

ON THE MARGINAL DISTRIBUTIONS OF THE LATENT
ROOTS OF THE MULTIVARIATE BETA MATRIX

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ABSTRACT

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The marginal distributions of the latent roots of the multivariate beta matrix are shown to constitute a complete system of solutions of an ordinary differential equation (d.e.), which is related to the author's d.e.'s for Hotelling's generalized T^2 and Pillai's $V^{(m)}$ statistics. Similar results are given for the latent roots of the multivariate F and Wishart matrices ($\Sigma=I$). Pillai's approximations to the distributions of the largest and smallest roots are interpreted as exact solutions, the contributions of higher order solutions being neglected.

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1. Introduction. Let $S(m \times m)$ and $T(m \times m)$ have independent Wishart distributions $W(q, \Sigma)$ and $W(n, \Sigma)$, respectively, where Σ is the population covariance matrix and $q, n \geq m$. The latent roots $\ell_1 > \dots > \ell_m > 0$ of the multivariate beta matrix $B = S(S+T)^{-1}$ are well known to have the joint density function

$$(1) \quad \phi_{m; q, n}(\underline{\ell}) = K(m; q, n) \prod_{i=1}^m \ell_i^{\frac{1}{2}(q-m-1)} \prod_{i=1}^m (1-\ell_i)^{\frac{1}{2}(n-m-1)} \prod_{i < j} (\ell_i - \ell_j),$$

where $\underline{\ell} = (\ell_1, \dots, \ell_m)'$ and

$$(2) \quad K(m; q, n) = \pi^{\frac{1}{2}m} \prod_{i=0}^{m-1} [\Gamma(\frac{1}{2}(q+n-i)) / \Gamma(\frac{1}{2}(m-i)) \Gamma(\frac{1}{2}(q-i)) \Gamma(\frac{1}{2}(n-i))].$$

The marginal distributions of the individual ℓ_i have been investigated by Roy [14], [15], who showed that the largest root ℓ_1 is of basic importance in testing hypotheses and constructing confidence regions in multivariate analysis of variance; also by Pillai [10], Khatri [8], Sugiyama and Fukutomi [17], Sugiyama [16], and Al-Ani [1]. Pillai [11] gave very accurate approximations to the upper and lower tails of the distributions of ℓ_1 and ℓ_m , respectively, and ℓ_1 has been extensively tabulated by Heck [7] for $m \leq 5$, using Pillai's approximation, and Pillai ([11], [12], etc.) for $m \leq 20$. Studies of the non-central distributions have been made by Khatri [9] and Pillai and Dotson [13].

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As $n \rightarrow \infty$, $nB \rightarrow W_I$, say, having the distribution $W(q, I)$ where $I (m \times m)$ is the unit matrix. Hanumara and Thompson [6] have tabulated the largest and smallest roots of W_I using limiting forms of Pillai's approximations, and discussed their application.

The present author [3], [5] has shown that the null distributions of $\text{tr } B$ (Pillai's $V^{(m)}$) and $\text{tr } F$ (Hotelling's generalized T^2), where $F = ST^{-1}$, satisfy certain ordinary linear differential equations (d.e.'s) of order m which are related by a simple transformation. In Section 2 it is shown that the marginal distributions of the λ_i form a complete system of solutions of a similar d.e. Thus, the power-series of Sugiyama and Fukutomi are solutions at the regular singularities 0 and 1. Pillai's approximations are also shown in Section 4 to be exact solutions of the d.e., but approximations to the distributions insofar as contributions from higher-order solutions are neglected. Corresponding results for the latent roots of F and W_I are readily deduced (Sections 6 and 7).

2. The differential equation. Let $D^r(s, \ell) = \{0 < x_r < \dots < x_s < \ell < x_{s-1} < \dots < x_1 < 1\} \subset R^r$, where R is the real line. The marginal density function $f_s(\ell)$ of λ_s is given by

$$(3) \quad f_s(\ell) = \int_{D^{m-1}(s, \ell)} \phi_{m; q, n}(x_1, \dots, x_{s-1}, \ell, x_s, \dots, x_{m-1}) dx$$

where $dx = \prod_{i=1}^{m-1} dx_i$; it is proportional to

$$(4) \quad \ell^{\frac{1}{2}(q-m-1)} (1-\ell)^{\frac{1}{2}(n-m-1)} \int_{D^{m-1}(s, \ell)} \phi(x) \prod_{i=1}^{m-1} (\ell - x_i) dx,$$

in which ϕ denotes $\phi_{m-1; q-1, n-1}$. Define

$$(5) \quad \Psi_r(\ell; \underline{x}) = \Phi(\underline{x}) \Sigma_{\alpha} (\ell - x_{\alpha(1)}) \dots (\ell - x_{\alpha(m-1-r)}), \quad (r=0, 1, \dots, m-1),$$

the summation being extended over the $\binom{m-1}{r}$ selections of integers $\alpha(1) < \dots < \alpha(m-1-r)$ from the set $1, 2, \dots, m-1$. When $r=m-1$, the sum is taken to be unity. We now introduce the m functions

$$(6) \quad L_{s,r}(\ell) = \int_{D^{m-1}(s,\ell)} \Psi_r(\ell; \underline{x}) d\underline{x}, \quad (r=0, 1, \dots, m-1),$$

noting that $f_s(\ell)$ is proportional to $\ell^{\frac{1}{2}(q-m-1)} (1-\ell)^{\frac{1}{2}(n-m-1)} L_{s,0}$. Our object is to show that, for each s , the $L_{s,r}$ are related by a system of first-order differential equations which are independent of s . Differentiating (6),

$$(7) \quad L'_{s,r}(\ell) = -Z_{s,r}^{(1)} + Z_{s,r}^{(2)} + (r+1)L_{s,r+1},$$

where

$$(8) \quad Z_{s,r}^{(1)} = \int_{D^{m-2}(s-1,\ell)} \Psi_r(\ell; x_1, \dots, x_{s-2}, \ell, x_{s-1}, \dots, x_{m-2}) d\underline{x},$$

$$Z_{s,r}^{(2)} = \int_{D^{m-2}(s,\ell)} \Psi_r(\ell; x_1, \dots, x_{s-1}, \ell, x_s, \dots, x_{m-2}) d\underline{x}.$$

Now let $\beta(1), \dots, \beta(r)$ denote the set of subscripts complementary to $\alpha(1), \dots, \alpha(m-1-r)$. We have

$$(9) \quad \begin{aligned} r\ell L_{s,r} &= \int_{D^{m-1}(s,\ell)} \Phi(\underline{x}) \Sigma_{\alpha} (\ell - x_{\alpha(1)}) \dots (\ell - x_{\alpha(m-1-r)}) [(\ell - x_{\beta(1)}) + \dots + \\ &\quad (\ell - x_{\beta(r)}) + (x_{\beta(1)} + \dots + x_{\beta(r)})] d\underline{x} \\ &= (m-r)L_{s,r+1} + \Theta_{s,r}, \end{aligned}$$

say. Integration by parts with respect to the $x_{\beta(i)}$ yields

$$(10) \quad \frac{1}{2}(q+n-2m+2)\Theta_{s,r} = \ell(1-\ell)[Z_{s,r}^{(1)} - Z_{s,r}^{(2)}] + \frac{1}{2}r(q-m+r)L_{s,r} + \Psi_{s,r},$$

where

$$(11) \quad \Psi_{s,r} = \int_{D^{m-1}(s,\ell)} \Phi(\underline{x}) \Sigma_{\alpha} (\ell - x_{\alpha(1)}) \dots (\ell - x_{\alpha(m-1-r)}) \prod_{j=1}^r x_{\beta(j)}^{1-x_{\beta(j)}} \prod_{k \neq \beta(j)} (x_{\beta(j)} - x_k)^{-1} d\underline{x}.$$

A term similar to (11) occurred in the derivation of a d.e. for Hotelling's generalized T_o^2 ([3], Equation (2.13)), and the same approach yields

$$(12) \quad \Psi_{s,r} = \frac{1}{2}(m-r)(m+r-3)L_{s,r-1} + \frac{1}{2}r(r-1)(1-2\ell)L_{s,r} + \frac{1}{2}r(r+1)\ell(1-\ell)L_{s,r+1}.$$

Finally, eliminating the Z's, Θ 's and Ψ 's from equations (7), (9), (10) and (12), we find that

$$(13) \quad \begin{aligned} \ell(1-\ell)L'_{s,r} &= \frac{1}{2}(m-r)(q+n-m+r-1)L_{s,r-1} + \frac{1}{2}r[(1-\ell)(q-m+r) - \ell(n-m+r)]L_{s,r} \\ &+ \frac{1}{2}(r+1)(r+2)\ell(1-\ell)L_{s,r+1}, \quad (r=0,1,\dots,m-1), \end{aligned}$$

where $L_{s,-1} \equiv L_{s,m} \equiv 0$.

We observe that the system (13) is independent of s , and in principle one could successively eliminate $L_{s,1}, \dots, L_{s,m-1}$, arriving at a homogeneous linear d.e. of order m having each $L_{s,0}$ as a solution. Clearly the f_s will be solutions of a similar d.e.; furthermore, they will constitute a linearly independent and hence complete system of solutions, since as $\ell \rightarrow 0+$

$$(14) \quad f_s(\ell)/\ell^{\frac{1}{2}(q-m-1)} \sim k_s(m; q, n)\ell^{\frac{1}{2}(m-s)(q-s+2)}, \quad (s=1, \dots, m),$$

where

$$(15) \quad k_s(m; q, n) = K(m; q, n) / [K(s-1; q+m-s+1, n-m+s-1)K(m-s; q-s, m-s+3)].$$

This is easily proved by writing $x_j = \ell w_j$ ($j=s, \dots, m-1$) in (4) and letting $\ell \rightarrow 0$.

We note in addition that (13) is invariant under

$$(16) \quad q \rightarrow n, \quad n \rightarrow q, \quad \ell \rightarrow 1-\ell,$$

provided that we also replace $L_{s,r}$ by $(-1)^r L_{s,r}$; this reflects the obvious result that (16) transforms $f_s(\ell)$ into $f_{m+1-s}(\ell)$.

3. Solutions of the d.e. It is convenient to introduce $H_r = (1-\ell)^{-r} L_{s,r}$ ($r=0, 1, \dots, m-1$) and to express (13) as a matrix d.e. for $H = (H_0, \dots, H_{m-1})'$:

$$(17) \quad dH/d\ell = [\ell^{-1}A + (1-\ell)^{-1}C]H,$$

where

$$(18) \quad A = \begin{bmatrix} a_0 & & & & 0 \\ & \ddots & & & \\ & b_1 & \ddots & & \\ & & \ddots & \ddots & \\ & & & b_{m-1} & a_{m-1} \\ 0 & & & & \end{bmatrix}, \quad C = \begin{bmatrix} c_0 & d_0 & & & 0 \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & d_{m-2} & \\ 0 & & & & \dots & c_{m-1} \end{bmatrix}$$

$$\begin{aligned} a_r &= \frac{1}{2}r(q-m+r), & b_r &= \frac{1}{2}(m-r)(q+n-m+r-1) \\ c_r &= -\frac{1}{2}r(n-m+r+2), & d_r &= \frac{1}{2}(r+1)(r+2). \end{aligned}$$

The d.e. (17) is of Fuchsian type, with regular singularities at $\ell=0, 1$ and infinity, and we refer to [2], Chapter 4, for the general theory of such d.e.'s. Assuming a series solution $H = \sum_{r=0}^{\infty} h_r \ell^{\rho+r}$ in $|\ell| < 1$, we obtain $Ah_0 = \rho h_0$, so that ρ must be one of the latent roots a_0, \dots, a_{m-1} of A , and h_0 the corresponding

latent vector. To relate this fundamental set of solutions to the $f_s(\ell)$, we first obtain a non-singular transformation $H=PM$, where $P(m \times m)$ is independent of ℓ , such that $P^{-1}AP = \text{diag}(a_r)$. A suitable choice is

$$(19) \quad P = \{p_{ij}\}, \quad p_{ij} = (-1)^{i-j} \binom{m-j-1}{i-j} \prod_{r=j}^{i-1} (q+n-m+r)/(q-m+j+r+1),$$

with inverse

$$(20) \quad P^{-1} = \{p_{ij}^*\}, \quad p_{ij}^* = \binom{m-j-1}{i-j} \prod_{r=j}^{i-1} (q+n-m+r)/(q-m+i+r).$$

Both P and P^{-1} are lower triangular, and $M_0 = H_0$. It may be shown that

$$(21) \quad P^{-1}CP = G = \begin{bmatrix} \mu_0 & v_0 & & 0 \\ \lambda_1 & \mu_1 & v_1 & \\ & \dots & \dots & \dots \\ 0 & & \lambda_{m-1} & \mu_{m-1} \end{bmatrix}$$

where

$$(22) \quad \begin{aligned} \lambda_i &= (m-i)(n-i)(q+i-1)(q-m+i-1)(q-m+i-2)(q+n-m+i-1)/[2(q-m+2i-2) \\ &\quad (q-m+2i-1)^2(q-m+2i)], \\ \mu_i &= i^2 - \frac{1}{2}i(m+n-3) - m + 1 + \frac{1}{2}i(i+1)(m-i)(n-i)/(q-m+2i-1) \\ &\quad - \frac{1}{2}(i+1)(i+2)(m-i-1)(n-i-1)/(q-m+2i+1), \\ v_i &= \frac{1}{2}(i+1)(i+2). \end{aligned}$$

The d.e. (17) now takes the form

$$(23) \quad dM/d\ell = [\ell^{-1} \text{diag}(a_r) + (1-\ell)^{-1}G]M,$$

and assuming a solution $M = \sum_{r=0}^{\infty} \eta_r \ell^{a+r}$ corresponding to the latent root a_p of A , we obtain the following recurrence relations for the components

$(\eta_{0,r}, \dots, \eta_{m-1,r})$ of the η_r :

$$\eta_{p,0} = 1, \quad \eta_{i,0} = 0 \quad (i \neq p),$$

$$(24) \quad (r - a_i + a_p) \eta_{i,r} = \lambda_i \eta_{i-1,r-1} + [\mu_i + (r-1) - a_i + a_p] \eta_{i,r-1} + \nu_i \eta_{i+1,r-1},$$

$$(i=0, \dots, m-1; r=1, 2, \dots).$$

This form of solution unfortunately breaks down if $a_i - a_p$ is a positive integer for some i . In fact, $a_{p+1} - a_p = \frac{1}{2}(q-m+1)+p$ ($p \leq m-2$), which is an integer if $q-m$ is odd, while $a_{p+2} - a_p = q-m+2(p+1)$ ($p \leq m-3$) is always an integer. Generally in such situations the solution must be obtained by limiting procedures which may produce logarithmic terms. However, it may be seen from (6) that the $L_{s,r}$ are in fact representable by power series, and it appears that if $a_i - a_p$ is a positive integer for $i > p$, then the right-hand side of the i th equation in (24) vanishes identically when $r = a_i - a_p$. Thus $\eta_{i,r}$ is an undetermined constant introducing the a_i -solution at this stage, and the power series form is preserved.

We also see from (24) that the $\eta_{0,r}$ are zero for $r < p$ in the a_p -solution, while

$$(25) \quad \eta_{0,p} = (p+1)! / \prod_{i=1}^p (q-m+p+i+1) = \xi_p, \text{ say.}$$

Hence $M_0(\ell) = O(\ell^{a+p})$ as $\ell \rightarrow 0+$, and since $a_{m-s} + (m-s) = \frac{1}{2}(m-s)(q-s+2)$, it follows from (14) that $L_{0,s}$ must be some linear combination of the $a_{m-s}, a_{m-s+1}, \dots$, and a_{m-1} -solutions. The coefficient of the a_{m-s} -solution is clearly $k_s(m; q, n) / \xi_{m-s}$, but the remaining coefficients have not been determined for general s . However, the density function $f_1(\ell)$ of the largest root corresponds to the largest root a_{m-1} of A , and is thus completely specified by (24). The resulting power series coincides with the result of Sugiyama and Fukutomi [17].

4. Pillai's approximations. A particular solution corresponding to the smallest root $a_0=0$ of A may be given explicitly as an $(m-1)$ th degree polynomial. Writing $(z)_i = z(z+1)\dots(z+i-1)$, $(z)_{-i} = z(z-1)\dots(z-i+1)$, it may be shown that

$$(26) \quad \eta_{i,r} = (-1)^r \binom{m-1}{r} \binom{r}{i} (q)_i (n-1)_{-i} (q+n-m)_r / [(q-m+1)_{i+r} (q-m+i)_i].$$

Thus we obtain the following approximation to the lower tail of $f_m(\lambda)$ for large q by neglecting the a_1, \dots, a_{m-1} solutions (i.e., terms of order λ^{q-m+1} at least):

$$(27) \quad f_m(\lambda) \approx k(m; q, n) \lambda^{\frac{1}{2}(q-m-1)} (1-\lambda)^{\frac{1}{2}(n-m-1)} \sum_{r=0}^{m-1} \binom{m-1}{r} (q+n-m)_r (q-1)_{-(m-1-r)} (-\lambda)^r,$$

where

$$(28) \quad k(m; q, n) = \pi^{\frac{1}{2}} \Gamma(\frac{1}{2}(q+n-m+1)) / [2^{m-1} \Gamma(\frac{1}{2}m) \Gamma(\frac{1}{2}q) \Gamma(\frac{1}{2}n)].$$

Using (16), a corresponding approximation to the upper tail of $f_1(\lambda)$ for large n (near the regular singularity $\lambda=1$) is obtained. The result is found to be simply the right-hand side of (27) multiplied by $(-1)^{m-1}$.

The integrated form of the approximation was arrived at by Pillai [11] using a different approach, and used in a series of tabulations of the upper 5% and 1% points of λ_1 . Its accuracy to essentially five places of decimals when $n_2 \geq m+11$ was demonstrated at least for $m \leq 10$ by substituting in explicit expressions for the distribution function [10]. In order to investigate the usefulness of the d.e. (23), some percentage points were calculated by following the a_{m-1} -solution out from the origin, using the same computation procedure as in [4]. The method appeared to be effective at least up to $m=7$, since on

comparing the 1% points, i.e., the less accurate results of the d.e. and the more accurate results of the approximation, these were generally found to differ by no more than a unit in the fifth decimal place. On the other hand, the 5% points obtained from the d.e. tended to exceed Pillai's by about three units in the fifth decimal place. The d.e. approach should be more accurate at lower significance levels, and a tabulation of upper 10% points has been made.

5. The median root for $m=3$. The success of the Pillai approximation suggests a similar approach to the tails of the distributions of the other roots, approximating the lower tail of f_s by the a_{m-s} -solution for large q , and deducing a corresponding result for the upper tail of f_{m-s+1} when n is large using (16). However, so far it has proved difficult to obtain the solutions in closed forms analogous to (27), except in the case of the median root ℓ_2 when $m=3$. The a_1 -solution is

$$(29) \quad M_0 = \ell^{\frac{1}{2}q}(1-\ell)^{\frac{1}{2}n}; \quad M_1 = (\frac{1}{2}q + \ell[2(n-1)/(q-2) - \frac{1}{2}(q+n-4)])\ell^{\frac{1}{2}q-1}(1-\ell)^{\frac{1}{2}n},$$

$$M_2 = -[(n-2)(q-3)(q+n-2)/2q(q-1)]\ell^{\frac{1}{2}q}(1-\ell)^{\frac{1}{2}n}.$$

Hence, for large q and ℓ near zero,

$$(30) \quad f_2(\ell) \approx [B(q-1, n-1)]^{-1} \ell^{q-2} (1-\ell)^{n-2},$$

the beta density with parameters $q-1$ and $n-1$. The same approximation holds for the upper tail and large n , and has been used to compute upper 5% and 1% points of ℓ_2 . The results are identical to five decimal places with those published by Pillai and Dotson [13], except where the latter have employed extrapolation, in which case differences of up to 0.006 occur for the 5% points and up to .003 for the 1% points.

6. The latent roots of the multivariate F matrix. Substituting $\ell = v/(v+1)$ in (23), we obtain the d.e.

$$(31) \quad dM^*/dv = (v^{-1} \text{diag}(a_r) + (1+v)^{-1} [G - \text{diag}(a_r)])M^*,$$

which has regular singularities at 0, -1 and infinity. The density function $f_s^*(v)$ of the sth largest root v_s of F is a certain linear combination of the a_{m-s}, \dots, a_{m-1} -solutions of (31), multiplied by the factor $v^{\frac{1}{2}(q-m-1)}/(v+1)^{\frac{1}{2}(q+n)-m+1}$. As $v \rightarrow 0+$

$$(32) \quad f_s^*(v)/v^{\frac{1}{2}(q-m-1)} \sim k_s(m; q, n) v^{a_{m-s} + (m-s)},$$

where k_s is defined by (14).

7. The latent roots of the Wishart matrix W_I . As $n \rightarrow \infty$, the densities of $n\lambda_s$ and nv_s converge to $\bar{f}_s(u)$, say, the density function of the sth largest root u_s of W_I . To obtain a d.e. for the \bar{f}_s , we substitute $\ell = u/n$ and $M_i = n^i \bar{M}_i$ ($i=0, \dots, m-1$) in (23); letting $n \rightarrow \infty$ it is found that

$$(33) \quad d\bar{M}/du = [u^{-1} \text{diag}(a_r) + \bar{G}] \bar{M},$$

where $\bar{M} = (\bar{M}_0, \dots, \bar{M}_{m-1})'$, and

$$(34) \quad \bar{G} = \begin{bmatrix} \bar{\mu}_0 & v_0 & & & 0 \\ \bar{\lambda} & \bar{\mu} & v_1 & & \\ & \ddots & \ddots & \ddots & \\ & & & v_{m-2} & \\ 0 & & & \bar{\lambda}_{m-1} & \bar{\mu}_{m-1} \end{bmatrix}$$

where

$$\bar{\lambda}_i = (m-i)(q+i-1)(q-m+i-1)(q-m+i-2)/[2(q-m+2i-2)(q-m+2i-1)^2(q-m+2i)] \quad (35)$$

$$\bar{\mu}_i = -[i(q-m+i)(q+m-5)+2(m-1)(q-m-1)]/[2(q-m+2i-1)(q-m+2i+1)].$$

The d.e. (33) has a regular singularity at $u=0$, but an irregular singularity at infinity. As before, \bar{f}_s is a linear combination of the a_{m-s}, \dots, a_{m-1} -solutions at the origin, multiplied by $e^{-\frac{1}{2}u} u^{\frac{1}{2}(q-m-1)}$. In particular, as $u \rightarrow 0+$,

$$\bar{f}_s(u)/u^{\frac{1}{2}(q-m-1)} \sim \bar{k}_s(m;q) u^{a_{m-s} + (m-s)}, \quad (36)$$

where

$$\bar{k}_s(m;q) = \bar{K}(m;q)/[\bar{K}(s-1;q+m-s+1)K(m-s;q-s,m-s+3)] \quad (37)$$

$$\bar{K}(m;q) = \pi^{\frac{1}{2}m}/[2^{\frac{1}{2}mq} \prod_{i=0}^{m-1} \Gamma(\frac{1}{2}(m-i))\Gamma(\frac{1}{2}(q-i))].$$

Taking limits in (27), we find that $\bar{f}_1(u) \approx (-1)^{m-1} g_{m,q}(u)$ for large u , and $\bar{f}_m(u) \approx g_{m,q}(u)$ for u near zero, where

$$g_{m,q}(u) = \kappa(m;q) e^{-\frac{1}{2}u} u^{\frac{1}{2}(q-m-1)} \sum_{r=0}^{m-1} \binom{m-1}{r} (q-1)_{-(m-1-r)} (-u)^r, \quad (38)$$

$$\kappa(m;q) = \pi^{\frac{1}{2}}/[2^{\frac{1}{2}(q+m-1)} \Gamma(\frac{1}{2}m)\Gamma(\frac{1}{2}q)].$$

Again, $g_{m,q}$ corresponds to a particular a_0 -solution of (33) at the origin. Hanumara and Thompson [6] used integrated forms of (38) in their tabulation of u_1 and u_m . Some percentage points of u_1 were calculated using the a_{m-1} -solution of the d.e., and these differed from the results of the approximation by no more than a unit in the second decimal place.

The d.e. (33) is in fact closely connected with the author's d.e. [5] for the moment generating function of Pillai's $V^{(m)} = \text{tr } B$. If we write

$\lambda_{m;q,n}(s) = k \exp(-s V^{(m)})$, then it is easily seen that $\bar{f}_1(u)$ is proportional to $e^{-\frac{1}{2}u} u^{\frac{1}{2}mq-1} \lambda_{m-1;q-1,m+2}(\frac{1}{2}u)$.

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