Distribution of ratio of two Wishart matrices and
evaluation of cumulative probability by holonomic
gradient method

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Abstract

We study the distribution of the ratio of two central Wishart matrices with different
covariance matrices. We first derive the density function of a particular matrix form of
the ratio and show that its cumulative distribution function can be expressed in terms
of the hypergeometric function \( _2F_1 \) of a matrix argument. Then we apply the holonomic
gradient method for numerical evaluation of the hypergeometric function. This approach
enables us to compute the power function of Roy’s maximum root test for testing the
equality of two covariance matrices.

Keywords and phrases: D-modules, equality of covariance matrices, Gröbner basis, hypergeometric function of a matrix argument, Roy’s maximum root test, zonal polynomial

1 Introduction

Let \( W_1 \) and \( W_2 \) be two independent Wishart matrices having the distribution \( W_m(n_1, \Sigma_1) \) and
\( W_m(n_2, \Sigma_2) \), respectively, where \( W_m(n, \Sigma) \) denotes the \( m \times m \) Wishart distribution with \( n \)
degrees of freedom and the covariance matrix \( \Sigma \). We assume \( n_1, n_2 \geq m \) and \( \Sigma_1, \Sigma_2 \) are positive
definite. For testing the equality of covariance matrices

\[ H_0 : \Sigma_1 = \Sigma_2 \tag{1} \]

we usually use test statistics based on the roots of \( W_1 W_2^{-1} \). \( W_1 W_2^{-1} \) (or some symmetric variant
of \( W_1 W_2^{-1} \)) is often called the \( F \) matrix. In this paper we are particularly interested in the
largest root \( l_1(W_1 W_2^{-1}) \) of \( W_1 W_2^{-1} \), which is Roy’s maximum root statistic for testing \( H_0 \). It is
a natural test statistic for testing against the one-sided alternative hypothesis

\[ H_1 : \Sigma_1 \geq \Sigma_2 , \]

where the inequality is in the sense of Loewner order. Kuriki [11] studied the likelihood ratio
statistic against this one-sided alternative.

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In order to compute the power function of Roy’s maximum root test, we need to evaluate the probability \( P(l_1(W_1W_2^{-1}) \leq x) \) for the general case \( \Sigma_1 \neq \Sigma_2 \). The event \( l_1(W_1W_2^{-1}) \leq x \) can be written as

\[
l_1(W_1W_2^{-1}) \leq x \iff W_1 \leq xW_2 \iff W_2^{-1/2}W_1W_2^{-1/2} \leq xI_m,
\]

where we specifically take \( W_2^{1/2} \) to be the unique positive definite square root of \( W_2 \). Note that in considering the distribution of the roots of \( W_1W_2^{-1} \), we can assume \( \Sigma_1 = I_m \) without loss of generality, because the distribution of the roots of \( W_1W_2^{-1} \) depends only on the roots of \( \Sigma_1 \Sigma_2^{-1} \). Under this additional assumption \( \Sigma_1 = I_m \), we derive the density function of the matrix

\[
U = W_2^{-1/2}W_1W_2^{-1/2}
\]

and its cumulative distribution function \( P(U \leq \Omega) \), which involves the hypergeometric function \( _2F_1 \) of a matrix argument. Then by specifying \( \Omega = xI_m \) we obtain \( P(l_1(W_1W_2^{-1}) \leq x) \).

By expressing the cumulative distribution function of the maximum root in terms of \( _2F_1 \), we can apply the holonomic gradient method (HGM, see e.g. Nakayama et al. \[14\]) to numerically evaluate \( _2F_1 \). In Hashiguchi et al. \[4\] we have already shown that HGM works very well for \( _1F_1 \), which appears in Roy’s maximum root test for the one-sample problem \( H_0 : \Sigma = \Sigma_0 \). Hence this paper is continuation of Hashiguchi et al. \[3\] and demonstrates that HGM works well also for \( _2F_1 \) unless the parameter values are extreme.

The organization of this paper is as follows. In Section 2 we derive the density function and the cumulative distribution function of \( W_2^{-1/2}W_1W_2^{-1/2} \). In Section 3 we discuss relations of our results to earlier results on the \( F \) matrix. In Section 4 we study HGM for \( _2F_1 \), based on the partial differential equation of Muirhead (Muirhead \[12\], Muirhead \[13\]). In Section 5 we present results on numerical experiments of HGM. We end the paper with some discussion of open problems in Section 6.

### 2 Distribution of ratio of two Wishart matrices

In this section we derive results on the density and the cumulative distribution function of \( U \) in \( \Sigma \).

First we present the following theorem concerning the density of \( U \).

**Theorem 1.** Under the assumption of \( \Sigma_1 = I_m \), the density function of \( U = W_2^{-1/2}W_1W_2^{-1/2} \geq 0 \) is given by

\[
f(U) = \frac{\Gamma_m\left(\frac{n_1+n_2}{2}\right)|\Sigma_2|^{n_1/2}I + \Sigma_2U|^{-(n_1+n_2)/2}|U|^{(n_1-m-1)/2}}{\Gamma_m\left(\frac{n_1}{2}\right)\Gamma_m\left(\frac{n_2}{2}\right)}.
\]

**Proof.** Consider the transformation \( (W_1, W_2) \rightarrow (U, W_2) \) with the Jacobian

\[
dW_1dW_2 = |W_2|^{(m+1)/2}dUdW_2.
\]

The joint density of \((W_1, W_2)\) is given as

\[
\frac{1}{2^{mn_1}\Gamma_m\left(\frac{n_1}{2}\right)}|W_1|^{(n_1-m-1)/2}\exp\left(-\frac{1}{2}\text{tr}W_1\right)\frac{1}{2^{mn_2}\Gamma_m\left(\frac{n_2}{2}\right)}|\Sigma_2|^{n_2/2}|W_2|^{(n_2-m-1)/2}\exp\left(-\frac{1}{2}\text{tr}\Sigma_2^{-1}W_2\right).
\]

Therefore, letting

\[
C_1 = \frac{1}{2^{mn_1}\Gamma_m\left(\frac{n_1}{2}\right)2^{mn_2}\Gamma_m\left(\frac{n_2}{2}\right)|\Sigma_2|^{n_2/2}},
\]

we can write

\[
f(U) = \frac{\Gamma_m\left(\frac{n_1+n_2}{2}\right)|\Sigma_2|^{n_1/2}I + \Sigma_2U|^{-(n_1+n_2)/2}|U|^{(n_1-m-1)/2}}{\Gamma_m\left(\frac{n_1}{2}\right)\Gamma_m\left(\frac{n_2}{2}\right)}.
\]
the joint density of \((U, W_2)\) is

\[
f(U, W_2) = C_1 |W_2|^{(m+1)/2} \times |W_2^{1/2}UW_2^{1/2}|^{(n_1-m-1)/2} \exp\left(-\frac{1}{2} \text{tr} W_2^{1/2}UW_2^{1/2}\right)
\]

\[
\times |W_2|^{(n_2-m-1)/2} \exp\left(-\frac{1}{2} \text{tr} \Sigma_2^{-1} W_2\right)
\]

\[
= C_1 |W_2|^{(n_1+n_2-m-1)/2} |U|^{(n_1-m-1)/2} \exp\left(-\frac{1}{2} \text{tr} \left(W_2^{1/2}UW_2^{1/2} + \Sigma_2^{-1} W_2\right)\right)
\]

\[
= C_1 |W_2|^{(n_1+n_2-m-1)/2} |U|^{(n_1-m-1)/2} \exp\left(-\frac{1}{2} \text{tr}(U + \Sigma_2^{-1}) W_2\right). \quad (5)
\]

Integrating this with respect to \(W_2\) gives \(\mathcal{I}\).

\[\square\]

Remark 1. In Theorem 1 the positive definite square root \(W_2^{-1/2}\) is essential. Other square roots do not work because of non-commutativity. Herz uses the positive definite square root for deriving the integral expression of \(2F_1\) from that of \(1F_1\) and the argument of Theorem 1 follows Herz’s derivation.

From Theorem 1 we have the following expression for the cumulative distribution function of \(U\), which involves the hypergeometric function \(2F_1\) of a matrix argument.

**Theorem 2.** Under the same assumption above, the cumulative probability \(P(U \leq \Omega)\) is given by

\[
P(U \leq \Omega) = \frac{\Gamma_m(\frac{n_1+1}{2})\Gamma_m(\frac{n_1+n_2}{2})}{\Gamma_m(\frac{n_1+m+1}{2})\Gamma_m(\frac{n_2}{2})} |\Sigma_2\Omega|^{n_1/2} 2F_1\left(\begin{array}{c} n_1, n_1 + n_2, n_1 + m + 1 \\ n_2 \end{array}; \frac{-\Sigma_2 \Omega}{2}\right). \quad (6)
\]

**Proof.** Let \(C_2 = \frac{\Gamma_m(\frac{n_1+1}{2})\Gamma_m(\frac{n_1+n_2}{2})}{\Gamma_m(\frac{n_1+m+1}{2})\Gamma_m(\frac{n_2}{2})}\). Then

\[
P(U \leq \Omega) = C_2 \int_{0 \leq U \leq \Omega} |I_m + \Sigma_2 U|^{-(n_1+n_2)/2} |U|^{(n_1-m-1)/2} dU.
\]

Let \(\tilde{U} = \Omega^{-1/2}U\Omega^{-1/2}\). Then \(P(U \leq \Omega) = P(\tilde{U} \leq I_m)\). The Jacobian of the transformation is \(dU = |\Omega|^{(m+1)/2}d\tilde{U}\). Hence

\[
P(U \leq \Omega) = C_2 |\Omega|^{n_1/2} \int_{0 \leq U \leq I_m} |I_m + \Sigma_2 \Omega^{1/2} \tilde{U} \Omega^{1/2}|^{-(n_1+n_2)/2} |\tilde{U}|^{(n_1-m-1)/2} d\tilde{U}
\]

\[
= C_2 |\Omega|^{n_1/2} \int_{0 \leq U \leq I_m} |I_m + \Omega^{1/2} \Sigma_2 \Omega^{1/2} \tilde{U}|^{-(n_1+n_2)/2} |\tilde{U}|^{(n_1-m-1)/2} d\tilde{U}
\]

\[
= C_2 |\Omega|^{n_1/2} \frac{\Gamma_m(\frac{n_1+1}{2})\Gamma_m(\frac{n_1+n_2}{2})}{\Gamma_m(\frac{n_1+m+1}{2})} 2F_1\left(\begin{array}{c} n_1, n_1 + n_2, n_1 + m + 1 \\ n_2 \end{array}; \frac{-\Omega^{1/2} \Sigma_2 \Omega^{1/2}}{2}\right)
\]

The last equality holds from the fact that the roots of \(\Omega^{1/2} \Sigma_2 \Omega^{1/2}\) is the same as the roots of \(\Sigma_2 \Omega^{1/2} \Omega^{1/2} = \Sigma_2 \Omega\), including multiplicities, and the hypergeometric function only depends on the roots of the matrix argument. Rewriting the constants yields \(\mathcal{I}\).

\[\square\]

Remark 2. Unlike Theorem 1 in the above proof, \(\Omega^{1/2}\) can be any square root of \(\Omega\), i.e., it does not have to be the positive definite square root of \(\Omega\).
By setting $\Omega = xI_m$ we have the following corollary. We state this corollary without assuming $\Sigma_1 = I_m$ for the purpose of easier reference.

**Corollary 1.** Let $W_1$ and $W_2$ be two independent Wishart matrices having the distribution $W_m(n_1, \Sigma_1)$ and $W_m(n_2, \Sigma_2)$, respectively. The probability $P(l_1(W_1W_2^{-1}) \leq x)$ is expressed as

$$
P(l_1(W_1W_2^{-1}) \leq x) = \frac{\Gamma_m\left(\frac{n_1+1}{2}\right)\Gamma_m\left(\frac{n_2+n_a}{2}\right)}{\Gamma_m\left(\frac{n_2+1}{2}\right)\Gamma_m\left(\frac{n_1+n_a}{2}\right)} x^{mn_2/2}\middle|\Sigma_2^{-1}\Sigma_1^{-1/2}
\cdot 2F_1\left(\frac{n_1}{2}, \frac{n_1+n_2}{2}, \frac{n_1+m+1}{2}; -x\Sigma_1^{-1}\Sigma_2\right).$$

(7)

Chikuse [1] already obtained the expression (7). Kummer relations for $2F_1$ (see e.g. James [6], Muirhead [13]) are referred as

$$2F_1(a, b; c; X) = |I_m - X|^{c-a-b} 2F_1(c - a - b, c - b; c; X),$$

(8)

$$2F_1(a, b; c; X) = |I_m - X|^{-b} 2F_1(c - a, b; c; -X(I_m - X)^{-1}),$$

(9)

and we apply (8) to (7) to obtain

$$\Pr(l_1(W_1W_2^{-1}) < x) = \frac{\Gamma_m\left(\frac{n_1}{2} + \frac{n_2}{2}\right)\Gamma_m\left(\frac{n_1+1}{2}\right)}{\Gamma_m\left(\frac{n_2}{2}\right)\Gamma_m\left(\frac{n_1+n_2}{2}\right)} x^{n_1/2}\middle|\Sigma_2^{-1}\Sigma_1^{-1/2} + xI_m|^{-n_1/2}
\cdot 2F_1\left(\frac{m+1}{2}, \frac{n_1+n_2}{2}, \frac{n_1+m+1}{2}; x\Sigma_2^{-1}\Sigma_1 + xI_m^{-1}\right).$$

(10)

In addition, we also have

$$\Pr(l_1(W_1W_2^{-1}) < x) = \frac{\Gamma_m\left(\frac{n_1}{2} + \frac{n_2}{2}\right)\Gamma_m\left(\frac{m+1}{2}\right)}{\Gamma_m\left(\frac{n_2}{2}\right)\Gamma_m\left(\frac{n_1+m+1}{2}\right)} x^{n_1/2}\middle|\Sigma_2^{-1}\Sigma_1 + xI_m|^{-n_1/2}
\cdot 2F_1\left(\frac{n_1}{2}, \frac{-n_2}{2} + \frac{m+1}{2}, \frac{n_1+m+1}{2}; x\Sigma_2^{-1}\Sigma_1 + xI_m^{-1}\right).$$

(11)

by applying (9) to (10). If $r = \frac{n_2}{2} - \frac{m+1}{2}$ is a non-negative integer, we see that (11) is terminated as a finite series. Both (7) and (11) are alternating series, while (10) is a series of nonnegative terms. In Section 5 we use (10) for numerical stability in evaluating the initial value for HGM.

Chikuse [1] mentioned that the upper probability of the smallest root $l_m(W_1W_2^{-1})$ can be obtained from (7) by replacing $n_1, n_2, x, \Sigma_1$ and $\Sigma_2$ by $n_2, n_1, x^{-1}, \Sigma_2$ and $\Sigma_1$, respectively.

$$\Pr(l_m(W_1W_2^{-1}) \geq x) = \frac{\Gamma_m\left(\frac{m+1}{2}\right)\Gamma_m\left(\frac{n_1+n_2}{2}\right)}{\Gamma_m\left(\frac{n_2}{2}\right)\Gamma_m\left(\frac{n_1+n_2+m+1}{2}\right)} \left|\frac{1}{x} \Sigma_2^{-1}\Sigma_1\right|^{n_2/2}
\cdot 2F_1\left(\frac{n_2}{2}, \frac{n_1+n_2}{2}, \frac{n_2+m+1}{2}; -\frac{1}{x}\Sigma_2^{-1}\Sigma_1\right).$$

(12)

The equation (12) can be obtained form the integral of (11) because of

$$\int_{U > \Omega} |U|^\frac{n_2}{2} - \frac{m+1}{2} |I_m + \Sigma_2 U|^{-\frac{n_1+n_2}{2}} dU$$

$$= \frac{\Gamma_m\left(\frac{n_2}{2}\right)\Gamma_m\left(\frac{m+1}{2}\right)}{\Gamma_m\left(\frac{n_2+m+1}{2}\right)} |\Sigma_2|^{-\frac{n_1+n_2}{2}} |\Omega|^{-\frac{n_2}{2}} 2F_1\left(\frac{n_2}{2}, \frac{n_1+n_2}{2}, \frac{n_2+m+1}{2}; -\left(\Omega\Sigma_2\right)^{-1}\right),$$

Pr($l_m(W_1W_2^{-1}) > x$) = Pr($U > xI_m$) and the substitution of $\Sigma_2$ by $\Sigma_1^{-1}\Sigma_2$. The above integral can be found in Problem 1.17 in p.50 of Gupta and Nagar [3].
3 Relations to known results on the $F$ matrix and the beta matrix

In this section we discuss the relationships between our results and earlier results. We mainly consider the null case $\Sigma_1 = \Sigma_2$.

Constantine [2] gave the cumulative distribution functions of the Wishart and the multivariate beta distributions. Let $B = (W_1 + W_2)^{-1/2}W_1(W_1 + W_2)^{-1/2}$ where $W_1 \sim W_m(n_1, \Sigma)$, $W_2 \sim W_m(n_2, \Sigma)$, $n_1, n_2 \geq m$ and $\Sigma > 0$. Then the random matrix $B$ follows the multivariate beta distribution of the first kind with parameters $\frac{n_1}{2}$ and $\frac{n_2}{2}$. Note that in the null case $(W_1 + W_2)^{-1/2}$ does not have to be the positive definite square root, because of the orthogonal invariance of the beta distribution. The cumulative distribution function of $B$ is given by

$$
\text{Pr}(B < \Omega) = \frac{\Gamma_m(\frac{n_1+m}{2})\Gamma_m(\frac{n_2+m+1}{2})}{\Gamma_m(\frac{n_1}{2})\Gamma_m(\frac{n_2}{2})\Gamma_m(\frac{n_1+m+1}{2})} \left[ \frac{1}{2} \right]_{2} F_{1} \left( \frac{n_1}{2}; -\frac{n_2}{2}, \frac{m+1}{2}, \frac{n_1+m+1}{2}; \Omega \right),
$$

for $0 < \Omega < I_m$. Therefore the cumulative distribution function of the largest root $b_1(B)$ of $B$ is given as $\text{Pr}(b_1(B) \leq x) = \text{Pr}(B \leq xI_m)$ and, from the relationship

$$
\text{Pr}(l_1(W_1W_2^{-1}) \leq x) = \text{Pr} \left( b_1(B) \leq \frac{x}{1+x} \right),
$$

we also have

$$
\text{Pr}(l_1(W_1W_2^{-1}) \leq x) = \frac{\Gamma_m(\frac{n_1+m}{2})\Gamma_m(\frac{n_1+m+1}{2})}{\Gamma_m(\frac{n_1}{2})\Gamma_m(\frac{n_1+m}{2})} \left( \frac{1}{x+1} \right)^{\frac{n_1+m}{2}} \cdot 2F_1 \left( \frac{n_1}{2}; -\frac{n_2}{2}, \frac{m+1}{2}, \frac{n_1+m+1}{2}; \frac{x}{1+x}I_m \right),
$$

for $x \geq 0$. The above equation is the same as (11) by substitutions of $\Sigma_1 = \Sigma_2$

Based on the results of Khatri [8], for the case that $r = \frac{n_1}{2} - \frac{m+1}{2}$ is a nonnegative integer, Venables [17] obtained another expression of $\text{Pr}(b_1(B) < x)$ which is equivalent to

$$
\text{Pr} \left( l_1(W_1W_2^{-1}) \leq x \right) = \left( \frac{x}{1+x} \right)^{\frac{n_1+m}{2}} \sum_{k=0}^{r_m} \frac{(1+x)^{-k}}{k!} \sum_{\kappa \vdash k} \left( \frac{1}{2} \right)^{\kappa_1} \kappa \cdot C_\kappa (I_m)
$$

(14)

where $r = \frac{n_1-m-1}{2}$ is a positive integer and $\sum^*$ denotes the summation over all partitions $\kappa = (\kappa_1, \ldots, \kappa_\ell)$ of $k$ with $\kappa_1 \leq r$. For example, $m = 3, n_1 = 6$ and $n_2 = 10$, the equation (13) is

$$
\begin{align*}
2145x^9 (x+1)^9 & \frac{2x^9}{143(x+1)^9} + \frac{27x^8}{143(x+1)^8} - \frac{166x^7}{143(x+1)^7} + \frac{914x^6}{2145(x+1)^6} - \frac{113x^5}{11(x+1)^5} \\
+ 184x^4 & \frac{55x^3}{3(x+1)^3} + \frac{13x^2}{(x+1)^2} - \frac{27x}{5(x+1)} + 1 \\
+ \frac{53x^3}{3(x+1)^3} & + \frac{360}{(x+1)^4} + \frac{165}{(x+1)^3} + \frac{45}{(x+1)^2} + \frac{9}{x+1} + 1
\end{align*}
$$

and (14) gives

$$
\begin{align*}
\frac{x^9}{(x+1)^9} & \left( \frac{30}{(x+1)^9} + \frac{135}{(x+1)^8} + \frac{330}{(x+1)^7} + \frac{539}{(x+1)^6} \\
+ \frac{531}{(x+1)^5} + \frac{360}{(x+1)^4} + \frac{165}{(x+1)^3} + \frac{45}{(x+1)^2} + \frac{9}{x+1} + 1 \right).
\end{align*}
$$
We find that they are the same by their subtraction by symbolic computation. In general, it seems to be difficult to show that (13) and (14) are equivalent, as pointed out in the concluding remarks of Venables [17].

Finally we mention a result of Khatri [7] in the nonnull case. Section 3.4 of Khatri [7] gives the density function of \( l_1(W_1W_2^{-1}) \) in terms of \( _3F_2 \):

\[
f(l_1) = c_2 |\Lambda|^{-\frac{n_1+n_2}{2}} |I_m + l_1\Lambda^{-1}|^{-\frac{n_1+n_2}{2}} \cdot _3F_2\left(\frac{n_1+n_2}{2}, \frac{m}{2} + 1, \frac{m-1}{2}; \frac{n_1+m+1}{2}; l_1(\Lambda + l_1 I_m)^{-1}\right),
\]

where \( \Lambda = \Sigma_1 \Sigma_2^{-1} \) and

\[
c_2 = \frac{\Gamma\left(\frac{1}{2}\right) \Gamma_m\left(\frac{n_1+n_2}{2}\right) \Gamma_{m-1}\left(\frac{m}{2} + 1\right)}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n_1+n_2}{2}\right) \Gamma\left(\frac{m-1}{2}\right) \Gamma\left(\frac{n_1+m+1}{2}\right)}.
\]

Differentiation of (9) should yield (15), but it does not seem to be obvious.

4 Holonomic gradient method for \( _2F_1 \)

Applying the HGM for a numerical evaluation of the matrix hypergeometric function \( _2F_1 \) is analogous to the case of \( _1F_1 \) of Hashiguchi et al. [4]. We explain mainly the differences briefly. Put

\[
g_i = \partial_i^2 + [p(x_i) + \sum_{j \neq i} q_2(x_i, x_j) \partial_i - \sum_{j \neq i} q(x_i, x_j) \partial_j - r(x_i), \quad i = 1, \ldots, m,
\]

where

\[
p(x_i) = \frac{c - (m - 1)/2 - (a + b + 1 - (m - 1)/2)x_i}{x_i(1 - x_i)},
\]

\[
q_2(x_i, x_j) = \frac{1}{2(x_i - x_j)},
\]

\[
q(x_i, x_j) = \frac{x_j(1 - x_j)}{2x_i(1 - x_i)(x_i - x_j)},
\]

\[
r(x_i) = \frac{ab}{x_i(1 - x_i)}.
\]

The matrix hypergeometric function \( _2F_1(a, b, c; x_1, \ldots, x_m) \) is annihilated by the linear partial differential operator \( g_i \)’s by Muirhead [12].

**Theorem 3.** The set \( \{g_i\}_{i=1}^m \) is a Gröbner basis in the ring of differential operators with rational function coefficients \( R_m = \mathbb{C}(x_1, \ldots, x_m)\langle \partial_1, \ldots, \partial_m \rangle \).

**Proof.** Put \( G_i = x_i(1 - x_i)g_i \). Then, we can see

\[
[G_i, G_j] = \frac{1}{2} \frac{2x_i x_j - x_i - x_j}{(x_i - x_j)^2} (G_i - G_j)
\]

by calculation. Let us consider the graded reverse lexicographic order among the monomials of \( \partial_1, \ldots, \partial_m \). Then, the leading term of \( G_i \) is \( x_i(1 - x_i) \partial_i^2 \) and the leading term of \( G_i \) and \( G_j \) are coprime when \( i \neq j \). Therefore, the commutator \( [G_i, G_j] \) can be regarded as an \( S \)-pair and the relation above leads the \( S \)-pair criterion \( [G_i, G_j] \rightarrow 0 \) by \( \{G_i\} \). Hence, \( \{g_i\} \) is a Gröbner basis. \( \square \)
Let $M$ be the left ideal of $R_m$ generated by $g_i, i = 1, \ldots, m$. The important conclusion of this theorem is that the system can be transformed into a completely integrable Pfaffian system

$$
\partial_i F \equiv P_i(x) F \mod M
$$

where $P_i(x)$ is a $2^m \times 2^m$ matrix and $F$ is a column vector of length $2^m$ whose $i$-th entry $(i = 0, 1, \ldots, 2^m - 1)$ is $\partial^\alpha = \prod_{k=1}^m \partial_k^{\alpha_k}$, $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m)$. Here, $\alpha$ is a vector obtained by the binary expansion of $i$ as $i = \sum_{k=0}^{m-1} \alpha_k 2^k$, $\alpha_k \in \{0, 1\}$. We use this Pfaffian system for a numerical evaluation of $2F_I$.

We derive an explicit expression of the matrix $P_i$ and we utilize a sparsity of the matrix $P_i$ in our implementation as follows. Let $[m] = \{1, 2, \ldots, m\}$. Suppose that $J \subset [m]$. The set $J$ is encoded into a binary number $jj$; if $k \in J$, then the $k$-th bit of $jj$ is 1 and if $k \notin J$, then the $k$-th bit of $jj$ is 0. Note that when $jj$ is the encoding of the set $J$, the encoding of $\{k\} \cup J$ is $((1 \ll (k-1)) | jj)$ in the language C. The operator $\partial_j$ is defined as $\prod_{k \in J} \partial_k$. Note that any element of $F$ can be written in this form. Let us describe the matrix $P_i$ in terms of $\partial_j$.

Let $I$ be a subset of $[m]$. When $i \notin I$, we have $\partial_i \partial_I = \partial_I$ where $I' = \{i\} \cup I$ and $\partial_I$ is again an element of $F$. Then, the corresponding row of the matrix $P_i$ is a unit vector. Suppose $i \notin J$ and put $I = \{i\} \cup J$. We want to express $\partial_i \partial_I$ in terms of the elements of $F$ modulo the left ideal $M$. Apply $\partial_j$ to the operator $g_i$ as

$$
\partial_j g_i = \partial_i^2 \partial_j + p(x_i) \partial_i \partial_j + \sum_{j \neq i} q_2(x_i, x_j) \partial_i - \partial_j \sum_{j \neq i} q(x_i, x_j) \partial_j - r(x_i) \partial_j.
$$

When $k \notin J$, we have $\partial_j q_2(x_i, x_k) \partial_i = q_2(x_i, x_k) \partial_i$,

When $k \in J$, we have $\partial_j q_2(x_i, x_k) \partial_i = q_2(x_i, x_k) \partial_i + \partial q_2(x_i, x_k) \partial_I \partial_I\{k\}$,

When $k \notin J$, we have $\partial_j q(x_i, x_k) \partial_k = q(x_i, x_k) \partial_I \partial_J\{k\}$,

When $k \in J$, we have $\partial_j q(x_i, x_k) \partial_k = q(x_i, x_k) \partial_I \partial_J\{k\} \partial_k^2 + \partial q(x_i, x_k) \partial_k \partial_j$.

In summary, when $i \notin J$, we have

$$
\partial_i^2 \partial_j + p(x_i) \partial_I + \sum_{k \neq i} q_2(x_i, x_k) \partial_I + \sum_{k \neq i, k \in J} \frac{\partial q_2(x_i, x_k)}{\partial x_k} \partial_I \partial_J\{k\}
$$

$$
- \sum_{k \neq i, k \notin J} q(x_i, x_k) \partial_I \partial_J\{k\} - \sum_{k \neq i, k \in J} q(x_i, x_k) \partial_I \partial_J\{k\} \partial_k^2 - \sum_{k \neq i, k \in J} \frac{\partial q(x_i, x_k)}{\partial x_k} \partial_j - r(x_i) \partial_j \equiv 0
$$

modulo the left ideal $M$ generated by $g_i, i = 1, \ldots, m$. It follows from this relation that the operator $\partial_i^2 \partial_j$ can be expressed in terms of the element of $F$ inductively with respect to $\sharp J$ (the cardinality of $J$).

### 5 Numerical experiments

The numerical evaluation by HGM consists of two steps. The first step is an approximate evaluation of $2F_I$ and its derivatives $\partial_{I' \bullet 2F_I}, I \subset [m]$ by Koev and Edelman \cite{Koev} at an initial \footnote{Here, we count 1-th bit, 2-th bit, \ldots instead of counting 0-th bit, 1-th bit, \ldots of the convention of programming.}
point \( x = x_0 \) (\( x_0 \) is \( q_0 \) in our package) which is close to the origin. The second step is the application of the Runge-Kutta method to the ordinary differential equation obtained from the Pfaffian system.

We find that the numerical evaluation of \( 2F_1 \) is more challenging than \( 1F_1 \) in Hashiguchi et al. [4]. Hence we employ some heuristics for the numerical evaluation.

1. We use the formula (10) for the step one, because all terms of \( 2F_1 \) is non-negative when \( x \) is positive. Convergence of series whose entries have alternating signs as (6) in Theorem 2 is slow in general.

2. For small positive number \( x_0 \), we evaluate \( 2F_1 \) at \( x_0 \left( \Sigma^{-1}_2 \Sigma_1 + x_0 I_m \right)^{-1} \). Let \( f_k \) be the \( k \)-th approximation of this series, which is the truncation of the series more than degree \( k = |\lambda| \) terms where \( \lambda \) is a partition. When \( |(f_k - f_{k-1})/f_{k-1}| \) is smaller than assigned_series_error, of which default value is \( 10^{-5} \) in our implementation, we use the \( k \)-th approximation as the value of the step one. When the value \( \Pr(\ell_1 < x_0) \) is smaller than the assigned value \( x_0value_{\text{min}} \), of which default value is \( 10^{-60} \) in our implementation, we increase \( x_0 \) and retry the evaluation. Too small initial value is not acceptable for the Runge-Kutta method by the double precision.

3. We use the adaptive version of the Runge-Kutta method by the default value of relative and absolute errors are \( 10^{-10} \) and \( |f_k - f_{k-1}| \times \Pr(\ell_1 < x_0)/f_k \) in our implementation.

4. When one of the entry of the initial evaluation point \( x_0 \left( \Sigma^{-1}_2 \Sigma_1 + x_0 I_m \right)^{-1} \) is close to 1, the convergence of series \( 2F_1 \) becomes very slow. In this case, we should decrease \( x_0 \) and the absolute error for the Runge-Kutta method.

Under the above heuristics, numerical evaluation works well unless the parameters are extreme, for example when \( n_i \)'s are large, or the ratio of eigenvalues of \( \Sigma^{-1}_2 \Sigma_1 \) is large. Systematic experiments and studies on parameter spaces for which the HGM works well and improved algorithms will be future research topics.

Let us present some numerical examples to illustrate some border cases of performance of HGM. We use our implementation of the package hgm for the system R. The command hgm.p2wishart evaluates the cumulative distribution function in (10). The arguments are \( m=m \) (the dimension), \( \text{beta} = \) the eigenvalues of \( \Sigma^{-1}_2 \Sigma_1 \), \( n1 = n_1 \), \( n2 = n_2 \) (the degrees of freedom of two Wishart distributions respectively), \( q \) (the last point of the evaluation interval) and \( q_0 \) (the point for the initial value).

**Example 1.** We evaluate \( \Pr(\ell_1 < x) \) for \( m = 10 \), \( n_1 = 11 \), \( n_2 = 12 \), and

\[
\Sigma^{-1}_2 \Sigma_1 = \text{diag}(1, 2, 3, 4, 5, 6, 7, 8, 9, 10)
\]

by our implementation. The starting point \( x_0 \) is 0.1 and the approximation by the zonal polynomial expansion is truncated at the degree 28, which is automatically determined by the heuristics above. It takes 13 minutes and 15 seconds to obtain Figure 1 on a machine with Intel Xeon CPU (2.70GHz) with 256 G memory.

Let us see the behavior of our algorithm when the eigenvalues of \( \Sigma^{-1}_2 \Sigma_1 \) are a mixture of relatively small numbers and large numbers.

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2The demonstration in this paper was performed on the version 1.16. It is newer than the version on cran. This version can be obtainable from [http://www.math.kobe-u.ac.jp/OpenXM/Math/hgm](http://www.math.kobe-u.ac.jp/OpenXM/Math/hgm)
Example 2. The command

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,2,3),q=300,n1=10,n2=20,autoplot=1))}
\]

works fine (no graph shown), but when we increase the eigenvalues 2 and 3 to 20 and 300 as

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,300),q=500,}
\]

\[
\text{n1=10,n2=20,autoplot=1),ylim=c(0,0.3))}
\]

we get a warning “abserr seems not to be small enough”, which means that the control parameter for the absolute error for the adaptive Runge-Kutta method is not small enough. The default value of the absolute error is \(1 \times 10^{-10}\). The output is the left graph of Figure 2 and it looks like a wrong evaluation. The trouble occurs when the initial value for the HGM is very small. We should make the absolute error smaller or the initial evaluation point \(q_0\), of which default value is 0.3, larger. Note that making \(q_0\) larger requires a lot of resources for approximate evaluation of the series expansion of \(\text{I}_1\). Then, we retry the command with a new \textbf{err} parameter vector, which specifies the absolute error and the relative error for the adaptive Runge-Kutta method, as

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,300),q=500,}
\]

\[
\text{n1=10,n2=20,autoplot=1),err=c(1e-30,1e-10),}
\]

\[
\text{ylim=c(0,0.3))}
\]

The output is the right graph of Figure 2 and looks a correct evaluation. This example illustrates that inappropriate setting of the control parameter for the adaptive Runge-Kutta method used in the hgm leads to a wrong answer. The computation time is a few seconds for these examples, then we do not show detailed timing data.

The next example illustrates the behavior of our algorithm and an implementation for \texttt{R} when the degrees of freedom becomes larger.

Example 3. We make the degrees of freedom \(n_2\) to 200.

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,300),q=50,}
\]

\[
\text{n1=10,n2=200,autoplot=1))}
\]
This execution does not finish in a few seconds and takes 19 seconds on Mac OS X 10.9 with 2.4GHz Intel Core i7 and 8G memory. The output is the left graph of Figure 3. A good choice of \( q_0 \), which is the initial evaluation point for the HGM and of which default value is 0.3, improves the performance. For example, the same evaluation with a different \( q_0 \) as

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,300),q=300,q0=0.1,n1=10,n2=200,err=c(1e-40,1e-10),autoplot=1,q0=0.1,verbose=1))}
\]

finishes in 0.248 seconds.

We make the degrees of freedom \( n_1 \) to 300.

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,300),q=300,q0=0.1,n1=300,n2=200,err=c(1e-30,1e-10),autoplot=1));}
\]

This execution stops with an error that the initial value is zero, because the factor of \( 2F_1 \) in \( (10) \) is too small.

Let us try other degrees of freedom \( n_1 = 40 \) with fixing the other parameters. The output of

\[
\text{plot(hgm.p2wishart(m=3,beta=c(1,20,150),q=300,q0=0.1,n1=40,n2=200,err=c(1e-60,1e-10),autoplot=1));}
\]
is the right graph of Figure 3. The execution takes 127.5 seconds.

6 Discussion

Some open problems remain in this paper. We already mentioned difficulties in proving that (13) and (14) are equivalent. Similarly differentiation of (9) should yield (15), but it does not seem to be obvious.

Another mathematically important question is the singularity of the differential operator \( g_i \) in (16). Note that \( g_i \) has singularity in the diagonal region \( x_i = x_j, i \neq j \). Therefore HGM cannot be used when there are multiple roots of \( \Sigma_1 \Sigma_2^{-1} \). The same problem was discussed in Hashiguchi et al. [4] for the case of \( 1F_1 \). In the case of \( 1F_1 \), Muirhead’s differential operator \( P_i \) annihilating \( 1F_1 \) is

\[
P_i = y_i \partial_i^2 + \left\{ c - \frac{m-1}{2} - y_i + \frac{1}{2} \sum_{j=1, j \neq i}^{m} \frac{y_i}{y_i - y_j} \right\} \partial_i - \frac{1}{2} \sum_{j=1, j \neq i}^{m} \frac{y_j}{y_i - y_j} \partial_j - a, \quad i = 1, \ldots, m.
\]

In Hashiguchi et al. [3] it was conjectured that \( y_i \prod_{j \neq i} (y_i - y_j) P_i, \; i = 1, \ldots, m \), generate a holonomic left ideal in the Weyl algebra \( D_m \). A proof for \( m = 2 \) was given in Appendix A of Hashiguchi et al. [4]. If this were the case for general \( m \), then differential equations for the diagonal region could be computed by restriction algorithm for holonomic \( D \)-modules. In Hashiguchi et al. [4] restriction algorithm was tried but failed for \( m = 4 \). In fact Kondo [10] proved that the left \( D \)-ideal generated by \( y_i \prod_{j \neq i} (y_i - y_j) P_i \) is not holonomic for \( m = 4 \). On the other hand Noro [15] showed the use of l’Hôpital’s rule in Hashiguchi et al. [4] can be generalized for computing a system of PDEs for various patterns of diagonalizations of variables. By symbolic computations using Risa/Asir([16]), it seems that the similar phenomenon occurs with \( 2F_1 \). However symbolic computations are heavier for \( 2F_1 \) than for \( 1F_1 \). Hence further investigation is needed to clarify the singularity of \( g_i \) in the diagonal region \( x_i = x_j, i \neq j \).

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