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COMPUTATIONALLY EFFICIENT RECURSIONS FOR TOP-ORDER INVARIANT POLYNOMIALS WITH APPLICATIONS

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The top-order zonal polynomials $C_k(A)$, and top-order invariant polynomials $C_{k_1,\ldots,k_r}(A_1,\ldots,A_r)$ in which each of the partitions of k_i, $i=1,\ldots,r$, has only one part, occur frequently in multivariate distribution theory, and econometrics — see, for example, Phillips (1980, *Econometrica* 48, 861–878; 1984, *Journal of Econometrics* 26, 387–398; 1985, *International Economic Review* 26, 21–36; 1986, *Econometrica* 54, 881–896), Hillier (1985, *Econometric Theory* 1, 53–72; 2001, *Econometric Theory* 17, 1–28), Hillier and Satchell (1986, *Econometric Theory* 2, 66–74), and Smith (1989, *Journal of Multivariate Analysis* 31, 244–257; 1993, *Australian Journal of Statistics* 35, 271–282). However, even with the recursive algorithms of Ruben (1962, *Annals of Mathematical Statistics* 33, 542–570) and Chikuse (1987, *Econometric Theory* 3, 195–207), numerical evaluation of these invariant polynomials is extremely time consuming. As a result, the value of invariant polynomials has been largely confined to analytic work on distribution theory. In this paper we present new, very much more efficient, algorithms for computing both the top-order zonal and invariant polynomials. These results should make the theoretical results involving these functions much more valuable for direct practical study. We demonstrate the value of our results by providing fast and accurate algorithms for computing the moments of a ratio of quadratic forms in normal random variables.

Most of the main results in the paper appeared in an earlier paper by Kan and Wang entitled "Fast Evaluation of Top-Order Invariant Polynomials and Moments of Ratio of Quadratic Forms in Normal Random Variables." Hillier first became involved as a referee of that earlier paper. His contribution has been confined mainly to suggesting the generating function approach, simplifying some of the proofs, and contributing a few additional results. We are grateful to Plamen Koev, Peter Phillips, Serge Provost, Marko Riedel, and two anonymous referees for helpful comments and suggestions. Kan gratefully acknowledges financial support from the National Bank Financial of Canada. Address correspondence to Raymond Kan, Joseph L. Rotman School of Management, University of Toronto, 105 St. George Street Toronto, ON M5S 3E6, Canada; e-mail: kan@chass.utoronto.ca.

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1. INTRODUCTION

Many distribution-theoretic problems in statistics and econometrics involve quite strong group-invariance properties. This fact means that analytical results are naturally expressed in terms of functions invariant under the relevant group action. Prominent among such functions are the zonal polynomials of the real symmetric matrices, first introduced and studied by James (1954, 1961) (for a more recent treatment see Muirhead, 1982). These arise, in particular, in the study of the properties of statistics that are functions of standard normal vectors, because the joint density function of n such variates is invariant under the action of the orthogonal group (see James, 1954).

As an example of this, if A is a real $n \times n$ symmetric matrix, and $z \sim N(0_n, I_n)$, the moment generating function of $q = z'Az$ is easily seen to be

$$M_q(t) = |I_n - 2tA|^{-1/2}. \tag{1}$$

This is clearly a function only of the characteristic roots $\lambda_1, \ldots, \lambda_n$, say, of A, and is invariant under permutations of those roots. That is, $M_q(t)$ is a symmetric function of the λ_i and thus will have an expansion in terms of any of the symmetric functions in n variables (for general background on such functions, see Macdonald, 1979). The zonal polynomials belong to the ring of all such symmetric functions and provide a parsimonious means of expressing results such as this: $M_q(t)$ has a simple series expansion in terms of zonal polynomials (see eqn. (4) in Section 2.1). The density function of q also has an expansion of the same type (see James, 1964, eqn. (133)). The first use of the zonal polynomials in econometrics seems to have been by Sargan (1976).

Motivated by a variety of similar, higher dimensional, multivariate distribution problems, Davis (1979, 1981) and Chikuse (1980) developed a family of invariant polynomials with several matrix arguments, extending the zonal polynomials. These invariant polynomials with multiple matrix arguments play an important role in finite-sample distribution theory in both multivariate statistical theory and econometrics. As an example of this type, the joint moment generating function of r statistics $q_i = z'A_i z$, with the A_i, $i = 1, \ldots, r$, each $n \times n$ symmetric, and $z \sim N(0_n, I_n)$ again, is

$$M_{q_1,\ldots,q_r}(t_1, \ldots, t_r) = |I_n - 2A(\boldsymbol{t})|^{-1/2}, \tag{2}$$

where $A(\boldsymbol{t}) = t_1 A_1 + \cdots + t_r A_r$. This is clearly invariant under the simultaneous transformations $A_i \to H'A_i H$, with H an $n \times n$ orthogonal matrix, and thus will have an expansion in terms of any family of functions invariant under this action. Again, the Davis–Chikuse invariant polynomials provide a parsimonious expansion of this type (see the subsequent discussion for more details).

Now, in both of the preceding examples, and a number of other cases of interest, only special cases of the relevant invariant polynomials occur in the expressions

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that are of interest (moment generating functions, moments, or densities), the so-called top-order polynomials, and it is to these special cases that this paper is addressed. These special cases of the polynomials also arise in statistical problems involving the expectation of a ratio of quadratic forms in normal variables (Smith, 1989; Hillier, 2001; Forchini, 2002), the distribution of the Wald test statistic in multivariate regressions (Phillips, 1986), and the finite-sample distribution of estimators in seemingly unrelated regressions (Hillier and Satchell, 1986), among others. In econometrics, Phillips (1980) appears to be the first paper to use invariant polynomials with multiple matrix arguments, and Phillips's, subsequent work (Phillips, 1984, 1985) also uses these polynomials in analyzing the exact properties of instrumental variable estimators, exogenous variable coefficient estimators, and limited information maximum likelihood (LIML) estimators. See also Hillier (1985), and Hillier, Kinal, and Srivastava (1984) for other examples.

Although many of their properties are well understood, no general formulas are known for either the zonal polynomials or the Davis–Chikuse invariant polynomials. This has limited their usefulness to analytical work. However, for the top-order polynomials of both types, explicit formulas are available. In the case of the top-order zonal polynomials, Ruben (1962) gives both an explicit formula and a recursive relation that permits their direct computation (see eqn. (18) in Section 2.2). However, this is fairly inefficient: the computation time of Ruben's recursive algorithm for a kth degree top-order zonal polynomial is $O(k^2)$, which can be very time consuming when k is large. One of our main results in this paper is a new recursive algorithm for the top-order zonal polynomials that has a computation time of order only $O(k)$, a substantial improvement on that hitherto available.

For the case of the top-order invariant polynomials with several arguments, Chikuse (1987) presents both explicit and recursive expressions for the polynomials. Unlike the recursive relation for top-order zonal polynomials, the expressions in Chikuse (1987) are difficult to implement and also very time consuming. For the two matrix arguments case, Smith (1993) simplifies the explicit expression of top-order invariant polynomials when the order in one of the terms is just 1 or 2. For the general case, we are unaware of any practical method for the numerical evaluation of the top-order invariant polynomials.

A second main contribution of this paper is to present two effective ways of dealing with this problem. The first method is based on a generalization of the algorithm provided for top-order zonal polynomials. This allows us to express a top-order invariant polynomial as a linear function of at most $(n+r)!/(n!r!)-1$ other top-order invariant polynomials (of lower degree), where n is the dimension of the matrices and r matrices are involved. When either n or r is small, this recursive method is extremely efficient. For the case when both n and r are large, we introduce a second method to evaluate the top-order invariant polynomial. This method relies on a new identity between top-order invariant polynomials and top-order zonal polynomials that is based on the results in Kan (2008) and has

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its roots in a lemma by Magnus (1978). Using this identity and our fast method of computing top-order zonal polynomials, we can evaluate top-order invariant polynomials with many matrix arguments with ease even when n is reasonably large.

To illustrate the value of our fast algorithms for evaluating top-order invariant polynomials, we consider the problem of computing the moments of a ratio of quadratic forms of normal random variables. Because many estimators and test statistics have this structure, the problem of finding their moments has attracted the attention of many researchers. Most of this literature makes use of an expression for the moments as one-dimensional integrals that can be evaluated by numerical integration (for details, see, e.g., Magnus, 1986, and references therein). The problem with this approach is that, for high-order moments particularly, the required numerical integration is very time consuming and often numerically unstable. More importantly, except for some special cases, there is no analysis of the approximation error from this numerical integration, so we cannot be sure how accurate the answer produced is. Using our fast algorithms for evaluating top-order invariant polynomials of two matrix arguments, we develop a new method for evaluating the moments of ratio of quadratic forms in normal random variables. Besides being efficient, our method also allows us to control the approximation error, so we can evaluate the moments up to any desired level of accuracy.

The rest of the paper is organized as follows. Section 2 provides the main recursive algorithm for computing top-order zonal polynomials. Recursions of the type we present are typically derived from relations between generating functions, and this is also the methodology that we use in the paper. For the zonal polynomials themselves, Ruben's recursion expresses the top-order zonal polynomials in terms of the power-sum symmetric functions, whereas our new recursion uses the elementary symmetric functions. The generating functions and the relations that produce the recursions are defined in Section 2.1. Section 2 also presents some additional formulas for various special cases of interest and discusses further applications. Section 3 generalizes the recursive algorithms that hold for top-order zonal polynomials to the case of top-order invariant polynomials. The implementation of these algorithms requires evaluation of multiple-argument analogs of the elementary and power-sum symmetric functions. In Section 3 we therefore also provide, apparently for the first time, recursive procedures for evaluating these multiple-argument symmetric functions. In addition, we present an identity between top-order invariant polynomials and top-order zonal polynomials that allows us to efficiently compute top-order invariant polynomials with multiple matrix arguments. Section 4 describes a new method for computing the moments of a ratio of quadratic forms in normal random variables. Section 5 concludes the paper. The Appendix contains proofs of all propositions and lemmas. Throughout the paper we use the standard notation for the forward factorial (or Pochhammer symbol): $(a)_s = a(a+1)\cdots(a+s-1)$.

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2. TOP-ORDER ZONAL POLYNOMIALS

2.1. Generating Functions

From von Neumann (1941) and James (1964), the function

$$D(t) = |I_n - tA|^{-1/2} \tag{3}$$

has an expansion in terms of top-order zonal polynomials $C_k(A)$ given by

$$D(t) = \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\right)_k C_k(A)}{k!} t^k \tag{4}$$

and so may be regarded as a generating function for the top-order zonal polynomials.[1]

To simplify the results to follow we define a normalized version of $C_k(A)$:

$$d_k(A) = \frac{1}{k!}\left(\frac{1}{2}\right)_k C_k(A), \tag{5}$$

so that, suppressing from now on when there is no source of confusion, the argument matrix A,

$$D(t) = |I_n - tA|^{-1/2} = \sum_{k=0}^{\infty} d_k t^k \tag{6}$$

is an ordinary generating function for the d_k.

Remark 1. Note that, comparing (1) and (4), the moments of $q = z'Az$, $\mu_k(A) = \mathrm{E}[q^k]$, can be expressed very simply in terms of either the $C_k(A)$ or the d_k:

$$\mu_k(A) = 2^k \left(\frac{1}{2}\right)_k C_k(A) = k! 2^k d_k. \tag{7}$$

There are at least two explicit expressions available for the d_k. Suppose A has eigenvalues λ_1 to λ_n. The first explicit expression of d_k was given by Ruben (1962)[2]:

$$d_k = \sum_{\substack{k_1,\ldots,k_n \geq 0 \\ k_1+\cdots+k_n=k}} \prod_{i=1}^{n} \frac{\left(\frac{1}{2}\right)_{k_i} \lambda_i^{k_i}}{k_i!}. \tag{8}$$

The second explicit expression of d_k is also given by Ruben (1962):

$$d_k = \sum_{\boldsymbol{\eta}} \prod_{j=1}^{k} \frac{(\mathrm{tr} A^j)^{\eta_j}}{\eta_j! (2j)^{\eta_j}}, \tag{9}$$

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where the summation is over all k-vectors $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_k)$ whose elements are nonnegative integers satisfying $\sum_{j=1}^{k} \eta_j j = k$. However, these two explicit expressions are both inefficient for computation purposes, especially when k is large.

It is clear from the generating function that d_k is a function only of the characteristic roots $\lambda_1, \ldots, \lambda_n$ of A and is a symmetric function of those roots, invariant under permutations of them. Various other such symmetric functions are used in the results to follow. These are, together with their generating functions (see MacDonald, 1979):

1. The *elementary symmetric functions* e_k, with generating function

$$E(t) = |I_n - tA| = \sum_{k=0}^{n} e_k t^k, \tag{10}$$

2. the *power-sum symmetric functions* p_k, with generating function

$$P(t) = \operatorname{tr}(tA(I_n - tA)^{-1}) = \sum_{k=1}^{\infty} p_k t^k, \tag{11}$$

and

3. the *complete homogeneous symmetric functions* h_k, with generating function

$$H(t) = |I_n - tA|^{-1} = \sum_{k=0}^{\infty} h_k t^k. \tag{12}$$

Note that for notational convenience, we define e_k here as the elementary symmetric functions of the eigenvalues of $-A$, rather than the eigenvalues of A. By definition, $d_0 = e_0 = h_0 = 1$. Also, because $(I_n - tA)^{-1} = \sum_{k=0}^{\infty} A^k t^k$ for t sufficiently small, $p_k = \operatorname{tr}(A^k)$.

2.2. Recursions: First Main Result

There are some well-known connections among these symmetric functions and d_k, and these relations can be obtained by differentiating $E(t)$ and $D(t)$. Using Bellman's trick of writing (for any symmetric positive definite $n \times n$ matrix Σ),

$$|\Sigma|^{-1/2} = \int_{\mathbb{R}^n} (2\pi)^{-n/2} \exp\left(-\frac{1}{2} x' \Sigma x\right) (\mathrm{d}x), \tag{13}$$

setting $\Sigma = I_n - tA$, differentiating and using the fact that $\mathrm{E}[x'Ax] = \operatorname{tr}(A(I_n - tA)^{-1})$ when $x \sim N(0_n, (I_n - tA)^{-1})$, we get

$$tE'(t) = -E(t)P(t). \tag{14}$$

Using this result, we can easily obtain

$$tD'(t) = \frac{1}{2} D(t)P(t). \tag{15}$$

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Equating coefficients of like powers of t on both sides, (14) yields the well-known Newton–Girard identities relating the e_k and p_k.[3]

$$\sum_{i=1}^{k} p_i e_{k-i} = -k e_k, \quad \text{if } k \le n, \tag{16}$$

$$\sum_{i=k-n}^{k} p_i e_{k-i} = 0, \quad \text{if } k > n. \tag{17}$$

Similarly, comparing the coefficients of like powers of t on both sides of (15), we obtain the following identity relating the d_k and p_k:

$$d_k = \frac{1}{2k} \sum_{i=1}^{k} p_i d_{k-i}. \tag{18}$$

Together with the boundary condition of $d_0 = 1$, this yields a recursive algorithm for computing d_k that is due to Ruben (1962) (see also James, 1964; Smith, 1993). Currently, this is probably the most efficient algorithm for computing the d_k. Although this recursive algorithm is more efficient than the explicit formulas (8) and (9), it still requires a computation time of $O(k^2)$, so it is not ideal to use when k is large, or when the d_k are required for many values of k, as is the case when the result under study is expressed in terms of series involving the d_k.

To overcome this problem, we shall now show that there is an analogous but shorter recursive relation expressing the d_k in terms of the elementary symmetric functions e_k. Let

$$F(t) = E(t)D(t) = \sum_{k=0}^{\infty} f_k t^k, \tag{19}$$

where

$$f_k = \sum_{i=0}^{\min[k,n]} e_i d_{k-i}. \tag{20}$$

Then

$$F'(t) = E'(t)D(t) + E(t)D'(t) = \left[E'(t) + \frac{1}{2t}E(t)P(t)\right] D(t) = \frac{1}{2}E'(t)D(t), \tag{21}$$

on using (14) and (15). Hence,

$$\sum_{k=1}^{\infty} k f_k t^{k-1} = \frac{1}{2}\left(\sum_{i=1}^{n} i e_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right). \tag{22}$$

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Equating the coefficients of t^{k-1} on both sides gives

$$kf_k = \frac{1}{2}\sum_{i=1}^{\min[k,n]} i e_i d_{k-i}. \tag{23}$$

Then, using (20) and rearranging terms, we obtain the following new recursive relation for the d_k:

$$d_k = \sum_{i=1}^{\min[k,n]} \left(\frac{i}{2k} - 1\right) e_i d_{k-i}. \tag{24}$$

The key advantage of (24) over Ruben's recursion (18) is that at most n terms are needed to continue the recursion, because $e_k = 0$ for $k > n$, a property that does not hold for the power sums p_k. In Theorem 1 in Section 2.3 we will see that even this result can be improved upon when some roots are repeated.

2.3. Repeated Roots

Equation (24) holds whatever the λ_i's. However, for certain problems the λ_i's are not distinct but occur with multiplicity greater than one. For example, we are often interested in a linear combination of s independent $\chi^2_{n_i}$ random variables w_i, say,

$$w = \lambda_1 w_1 + \ldots + \lambda_s w_s \tag{25}$$

(see Robbins, 1948; Pachares, 1955; Ruben, 1962). We may obviously express w as a quadratic form in $n = \sum_{i=1}^{s} n_i$ standard normal random variables, with the matrix of the quadratic form having roots λ_i, each with multiplicity n_i. The following theorem shows that in this case a recursion analogous to (24), but of length s rather than n, can be obtained.[4]

THEOREM 1. *Suppose that A has s distinct eigenvalues $\lambda_1, \ldots, \lambda_s$, with multiplicities $n_1, \ldots, n_s$ ($n_1 + n_2 + \cdots + n_s = n$), respectively. Let $\tilde{e}_i$, $i = 0, \ldots, s$, be the coefficients of t^i in the following polynomial:*

$$\prod_{i=1}^{s}(1 - t\lambda_i) = \sum_{i=0}^{s} \tilde{e}_i t^i. \tag{26}$$

Then, the d_k satisfy the recursive relation

$$d_k = \sum_{i=1}^{\min[k,s]} \left(\frac{c_i}{k} - \tilde{e}_i\right) d_{k-i}, \qquad d_0 = 1, \tag{27}$$

where

$$c_i = i\tilde{e}_i + \frac{\sum_{j=0}^{i-1} \tilde{e}_j p_{i-j}}{2}, \qquad i = 1, \ldots, s. \tag{28}$$

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When $n_i = m$ for $i = 1, \ldots, s$, the recursive relation can be simplified to

$$d_k = \sum_{i=1}^{\min[k,s]} \left[\frac{(2-m)i}{2k} - 1 \right] \tilde{e}_i d_{k-i}, \quad d_0 = 1. \tag{29}$$

For the case that all the eigenvalues of A are distinct (i.e., $s = n$ and $m = 1$), we have $\tilde{e}_i = e_i$ and

$$d_k = \sum_{i=1}^{\min[k,n]} \left(\frac{i}{2k} - 1 \right) e_i d_{k-i}, \quad d_0 = 1. \tag{30}$$

Theorem 1 provides a recursive relation for the d_k that has length at most s, the number of distinct eigenvalues of A, and it is independent of k, so the computation time for d_k is only $O(k)$, as claimed.[5]

2.4. Roots with Even Multiplicities

When the distinct eigenvalues of A all have even multiplicities, the problem of evaluating zonal polynomials d_k can be reduced to the problem of evaluating complete homogeneous symmetric functions. To see this, assume that each λ_i occurs with even multiplicity $n_i = 2m_i$ for $i = 1, \ldots, s$, so $n = n_1 + \cdots + n_s = 2(m_1 + \cdots + m_s) = 2m$, say. The generating function for the d_k can be written as

$$D(t) = |I_n - tA|^{-1/2} = \frac{1}{\prod_{i=1}^{s}(1 - t\lambda_i)^{m_i}} = |I_m - t\tilde{A}|^{-1} = \sum_{k=0}^{\infty} h_k(\tilde{A}) t^k, \tag{31}$$

where $\tilde{A}$ has s distinct eigenvalues $\lambda_1, \ldots, \lambda_s$, with multiplicities $m_1, \ldots, m_s$, respectively, and $h_k(\tilde{A})$ is the kth-order complete homogeneous symmetric function of the eigenvalues of $\tilde{A}$. Equating coefficients of powers of t, it is clear that

$$d_k(A) = h_k(\tilde{A}). \tag{32}$$

Thus, computing the $d_k(A)$ is equivalent to computing the $h_k(\tilde{A})$.

Various recursive relations for, and explicit formulas for, the homogeneous symmetric functions are well known—see MacDonald (1979), for instance. However, we shall now present a new, nonrecursive, relation that provides an extremely efficient method of computing the $h_k(\tilde{A})$ and hence the $d_k(A)$. This is based on a partial fractions expansion of the generating function for the $h_k(\tilde{A})$, $\tilde{H}(t)$. This is much faster than the known recursive algorithms hitherto available. Before giving the general result it is helpful to consider the case where $s = m$, that is, the roots of $\tilde{A}$ are distinct. In this case, if we write

$$\tilde{H}(t) = \frac{1}{\prod_{i=1}^{m}(1 - t\lambda_i)} = \sum_{i=1}^{m} \frac{a_i}{(1 - t\lambda_i)}, \tag{33}$$

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then, on expanding each geometric series and equating coefficients of powers of t, we obtain

$$h_k(\tilde{A}) = \sum_{i=1}^{m} a_i \lambda_i^k. \tag{34}$$

Multiplying both sides of (33) by $(1 - t\lambda_i)$ and then setting $t = \lambda_i^{-1}$, it is easy to see that

$$a_i = \prod_{\substack{j=1 \\ j \neq i}}^{m} \left(\frac{\lambda_i}{\lambda_i - \lambda_j} \right), \qquad i = 1, \ldots, m, \tag{35}$$

which are straightforward to compute. Thus, all of the $h_k(\tilde{A})$ may be computed (nonrecursively) from (34).

In the general case, where some of the m_i may be greater than one, the analog of (33) will be of the form

$$\tilde{H}(t) = \sum_{i=1}^{s} \sum_{j=1}^{m_i} \frac{a_{i,j}}{(1 - t\lambda_i)^j}. \tag{36}$$

In this case the coefficients $a_{i,j}$ are more complicated. The general result is given in the following theorem.

THEOREM 2. *When some of the roots of $\tilde{A}$ occur with multiplicity $m_i > 1$, then*

$$h_k(\tilde{A}) = \frac{1}{k!} \sum_{i=1}^{s} \left[\sum_{j=1}^{m_i} (j)_k a_{i,j} \right] \lambda_i^k. \tag{37}$$

In this expression the coefficients $a_{i,j}$ are given by

$$a_{i,m_i - r} = \prod_{\substack{j=1 \\ j \neq i}}^{s} \left(\frac{\lambda_i}{\lambda_i - \lambda_j} \right)^{m_i} h_r(B_i), \quad r = 0, \ldots, m_i - 1, \tag{38}$$

where $h_r(B_i)$ denotes the rth-order complete homogeneous symmetric function of B_i and B_i is a matrix that has distinct eigenvalues $\lambda_j/(\lambda_j - \lambda_i)$ with multiplicity m_j for $j = 1, \ldots, s$ and $j \neq i$.

It follows that, when n_i's are all even, once the $a_{i,j}$'s are obtained, the $d_k(A)$ can be computed for any k without first computing d_0 to d_{k-1}. As a result, in the special case of roots with even multiplicities, (37) is more efficient for computing the d_k than the recursive algorithm given in Theorem 1.[6]

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2.5. Hypergeometric Functions

The hypergeometric functions of matrix argument are, in general, defined in terms of the zonal polynomials as follows (see Muirhead, 1982, Ch. 7):

$$ {}_pF_q(\alpha_1,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;A) = \sum_{k=0}^{\infty}\sum_{\boldsymbol{\kappa}} \frac{(\alpha_1)_{\boldsymbol{\kappa}}\ldots(\alpha_p)_{\boldsymbol{\kappa}}}{(\beta_1)_{\boldsymbol{\kappa}}\ldots(\beta_q)_{\boldsymbol{\kappa}}}\frac{C_{\boldsymbol{\kappa}}(A)}{k!}, \tag{39} $$

where A is an $n\times n$ symmetric matrix, $\sum_{\boldsymbol{\kappa}}$ denotes summation over all partitions $\boldsymbol{\kappa}=(k_1,\ldots,k_n)$, $k_1\geq\cdots\geq k_n\geq 0$ of k, $C_{\boldsymbol{\kappa}}(A)$ is the zonal polynomial of A corresponding to $\boldsymbol{\kappa}$, and $(\alpha)_{\boldsymbol{\kappa}}=\prod_{i=1}^{n}(\alpha-(i-1)/(2))_{k_i}$. The moment generating function for $z'Az$ in (1) is an example of such a function, corresponding to the case $p=1$, $q=0$, $\alpha_1=1/2$, with argument matrix $2A$. In addition, both the cumulative density function (c.d.f.) and the probability density function (c.d.f.) of $z'Az$ can also be written using such function with $p=q=1$, $\alpha_1=1/2$, and $\beta_1=n/2+1$ or $n/2$ (see (42) and (44) in Section 2.6). Other examples occur in the literature mentioned in the Introduction.

Now, when one of the α_i's in the numerator is $1/2$, the expression for ${}_pF_q$ is significantly simplified because only the top-order zonal polynomial is involved for each k. Without loss of generality, we assume that $\alpha_1=1/2$, and we have

$$ \begin{aligned} {}_pF_q\left(\frac{1}{2},\alpha_2,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;A\right) &= \sum_{k=0}^{\infty}\frac{(\frac{1}{2})_k(\alpha_2)_k\ldots(\alpha_p)_k}{(\beta_1)_k\ldots(\beta_q)_k}\frac{C_k(A)}{k!} \\ &= \sum_{k=0}^{\infty}\frac{(\alpha_2)_k\ldots(\alpha_p)_k}{(\beta_1)_k\ldots(\beta_q)_k}d_k. \end{aligned} \tag{40} $$

Therefore, our fast recursive algorithm for computing d_k also allows us to efficiently compute hypergeometric functions in this special, but important, case—or at least finite truncations of their series expansions.[7]

In general, there is no known relation between hypergeometric functions of matrix argument and hypergeometric functions of scalar argument. However, when all the eigenvalues of A have even multiplicities, the following lemma shows that the hypergeometric function in (40) can be written as a linear combination of hypergeometric functions with scalar arguments.

LEMMA 1. *Suppose that n_i's are all even and let $m_i=n_i/2$, $i=1,\ldots,s$. Then, we have*

$$ {}_pF_q\left(\frac{1}{2},\alpha_2,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;A\right) = \sum_{i=1}^{s}\sum_{j=1}^{m_i} a_{i,j}\,{}_pF_q(j,\alpha_2,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;\lambda_i), $$

where $a_{i,j}$'s are defined in (38).

As the hypergeometric functions with scalar argument are widely available in most modern mathematical software, Lemma 1 provides us with a convenient

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way to compute hypergeometric functions of matrix argument when one of the parameters in the numerator is $1/2$ and the matrix has eigenvalues with even multiplicities.

2.6. Some Applications

We have already seen (in (7)) that, if $z \sim N(0_n, I_n)$, $\mathrm{E}[(z'Az)^k] = 2^k k! d_k$. A slightly more general result is implied by this: it is well known that, if $z \sim N(0_n, I_n)$, then $v = (z'z)^{-1/2}z$ and $q = z'z$ are independent, v is uniformly distributed on the unit n-sphere, and $q \sim \chi^2_n$. It follows from these facts and (7) that

$$\mathrm{E}\left[\left(\frac{z'Az}{z'z}\right)^k\right] = \int_{v'v=1} (v'Av)^k (\mathrm{d}v) = \frac{k!}{\left(\frac{n}{2}\right)_k} d_k, \tag{41}$$

where $(\mathrm{d}v)$ denotes normalized Haar measure on the surface of the unit n-sphere (see Muirhead, 1982, Ch. 2). This is an example of more general results discussed, for instance, in Muirhead 1982, Ch. 7 for integrals over the orthogonal group. The result holds for any spherically symmetric distribution for z, not just the $N(0_n, I_n)$ (for more on this statistic, see Hillier, 2001). Our recursive formula for d_k is useful for all such calculations of moments, and generalizations of these results will be given in Section 4.

Solutions to a number of other distribution problems in statistics can be expressed as linear functions of d_k. We have already seen from Remark 1 that the computation of the moments of a linear combination of independent χ^2 random variables, w in (25), is the same as computing d_k. In addition, the c.d.f. and p.d.f. of w are both closely related to d_k. For example, when $\lambda_i > 0$ for $i = 1, \ldots, s$, Robbins (1948) and Pachares (1955) show that for $c \geq 0$,

$$P[w < c] = \frac{c^{n/2}}{2^{n/2}\Gamma\left(\frac{n}{2}+1\right)|A|^{1/2}} {}_1F_1\left(\frac{1}{2}; \frac{n}{2}+1; -\frac{c}{2}A^{-1}\right), \tag{42}$$

where $A = \mathrm{Diag}(\lambda_1 1'_{n_1}, \ldots, \lambda_s 1'_{n_s})$ and $n = n_1 + \cdots + n_s$. Ruben (1962) provides a different expression for this probability:

$$P[w < c] = \left[\prod_{i=1}^{s}\left(\frac{\beta}{\lambda_i}\right)^{n_i/2}\right] \sum_{k=0}^{\infty} d_k(I_n - \beta A^{-1}) P\left[\chi^2_{n+2k} < \frac{c}{\beta}\right], \tag{43}$$

where β is an arbitrary positive constant.[8] By differentiating (42), we can easily obtain the density of w as

$$pdf(w) = \frac{w^{(n/2)-1}}{2^{n/2}\Gamma(\frac{n}{2})|A|^{1/2}} {}_1F_1\left(\frac{1}{2}; \frac{n}{2}; -\frac{w}{2}A^{-1}\right) \tag{44}$$

(see James, 1964).

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Our earlier results thus provide efficient procedures for computing the various functions involved in all these expressions. When the n_i's are all even, we can use Lemma 1 to write (42) and (44) as a linear combination of $n/2$ confluent hypergeometric functions. For the general case, we need to approximate the c.d.f. and p.d.f. of w by summing a finite number of terms. In many cases, a large number of terms is required to achieve a desirable accuracy, so our new recursive algorithm for computing d_k can help to substantially reduce the computation time.[9] As an illustration, we consider an example with $w = w_1 + 2w_2 + 3w_3$, where $w_1 \sim \chi^2_{20}$, $w_2 \sim \chi^2_{40}$, and $w_3 \sim \chi^2_{60}$. Using Ruben's algorithm (with $\beta = 1$ and a precision of 10^{-10}), it takes Mathematica 0.313 second to compute $P[w < 400]$. However, using our new recursive algorithm, it takes only 0.109 second to get the same answer.

3. TOP-ORDER INVARIANT POLYNOMIALS

3.1. Definitions

Let A_1 to A_r be $n \times n$ symmetric matrices. We denote by $C_{k_1,\ldots,k_r}(A_1,\ldots,A_r)$ the top-order invariant polynomials in which each of the partitions of k_i, $i = 1,\ldots,r$, has only one part.[10] The generating function for the top-order invariant polynomials is the following generalization of the generating function for the d_k (see Chikuse, 1987, eqn. (2.1)):

$$D(t_1,\ldots,t_r) = |I_n - t_1A_1 - t_2A_2 - \cdots - t_rA_r|^{-1/2} = \sum_{k_1=0}^{\infty}\cdots\sum_{k_r=0}^{\infty}\frac{\left(\frac{1}{2}\right)_{k_1+\cdots+k_r} C_{k_1,\ldots,k_r}(A_1,\ldots,A_r)}{k_1!\ldots k_r!} t_1^{k_1}\ldots t_r^{k_r}. \quad (45)$$

As in the case of top-order zonal polynomials, it is more convenient to work with a normalized version of the top-order invariant polynomials:

$$d_{k_1,\ldots,k_r}(A_1,\ldots,A_r) = \frac{\left(\frac{1}{2}\right)_{k_1+\cdots+k_r} C_{k_1,\ldots,k_r}(A_1,\ldots,A_r)}{k_1!\ldots k_r!}. \quad (46)$$

For notational compactness, we suppress the arguments in $d_{k_1,\ldots,k_r}(A_1,\ldots,A_r)$ when there is no likelihood of confusion. In addition, we shall adopt the following notation: $A(\boldsymbol{t}) = t_1A_1 + \cdots + t_rA_r$, $\boldsymbol{\kappa} = (k_1,\ldots,k_r)$ with $k_i \geq 0$, $|\boldsymbol{\kappa}|$ will denote the sum of the parts of $\boldsymbol{\kappa}$, $|\boldsymbol{\kappa}| = \sum_{i=1}^r k_i$, $\boldsymbol{t}^{\boldsymbol{\kappa}} = \prod_{i=1}^r t_i^{k_i}$, and $\boldsymbol{\kappa}! = \prod_{i=1}^r k_i!$. With this notation, the generating function for the $d_{\boldsymbol{\kappa}}$ can be written as

$$D(\boldsymbol{t}) = |I_n - A(\boldsymbol{t})|^{-1/2} = \sum_{k=0}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} d_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}}. \quad (47)$$

Remark 2. From the joint moment generating function of the quadratic forms q_i in equation (2) we see that, for $z \sim N(0_n, I_n)$ and $k = |\boldsymbol{\kappa}|$,

$$\mu_{\boldsymbol{\kappa}}(A_1,\ldots,A_r) = \mathrm{E}[(z'A_1z)^{k_1}(z'A_2z)^{k_2}\ldots(z'A_rz)^{k_r}] = 2^k\boldsymbol{\kappa}!d_{\boldsymbol{\kappa}}, \quad (48)$$

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a generalization of (7) (see Chikuse, 1987, eqn. (2.17)). That is, computing top-order invariant polynomials is equivalent to computing the product moments of quadratic forms in standard normal random variables.

We shall also make use of generalizations of the generating functions $E(t)$ and $P(t)$ in (10) and (11). These are

$$E(\boldsymbol{t}) = |I_n - A(\boldsymbol{t})| = \sum_{k=0}^{n} \sum_{|\boldsymbol{\kappa}|=k} e_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}} \tag{49}$$

and

$$P(\boldsymbol{t}) = \operatorname{tr}(A(\boldsymbol{t})(I_n - A(\boldsymbol{t}))^{-1}) = \sum_{k=1}^{\infty} \operatorname{tr}(A(\boldsymbol{t})^k) = \sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} p_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}. \tag{50}$$

The $e_{\boldsymbol{\kappa}}$ are the multivariate versions of the elementary symmetric functions for the single matrix case, and the $p_{\boldsymbol{\kappa}}$ are multivariate versions of the power-sum symmetric functions for the single matrix case. Notice that, from the generating functions defining these polynomials, both the $e_{\boldsymbol{\kappa}}$ and the $p_{\boldsymbol{\kappa}}$ are invariant under precisely the same group of transformations as are the $d_{\boldsymbol{\kappa}}$, namely, $A_i \to H' A_i H$ for $i = 1, \ldots, r$, with H an $n \times n$ orthogonal matrix.

Chikuse (1987) provides an explicit expression for $d_{\boldsymbol{\kappa}}$ in terms of the $p_{\boldsymbol{\kappa}}$ as

$$d_{\boldsymbol{\kappa}} = \sum_{\boldsymbol{\eta}} \prod_{\substack{|\boldsymbol{\nu}|\geq 1, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} \frac{p_{\boldsymbol{\nu}}^{\eta_{\boldsymbol{\nu}}}}{\eta_{\boldsymbol{\nu}}! (2|\boldsymbol{\nu}|)^{\eta_{\boldsymbol{\nu}}}}, \tag{51}$$

where $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_r)$ is a vector of nonnegative integers and $\boldsymbol{\nu} \leq \boldsymbol{\kappa}$ means that $\nu_i \leq \kappa_i$ for $i = 1, \ldots, r$. In the preceding expression, the summation denotes summing over the set of nonnegative integers $\eta_{\boldsymbol{\nu}}$ that satisfies r linear constraints $\sum_{\boldsymbol{\nu} \leq \boldsymbol{\kappa}, |\boldsymbol{\nu}| \geq 1} \eta_{\boldsymbol{\nu}} \boldsymbol{\nu} = \boldsymbol{\kappa}$.

There are two hurdles with using this explicit expression to compute $d_{\boldsymbol{\kappa}}$. The first is to enumerate the set of integers $\eta_{\boldsymbol{\nu}}$ that satisfy the r constraints. The second is to compute $p_{\boldsymbol{\nu}}$. Both problems are nontrivial and computationally intensive. For the special case when the top-order invariant polynomial involves only two matrices (i.e., $r = 2$) and $k_1 = 1$ or 2, Smith (1993) provides the explicit expressions for d_{1,k_2} and d_{2,k_2}. When there are more than two matrices or when $k_1 > 2$ and $k_2 > 2$, the complexity of this explicit expression becomes overwhelming.

3.2. Recursive Algorithms

Similar to the top-order zonal polynomials, there are also recursive relations for the top-order invariant polynomials. To obtain these recursive relations, we need to understand the relationships between $d_{\boldsymbol{\kappa}}$, $p_{\boldsymbol{\kappa}}$, and $e_{\boldsymbol{\kappa}}$.

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For any analytic function $f(\boldsymbol{t})$,

$$f(\boldsymbol{t}) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} f_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{52}$$

we define

$$\dot{f}(\boldsymbol{t}) = \sum_{i=1}^{r} t_i \frac{\partial f(\boldsymbol{t})}{\partial t_i} = \sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} |\boldsymbol{\kappa}| f_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}. \tag{53}$$

To see the connections between $e_{\boldsymbol{\kappa}}$, $p_{\boldsymbol{\kappa}}$, and $d_{\boldsymbol{\kappa}}$, we need to compute $\dot{E}(\boldsymbol{t})$ and $\dot{D}(\boldsymbol{t})$. Just as in the single matrix case, it can be readily shown that

$$\dot{E}(\boldsymbol{t}) = -E(\boldsymbol{t})P(\boldsymbol{t}), \tag{54}$$

$$\dot{D}(\boldsymbol{t}) = \frac{1}{2} D(\boldsymbol{t})P(\boldsymbol{t}). \tag{55}$$

Comparing the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides of (54), we obtain the following relations between the $e_{\boldsymbol{\kappa}}$ and $p_{\boldsymbol{\kappa}}$:

$$\sum_{i=1}^{k} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \le \boldsymbol{\kappa}}} p_{\boldsymbol{\nu}} e_{\boldsymbol{\kappa}-\boldsymbol{\nu}} = -k e_{\boldsymbol{\kappa}} \quad \text{if } k \le n, \tag{56}$$

$$\sum_{i=k-n}^{k} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \le \boldsymbol{\kappa}}} p_{\boldsymbol{\nu}} e_{\boldsymbol{\kappa}-\boldsymbol{\nu}} = 0 \quad \text{if } k > n, \tag{57}$$

where $k = |\boldsymbol{\kappa}|$. These formulas provide a multivariate generalization of the Newton–Girard formulas for the single matrix case. Note that they permit the recursive computation of the $e_{\boldsymbol{\kappa}}$, given the $p_{\boldsymbol{\kappa}}$, or vice versa. We discuss the computation of these polynomials in Section 3.3.

Similarly, comparing the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides of (55) we obtain the following result relating the $d_{\boldsymbol{\kappa}}$ and $p_{\boldsymbol{\kappa}}$—a generalization of Ruben's recursion for the top-order zonal polynomials given in equation (18).

THEOREM 3. *When* $k = |\boldsymbol{\kappa}|$,

$$d_{\boldsymbol{\kappa}} = \frac{1}{2k} \sum_{i=1}^{k} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \le \boldsymbol{\kappa}}} p_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}. \tag{58}$$

Together with the boundary condition of $d_{\mathbf{0}} = 1$, this result yields a recursive algorithm for computing the $d_{\boldsymbol{\kappa}}$, given the $p_{\boldsymbol{\kappa}}$. Chikuse (1987) provides a recursive result of this type for the $d_{\boldsymbol{\kappa}}$, but (58) represents a much improved version of her results. In comparison with the explicit expression, the recursive expression is

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computationally more efficient. However, a drawback of this recursive algorithm is that we need to compute $d_{\boldsymbol{\kappa}}$ by using all the $p_{\boldsymbol{\nu}}$ and $d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}$ with $\boldsymbol{\nu} \leq \boldsymbol{\kappa}$, which is very time consuming when k_i's are large.

To overcome this problem, we now derive a more efficient recursive algorithm for the $d_{\boldsymbol{\kappa}}$ analogous to the result given in Theorem 1 for the d_k. As in the single matrix case, we first define

$$F(\boldsymbol{t}) = E(\boldsymbol{t})D(\boldsymbol{t}) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} f_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{59}$$

where

$$f_{\boldsymbol{\kappa}} = \sum_{i=0}^{\min[|\boldsymbol{\kappa}|,n]} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} e_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}. \tag{60}$$

Then,

$$\dot{F}(\boldsymbol{t}) = \dot{E}(\boldsymbol{t})D(\boldsymbol{t}) + E(\boldsymbol{t})\dot{D}(\boldsymbol{t}) = \left[\dot{E}(\boldsymbol{t}) + \frac{1}{2}E(\boldsymbol{t})P(\boldsymbol{t})\right] D(\boldsymbol{t}) = \frac{1}{2}\dot{E}(\boldsymbol{t})D(\boldsymbol{t}) \tag{61}$$

on using (54) and (55). Hence

$$\sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} |\boldsymbol{\kappa}| f_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}} = \frac{1}{2} \left(\sum_{i=1}^{n} \sum_{|\boldsymbol{\nu}|=i} |\boldsymbol{\nu}| e_{\boldsymbol{\nu}} \boldsymbol{t}^{\boldsymbol{\nu}} \right) \left(\sum_{i=0}^{\infty} \sum_{|\boldsymbol{\nu}|=i} d_{\boldsymbol{\nu}} \boldsymbol{t}^{\boldsymbol{\nu}} \right). \tag{62}$$

Equating the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides gives us

$$|\boldsymbol{\kappa}| f_{\boldsymbol{\kappa}} = \frac{1}{2} \sum_{i=1}^{\min[|\boldsymbol{\kappa}|,n]} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} |\boldsymbol{\nu}| e_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}. \tag{63}$$

Finally, using (60) and rearranging terms gives us an efficient recursive algorithm for computing top-order invariant polynomials, as given in the following theorem.

THEOREM 4. *The top-order invariant polynomials $d_{\boldsymbol{\kappa}}$, with $|\boldsymbol{\kappa}| = k$, can be recursively obtained from the following relation:*

$$d_{\boldsymbol{\kappa}} = \sum_{i=1}^{\min[k,n]} \sum_{\substack{|\boldsymbol{\nu}|=i, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} \left(\frac{i}{2k} - 1 \right) e_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}} \tag{64}$$

and the boundary condition of $d_{\mathbf{0}} = 1$.

In contrast to the earlier recursive relation in terms of the $p_{\boldsymbol{\kappa}}$, our new recursive relation only involves the $e_{\boldsymbol{\kappa}}$, and these vanish for $|\boldsymbol{\kappa}| > n$. Regardless of the value

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of $\boldsymbol{\kappa}$, Theorem 4 suggests that $d_{\boldsymbol{\kappa}}$ can be expressed as a linear combination of at most $(n+r)!/(n!r!)-1$ other top-order invariant polynomials of lower degree. For large k_i's, this fast recursive algorithm significantly reduces the computation time and memory requirement when compared with the recursive algorithms in (58).

Remark 3. In view of (48), the formulas in (58) and (64) give recursive relations for the product moments of quadratic forms in standard normal variables. Ghazal (1996) also provides a recursive relation for these product moments, but his formula is less efficient than ours.

3.3. An Algorithm for Computing the $p_{\boldsymbol{\kappa}}$

To use the recursive algorithm (58) or (64) to compute $d_{\boldsymbol{\kappa}}$, we need to first obtain the coefficients $p_{\boldsymbol{\kappa}}$ and $e_{\boldsymbol{\kappa}}$. When n is very small, we can use a symbolic mathematics program to compute $p_{\boldsymbol{\kappa}}$ and $e_{\boldsymbol{\kappa}}$.[11] However, this is extremely time consuming even when n is only moderately large. Therefore, it is crucial that we have efficient numerical algorithms for computing the $p_{\boldsymbol{\kappa}}$ and $e_{\boldsymbol{\kappa}}$. Because $e_{\boldsymbol{\kappa}}$ can be easily obtained from the $p_{\boldsymbol{\kappa}}$ by using (56)–(57), we focus our attention on a numerical algorithm for computing the $p_{\boldsymbol{\kappa}}$.

Our objective is to compute the coefficients $p_{\boldsymbol{\kappa}}$ in the following expansion:

$$\operatorname{tr}(A(\boldsymbol{t})^k) = \sum_{|\boldsymbol{\kappa}|=k} p_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}. \tag{65}$$

3.3.1. A Naive Approach. One approach is simply to use a multinomial-like expansion for the term $\operatorname{tr}(A(\boldsymbol{t})^k)$ but taking account of the fact that the matrices involved do not, in general, commute. This yields an explicit expression for $p_{\boldsymbol{\kappa}}$ as a linear combination of the traces of various products of A_i's, but is numerically inefficient to use, as we shall now argue.

In expanding the left-hand side of (65), there are $M(\boldsymbol{\kappa}) \equiv k!/\boldsymbol{\kappa}!$ terms that contain $\boldsymbol{t}^{\boldsymbol{\kappa}}$. A naive way of computing $p_{\boldsymbol{\kappa}}$ is to simply enumerate all the $M(\boldsymbol{\kappa})$ permutations of the multiset with k_i occurrences of i, $i = 1, \ldots, r$, and then sum up the trace of the corresponding products of k matrices in each term. However, many of the $M(\boldsymbol{\kappa})$ terms have the same trace. This is because if A, B, and C are symmetric matrices, we have $\operatorname{tr}(ABC) = \operatorname{tr}(CAB) = \operatorname{tr}(BCA) = \operatorname{tr}(CBA) = \operatorname{tr}(BAC) = \operatorname{tr}(ACB)$, so the trace of a product of k symmetric matrices is invariant to rotation and reversion of the sequence of the k matrices. The number of unique traces is the same as the number of bracelets with length k and fixed contents of k_i beads in color i, $i = 1, \ldots, r$.[12] Using the Pólya enumeration theorem, it can be shown that the number of elements in this set is given by[13]

$$B(\boldsymbol{\kappa}) = \begin{cases} \frac{1}{2}N(\boldsymbol{\kappa}) + \frac{1}{2}M\left(\left\lfloor \frac{\boldsymbol{\kappa}}{2} \right\rfloor\right) & \text{if the number of odd } k_i \\ & \text{is less than or equal to 2,} \\ \frac{1}{2}N(\boldsymbol{\kappa}) & \text{otherwise,} \end{cases} \tag{66}$$

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where $\lfloor x \rfloor$ is the integral part of x and

$$N(\boldsymbol{\kappa}) = \frac{1}{k} \sum_{d|\gcd(\boldsymbol{\kappa})} \phi(d) M\left(\frac{\boldsymbol{\kappa}}{d}\right), \tag{67}$$

with $d|\gcd(\boldsymbol{\kappa})$ as the set of integer divisors of the greatest common divisor of k_1 to k_r, and $\phi(d)$ is the totient function, which is the number of positive integers (including 1) less than or equal to d that are relative prime to d. For example, if $\gcd(\boldsymbol{\kappa}) = 1$ and more than two k_i's are odd, then we have $B(\boldsymbol{\kappa}) = M(\boldsymbol{\kappa})/(2k)$, so we can reduce the number of traces to be computed by a factor of $2k$.

A fast algorithm for generating bracelets with fixed contents can be obtained by combining the algorithms of Sawada (2001, 2003). Then, for each bracelet that we generate, we just need to know how many different multiset permutations that the bracelet corresponds to, and we can then multiply the corresponding trace by this number. As it turns out, this number depends on the primitive (i.e., smallest) period of the bracelet and whether the reverse of the bracelet is the same as the original bracelet (after possible rotation). If the bracelet has a primitive period of h, then it corresponds to either h or $2h$ multiset permutations, depending on whether the reverse of the bracelet is the same as the original bracelet or not. This information is readily available in the algorithms of Sawada (2001, 2003). A Matlab program for implementing this algorithm to compute $p_{\boldsymbol{\kappa}}$ is available from the authors upon request.

The problem with this approach is that even with small r and moderately small k_i's, there are just too many unique traces to compute. For example, when $\boldsymbol{\kappa} = (10, 10, 10)$, we need to enumerate 9.2517×10^{10} different traces to obtain $p_{\boldsymbol{\kappa}}$, so this approach is clearly unsuitable for computation purposes.

3.3.2. An Efficient Recursive Algorithm. To derive an efficient method of computing the $p_{\boldsymbol{\kappa}}$, first note that we are only interested in the diagonal elements of $A(\boldsymbol{t})^k$, so we can write

$$\operatorname{tr}(A(\boldsymbol{t})^k) = \sum_{i=1}^{n} e_i' A(\boldsymbol{t})^k e_i, \tag{68}$$

where e_i is an n-vector with ith element equal to one and zeros elsewhere. Each term $e_i' A(\boldsymbol{t})^k e_i$ here admits an expansion of the form

$$e_i' A(\boldsymbol{t})^k e_i = \sum_{|\boldsymbol{\kappa}|=k} p_{\boldsymbol{\kappa},i} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{69}$$

so that the term we require is simply $p_{\boldsymbol{\kappa}} = \sum_{i=1}^{n} p_{\boldsymbol{\kappa},i}$.[14] Hence, we can concentrate on an expansion for a term of the form $e_i' A(\boldsymbol{t})^k e_i$. The expansion we seek contains

$$f_{k,r} = \binom{k+r-1}{k} \tag{70}$$

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distinct terms, the number of compositions of k with r nonnegative parts. Let $C(k,r)$ denote this set of compositions.

The recursion we present subsequently relies on the following observation. If we denote by $a_{k,i}$ the ith column of $A(\boldsymbol{t})^k$, we will have an expansion

$$a_{k,i} = \sum_{\boldsymbol{\kappa}\in C(k,r)} a_{\boldsymbol{\kappa},i}\boldsymbol{t}^{\kappa} \tag{71}$$

for some set of n-vectors $a_{\boldsymbol{\kappa},i}$, $\boldsymbol{\kappa} \in C(k,r)$. On multiplying by $A(\boldsymbol{t})$ again we therefore will have

$$a_{k+1,i} = \sum_{j=1}^{r} \sum_{\boldsymbol{\kappa}\in C(k,r)} A_j a_{\boldsymbol{\kappa},i}(t_j\boldsymbol{t}^{\kappa}), \tag{72}$$

and this must be of the form

$$a_{k+1,i} = \sum_{\boldsymbol{\nu}\in C(k+1,r)} a_{\boldsymbol{\nu},i}\boldsymbol{t}^{\boldsymbol{\nu}}, \tag{73}$$

for some set of n-vectors $a_{\boldsymbol{\nu},i}$, with $\boldsymbol{\nu} \in C(k+1,r)$. Thus, for $\boldsymbol{\nu} \in C(k+1,r)$, $a_{\boldsymbol{\nu},i}$ will be a sum of products $A_j a_{\boldsymbol{\kappa},i}$ containing the terms corresponding to pairs $(j,\boldsymbol{\kappa})$, with $j \in \{1,\ldots,r\}$ and $\boldsymbol{\kappa} \in C(k,r)$, that yield the same $\boldsymbol{\nu} \in C(k+1,r)$. This suggests a recursive algorithm for computing the columns $a_{\boldsymbol{\kappa},i}$: if X_k is the $n \times f_{k,r}$ matrix with columns $a_{\boldsymbol{\kappa},i}$ in some definite order, then provided we can identify (efficiently) which sets of pairs $(j,\boldsymbol{\kappa})$, with $\boldsymbol{\kappa} \in C(k,r)$, appear in which column of X_{k+1}, the recursion will be well defined.

The ability to make the required identification of columns efficiently depends on the result given in the following lemma. This provides, for any k and r, a mapping from the set $C(k,r)$ onto the integers $\{1,2,\ldots,f_{k,r}\} = N(k,r)$, say, and therefore provides a labeling of the columns of X_k for each k. The lemma has a number of other applications and appears to be new.

LEMMA 2. *For each* $\boldsymbol{\kappa} = (k_1,\ldots,k_r) \in C(k,r)$, *let*

$$s_i(\boldsymbol{\kappa}) = \sum_{j=1}^{i} k_j, \qquad i = 1,\ldots,r-1, \tag{74}$$

and define

$$n_k(\boldsymbol{\kappa}) = 1 + \sum_{i=1}^{r-1} \binom{i + s_i(\boldsymbol{\kappa}) - 1}{i}. \tag{75}$$

Then, $n_k(\boldsymbol{\kappa}) \in N(k,r)$ *for all* $\boldsymbol{\kappa} \in C(k,r)$, *and the map* $C(k,r) \to N(k,r)$ *defined by* $n_k(\boldsymbol{\kappa})$ *is* 1–1.

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Now, adopting the numbering described previously in $C(k+1,r)$, it is easy to see that the sequence $\boldsymbol{\kappa}(j) = (k_1, \ldots, k_j + 1, \ldots, k_r) \in C(k+1,r)$ produced by the preceding updating process has the number

$$n_{k+1}(\boldsymbol{\kappa}(j)) = n_k(\boldsymbol{\kappa}) + \sum_{i=j}^{r-1} \binom{i + s_i(\boldsymbol{\kappa}) - 1}{s_i(\boldsymbol{\kappa})} \in N(k+1,r). \tag{76}$$

There can be a number of pairs $(j, \boldsymbol{\nu})$ that map into the same number $n_{k+1}(\boldsymbol{\kappa}(j))$. Let this set be $S(\boldsymbol{\kappa}(j))$, an easily identified subset of $\{1, \ldots, r\} \times C(k,r)$. Then, we have the recursive relation for moving between the matrices X_k and X_{k+1}:

$$X_{k+1, n_{k+1}(\boldsymbol{\kappa}(j))} = \sum_{(j,\boldsymbol{\nu}) \in S(\boldsymbol{\kappa}(j))} A_j X_{k, n_k(\boldsymbol{\nu})}, \tag{77}$$

where $X_{i,j}$ stands for the jth column of X_i. The algorithm is very efficient: with $r = 3$ and $n = 60$, it takes less than 1 second in Matlab to compute the $p_{\boldsymbol{\kappa}}$'s for all $\boldsymbol{\kappa} \leq (10, 10, 10)$ using an Opteron 165 machine.

3.4. An Alternative Formula for the $d_{\boldsymbol{\kappa}}$

Motivated by a lemma in Magnus (1978), Kan (2008) presents an identity that allows us to express the product moments of a set of random variables as a linear combination of the moments of various weighted sums of the random variables. The identity is, for a sequence $\boldsymbol{\kappa} = (k_1, \ldots, k_r)$ with $|\boldsymbol{\kappa}| = k$,

$$\prod_{i=1}^{r} x_i^{k_i} = \frac{1}{k!} \sum_{\mathbf{0} \leq \boldsymbol{\nu} \leq \boldsymbol{\kappa}} (-1)^{|\boldsymbol{\nu}|} \binom{\boldsymbol{\kappa}}{\boldsymbol{\nu}} \left(\sum_{i=1}^{r} h_i(\boldsymbol{\kappa}, \boldsymbol{\nu}) x_i \right)^k, \tag{78}$$

where

$$\binom{\boldsymbol{\kappa}}{\boldsymbol{\nu}} = \prod_{i=1}^{r} \frac{k_i!}{\nu_i!(k_i - \nu_i)!} \tag{79}$$

and $h_i(\boldsymbol{\kappa}, \boldsymbol{\nu}) = (k_i/2) - \nu_i$. Applying this identity to the random variables $x_i = z' A_i z$, $i = 1, \ldots, r$, and taking expectations on both sides yields the following theorem.

THEOREM 5. *Let* $B(\boldsymbol{\kappa}, \boldsymbol{\nu}) = \sum_{i=1}^{r} (k_i/2) - \nu_i) A_i$ *and* $k = |\boldsymbol{\kappa}|$. *We have*

$$d_{\boldsymbol{\kappa}}(A_1, \ldots, A_r) = \sum_{\mathbf{0} \leq \boldsymbol{\nu} \leq \boldsymbol{\kappa}} (-1)^{|\boldsymbol{\nu}|} \frac{d_k(B(\boldsymbol{\kappa}, \boldsymbol{\nu}))}{\boldsymbol{\nu}!(\boldsymbol{\kappa} - \boldsymbol{\nu})!}. \tag{80}$$

As noted in Kan (2008), half of the terms on the right-hand side of (80) are repeated, so one can compute the top-order invariant polynomial by using $\left\lfloor \prod_{i=1}^{r} (k_i + 1)/2 \right\rfloor$ different top-order zonal polynomials, where $\lfloor x \rfloor$ stands for the

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integral part of x. The advantage of this algorithm is that the computation of top-order zonal polynomials is extremely efficient, especially with our new recursive algorithm in Theorem 1. When n and r are both large, this algorithm can significantly outperform the recursive algorithm in Theorem 4. However, when n is small, the algorithm in Theorem 4 gives us a short recursive relation, and it can be more efficient than (80), especially when r is small.

3.5. Some Applications

We have seen in (48) that product moments of quadratic forms in standard normal variables can be expressed in terms of the $d_{\boldsymbol{\kappa}}$, and we will see in the next section that these polynomials also arise in expressions for the moments of more complicated functions of quadratic forms. Other applications have already been mentioned in the Introduction.

As in the case $r = 1$, the top-order invariant polynomials also arise in the evaluation of certain integrals over the surface of the unit n-sphere. For example, it follows from (48) and the properties noted in obtaining (41) that

$$\mathrm{E}\left[\prod_{i=1}^{r}\left(\frac{z'A_iz}{z'z}\right)^{k_i}\right] = \int_{v'v=1}\left[\prod_{i=1}^{r}(v'A_iv)^{k_i}\right](\mathrm{d}v) = \frac{\boldsymbol{\kappa}!}{\left(\frac{n}{2}\right)_k}d_{\boldsymbol{\kappa}}, \tag{81}$$

where, as defined in Section 3.1, $\boldsymbol{\kappa} = (k_1, \ldots, k_r)$, $k = |\boldsymbol{\kappa}|$, and $\boldsymbol{\kappa}! = \prod_{i=1}^{r} k_i!$. This generalizes (41) and again holds under any spherically symmetric density for z.

4. RATIOS OF QUADRATIC FORMS IN NORMAL RANDOM VARIABLES

4.1. The Problem

With Theorems 4 and 5, we now have practical ways of computing top-order invariant polynomials. These new algorithms allow us to efficiently compute the p.d.f., the c.d.f., and the moments of ratios of quadratic forms in normal random variables. In this section, we demonstrate the value of our new algorithms by presenting an efficient method for computing the moments of ratios of quadratic forms in normal random variables. Let $z \sim N(0_n, I_n)$, A be a symmetric $n \times n$ matrix, and B be a positive definite $n \times n$ matrix. In this section, we are interested in obtaining an efficient algorithm for computing the expectation of

$$\frac{(z'Az)^p}{(z'Bz)^q}, \tag{82}$$

where p is a nonnegative integer and q is a positive real number.[15] As discussed in Section 2.5, the expression for this expectation holds for any spherically symmetric distribution for z, not just the $N(0_n, I_n)$.

Many estimators in statistics take the form of ratio of quadratic forms in normal random variables. As a result, the problem of computing the expectation

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of (82) has attracted the attention of many researchers.[16] A majority of the literature applies the Sawa (1972) lemma and presents formulas that are in the form of one-dimensional integrals. For the development of this type of formula, see the excellent papers of Magnus (1986) and Meng (2005) and the references therein. Suppose that $B = P\Lambda P'$, where Λ is a diagonal matrix of the eigenvalues of B and P is a matrix of the corresponding eigenvectors of B. When $(n/2) + p > q$, the expectation of (82) exists. By combining the results of Theorem 6 of Magnus (1986) and Lemma 1 of Meng (2005), we obtain

$$\mathrm{E}\left[\frac{(z'Az)^p}{(z'Bz)^q}\right] = \frac{1}{\Gamma(q)}\int_0^\infty t^{q-1}|\Delta|\mathrm{E}[(w'Rw)^p]\mathrm{d}t, \tag{83}$$

where $\Delta = (I_n + 2t\Lambda)^{-1/2}$, $R = \Delta P' A \Delta$, and $w \sim N(0_n, I_n)$.

Currently, this is the only practical method that can be used for numerical evaluation of $\mathrm{E}[(z'Az)^p/(z'Bz)^q]$. However, there are two problems associated with the use of this formula. The first problem is in the computation of $\mathrm{E}[(w'Rw)^p]$. Although an explicit formula of this expression is readily available (see, e.g., Magnus, 1986, Lem. 3), it is computationally expensive to evaluate this expectation even for moderately large p (say, $p > 4$), especially when this expectation has to be evaluated many times because its value changes with t inside the integral. The second problem is that it is difficult to control for the accuracy of the numerical integration. Besides some special cases, we are unaware of a general result in the literature that allows us to analyze and control the errors in the numerical integration of (83).[17]

Smith (1989) provides a very different expression for $\mathrm{E}[(z'Az)^p/(z'Bz)^q]$ for the more general case of $z \sim N(\mu, I_n)$. He expresses it in terms of infinite sums of top-order invariant polynomials. In our notation, his expression is

$$\mathrm{E}\left[\frac{(z'Az)^p}{(z'Bz)^q}\right] = \frac{2^{p-q}\Gamma\left(\frac{n}{2}+p-q\right)\beta^q e^{-\lambda/2}p!}{\Gamma\left(\frac{n}{2}\right)} \times \sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{(q)_j\left(\frac{n}{2}+p-q\right)_k}{\left(\frac{1}{2}\right)_k\left(\frac{n}{2}\right)_{p+j+k}2^k}d_{p,j,k}(A, I_n - \beta B, \mu\mu'), \tag{84}$$

where $\lambda = \mu'\mu$ and β is a constant that satisfies $0 < \beta < 2/b$, with b the largest eigenvalue of B. Because it involves a doubly infinite series, and the difficulty in evaluating top-order invariant polynomials with three matrix arguments, Smith's formula has not been of much practical use. Smith (1993) makes an attempt to use this formula for the case of $p = 1$ and with either $\mu = 0_n$ or $B = I_n$. However, it appears that there is great difficulty in using this formula in the general case.

In this section, for the case $\mu = 0_n$ we show how our recursive algorithms for top-order invariant polynomials can greatly simplify the evaluation of $\mathrm{E}[(z'Az)^p/(z'Bz)^q]$. In addition to numerical efficiency, our method also provides error control, so we can compute the expectation up to any desired level of accuracy. The nonzero mean case will be dealt with in a separate paper.

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4.2. Computational Method

We first study the case $B = I_n$. For this case, the result is well known—it is a straightforward extension of equation (41). From equation (2.13) of Smith (1989) we have, provided $(n/2) + p - q > 0$,

$$\mathrm{E}\left[\frac{(z'Az)^p}{(z'z)^q}\right] = \frac{2^{p-q}\Gamma\left(\frac{n}{2}+p-q\right)p!}{\Gamma\left(\frac{n}{2}+p\right)}d_p(A). \tag{85}$$

It is straightforward to show that this equation also holds for $q \leq 0$. Given our recursive algorithm for computing $d_p(A)$, we can easily compute this expectation for all values of p and q.

For the more general case that B is not proportional to an identity matrix, Smith (1993) provides the following expression (using our notation):

$$\mathrm{E}\left[\frac{(z'Az)^p}{(z'Bz)^q}\right] = \frac{2^{p-q}\Gamma\left(\frac{n}{2}+p-q\right)p!\beta^q}{\Gamma\left(\frac{n}{2}+p\right)}\sum_{j=0}^{\infty}\frac{(q)_j}{\left(\frac{n}{2}+p\right)_j}d_{p,j}(A, I_n - \beta B), \tag{86}$$

where β is a constant that may be freely chosen in the interval $0 < \beta < 2/b$, with b the largest eigenvalue of B. Again, we require $(n/2) + p - q > 0$. Given our algorithm for evaluating top-order invariant polynomials with two matrix arguments, it is rather straightforward to evaluate this series if we stop the summation at $j = M$. The only issue is to bound the truncation error if we truncate at $j = M$. In the following theorem, we provide a bound for this truncation error.

THEOREM 6. *Assume that* $0 < \beta \leq 1/b$, *where* b *is the largest eigenvalue of* B. *A bound on the truncation error is given by*

$$\sum_{j=M+1}^{\infty}\frac{(q)_j}{\left(\frac{n}{2}+p\right)_j}d_{p,j}(A, I_n - \beta B) \leq \frac{(q)_{M+1}}{\left(\frac{n}{2}+p\right)_{M+1}}$$

$$\times\left[\frac{d_p(B^{-1/2}\tilde{A}B^{-1/2})}{\beta^{n/2+p}|B|^{1/2}} - \sum_{j=0}^{M}d_{p,j}(\tilde{A}, I_n - \beta B)\right], \tag{87}$$

where $\tilde{A} = A$ *if* A *is positive semidefinite or* p *is even and* $\tilde{A} = P\tilde{D}P'$ *otherwise, with* P *as the matrix of the eigenvectors of* A *and* $\tilde{D}$ *as a diagonal matrix of the absolute eigenvalues of* A.

For illustrative purposes, we consider an example with $n = 20$, A a Toeplitz matrix with (i, j)th element given by $(|i - j| - 1)/n^2$, and B a diagonal matrix with ith diagonal element $b_{ii} = i/n^2$. Using the choice of $\beta = n$ (i.e., the reciprocal of the largest eigenvalue of B), Table 1 reports the value of $\mathrm{E}[(z'Az)^p/(z'Bz)^q]$ for various combinations of p and q, with approximation errors less than 10^{-5}. In the table, we also report in parentheses the number of terms (M) that we need to compute to achieve the desired level of accuracy. When

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TABLE 1. Expectation of ratio of quadratic forms in central normal random variables

	$q=1$	$q=2$	$q=3$	$q=4$	$q=5$	$q=10$
$p=0$	2.17970	5.52039	16.55785	60.28059	275.30455	n/a
	(30)	(44)	(64)	(91)	(130)	
$p=1$	−0.09809	−0.22082	−0.57952	−1.80842	−6.88261	−904,575.08083
	(30)	(44)	(63)	(89)	(125)	(530)
$p=2$	0.48712	0.98413	2.28489	6.19428	20.00257	380,477.23086
	(26)	(37)	(52)	(71)	(98)	(420)
$p=3$	0.16653	0.30414	0.62963	1.49641	4.14679	17,399.85368
	(36)	(51)	(70)	(95)	(128)	(468)
$p=4$	0.99067	1.66089	3.13318	6.72564	16.65035	2,8182.05694
	(29)	(39)	(52)	(68)	(89)	(333)
$p=5$	1.38677	2.13748	3.67192	7.09659	15.60182	9,986.85442
	(47)	(64)	(84)	(109)	(142)	(446)
$p=10$	2,321.96818	2,564.18967	3,069.43017	4,003.06705	5,720.63501	174,918.10486
	(51)	(63)	(76)	(90)	(107)	(257)

Note: The table presents $\mathrm{E}[(z'Az)^p/(z'Bz)^q]$ for various values of p and q, where $z \sim N(0_n, I_n)$, $n=20$, A is a Toeplitz matrix with its (i,j)th element as $a_{ij}=(|i-j|-1)/n^2$, and B is a diagonal matrix with its ith diagonal element as $b_{ii}=i/n^2$. The approximation error is set to be less than 10^{-5}, and the number of terms required to achieve this level of accuracy is reported in the parentheses. n/a = not applicable.

the error is set to be 10^{-5}, the number of terms is quite manageable. In fact, the number of terms is not exceedingly large even for very high accuracy. For example, when the approximation error is set to be less than 10^{-10} (10^{-20}), the number of terms required for $p = q = 10$ is $M = 421$ (797) instead of $M = 257$, so the algorithm is quite efficient.[18]

5. CONCLUSION

Despite the importance of top-order invariant polynomials in finite-sample theory in multivariate statistics, their use in practical applications has been greatly limited by the difficulties of their numerical evaluation. In this paper, we overcome this problem by proposing two efficient algorithms for computing top-order invariant polynomials. With our new algorithms, the use of top-order invariant polynomials in applied work can now become a reality.[19] As an application, we use our new algorithm to develop an efficient method for computing the moments of ratio of quadratic forms in normal random variables. Unlike existing methods, which typically rely on numerical integration, our method has the advantages of being both fast and reliable even for very high-order moments. For future research, we plan to extend the recursive algorithms in this paper to other applications such as the numerical evaluation of p.d.f. of ratio of quadratic forms in normal random variables.

NOTES

1. In general the zonal polynomials of degree k are indexed by partitions of k with n or fewer parts, $\boldsymbol{\kappa} = (k_1, \ldots, k_n)$, where $k_1 \geq k_2 \geq \ldots \geq k_n \geq 0$ and $\sum_{i=1}^{n} k_i = k$. When $k_1 = k$ is the only nonzero part of the partition, so that $\boldsymbol{\kappa} = (k, 0, \ldots, 0)$ is the top-order partition of k, we denote $C_{\boldsymbol{\kappa}}(A)$ simply by $C_k(A)$.

2. Hillier (2001) provides a different expression for d_k when some of the eigenvalues are repeated.

3. We use here the familiar Newton identity relating the terms in a product of two power series to the terms in the component series:

$$\left(\sum_{i=0}^{\infty} a_i t^i\right)\left(\sum_{j=0}^{\infty} b_j t^j\right) = \left(\sum_{j=0}^{\infty} c_j t^j\right)$$

with $c_j = \sum_{i=0}^{j} a_i b_{j-i}$. In addition, using the fact that $H(t) = D(t)^2$ and the Newton identity, we have $h_k = \sum_{i=0}^{k} d_i d_{k-i}$.

4. Theorem 1 can be easily generalized to provide fast recursive algorithms for computing top-order Jack polynomials, which are generalizations of the zonal polynomials. See Stanley (1989, Prop. 2.2) for various explicit expressions of top-order Jack polynomials.

5. In addition, there is also less memory requirement for our algorithm because we only need to store d_{k-s} to d_{k-1} for the recursion to continue. In contrast, Ruben's algorithm requires the storage of d_0 to d_{k-1}, so memory requirement goes up with k.

6. Mahoney and Sivazlian (1983) provide a review and comparison of various computational methods for performing partial fractions expansions for contexts similar to that discussed here. Using our

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fast recursive algorithm in Theorem 1 to compute $h_r(B_i)$, we can compute all the $a_{i,j}$'s with $O(ms)$ arithmetic operations. In comparison, the most efficient method described in Mahoney and Sivazlian (1983) takes $O(m^2)$ arithmetic operations to compute the partial fractions expansion, so our method is faster especially when s is small relative to m. In addition, our algorithm is suitable for parallel computing because $a_{i,j}$'s can be calculated independently across i.

7. An efficient algorithm for evaluating hypergeometric function of matrix argument has been recently developed by Koev and Edelman (2006). However, for the special kind of hypergeometric function in (40), our algorithm is significantly faster.

8. Although the probability is independent of β, the choice of βcan affect the speed of convergence. Ruben (1962) recommends using $\beta = 2/(\lambda_1^{-1} + \lambda_s^{-1})$, but the optimal choice of β is not well understood.

9. Using Ruben's recursive algorithm for computing d_k, Farebrother (1984) develops a computer program for approximating the c.d.f. of w based on (43).

10. In the literature, the standard notation for top-order invariant polynomials is $C_{k_1+\cdots+k_r}^{k_1,\ldots,k_r}(A_1,\ldots,A_r)$. Because we are only dealing with top-order invariant polynomials in this paper, we suppress $k_1+\cdots+k_r$ to economize on notation.

11. For example in Mathematica, we can obtain the coefficients $e_{\boldsymbol{\kappa}}$ using the following command:
CoefficientList[Det[IdentityMatrix[n]-t1*A1-$\cdots$-tr*Ar],{t1,...,tr}].

12. In combinatorics, a bracelet is the lexicographically smallest element in an equivalence class of strings under string rotation and reversal.

13. Details of the proof are available upon request.

14. We can also use our approach to evaluate the expansion $A(\boldsymbol{t})^k = \sum_{|\boldsymbol{\kappa}|=k} A_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}$ and obtain $p_{\boldsymbol{\kappa}}$ directly using $p_{\boldsymbol{\kappa}} = \mathrm{tr}(A_{\boldsymbol{\kappa}})$. The reason why we do the expansion of $\sum_{i=1}^n e_i' A(\boldsymbol{t})^k e_i$ instead is because it allows us to save memory space by a factor of n.

15. If $z \sim N(0_n, \Sigma)$, where Σ is a positive definite matrix, then it can be easily converted into our problem by writing $(z'A_z)^p/(z'B_z)^q = (\tilde{z}\tilde{A}\tilde{z})^p/(\tilde{z}'\tilde{B}\tilde{z})^q$, where $\tilde{z} = \Sigma^{1/2}z \sim N(0_n, I_n)$, $\tilde{A} = \Sigma^{1/2}A\Sigma^{1/2}$, and $\tilde{B} = \Sigma^{1/2}B\Sigma^{1/2}$.

16. Mathai and Provost (1992, Sect. 4.5) provide a good review of the existing literature on ratios of quadratic forms in normal random variables.

17. A notable exception is De Gooijer (1980), in which the author gives bounds on the numerical integration error for the special case of $p = q = 1$ or 2.

18. The numbers in Table 1 are computed using Mathematica with infinite precision. Even with approximation errors of less than 10^{-20}, none of the numbers in the table take more than 1 minute to compute using an Opteron 165 machine.

19. A set of Matlab programs that implement the algorithms in the paper is available from the authors upon request.

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APPENDIX

Proof of Theorem 1. Define

$$F(t) = \left(\prod_{i=1}^{s}(1-t\lambda_i)\right)|I_n - tA|^{-1/2} = \left(\sum_{i=0}^{s}\tilde{e}_i t^i\right)\left(\sum_{i=0}^{\infty} d_i t^i\right) \equiv \sum_{i=0}^{\infty} f_i t^i \tag{A.1}$$

for t sufficiently small such that $1-t\lambda_i$ is positive. Comparing the coefficient of t^i, it is easy to see that

$$f_i = \sum_{j=0}^{\min[i,s]} \tilde{e}_j d_{i-j}. \tag{A.2}$$

Differentiating $F(t)$ with respect to t, we have

$$\begin{aligned} F'(t) &= \left(\sum_{i=1}^{s} i\tilde{e}_i t^{i-1}\right)|I_n - tA|^{-1/2} + \left(\sum_{i=0}^{s}\tilde{e}_i t^i\right)\frac{1}{2}\mathrm{tr}(A(I_n - tA)^{-1})|I_n - tA|^{-1/2} \\ &\Rightarrow \sum_{i=1}^{\infty} i f_i t^{i-1} = \left(\sum_{i=1}^{s} i\tilde{e}_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right) \\ &\quad + \frac{1}{2}\left(\sum_{i=0}^{s}\tilde{e}_i t^i\right)\left(\sum_{i=1}^{\infty} p_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right) \\ &\Rightarrow \sum_{i=1}^{\infty} i f_i t^{i-1} = \left(\sum_{i=1}^{s} i\tilde{e}_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right) + \frac{1}{2}\left(\sum_{i=1}^{\infty}\tau_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right), \end{aligned} \tag{A.3}$$

where

$$\tau_i = \sum_{j=0}^{\min[i-1,s]} \tilde{e}_j p_{i-j}. \tag{A.4}$$

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The second equality follows because $\operatorname{tr}(A(I_n - tA)^{-1}) = P(t)/t = \sum_{i=1}^{\infty} p_i t^{i-1}$. Note that

$$\sum_{i=1}^{\infty} \tau_i t^{i-1} = \left[\prod_{i=1}^{s}(1-t\lambda_i)\right] \operatorname{tr}(A(I_n - tA)^{-1}) = \left[\prod_{i=1}^{s}(1-t\lambda_i)\right] \sum_{i=1}^{n} \frac{\lambda_i}{1-t\lambda_i}, \tag{A.5}$$

and because the right-hand side is a polynomial of order $s-1$ in t, we have $\tau_i = 0$ for $i > s$. Therefore, (A.3) can be written as

$$\sum_{i=1}^{\infty} i f_i t^{i-1} = \left(\sum_{i=1}^{s} i\tilde{e}_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right) + \frac{1}{2}\left(\sum_{i=1}^{s} \tau_i t^{i-1}\right)\left(\sum_{i=0}^{\infty} d_i t^i\right). \tag{A.6}$$

Comparing the coefficients of t^{k-1} on both sides of (A.6), we obtain the following identity:

$$\begin{aligned} k f_k &= \sum_{i=1}^{\min[k,s]} i\tilde{e}_i d_{k-i} + \frac{1}{2}\sum_{i=1}^{\min[k,s]}\left(\sum_{j=0}^{i-1} \tilde{e}_j p_{i-j}\right) d_{k-i} \\ &\Rightarrow k \sum_{i=0}^{\min[k,s]} \tilde{e}_i d_{k-i} = \sum_{i=1}^{\min[k,s]}\left(i\tilde{e}_i + \frac{\sum_{j=0}^{i-1}\tilde{e}_j p_{i-j}}{2}\right) d_{k-i} \\ &\Rightarrow d_k = \sum_{i=1}^{\min[k,s]}\left(\frac{c_i}{k} - \tilde{e}_i\right) d_{k-i}, \end{aligned} \tag{A.7}$$

where

$$c_i = i\tilde{e}_i + \frac{\sum_{j=0}^{i-1}\tilde{e}_j p_{i-j}}{2}. \tag{A.8}$$

When $n_i = m$ for $i = 1, \ldots, s$, we can use the fact that $p_i = m\sum_{j=1}^{s}\lambda_j^i$ and the Newton–Girard formula to show that $\sum_{j=0}^{i-1}\tilde{e}_j p_{i-j} = -mi\tilde{e}_i$ and hence $c_i = (1-(m/2))i\tilde{e}_i$. In this case, the recursive relation can be simplified to

$$d_k = \sum_{i=1}^{\min[k,s]}\left[\frac{(2-m)i}{2k} - 1\right]\tilde{e}_i d_{k-i}. \tag{A.9}$$

The proof of the result for the case of distinct roots is given in the text in Section 2.2. ■

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Proof of Theorem 2. We first multiply both sides of (36) by $(1-t\lambda_i)^{m_i}$ and denote the function $(1-t\lambda_i)^{m_i}\tilde{H}(t)$ on the left by

$$P_i(t) = \prod_{\substack{j=1 \\ j\neq i}}^{s} (1-t\lambda_j)^{-m_j} \tag{A.10}$$

and the terms on the right that do not involve λ_i by $\tilde{H}_i(t)$. Then

$$P_i(t) = [a_{i,m_i} + a_{i,m_i-1}(1-t\lambda_i) + \cdots + a_{i,1}(1-t\lambda_i)^{m_i-1}] + (1-t\lambda_i)^{m_i}\tilde{H}_i(t). \tag{A.11}$$

Setting $t = \lambda_i^{-1}$ gives at once

$$a_{i,m_i} = \prod_{\substack{j=1 \\ j\neq i}}^{s} \left(\frac{\lambda_i}{\lambda_i - \lambda_j}\right)^{m_j}. \tag{A.12}$$

Next, differentiating both sides of (A.11) with respect to t r times and setting $t = \lambda_i^{-1}$ gives

$$r!(-\lambda_i)^r a_{i,m_i-r} = \left.\frac{\partial^r P_i(t)}{\partial t^r}\right|_{t=\lambda_i^{-1}}. \tag{A.13}$$

Now, because

$$1-t\lambda_j = \left(\frac{\lambda_i-\lambda_j}{\lambda_i}\right)\left(1-(t-\lambda_i^{-1})\frac{\lambda_i\lambda_j}{\lambda_i-\lambda_j}\right) = \left(\frac{\lambda_i-\lambda_j}{\lambda_i}\right)\left(1-\tilde{t}\,\frac{\lambda_i\lambda_j}{\lambda_i-\lambda_j}\right), \tag{A.14}$$

where $\tilde{t} = t - \lambda_i^{-1}$, we can write

$$P_i(t) = \prod_{\substack{j=1 \\ j\neq i}}^{s} \left(\frac{\lambda_i}{\lambda_i-\lambda_j}\right)^{m_j} \left[\prod_{\substack{j=1 \\ j\neq i}}^{s} \left(1-\tilde{t}\,\frac{\lambda_i\lambda_j}{\lambda_i-\lambda_j}\right)^{-m_j}\right]. \tag{A.15}$$

But, by definition, the second term is the generating function of the complete homogeneous symmetric functions of the eigenvalues of $-\lambda_i B_i$. The coefficient of the term $\tilde{t}^r$ is thus $(-\lambda_i)^r h_r(B_i)$. Therefore,

$$\left.\frac{\partial^r P_i(t)}{\partial t^r}\right|_{t=\lambda_i^{-1}} = \left.\frac{\partial^r P_i(t)}{\partial \tilde{t}^r}\right|_{\tilde{t}=0} = r!(-\lambda_i)^r \prod_{\substack{j=1 \\ j\neq i}}^{s} \left(\frac{\lambda_i}{\lambda_i-\lambda_j}\right)^{m_j} h_r(B_i), \tag{A.16}$$

and so

$$a_{i,m_i-r} = \prod_{\substack{j=1 \\ j\neq i}}^{s} \left(\frac{\lambda_i}{\lambda_i-\lambda_j}\right)^{m_j} h_r(B_i). \tag{A.17}$$

■

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Proof of Lemma 1. Substituting (37) in (40), we have

$$
{}_pF_q\left(\frac{1}{2},\alpha_2,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;A\right)=\sum_{k=0}^{\infty}\frac{(\alpha_2)_k\ldots(\alpha_p)_k}{(\beta_1)_k\ldots(\beta_q)_k}\sum_{i=1}^{s}\sum_{j=1}^{m_i}a_{i,j}\frac{(j)_k\lambda_i^k}{k!}
$$

$$
=\sum_{i=1}^{s}\sum_{j=1}^{m_i}a_{i,j}\,{}_pF_q(j,\alpha_2,\ldots,\alpha_p;\beta_1,\ldots,\beta_q;\lambda_i). \tag{A.18}
$$

■

Proof of Lemma 2. First define, for each $\boldsymbol{\kappa}\in C(k,r)$, the sequence of partial sums in reverse order:

$$
s(\boldsymbol{\kappa})=(s_{r-1}(\boldsymbol{\kappa}),\ldots,s_1(\boldsymbol{\kappa})), \tag{A.19}
$$

with $s_i(\boldsymbol{\kappa})=\Sigma_{j=1}^{i}k_j$. It is easy to check that the map $\boldsymbol{\kappa}\to s(\boldsymbol{\kappa})$ is 1–1. We can define a total order on $C(k,r)\times C(k,r)$—lexicographic order on the $s(\boldsymbol{\kappa})$—as follows: first order in ascending order of the $s_{r-1}(\boldsymbol{\kappa})$, then in ascending order of the $s_{r-2}(\boldsymbol{\kappa})$, and so on. That is, $s_{r-1}(\boldsymbol{\nu})<s_{r-1}(\boldsymbol{\kappa})$ implies that $\boldsymbol{\nu}$ precedes $\boldsymbol{\kappa}$ (written as $\boldsymbol{\nu}<\boldsymbol{\kappa}$). The number of $\boldsymbol{\nu}$'s that satisfy $s_{r-1}(\boldsymbol{\nu})<s_{r-1}(\boldsymbol{\kappa})$ is the same as the number of nonincreasing sequences of length $r-1$ with terms chosen from $\{0,1,\ldots,s_{r-1}(\boldsymbol{\kappa})-1\}$, namely,

$$
f_{s_{r-1}(\boldsymbol{\kappa}),r-1}=\binom{r+s_{r-1}(\boldsymbol{\kappa})-2}{r-1}.
$$

But also, $\boldsymbol{\nu}<\boldsymbol{\kappa}$ if $s_{r-1}(\boldsymbol{\kappa})=s_{r-1}(\boldsymbol{\nu})$ and $s_{r-2}(\boldsymbol{\nu})<s_{r-2}(\boldsymbol{\kappa})$, and the number of these is the number of nonincreasing sequences of length $r-2$ with terms chosen from $\{0,1,\ldots,s_{r-2}(\boldsymbol{\kappa})-1\}$, namely,

$$
f_{s_{r-2}(\boldsymbol{\kappa}),r-2}=\binom{r+s_{r-2}(\boldsymbol{\kappa})-3}{r-2}.
$$

Continuing in this way, $\boldsymbol{\nu}$ precedes $\boldsymbol{\kappa}$ if the first nonvanishing term in $s(\boldsymbol{\nu})-s(\boldsymbol{\kappa})$ is negative, and the total number of sequences $\boldsymbol{\nu}$ that precede $\boldsymbol{\kappa}$ in this ordering is

$$
\sum_{i=1}^{r-1}\binom{i+s_i(\boldsymbol{\kappa})-1}{i}. \tag{A.20}
$$

Hence, in this ordering, $\boldsymbol{\kappa}$ is assigned the number $n_k(\boldsymbol{\kappa})$ given in the lemma. ■

Proof of Theorem 6. Under the assumption of $0<\beta\le 1/b$, $I_n-\beta B$ is positive semidefinite. Therefore, when A is positive semidefinite or p is even, the remainder terms are positive. Using the fact that $(n/2)+p>q$, we have $(q)_j/((n/2)+p)_j\le(q)_{M+1}/((n/2)+p)_{M+1}$ for $j>M$. It follows that

$$
\sum_{j=M+1}^{\infty}\frac{(q)_j}{\left(\frac{n}{2}+p\right)_j}d_{p,j}(A,I_n-\beta B)\le\frac{(q)_{M+1}}{\left(\frac{n}{2}+p\right)_{M+1}}\sum_{j=M+1}^{\infty}d_{p,j}(A,I_n-\beta B). \tag{A.21}
$$

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The generating function of $d_{i,j}(A, I_n - \beta B)$ is given by

$$|I_n - t_1 A - t_2(I_n - \beta B)|^{-1/2} = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} d_{i,j}(A, I_n - \beta B) t_1^i t_2^j. \tag{A.22}$$

Putting $t_2 = 1$, the equation becomes

$$|\beta B|^{-1/2}\left|I_n - t_1 \frac{B^{-1/2}AB^{-1/2}}{\beta}\right|^{-(1/2)} = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} d_{i,j}(A, I_n - \beta B) t_1^i. \tag{A.23}$$

Comparing the coefficient of t_1^p on both sides, we get

$$\sum_{j=0}^{\infty} d_{p,j}(A, I_n - \beta B) = |\beta B|^{-1/2} d_p\left(\frac{B^{-1/2}AB^{-1/2}}{\beta}\right) = \frac{d_p(B^{-1/2}AB^{-1/2})}{\beta^{(n/2)+p}|B|^{1/2}}. \tag{A.24}$$

It follows that

$$\begin{aligned}\sum_{j=M+1}^{\infty} d_{p,j}(A, I_n - \beta B) &= \sum_{j=0}^{\infty} d_{p,j}(A, I_n - \beta B) - \sum_{j=0}^{M} d_{p,j}(A, I_n - \beta B) \\ &= \frac{d_p(B^{-1/2}AB^{-1/2})}{\beta^{(n/2)+p}|B|^{1/2}} - \sum_{j=0}^{M} d_{p,j}(A, I_n - \beta B).\end{aligned} \tag{A.25}$$

When A is not positive semidefinite and p is odd, we have $|z'Az| = |z'PDP'z| \leq z'P\tilde{D}P'z = z'\tilde{A}z$. Using the fact that $z'(I_n - \beta B)z \geq 0$, we have $|(z'Az)^p(z'(I_n - \beta B)z)^j| \leq (z'\tilde{A}z)^p(z'(I_n - \beta B)z)^j$, and it follows that

$$\left|\sum_{j=M+1}^{\infty} \frac{(q)_j}{\left(\frac{n}{2}+p\right)_j} d_{p,j}(A, I_n - \beta B)\right| \leq \sum_{j=M+1}^{\infty} \frac{(q)_j}{\left(\frac{n}{2}+p\right)_j} d_{p,j}(\tilde{A}, I_n - \beta B), \tag{A.26}$$

and the bound is obtained using the same derivation as before because $\tilde{A}$ is positive semidefinite. ■

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