V^TI_mV = \frac{1}{pb}W_m(0, I_q),
\]

\( W_m(0, I_q) \) is a Wishart distribution, possibly singular, since typically \( m > q. \)

As the eigenvalues of matrices \( VTV \) and \( VVT \) are identical, our result could be stated as:

\[
\lim_{p \to \infty} \lambda_{\text{max}} = \max \text{eig}\{\frac{1}{pb}W_q(0, I_m)\},
\]

which constitutes the statement of Theorem 2. Theorem 1 is recovered at \( \Sigma = I_p. \)
4. Proof of the Theorem 3

Observing that in (7) diagonal matrix $L$ of roots of Wishart-distributed matrix $W_m(\Sigma,p)$ is approximated by identity matrix, we make a conclusion that the approximation in Theorem 1 can be improved to derive the exact distribution. Namely, instead of using equality $\lim_{p \to \infty} (CLC)^{-1} = \frac{1}{p^b} I_m$ we take into account that $L$ is a matrix of roots of $W_m(\Sigma,p)$.

Let us set $\Sigma = I$, then $C = (H^T H)^{-1/2} = I_m$, hence

$$\text{eig}\{BA^+\} = \text{eig}\{V^T L^{-1} V\} = \text{eig}\{V^T L^{-1} V\} = \text{eig}\{V^T O^T O^{-1} O^T O V\},$$

where $O$ is random orthogonal matrix such that $L^{-1} = O^T W_m(p,I)^{-1} O$, $W_m(p,I)^{-1}$ is inverse Wishart distribution. Next, permuting terms under eig we get:

$$\text{eig}\{BA^+\} = \text{eig}\{V^T O^T W_m(p,I)^{-1} O V\} = \text{eig}\{O V^T O^T W_m(p,I)^{-1}\} = \text{eig}\{W_m(q,I) W_m(p,I)^{-1}\},$$

which leads to (3).

5. Appendix

Here we present some numerical illustrations of existing approximations introduced in section 2. Asymptotics presented in Theorems 1 and 2 are expressed in terms of Wishart ensemble. CDF of the largest root of Wishart matrix is computed using exact result [8].

Figure 3 compares exact CDF with the approximation of Theorem 1. We run 10000 simulations with unit scale matrix for set of values of $p$ between 500 and 2000 to obtain the empirical CDF.

Figure 4 demonstrates how the correction for the non-identity scale matrix works, see Theorem 2. Each simulation has its own scale matrix, 100 simulations per each of 5 values of $p$ are done.

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Figure 3: Approximation CDF of the largest root of doubly singular beta ensemble with identity scale matrix. Black lines are the exact CDF, red lines are the approximations. The largest roots (the x-axis) are multiplied by $p$ to bring all plots in the same coordinates. Here $m = 96, q = 4$
Figure 4: Comparison of the CDF calculation with and without correction for the scale matrix. Black lines are the exact CDF of the doubly singular beta ensemble with randomly generated scale matrix scale matrix, red lines are the approximations. The largest roots (the x-axis) are multiplied by $p$ to bring all plots in the same coordinates. Here $m = 96, q = 4$. In the top row red curve represent the approximated CDF with the correction for scale matrix described in Theorem 2, red curve in the bottom row is the CDF approximation without correction from Theorem 1.