DISTRIBUTION THEORY OF A POSITIVE DEFINITE QUADRATIC FORM WITH MATRIX ARGUMENT¹

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1. Introduction and summary. Let $x: 1 \times n$ be a row vector of random variables such that each x_i ($i = 1, 2, \dots, n$) is independently normally distributed with mean μ_i and variance one. Many authors have studied the distribution of what we shall call a univariate quadratic form xAx', where A is a positive definite $n \times n$ matrix. Three types of representation of the distribution have been developed, namely (i) power series about the origin, (ii) mixtures of chi-squares (we refer to these as Ruben-type representations), and (iii) series of Laguerre polynomials. Though all three types of expansion yield correct convergent representations, it has been found that the Laguerre series representation is computationally the most convenient and effective throughout the range of interesting values of the argument.

Let $X: p \times n$ be a matrix whose column vectors are independently and identically distributed in multivariate normal distributions having zero mean vector and variance covariance matrix Σ . If L is a positive definite $n \times n$ matrix, we refer to the $p \times p$ matrix S = XLX' as a positive definite quadratic form with matrix argument. Khatri [11] has given a representation of the density function of the distribution of S, somewhat similar to the Ruben-type expansion for the univariate case. In this paper we express the density function of S in terms of Laguerre polynomials with matrix argument. Our results can be easily extended to quadratic forms in a matrix argument when the common multivariate distribution of the column vectors is complex. In Section 2, we give definitions and notations. Section 3 gives some results on integration over orthogonal groups, and in Section 4 we derive the main results.

2. Notations and preliminary results. In this section we will give definitions of various functions already given by James [8], Constantine [1], and Herz [4].

(1)
$${}_{p}F_{q}(a_{1},\cdots,a_{p};b_{1},\cdots,b_{q};S) = \sum_{k=0}^{\infty} \sum_{\kappa} \frac{(a_{1})_{\kappa}\cdots(a_{p})_{\kappa}}{(b_{1})_{\kappa}\cdots(b_{q})_{\kappa}} \frac{C_{\kappa}(S)}{k!},$$

where $a_1, \dots, a_p, b_1, \dots, b_q$ are real or complex constants and the multivariate hypergeometric quantity $(a)_{\kappa}$ is given by

(2)
$$(a)_{\kappa} = \prod_{i=1}^{m} \left\{ a - \frac{1}{2}(i-1) \right\}_{k_i},$$

where $(x)_k = x(x+1)\cdots(x+k-1)$, with $(x)_0 = 1$, and the summation \sum_{k} in (1)

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is taken over all the partitions $\kappa = (k_1, \dots, k_m)$, $k_1 \ge k_2 \ge \dots \ge k_m \ge 0$, such that $k_1 + \dots + k_m = k$. In (1) $C_{\kappa}(S)$ is a symmetric homogeneous polynomial of degree k in the latent roots of the matrix S. Further let

(3)
$$\Gamma_m(x) = \pi^{\frac{1}{2}m(m-1)} \prod_{j=1}^m \Gamma\{x - \frac{1}{2}(j-1)\}$$
 and

(4)
$$\Gamma_m(a,\kappa) = (a)_{\kappa}/\Gamma_m(a) \quad \text{with} \quad \Gamma_m(a,0) = \Gamma_m(a).$$

Let the density of the central Wishart distribution in p variates with n degrees of freedom be denoted by $W(n, p; \Sigma; S)$, i.e.

(5)
$$W(n, p; \Sigma; S) = |2\Sigma|^{-\frac{1}{2}n} \{ \Gamma_p(n/2) \}^{-1} |S|^{\frac{1}{2}(n-p-1)} \exp\{ -\frac{1}{2} \operatorname{tr} \Sigma^{-1} S \}, \text{ if } n \ge p.$$

3. Some results on integration. We shall write $X > \dot{X}_0$ meaning that $X - X_0$ is a positive definite matrix, O(m) for the orthogonal group of $m \times m$ orthogonal matrices, and R(Z) for the real part of Z.

LEMMA 1. Let $S: m \times m$ and $T: m \times m$ be symmetric matrices. Then

(6)
$$\int_{O(m)} C_{\kappa}(SH'TH) dH = C_{\kappa}(S)C_{\kappa}(T)/C_{\kappa}(I_m),$$

where the measure dH on O(m) is normalized to make its integral over the orthogonal group unity. (See James, A. T. [8].)

LEMMA 2. Let $Z:m \times m$ be a complex symmetric matrix whose real part is positive definite and $T:m \times m$ be an arbitrary complex symmetric matrix. Then the Laplace transform of the zonal polynomial is

(7)
$$\int_{R>0} \exp\left(-\operatorname{tr} RZ\right) |R|^{a-\frac{1}{2}(m+1)} C_{\kappa}(TR) dR = \Gamma_{m}(a,\kappa) |Z|^{-a} C_{\kappa}(TZ^{-1}).$$

(See Constantine [1].)

Lemma 3. Let $S: m \times m$ be a positive definite symmetric matrix. Then

(8)
$$\int_{S>0} \frac{\exp(-\operatorname{tr} SZ) |S|^{\gamma} L_{\kappa}^{\gamma}(S) dS}{\Gamma_{m}(\gamma + \frac{1}{2}(m+1), \kappa)} = |Z|^{-\gamma - \frac{1}{2}(m+1)} C_{\kappa}(I - Z^{-1}),$$

where $L_{\sigma}^{\gamma}(S)$ is a polynomial of the same degree as σ , and if σ ranges over a basis for the homogeneous symmetric polynomials, then the L_{σ}^{γ} form a complete set of polynomials in the L^2 -space of functions f(S) on S>0 with respect to the weight function $w(S)=\exp(-\operatorname{tr} S) |S|^{\gamma}, S>0$. Note that a constant times w(S) is the density function of the Wishart distribution. Constantine strongly conjectured in 1964 that Laguerre polynomials of matrix argument are orthogonal to the Wishart density function. He proved this important result in 1966 [2]. We may note here that in univariate theory Laguerre polynomials are orthogonal to the chi-square density function.

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Lemma 4. Let q be a positive scalar quantity and Σ be a positive definite symmetric matrix. Then

(9)
$$= \frac{(2\pi i)^{-\frac{1}{2}m(m+1)} \int_{R(Z)>0} \exp\left(\operatorname{tr} ZS\right) \left|\Sigma + Z\right|^{-t} C_{\kappa} \left[I - (\Sigma + Z)^{-1}\right] dZ}{2^{\frac{1}{2}m(m-1)} \Gamma_{m}(t,\kappa)} .$$

PROOF. Using Lemma 3, we have

(10)
$$\int_{S>0} \frac{\exp\left(-\operatorname{tr}\left(\Sigma S + ZS\right) \left|S\right|^{\gamma} L_{\kappa}^{\gamma}(S) dS}{\Gamma_{m}(t,\kappa)} = \left|\Sigma + Z\right|^{-t} C_{\kappa} \left[I - (\Sigma + Z)^{-1}\right],$$

where $t = \gamma + \frac{1}{2}(m+1)$.

Now taking the inverse transform of (10), we get

$$2^{\frac{1}{2}m(m-1)}(2\pi i)^{\frac{1}{2}m(m+1)}\int_{R(Z)>0}\exp(\operatorname{tr} ZS)|\Sigma+Z|^{-t}C_{\kappa}[I-(\Sigma+Z)^{-1}]dZ$$

$$=\exp(-\operatorname{tr} \Sigma S)|S|^{t-\frac{1}{2}(m+1)}L_{\kappa}^{t-\frac{1}{2}(m+1)}(S)\{\Gamma_{m}(t,\kappa)\}^{-1},$$

which proves Lemma 4. For detail of the Laplace transform and inverse transform of matrix argument over the real symmetric matrix see Herz [5].

Lemma 5. Let S = XLX'. Then

(11)
$$E[\exp(\operatorname{tr} ZS)] = \prod_{j=1}^{n} |I_m - 21_j Z\Sigma|^{-\frac{1}{2}}$$
$$= \sum_{k=0}^{\infty} \sum_{\kappa} (\frac{1}{2}n)_{\kappa} C_{\kappa}(L) C_{\kappa}(Z\Sigma) 2^k / (k! C_{\kappa}(I_n)),$$

where the 1_j 's are characteristic roots of L. (See Khatri [11] equation 39.)

4. Distribution of a multivariate of positive definite quadratic form.

Theorem 1. Let the matrix $X: m \times n$ be distributed as

(12)
$$(2\pi)^{-\frac{1}{2}nm} |\Sigma|^{-\frac{1}{2}n} \exp(-\frac{1}{2} \operatorname{tr} \Sigma^{-1} X X').$$

Then a moment generating function of S = XLX', where $L: n \times n$ is a positive definite matrix, is

(13)
$$E\{\exp(-\operatorname{tr} ZS)\} = |G|^{-\frac{1}{2}n} \sum_{k=0}^{\infty} \sum_{\kappa} (\frac{1}{2}n)_{\kappa} C_{\kappa} (I - q^{-1}L) C_{\kappa} (I - G^{-1}) / k! C_{\kappa} (I_{n}),$$

where q is a real positive quantity and $G = I_m + 2qZ\Sigma$. Note that we have introduced a minus sign in the expectation.

PROOF. Making the transformation $X \to \Sigma^{\frac{1}{2}} X(Lq^{-1})^{-\frac{1}{2}}$, of which the Jacobian is $|Lq^{-1}|^{-\frac{1}{2}m} |\Sigma|^{\frac{1}{2}n}$, we find

(14)
$$E\{\exp(-\operatorname{tr} ZS)\} = (2\pi)^{-\frac{1}{2}mn} |Lq^{-1}|^{-\frac{1}{2}m} \int_X \exp\left[\frac{1}{2}\operatorname{tr}(XTX' - GXX')\right] dX,$$

where $T = I_n - qL^{-1}$. Since XX' is invariant under post multiplication of X by an orthogonal matrix, we consider the matrix T to be a diagonal matrix with φ_j 's as diagonal elements. Let $X = (x_1, \dots, x_n)$. Then we have from (14)

$$E\{\exp(-\operatorname{tr} ZS)\} = |Lq^{-1}|^{-\frac{1}{2}m} \prod_{j=1}^{n} (2\pi)^{-\frac{1}{2}m} \int_{x_j} \exp\left[-\frac{1}{2}x_j' (G - \varphi_j I_m)x_j\right] dx_j.$$

The above integral is a multivariate normal integral with mean zero and variance covariance matrix $(G - \varphi_i I_m)^{-1}$. Hence

(15)
$$E\{\exp(-\operatorname{tr} ZS)\} = |Lq^{-1}|^{-\frac{1}{2}m}|G|^{-\frac{1}{2}n}\prod_{j=1}^{n}|I_m - \varphi_j G^{-1}|^{-\frac{1}{2}}$$

$$= |Lq^{-1}|^{-\frac{1}{2}m}|G|^{-\frac{1}{2}n}\left[\prod_{j=1}^{n}(1 - \varphi_j)^{-\frac{1}{2}m}\right]$$

$$\cdot \prod_{j=1}^{n}|I - (-\varphi_j/(1 - \varphi_j))(I - G^{-1})|^{-\frac{1}{2}}.$$

Equation (15) can be simplified as

(16)
$$E\{\exp(-\operatorname{tr} ZS)\} = |Lq^{-1}|^{-\frac{1}{2}m} |I - qL^{-1}|^{-\frac{1}{2}m} |G|^{-\frac{1}{2}n} \prod_{j=1}^{n} |I - l_j(I - G^{-1})|^{-\frac{1}{2}},$$
 where $l_j = -\varphi_j |(1 - \varphi_j)$, i.e. l_j 's are characteristic roots of $-(I - qL^{-1})$ $\{I - (I - qL^{-1})\}^{-1} = (qL^{-1} - I)q^{-1}L = I - q^{-1}L$, or
$$E\{\exp(-\operatorname{tr} ZS)\} = |q^{-1}L - I|^{-\frac{1}{2}m} |G|^{-\frac{1}{2}n} \prod_{i=1}^{n} |I - I_i(I - G^{-1})|^{-\frac{1}{2}}.$$

Now using Lemma 5, we have Theorem 1.

THEOREM 2. Let $X: m \times n$ be distributed as (12). Then a density function of S = XLX' is

(17)
$$\sum_{k=0}^{\infty} \sum_{\kappa} C_{\kappa} (I - q^{-1}L) L_{\kappa}^{\frac{1}{2}(n-m-1)} (\frac{1}{2} q \Sigma^{-1} S) (k!)^{-1} \{ C_{\kappa} (I_n) \}^{-1} \cdot W(n, m; q \Sigma; S).$$

PROOF. By inverse Laplace transform of (13), we can have

(18)
$$2^{\frac{1}{2}m(m-1)}(2\pi i)^{-\frac{1}{2}m(m+1)} \int_{R(Z)>0} \exp(\operatorname{tr} ZS) \left| I + 2qZ\Sigma \right|^{-\frac{1}{2}n} \\ \cdot \sum_{k=0}^{\infty} \sum_{\kappa} (\frac{1}{2}n)_{\kappa} C_{\kappa} (I - q^{-1}L) C_{\kappa} \left[I - (I + 2qZ\Sigma)^{-1} \right] (k!)^{-1} \left\{ C_{\kappa} (I_{n}) \right\}^{-1} dZ \\ = \sum_{k=0}^{\infty} \sum_{\kappa} (\frac{1}{2}n)_{\kappa} C_{\kappa} (I - q^{-1}L) (k!)^{-1} \left\{ C_{\kappa} (I_{n}) \right\}^{-1} B_{\kappa}(S),$$

where

(19)
$$B_{\kappa}(S) = 2^{\frac{1}{2}m(m-1)} (2\pi i)^{-\frac{1}{2}m(m+1)} \int_{R(Z)>0} \exp(\operatorname{tr} ZS) \left| I + 2qZ\Sigma \right|^{-\frac{1}{2}n} \cdot C_{\kappa} \left[I - (I + 2qZ\Sigma)^{-1} \right] dZ.$$

Now in Lemma 3, let $Z=(I+2qZ\Sigma)$, which does not change the integral over S>0. Making the transformation $\Sigma^{\frac{1}{2}}S\Sigma^{\frac{1}{2}}(2q)\to S$, of which the Jacobian is $|\frac{1}{2}q^{-1}\Sigma^{-1}|^{\frac{1}{2}n}$, and noting that $L_{\sigma}^{\gamma}(\Sigma S)=L_{\sigma}^{\gamma}(S\Sigma)$, since the matrices S and Σ are square and of the same dimensions (see Herz [5]), we have

(20)
$$|2q\Sigma|^{-\frac{1}{2}n} \int_{S>0} \exp\left[-\operatorname{tr}\left\{ (I+2qZ\Sigma)(2q\Sigma)^{-1}S\right\} \right] \\ \cdot |S|^{\frac{1}{2}(n-m-1)} L_{\kappa}^{\frac{1}{2}(n-m-1)} (\frac{1}{2}q^{-1}\Sigma^{-1}S) dS \\ = |I+2qZ\Sigma|^{-\frac{1}{2}n} C_{\kappa} [I-(I+2qZ\Sigma)^{-1}].$$

Now using the inverse Laplace transform of expression (20) we will get

$$B_{\kappa}(S) = \frac{\left|2q\Sigma\right|^{-\frac{1}{2}n} \exp\left[-\operatorname{tr}(2q\Sigma)^{-1}S\right] \left|S\right|^{\frac{1}{2}(n-m-1)} L_{\kappa}^{\frac{1}{2}(n-m-1)}(\frac{1}{2}q^{-1}\Sigma^{-1}S)}{\Gamma_{m}(\frac{1}{2}n,\kappa)} \; .$$

Hence, noting that $(\frac{1}{2}n)_{\kappa} = \Gamma_m(\frac{1}{2}n, \kappa)/\Gamma_m(\frac{1}{2}n)$, we get Theorem 2.

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When m=1, i.e. in the univariate case, \sum_{κ} drops out and κ is replaced by k. The Wishart density becomes a chi-square density, S is replaced by s, $L^{\frac{1}{2}(n-m-1)}(\frac{1}{2}q^{-1}\Sigma^{-1}S)$ becomes $L_k^{(\frac{1}{2}n-1)}(s/2\sigma^2q)$, $C_{\kappa}(I-q^{-1}L)$ $\{C_{\kappa}(I_n)\}^{-1}$ becomes the top order zonal polynomial in the latent roots of L, and we get the Gurland [4] expression. We may note that our q is Gurland's $\bar{\lambda}$.

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