Generating Functions and Short Recursions, with Applications to the Moments of Quadratic Forms in Noncentral Normal Vectors

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PROPOSED RUNNING HEAD: Generating Functions and Short Recursions

Abstract

Recursive relations for objects of statistical interest have long been important for computation, and remain so even with hugely improved computing power. Such recursions are frequently derived by exploiting relations between generating functions. For example, the top-order zonal polynomials that occur in much distribution theory under normality can be recursively related to other (easily computed) symmetric functions (power-sum and elementary symmetric functions, Ruben, 1962, *Annals of Mathematical Statistics* 33, 542–570), Hillier, Kan, and Wang, 2009, *Econometric Theory* 25, 211–242). Typically, in a recursion of this type the k-th object of interest, d_k say, is expressed in terms of all lower-order d_j's. In Hillier et al. (2009) we pointed out that, in the case of top-order zonal polynomials and other invariant polynomials of multiple matrix argument, a *fixed length* recursion can be deduced. We refer to this as a short recursion. The present paper shows that the main results in Hillier et al. (2009) can be generalized, and that short recursions can be obtained for a much larger class of objects/generating functions. As applications, we show that short recursions can be obtained for various problems involving quadratic forms in noncentral normal vectors, including moments, product moments, and expectations of ratios of powers of quadratic forms. For this class of problems, we also show that the length of the recursion can be further reduced by an application of a generalization of Horner's method (c.f. Brown, 1986, *SIAM Journal on Scientific and Statistical Computing* 7, 689–695), producing a super-short recursion that is significantly more efficient than even the short recursion.

1. INTRODUCTION

Relations between the generating functions for different mathematical objects can yield useful recurrence relations between those objects. This has long been appreciated in the theory of symmetric functions. In statistics, these relations can be exploited to yield recurrence relations between moments and cumulants (Smith, 1995). In addition, the top-order zonal polynomials that occur in much statistical distribution theory under normality can, by this device, be recursively related to other symmetric functions, in particular, the power-sum and elementary symmetric functions (Ruben, 1962; Hillier, Kan, and Wang, 2009 [henceforth HKW]).

Such results greatly facilitate the efficient computation of these functions, and hence our ability to compute moments, densities, distribution functions, etc., that are expressed in terms of the objects of interest d_k, say. However, such recursions typically express d_k in terms of all lower-order d_j's, and in HKW we pointed out that, in the case of top-order zonal polynomials (and invariant polynomials with several matrix arguments), a shorter (i.e., fixed length) recursion can also be deduced by exploiting the relations between several generating functions. In this paper we show that the argument in HKW applies much more generally. We first show that *any* generating function may be used to define an associated function that induces a recurrence relation of exactly the same form as holds between the top-order zonal polynomials and the power-sum symmetric functions. Then, we show that, under certain conditions on the associated function, there is a short recursion that can considerably improve the efficiency of the recursion for computational purposes. These results evidently have very general applicability, and in the present paper we apply them to various problems involving quadratic forms in noncentral normal vectors, including: moments, product moments, and expectations of ratios of powers of quadratic forms.

While the short recursion for the top-order zonal and invariant polynomials given in HKW is significantly more efficient than the traditional long recursion, the length of the short recursion can still be quite long when the dimension of the matrix involved is large. In addition, unlike the long recursion, the short recursion is often numerically unstable because the coefficients in the short recursion often have different signs that lead to cancellation error in the summation. In order to overcome these problems, we draw our inspiration from Brown (1986), and introduce in this paper what we call a "super-short" recursion algorithm for problems that involve quadratic forms in noncentral normal vectors. Our super-short recursion is essentially a multivariate generalization of Horner's method for evaluating polynomials. The most important feature of this new recursion is that the length of recursion depends only on the number of matrices involved and is independent of the dimension of the matrices. When only one matrix is involved, the super-short recursion allows us to update d_k from d_{k-1}. When r matrices are involved, the length of recursion is at most r. Another attractive feature of the super-short recursion is that it retains the numerical stability of the long recursion, making it perfectly suitable for numerical evaluation of top-order zonal polynomials and top-order invariant polynomials, among other problems that involve quadratic forms in normal random variables.

The rest of the paper is organized as follows. We begin in Section 2 with an extension of the results in HKW, first for univariate generating functions, then for the general multivariate case. In Section 3, we consider the problem of computing the moments of quadratic form in noncentral normal random variables. In particular, we introduce the super-short recursion and contrast it with the long and short recursions that were introduced in Section 2. Section 4 presents some analogous results for the product moments of several quadratic forms. Finally in Section 5, we study the expectation of a ratio of powers of two quadratic forms in noncentral normal vectors. Section 6 concludes. Throughout the paper we use the notation in Wilf (2005) for coefficients in generating functions: the expression $[t^k]f(t)$ denotes the coefficient of t^k in the formal expansion of the function $f(t)$ in powers of t.

2. GENERATING FUNCTIONS AND RECURSIONS

2.1 Background

The top-order zonal polynomials of a symmetric matrix A, $C_k(A)$, and the top-order invariant polynomials with several matrix arguments introduced by Davis (1979) (1981), $C_{k_1,k_2,\ldots,k_r}(A_1,\ldots,A_r)$, occur sufficiently frequently in multivariate calculations as to deserve special attention. For example, if $z \sim N(0_n, I_n)$, the moments of the quadratic form $q = z'Az$ are given by

$$\mu_k = \mathbb{E}[q^k] = 2^k \left(\frac{1}{2}\right)_k C_k(A), \tag{1}$$

and the product-moments of the several quadratic forms $q_i = z'A_iz$, $i = 1, \ldots, r$, are given by

$$\mu_{\boldsymbol{\kappa}} = \mathbb{E}[q_1^{k_1} q_2^{k_2} \cdots q_r^{k_r}] = 2^k \left(\frac{1}{2}\right)_k C_{\boldsymbol{\kappa}}(A_1, \cdots, A_r), \tag{2}$$

where $\boldsymbol{\kappa} = (k_1, \ldots, k_r)$, $k = \Sigma_{i=1}^r k_i$, and $(c)_k = c(c+1)\cdots(c+k-1)$ is the usual Pochhammer symbol. These expressions follow easily from the moment generating function (MGF) of q, and the joint moment generating function of the q_i, both of which have expansions in terms of these polynomials (see below). Ruben (1962) and James (1961) essentially give (1), while Chikuse (1987) gives (2). The density function of q may also be expressed as an infinite series in the $C_k(A)$; see James (1961) and Ruben (1962).

Many alternative expressions for these polynomials (or, equivalently, moments) have appeared in the literature, but for computation purposes the most efficient expressions have, until recently, been the recurrence relations due to Ruben (1962) for the $C_k(A)$, and Chikuse (1987) for the $C_{\boldsymbol{\kappa}}(A_1, \cdots, A_r)$. These recursions involve the power-sum symmetric functions, p_k say, in the eigenvalues of A, and, in the multivariate case, generalizations of them defined in terms of a multivariate generating function. Although superior to the explicit formulae for the polynomials, these recurrence relations have length k, and hence have computation complexity of order $O(k^2)$, which means that the recursions are computationally quite inefficient. However, in HKW, we have given new recurrence relations for both cases that involve, instead, the elementary symmetric functions, and appropriate generalizations of them for the multivariate case. These have length at most equal to n, the dimension of the matrix (or matrices) involved, and so do not increase with k. These new recursions therefore improve computational complexity to $O(k)$, and the fact that they involve only a fixed number of terms, whatever the degree of the polynomial, means that there is also a substantial saving on storage requirements.

The new recurrence relations in HKW were derived by exploiting properties of, and relations between, the various generating functions for the polynomials that are involved. If we normalize the top-order zonal polynomial $C_k(A)$ by writing

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

the (ordinary) generating function for the d_k is:

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

while the power sums p_k and elementary symmetric functions e_k have generating functions $P(t) = \mathrm{tr}(tA(I_n - tA)^{-1})$ and $E(t) = |I_n - tA|$, respectively,[1] where $\mathrm{tr}(\cdot)$ is the trace operator. Here, $d_0 = e_0 = 1$, and, crucially, $e_k = 0$ for $k > n$. Note that, in terms of the d_k, $\mu_k = 2^k k! d_k(A)$.

These generating functions may easily be shown to satisfy the differential equations:

$$tE'(t) = -E(t)P(t),$$

and

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

The second of these immediately yields (on equating coefficients of like powers of t on both sides) the recursion in Ruben (1962):

$$d_k = \frac{1}{2k}\sum_{j=1}^{k} p_j d_{k-j}, \tag{3}$$

while combining the two leads to the alternative recursion in terms of the e_k given in HKW:

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

In HKW, we show that these relations generalize in the obvious way to the multivariate case. For brevity we refer to the recursions involving the e_j as the "short" recursions, and those involving the p_j as the "long" recursions.

In Sections 2.2 and 2.3, we show that the generating function relationships that underpin the short recursions given in HKW for the polynomials d_k and $d_{\boldsymbol{\kappa}}$ can be extended to a larger class of problems, provided certain conditions are satisfied.

2.2 Generating Functions with a Single Variable

Let $D(t)$ be an arbitrary generating function for the objects d_k, which themselves will in general be functions of other variables,

$$D(t) = \sum_{k=0}^{\infty} d_k t^k.$$

In applications $D(t)$ will typically be the MGF of some random variable of interest or a more general generating function for moment-like quantities associated with one or more random variables.[2]

We define a second generating function $P(t)$ by the formula:

$$P(t) = t\frac{\partial \ln D(t)}{\partial t} = \frac{tD'(t)}{D(t)} = \sum_{k=1}^{\infty} p_k t^k, \tag{4}$$

so that

$$tD'(t) = D(t)P(t). \tag{5}$$

Equating coefficients of powers of t on both sides of this identity yields the recursion in (3), except for the factor 1/2:

$$d_k = \frac{1}{k}\sum_{j=1}^{k} p_j d_{k-j} = \frac{1}{k}\sum_{j=0}^{k-1} d_j p_{k-j}. \tag{6}$$

With the initial condition $d_0 = D(0)$, this recurrence relation allows us to recursively obtain the d_k from the p_k. The usefulness of this type of result depends, of course, on whether the functions p_k are significantly easier to compute than are the d_k themselves. And, unless $P(t)$ is a finite order polynomial, the length of the recursion increases with k, so it may be computationally inefficient to use this recurrence relation when k is large. In the case $D(t) = |I_n - tA|^{-\frac{1}{2}}$ (the MGF of $q/2 = z'Az/2$ when $z \sim N(0_n, I_n)$), $P(t) = \mathrm{tr}(tA(I_n - tA)^{-1})/2$, so that the $p_j = \mathrm{tr}(A^j)/2$ are essentially the power-sum symmetric functions, and these are indeed easily computed. However, it is now clear that this same recursion applies for any generating functions $D(t)$ and $P(t)$ related by (5).

Remark 1. *If $D(t) = \sum_{r=0}^{\infty} \mu_r t^r/r!$, say, is the moment generating function for a random variable with cumulant generating function $K(t) = \ln D(t) = \sum_{r=1}^{\infty} \kappa_r t^r/r!$, say, then $d_k = \mu_k/k!$ and $P(t) = tK'(t) = \sum_{r=1}^{\infty} \kappa_r t^r/(r-1)!$, so that $p_r = \kappa_r/(r-1)!$. Thus, (6) gives the well-known recursion for moments in terms of cumulants:*

$$\mu_k = \sum_{j=1}^{k} \binom{k-1}{j-1} \kappa_j \mu_{k-j} = \sum_{j=0}^{k-1} \binom{k-1}{j} \mu_j \kappa_{k-j}.$$

See, e.g., Smith (1995).

Now, suppose that $P(t)$, as defined in (4), is a rational function of t and can be written as

$$P(t) = \frac{G(t)}{E(t)},$$

where $G(t) = \sum_{k=1}^{m_1} g_k t^k$ and $E(t) = \sum_{k=0}^{m_2} e_k t^k$ are *both finite order polynomials* in t. Note that $g_0 = 0$ because $p_0 = 0$, and that g_k can be obtained by using the fact that $g_k = \sum_{i=0}^{k-1} e_i p_{k-i}$, which follows from the identity $G(t) = E(t)P(t)$. Without loss of generality, we normalize the two polynomials $G(t)$ and $E(t)$ so that $e_0 = 1$. The following result generalizes the result given in equation (24) in HKW:

LEMMA 1. *Suppose that the generating function $P(t)$ defined in (4) can be written as*

$$P(t) = \frac{G(t)}{E(t)},$$

with both $G(t)$ and $E(t)$ polynomials of finite order, say m_1 and m_2 respectively, and $e_0 = 1$. Then the d_k may be determined recursively from the relation

$$d_k = \sum_{j=1}^{\min[k,m]} \left(\frac{c_j}{k} - e_j \right) d_{k-j}, \tag{7}$$

together with the initial condition $d_0 = D(0)$, where $m = \max[m_1, m_2]$ and $c_j = je_j + g_j$.

Proof. Define

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

with

$$f_k = \sum_{j=0}^{\min[k,m_2]} e_j d_{k-j}. \tag{8}$$

Differentiating $F(t)$, and making use of the relationship in (5),

$$F'(t) = E'(t)D(t) + E(t)D'(t) = E'(t)D(t) + \frac{1}{t}E(t)P(t)D(t) = \left[E'(t) + \frac{G(t)}{t} \right] D(t).$$

Thus,

$$\sum_{k=1}^{\infty} k f_k t^{k-1} = \left(\sum_{j=1}^{m} (je_j + g_j) t^{j-1} \right) \left(\sum_{i=0}^{\infty} d_i t^i \right),$$

where $m = \max[m_1, m_2]$. Equating coefficients of like powers of t on both sides and using (8) we obtain:

$$k \sum_{j=0}^{\min[k,m_2]} e_j d_{k-j} = k f_k = \sum_{j=1}^{\min[k,m]} (je_j + g_j) d_{k-j}.$$

Rearranging this and using the fact that $e_0 = 1$ gives the stated relation. ■

The key advantage of (7) over (6) is that at most m terms are needed to compute d_k. As a result, the computation time for the d_k does not increase with k, and there is no need to store all previous values of the c_j, so the memory requirement also does not increase with k. Again, though, the usefulness of the result depends on whether or not the c_j are significantly easier to compute than the d_k themselves. As we shall see, this is certainly the case in the applications involving quadratic forms in normal variates that we discuss below.

Remark 2. *For the case* $D(t) = |I_n - tA|^{-\frac{1}{2}}$, $P(t) = \mathrm{tr}(tA(I_n - tA)^{-1})/2$ *and* $P(t)$ *can be written as* $G(t)/E(t)$, *where* $G(t) = \mathrm{tr}((tA)\mathrm{adj}(I_n - tA))/2$ *with* $\mathrm{adj}(I_n - tA)$ *denoting the adjoint matrix of* $I_n - tA$, *and* $E(t) = |I_n - tA|$. *Since the elements of* $\mathrm{adj}(I_n - tA)$ *are polynomials of degree* $n-1$ *in* t, *both* $G(t)$ *and* $E(t)$ *are polynomials of degree* n *in* t. *Thus,* $P(t)$ *satisfies the hypotheses of the Lemma.*

A number of known results that have statistical applications are simple consequences of Lemma 1. For example, well-known recurrence relations for both the Hermite and generalized Laguerre polynomials are easily deduced from the result given in Lemma 1.

2.3 Multivariate Generating Functions

We now extend the results in the previous subsection to deal with generating functions of more than one variable. Special cases of these results were given in Section 3 of HKW. For the rest of the paper, we shall adopt the following notation: $\boldsymbol{t} = (t_1, \ldots, t_r)$, $\boldsymbol{\kappa} = (k_1, \ldots, k_r)$, the k_i being nonnegative integers, $|\boldsymbol{\kappa}|$ will denote the sum of the parts of $\boldsymbol{\kappa}$, i.e., $|\boldsymbol{\kappa}| = \sum_{i=1}^r k_i$, $\boldsymbol{t}^{\boldsymbol{\kappa}} = \prod_{i=1}^r t_i^{k_i}$, and $\boldsymbol{\kappa}! = \prod_{i=1}^r k_i!$.

With this notation, we can also extend Wilf's notation for the coefficients in a generating function

$$G(\boldsymbol{t}) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} g_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}},$$

say, by writing

$$g_{\boldsymbol{\kappa}} = [\boldsymbol{t}^{\boldsymbol{\kappa}}] G(\boldsymbol{t}).$$

Also, generalizing the familiar relation between the coefficients in the product of two (formal) power series with those of the two constituent series, we have that, if $G(\boldsymbol{t}) = P(\boldsymbol{t})E(\boldsymbol{t})$, say, where $P(\boldsymbol{t})$

and $E(\boldsymbol{t})$ are at this stage arbitrary, then,

$$g_{\boldsymbol{\kappa}} = [\boldsymbol{t}^{\boldsymbol{\kappa}}]P(\boldsymbol{t})E(\boldsymbol{t}) = \sum_{j=0}^{|\boldsymbol{\kappa}|} \sum_{\substack{|\boldsymbol{\nu}|=j \\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} e_{\boldsymbol{\nu}} p_{\boldsymbol{\kappa}-\boldsymbol{\nu}},$$

where the notation $\boldsymbol{\nu} \leq \boldsymbol{\kappa}$ means that $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_r)$ is a sequence of nonnegative integers satisfying $0 \leq \nu_i \leq k_i$ for all i.

Next, for a given (ordinary) generating function

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

we define

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

as a generalization of $tf'(t)$ for the single variable case.

Assume given, as in the univariate case, an arbitrary multivariate generating function $D(\boldsymbol{t})$ for objects $d_{\boldsymbol{\kappa}}$, i.e.,

$$D(\boldsymbol{t}) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} d_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}.$$

Then, exactly as in the case with single variable, we define $P(\boldsymbol{t})$ by the equation

$$P(\boldsymbol{t}) = \frac{\dot{D}(\boldsymbol{t})}{D(\boldsymbol{t})} = \sum_{i=1}^{r} t_i \frac{\partial \ln D(\boldsymbol{t})}{\partial t_i}, \tag{9}$$

so that

$$\dot{D}(\boldsymbol{t}) = P(\boldsymbol{t})D(\boldsymbol{t}). \tag{10}$$

Since $P(\boldsymbol{0}) = 0$, we can write $P(\boldsymbol{t})$ as

$$P(\boldsymbol{t}) = \sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} p_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}$$

and rewrite (10) as

$$\sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} k d_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}} = \left(\sum_{i=1}^{\infty} \sum_{|\boldsymbol{\nu}|=i} p_{\boldsymbol{\nu}} \boldsymbol{t}^{\boldsymbol{\nu}} \right) \left(\sum_{j=0}^{\infty} \sum_{|\boldsymbol{\lambda}|=j} d_{\boldsymbol{\lambda}} \boldsymbol{t}^{\boldsymbol{\lambda}} \right).$$

Comparing the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides, we obtain the multivariate version of the recurrence relation (6):

$$d_{\boldsymbol{\kappa}} = \frac{1}{k}\sum_{j=1}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} p_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{11}$$

where $k = |\boldsymbol{\kappa}|$. Together with the initial condition $d_{\mathbf{0}} = D(\mathbf{0})$, this result provides a (long) recursive algorithm for computing the $d_{\boldsymbol{\kappa}}$, given the $p_{\boldsymbol{\nu}}$'s, and is a generalization of (6) for the single variable case. However, (11) expresses $d_{\boldsymbol{\kappa}}$ as a linear combination of $\prod_{i=1}^{r}(k_i+1)-1$ different $d_{\boldsymbol{\nu}}$'s, so it is extremely inefficient when any of the k_i's are large.

Before presenting the generalized version of (7), we note that a different and potentially slightly shorter recursive algorithm for the $d_{\boldsymbol{\kappa}}$ can be obtained by using a different generalization of the expression $tf'(t)$. Instead of computing $\dot{D}(\boldsymbol{t})$, we can pick an l such that $k_l > 0$ and consider just the derivative of $D(\boldsymbol{t})$ with respect to t_l. This gives us

$$t_l\frac{\partial D(\boldsymbol{t})}{\partial t_l} = t_l\frac{\partial \ln(D(\boldsymbol{t}))}{\partial t_l}D(\boldsymbol{t}),$$

which implies:

$$\sum_{k=1}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} k_l d_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}} = \left(\sum_{k=1}^{\infty}\sum_{|\boldsymbol{\kappa}|=k}\frac{k_l}{k}p_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}}\right)\left(\sum_{k=0}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} d_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}}\right),$$

because the coefficient of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ in $\ln(D(\boldsymbol{t}))$ is $p_{\boldsymbol{\kappa}}/k$. Comparing the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides, we obtain a second recursive algorithm for the $d_{\boldsymbol{\kappa}}$:

$$d_{\boldsymbol{\kappa}} = \frac{1}{k_l}\sum_{j=1}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} \frac{\nu_l}{j} p_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{12}$$

which can also be considered as a multivariate generalization of (6).

Equation (12) expresses $d_{\boldsymbol{\kappa}}$ as a linear combination of $[k_l/(k_l+1)]\prod_{i=1}^{r}(k_i+1)$ different $d_{\boldsymbol{\nu}}$'s with $\boldsymbol{\nu} < \boldsymbol{\kappa}$. While (12) works for any l with $k_l > 0$, it is best to pick the l with the smallest nonzero k_l in order to achieve the shortest recursion. When $k_l = 1$, the length of recursion in (12) is only half of that of (11). Nevertheless, there is no substantial computational advantage of using (12) over (11). This is because, while (12) requires summing fewer terms than (11), each term in the recursion entails an extra multiplication by ν_l/j.

As in the single variable case, we can obtain a shorter recurrence relation for the $d_{\boldsymbol{\kappa}}$ if $P(\boldsymbol{t})$ is a rational function of $\boldsymbol{t}$ and can be expressed as

$$P(\boldsymbol{t}) = \frac{G(\boldsymbol{t})}{E(\boldsymbol{t})}, \tag{13}$$

where both

$$G(\boldsymbol{t}) = \sum_{k=1}^{m_1} \sum_{|\boldsymbol{\kappa}|=k} g_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}$$

and

$$E(\boldsymbol{t}) = \sum_{k=0}^{m_2} \sum_{|\boldsymbol{\kappa}|=k} e_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}$$

are finite-order polynomials in $\boldsymbol{t}$ and $e_{\mathbf{0}} = 1$. Note that $g_{\mathbf{0}} = G(\mathbf{0}) = 0$ because $P(\mathbf{0}) = 0$, and that the coefficients $g_{\boldsymbol{\kappa}}$ in $G(\boldsymbol{t})$ can be obtained from

$$g_{\boldsymbol{\kappa}} = \sum_{j=0}^{k-1} \sum_{\substack{|\boldsymbol{\nu}|=j, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} e_{\boldsymbol{\nu}} p_{\boldsymbol{\kappa}-\boldsymbol{\nu}}$$

as in the single variable case. We have, in generalization of Lemma 1, the following result.

LEMMA 2. *Given an arbitrary multivariate generating function $D(\boldsymbol{t})$, defining $P(\boldsymbol{t})$ as in (9), and assuming that $P(\boldsymbol{t})$ is a rational function of $\boldsymbol{t}$ as in (13), with both $G(\boldsymbol{t})$ and $E(\boldsymbol{t})$ are finite-order polynomials of degrees m_1 and m_2, respectively, then the $d_{\boldsymbol{\kappa}}$ can be determined recursively from the short recurrence relation:*

$$d_{\boldsymbol{\kappa}} = \sum_{j=1}^{\min[k,m]} \sum_{\substack{|\boldsymbol{\nu}|=j, \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} \left(\frac{c_{\boldsymbol{\nu}}}{k} - e_{\boldsymbol{\nu}} \right) d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{14}$$

where $m = \max[m_1, m_2]$ and $c_{\boldsymbol{\nu}} = |\boldsymbol{\nu}| e_{\boldsymbol{\nu}} + g_{\boldsymbol{\nu}}$.

Proof. Defining, as in the single variable case,

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

where

$$f_{\boldsymbol{\kappa}} = \sum_{j=0}^{\min[k,m_2]} \sum_{\substack{|\boldsymbol{\nu}|=j \\ \boldsymbol{\nu} \leq \boldsymbol{\kappa}}} e_{\boldsymbol{\nu}} d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}. \tag{15}$$

Then

$$\dot{F}(\boldsymbol{t}) = \dot{E}(\boldsymbol{t})D(\boldsymbol{t}) + E(\boldsymbol{t})\dot{D}(\boldsymbol{t}) = [\dot{E}(\boldsymbol{t}) + G(\boldsymbol{t})]D(\boldsymbol{t})$$

on using (10) and (13). Hence

$$\sum_{k=1}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} kf_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}} = \left(\sum_{j=1}^{m}\sum_{|\boldsymbol{\nu}|=j}(je_{\boldsymbol{\nu}} + g_{\boldsymbol{\nu}})\,\boldsymbol{t}^{\boldsymbol{\kappa}}\right)\left(\sum_{k=0}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} d_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}}\right),$$

where $m = \max[m_1, m_2]$. Equating the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ on both sides gives us

$$kf_{\boldsymbol{\kappa}} = \sum_{j=1}^{\min[k,m]}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}}(je_{\boldsymbol{\nu}} + g_{\boldsymbol{\nu}})d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}.$$

Finally, using (15) and rearranging terms gives the stated result for the $d_{\boldsymbol{\kappa}}$. ■

As before — and in contrast to (11) and (12) — the short recurrence relation never uses at most $(m + r)!/(m!r!) - 1$ terms and so significantly reduces the computation time and memory requirement when compared with the long recurrence relation. In the remainder of the paper we present a variety of applications of these results to problems involving properties of quadratic forms in normal random variables. However, for many of these problems, the short recurrence relation is often numerically unstable. This is because unlike $p_{\boldsymbol{\nu}}$ in the long recurrence relation, the coefficients $c_{\boldsymbol{\nu}}/k - e_{\boldsymbol{\nu}}$ in the short recurrence relation often have different signs, which lead to serious cancellation errors especially when $|\boldsymbol{\kappa}|$ is large. In order to overcome this problem, we introduce in the following sections a new recurrence relation that is even shorter than the short recurrence relation, yet retains the numerical stability of the long recurrence relation.

From now on we reserve the notation $D(\boldsymbol{t})$ for the multivariate generating function for the top-order invariant polynomials $d_{\boldsymbol{\kappa}}$

$$D(\boldsymbol{t}) = |I_n - A(\boldsymbol{t})|^{-\frac{1}{2}} = \sum_{k=0}^{\infty}\sum_{|\boldsymbol{\kappa}|=k} d_{\boldsymbol{\kappa}}\boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{16}$$

where $A(\boldsymbol{t}) = t_1A_1 + ... + t_rA_r$, and $P(\boldsymbol{t})$ for the generalized power-sum generating function associated with it:

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

Also, we reserve $E(\boldsymbol{t})$ for the determinant $|I_n - A(\boldsymbol{t})|$. In all other applications of the results given in this Section we add a tilde to D, P, and E, and their associated coefficients $d_{\boldsymbol{\kappa}}$, $p_{\boldsymbol{\kappa}}$, and $e_{\boldsymbol{\kappa}}$, to indicate that these are not the basic forms. Beware, though, that this means that the same symbol will appear in different places with different meanings.

Remark 3. *$P(\boldsymbol{t})$ can be written as $G(\boldsymbol{t})/E(\boldsymbol{t})$, where $G(\boldsymbol{t}) = \mathrm{tr}\,(A(\boldsymbol{t})\mathrm{adj}\,(I_n - A(\boldsymbol{t})))$. Since the elements of* adj $(I_n - A(\boldsymbol{t}))$ *are polynomials of degree $n-1$, both $E(\boldsymbol{t})$ and $G(\boldsymbol{t})$ are polynomials of degree n. Therefore, $P(\boldsymbol{t})$ satisfies the hypotheses of Lemma 2.*

3. FIRST APPLICATION: MOMENTS OF QUADRATIC FORMS

3.1 Long and Short Recursions for the Noncentral Case

When $z \sim N(0_n, I_n)$ we have already noted that the moments of $q = z'Az$ are given by

$$\mu_k = \mathbb{E}[(z'Az)^k] = 2^k k! d_k(A).$$

Ruben (1962) provides the long recursion for computing the μ_k and HKW provide the corresponding short recursion. For the noncentral case with $z \sim N(\mu, I_n)$, it is easy to show that the MGF of q is given by

$$M_q(\tau) = |I_n - 2\tau A|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - 2\tau A)^{-1}\mu - \mu'\mu}{2}\right).$$

Letting

$$\tilde{D}(t) = |I_n - tA|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - tA)^{-1}\mu - \mu'\mu}{2}\right) = \sum_{k=0}^{\infty} \tilde{d}_k t^k, \tag{17}$$

the moments of q are given by

$$\mu_k = \mathbb{E}[q^k] = 2^k k! \tilde{d}_k,$$

an exact anolgue of the result for the central case, and we can use the results in Section 2 to derive recurrence relations for these moments.[3]

Using the fact that when t is sufficiently small, $(I_n - tA)^{-1} = \sum_{k=0}^{\infty} A^k t^k$, and $\ln|I_n - tA| = -\sum_{k=1}^{\infty} \frac{1}{k}\mathrm{tr}(A^k)t^k$, we can write $\ln(\tilde{D}(t))$ as

$$\ln(\tilde{D}(t)) = -\frac{1}{2}\ln|I_n - tA| + \frac{1}{2}\mu'[(I_n - tA)^{-1} - I_n]\mu = \frac{1}{2}\sum_{k=1}^{\infty}\left[\mu'A^k\mu + \frac{\mathrm{tr}(A^k)}{k}\right]t^k.$$

Defining $\tilde{P}(t)$ as in (4), we therefore have

$$\tilde{P}(t) = t\frac{\partial \ln(\tilde{D}(t))}{\partial t} = \frac{1}{2}\sum_{k=1}^{\infty}\left[k\mu'A^k\mu + \mathrm{tr}(A^k)\right]t^k, \tag{18}$$

so that, for this noncentral case,

$$\tilde{p}_k = \frac{1}{2}\left[k\mu' A^k \mu + \mathrm{tr}(A^k)\right].$$

Obviously, $\tilde{p}_k$ reduces to $p_k/2$ when $\mu = 0_n$.

To see that $\tilde{P}(t)$ is a rational polynomial with both numerator and denominator of finite degree, so that the result in Lemma 1 also applies, first note that, by definition,

$$\begin{aligned} \tilde{P}(t) &= t\frac{\partial \ln |I_n - tA|^{-\frac{1}{2}}}{\partial t} + \frac{1}{2}t\frac{\partial}{\partial t}\mu'(I_n - tA)^{-1}\mu \\ &= \frac{1}{2}\mathrm{tr}\left(tA(I_n - tA)^{-1}\right) + \frac{1}{2}\mu'(I_n - tA)^{-1}(tA)(I_n - tA)^{-1}\mu. \end{aligned} \tag{19}$$

Writing $(I_n - tA)^{-1} = \mathrm{adj}(I_n - tA)/|I_n - tA|$ we have $\tilde{P}(t) = \tilde{G}(t)/\tilde{E}(t)$, where

$$\tilde{G}(t) = \frac{1}{2}|I_n - tA|\mathrm{tr}(tA[\mathrm{adj}(I_n - tA)]) + \frac{1}{2}\mu'[\mathrm{adj}(I_n - tA)](tA)[\mathrm{adj}(I_n - tA)]\mu, \tag{20}$$

a polynomial of degree $2n$, and

$$\tilde{E}(t) = |I_n - tA|^2, \tag{21}$$

also of degree $2n$. We therefore have the following Theorem, which gives long and short recursions for the moments of a quadratic form in noncentral normal variates:

THEOREM 1. *The moments of a quadratic form $q = z'Az$, with $z \sim N(\mu, I_n)$, satisfy* ***exactly the same recurrence relations*** *— those given in (6) and (7) — whether μ is zero or not. In the central case $\tilde{D}(t) = D(t)$, $\tilde{P}(t) = P(t)/2$, and $\tilde{E}(t) = E(t)$, while in the noncentral case $\tilde{D}(t)$, $\tilde{P}(t)$, and $\tilde{E}(t)$ are as in (17), (19) and (21), respectively. That is, the $\tilde{d}_k$ satisfy both the long recursion*

$$\tilde{d}_k = \frac{1}{k}\sum_{j=1}^{k}\tilde{p}_j\tilde{d}_{k-j}, \tag{22}$$

and the short recursion

$$\tilde{d}_k = \sum_{j=1}^{\min[k,2n]}\left(\frac{\tilde{c}_j}{k} - \tilde{e}_j\right)\tilde{d}_{k-j}, \tag{23}$$

where $\tilde{c}_j = j\tilde{e}_j + \tilde{g}_j$.

Note again that the $\tilde{g}_k$ may be computed indirectly from the $\tilde{p}_k$ and $\tilde{e}_k$ by using the identity $\tilde{G}(t) = \tilde{P}(t)\tilde{E}(t)$ (rather than directly from the expansion of $\tilde{G}(t)$ in (20)), and, since $\tilde{E}(t) =$

$E(t)E(t)$, the $\tilde{e}_k$ may be computed from

$$\tilde{e}_k = \sum_{j=0}^{\min[k,n]} e_j e_{k-j},$$

where the e_k are the elementary symmetric functions of the eigenvalues of $-A$.

These results provide recursive procedures for computing moments in the noncentral case. To end this section, though, we note that a second expression for the moments of q that also leads to a simple recursion may be obtained from the MGF, as follows. Let

$$\phi(t) = \mu'(I_n - tA)^{-1}\mu - \mu'\mu = \sum_{i=1}^{\infty} \eta_i t^i,$$

where $\eta_i = \mu' A^i \mu$, and define functions $a_{r,l}$ by the equation

$$a_{r,l} = [t^r] D(t)\phi(t)^l. \tag{24}$$

Note that $a_{r,0} = d_r(A)$, and that the lowest-order term in $\phi(t)^l$ is t^l, so that $a_{r,l} = 0$ for $l > r$. From equation (17) we have the following expression for the μ_k:

$$\mu_k = 2^k k! [t^k] D(t) \exp\left(\frac{\phi(t)}{2}\right) = 2^k k! \sum_{l=0}^{k} \frac{a_{k,l}}{l! 2^l}.$$

That is,

$$\tilde{d}_k = \sum_{l=0}^{k} \frac{a_{k,l}}{l! 2^l}. \tag{25}$$

Now, it is easy to see that the $a_{k,l}$ themselves satisfy a very simple recurrence relation, which induces a simple recursion for the moments. To see this, simply note that

$$D(t)\phi(t)^l = \left[D(t)\phi(t)^{l-1}\right]\phi(t) = \left(\sum_{j=0}^{\infty} a_{j,l-1} t^j\right)\left(\sum_{i=1}^{\infty} \eta_i t^i\right).$$

Equating coefficients of like powers of t on both sides, and taking account of the fact that $a_{r,l} = 0$ for $r < l$, gives the following recursion for the $a_{r,l}$.

LEMMA 3. *For $l \geq 1$, the functions $a_{r,l}$ defined by (24) satisfy the recursion:*

$$a_{r,l} = \sum_{j=1}^{r-l+1} \eta_j a_{r-j,l-1}, \tag{26}$$

where $\eta_j = \mu' A^j \mu$ and we have the initial conditions $a_{r,0} = d_r(A)$.

These results provide an alternative procedure for the calculation of the noncentral moments. The functions $a_{r,l}$ will also be useful later in Section 5 where some low-order cases are given explicitly.

3.2 Super-short Recursion

While the short recursion for computing $\tilde{d}_k$ is numerically efficient, it is not numerically stable because the coefficients in the short recursion have different signs. In contrast, the long recursion is given by

$$\tilde{d}_k = \frac{1}{2k}\sum_{j=1}^{k}[\mathrm{tr}(A^j) + j\mu' A^j \mu]\tilde{d}_{k-j} = \frac{1}{2k}\sum_{j=1}^{k}\sum_{i=1}^{n}(\lambda_i^j + j\delta_i\lambda_i^j)\tilde{d}_{k-j}, \tag{27}$$

where λ_i's are the eigenvalues of A and $\delta_i = (h_i'\mu)^2$, with h_i being the eigenvector of A corresponding to the eigenvalue λ_i. It can be seen that when A is positive semi-definite, the coefficients in the long recursion are always positive and hence the long recursion is numerically stable.

We now present a new recursive algorithm on $\tilde{d}_k$ that is even shorter than the short recursion yet retains the numerical stability of the long recursion. The new algorithm is motivated by the work of Brown (1986), which provides an efficient method for computing the weights in an infinite series representation of the cumulative distribution function of q. It is obtained by exchanging the two summations in (27)

$$\tilde{d}_k = \frac{1}{2k}\sum_{i=1}^{n}\sum_{j=1}^{k}(\lambda_i^j + j\delta_i\lambda_i^j)\tilde{d}_{k-j} = \frac{1}{2k}\sum_{i=1}^{n}(u_{k,i} + v_{k,i}), \tag{28}$$

where

$$\begin{aligned} u_{k,i} &= \sum_{j=1}^{k}\lambda_i^j\tilde{d}_{k-j}, \\ v_{k,i} &= \delta_i\sum_{j=1}^{k} j\lambda_i^j\tilde{d}_{k-j}. \end{aligned}$$

It can be readily verified that $u_{k,i}$ and $v_{k,i}$ have the following recursions of length one:

$$u_{k,i} = \lambda_i\left(\tilde{d}_{k-1} + \sum_{j=2}^{k}\lambda_i^{j-1}\tilde{d}_{k-j}\right) = \lambda_i(\tilde{d}_{k-1} + u_{k-1,i}), \tag{29}$$

$$v_{k,i} = \delta_i\sum_{j=1}^{k}\lambda_i^j\tilde{d}_{k-j} + \lambda_i\delta_i\sum_{j=2}^{k}(j-1)\lambda_i^{j-1}\tilde{d}_{k-j} = \delta_i u_{k,i} + \lambda_i v_{k-1,i}, \tag{30}$$

with the initial conditions $u_{0,i} = 0$ and $v_{0,i} = 0$.

We call (28) and the corresponding recursions in (29) and (30) the super-short recursion for $\tilde{d}_k$. This is because in order to compute $\tilde{d}_k$ using this new recurrence algorithm, we only need to store $\tilde{d}_{k-1}$. There is no need to store $\tilde{d}_0$ to $\tilde{d}_{k-1}$ as in the long recursion or $\tilde{d}_{k-2n}$ to $\tilde{d}_{k-1}$ as in the short recursion. While we need $2n$ auxiliary variables $u_{k,i}$ and $v_{k,i}$ for the super-short recursion to proceed, they can be updated with a recursion of length one, so we only need $2n$ elements of memory space. This compares favorably even with the short recursion which requires $6n$ elements of memory space ($2n$ elements of $\tilde{p}_i$, $2n$ elements for $\tilde{e}_i$ and $2n$ elements for $\tilde{d}_{k-2n}$ to $\tilde{d}_{k-1}$). As far as efficiency is concerned, each update of $\tilde{d}_k$ in the short recursion requires $8n$ arithmetic operations whereas only $7n + 1$ arithmetic operations are required for the super-short recursion. Finally, in terms of numerical stability, $u_{k,i}$, $v_{k,i}$ as well as their corresponding updating coefficients are all positive when $\lambda_i > 0$. As a result, the super-short recursion has no cancellation error and it is numerically just as stable as the long recursion. In summary, the super-short recursion either dominates or is comparable with the long and short recursions along every aspect (memory space, speed, and numerical stability), so we strongly recommend the super-short recursion for the computation of $\tilde{d}_k$.

Similarly, a super-short recursion can be obtained for the $a_{r,l}$'s defined in Lemma 3. In order to do that, we rewrite (26) as

$$a_{r,l} = \sum_{j=1}^{r-l+1} \sum_{i=1}^{n} \delta_i \lambda_i^j a_{r-j,l-1} = \sum_{i=1}^{n} \delta_i \sum_{j=1}^{r-l+1} \lambda_i^j a_{r-j,l-1} = \sum_{i=1}^{n} \delta_i w_{r,i}, \tag{31}$$

where

$$w_{r,i} = \sum_{j=1}^{r-l+1} \lambda_i^j a_{r-j,l-1} = \lambda_i (a_{r-1,l-1} + w_{r-1,i}) \tag{32}$$

has a recursion of length one with initial conditions $w_{0,i} = 0$.

3.3 Special Cases: Repeated Eigenvalues and the Partially Central Case

The recurrence relations for moments given so far hold for any values of the eigenvalues of A, and any value of μ. However, some further improvement is possible if either some eigenvalues of A occur with multiplicity greater than one, and/or the noncentrality present is of dimension lower than n. To see this, first let $A = H\Lambda H'$, where $\Lambda = \mathrm{Diag}(\lambda_1, \cdots, \lambda_n)$ is a diagonal matrix containing the eigenvalues of A, and $H = [h_1, \ldots, h_n]$ is a matrix of the corresponding eigenvectors. Using this decomposition, we can write

$$q = z'Az = z'H\Lambda H'z = \tilde{z}'\Lambda\tilde{z},$$

where $\tilde{z} = H'z \sim N(H'\mu, I_n) = N(\tilde{\mu}, I_n)$, say.

Now, suppose that the eigenvalues λ_i are not distinct, but that the $s \leq n$ distinct eigenvalues λ_i occur with multiplicities n_i, where $n = \Sigma_{i=1}^{s} n_i$. Letting $\tilde{z}_i \sim N(\tilde{\mu}_i, I_{n_i})$ denote the sub-vector of $\tilde{z}$ associated with λ_i, we set $\delta_i = \tilde{\mu}_i'\tilde{\mu}_i$ for $i = 1, \ldots, s$ (generalizing the earlier definition). This setup occurs naturally in the context of much-studied statistics of the form

$$q = \lambda_1 q_1 + \cdots + \lambda_s q_s,$$

where the q_i are independent noncentral $\chi^2_{n_i}(\delta_i)$ random variables (see Ruben, 1962; Press, 1966). We wish to consider the case where, in addition to the possibility of repeated eigenvalues, some of the noncentrality parameters δ_i may also vanish. Without loss of generality, we assume that $\delta_i \neq 0$ for $i = 1, \ldots, r$, and $\delta_i = 0$ for $i = r+1, \ldots, s$.

With these assumptions and notation the MGF of $q/2$ in (17) becomes:

$$\tilde{D}(t) = \left[\prod_{i=1}^{s}(1 - t\lambda_i)^{-\frac{n_i}{2}}\right] \exp\left(\frac{1}{2}\sum_{i=1}^{r}\frac{t\delta_i\lambda_i}{1 - t\lambda_i}\right).$$

Thus, defining $\tilde{P}(t)$ as in (18), we have

$$\tilde{P}(t) = \frac{1}{2}\left[\sum_{i=1}^{s}\frac{tn_i\lambda_i}{1 - t\lambda_i} + \sum_{i=1}^{r}\frac{t\delta_i\lambda_i}{(1 - t\lambda_i)^2}\right] = \frac{1}{2}\sum_{k=1}^{\infty}\left(\sum_{i=1}^{s} n_i\lambda_i^k + k\sum_{i=1}^{r}\delta_i\lambda_i^k\right)t^k.$$

Hence, in this case,

$$\tilde{p}_k = \frac{1}{2}\left(\sum_{i=1}^{s} n_i\lambda_i^k + k\sum_{i=1}^{r}\delta_i\lambda_i^k\right), \tag{33}$$

and the recursion (22) applies with these $\tilde{p}_k$. However, as before, $\tilde{P}(t)$ is a rational polynomial with both denominator polynomial

$$\tilde{E}(t) = \left(\prod_{i=1}^{r}(1 - t\lambda_i)^2\right)\left(\prod_{i=r+1}^{s}(1 - t\lambda_i)\right) = \sum_{k=0}^{r+s}\tilde{e}_k t^k, \tag{34}$$

say, and numerator polynomial

$$\tilde{G}(t) = \frac{1}{2}\left[\left(\prod_{i=1}^{r}(1 - t\lambda_i)\right)\left(\sum_{i=1}^{s} tn_i\lambda_i\prod_{\substack{j=1\\j\neq i}}^{s}(1 - t\lambda_j)\right) + \left(\prod_{i=r+1}^{s}(1 - t\lambda_i)\right)\left(\sum_{i=1}^{r} t\delta_i\lambda_i\prod_{\substack{j=1\\j\neq i}}^{r}(1 - t\lambda_j)^2\right)\right]$$

of finite degree. Applying Lemma 1, $\tilde{d}_k$ can then be computed from the short recursion given in (7), with the $\tilde{p}_k$ as given in (33), and the $\tilde{e}_k$ as defined by (34). The recursion has length at most $r + s$ (rather than $2n$ as in the case where $r = s = n$).

Remark 4. *To illustrate the improvement afforded by the short recursion, we consider an example with $A = I_n$, so that $q = z'z \sim \chi^2_n(\delta)$ is a noncentral chi-square variate. Using (22), we obtain the following recurrence relation for the $\mu_k \equiv \mathbb{E}[q^k]$:*

$$\mu_k = \frac{1}{2k}\sum_{i=1}^{k}(k-i+1)_i 2^i (n+i\delta)\mu_{k-i} \quad \text{for } k > 0.$$

However, applying the shorter recursion (with $r = s = 1$), we obtain the following two-term recurrence relation:

$$\mu_k = (4k+\delta+n-4)\mu_{k-1} - 2(k-1)(2k+n-4)\mu_{k-2} \quad \text{for } k > 1,$$

with the initial conditions $\mu_0 = 1$ and $\mu_1 = n + \delta$. This recurrence relation is also shorter than the one provided by Withers and Nadarajah (2007).[4]

Similarly, the super-short recursion of $\tilde{d}_k$ can also be improved when there are repeated eigenvalues and/or some of the noncentrality parameters are zero. Using $\tilde{p}_k$ in (33), we can easily show that

$$\tilde{d}_k = \frac{1}{2k}\left(\sum_{i=1}^{s} n_i u_{k,i} + \sum_{i=1}^{r} v_{k,i}\right),$$

with $u_{k,i}$ and $v_{k,i}$ as defined in (29) and (30) respectively. Unlike the general case, which requires n elements of $u_{k,i}$'s and n elements of $v_{k,i}$'s, we now only need s of the $u_{k,i}$'s and r of the $v_{k,i}$'s.

4. SECOND APPLICATION: PRODUCT MOMENTS OF SEVERAL QUADRATIC FORMS

Let A_1 to A_r be r $n \times n$ real symmetric matrices, and let $q_i = z'A_i z$, $i = 1, \ldots, r$, denote the variates of interest, with $z \sim N(\mu, I_n)$. Explicit expressions for the product moments $\mu_{\boldsymbol{\kappa}}$ have, at least for low-order cases, long been available in the statistics literature. However, most of the existing work expresses $\mu_{\boldsymbol{\kappa}}$ as a sum of various products of the traces of $|\boldsymbol{\kappa}|$ matrices related to A_i's and are extremely inefficient for computational purposes. Kan (2008) provides a review of this literature, and a discussion of why current methods are impractical for computing $\mu_{\boldsymbol{\kappa}}$ even for moderately large $|\boldsymbol{\kappa}|$. See also Mathai and Provost (1992) for an excellent review of quadratic forms in random variables.

For the central normal case, i.e., $z \sim N(0_n, I_n)$, $\mu_{\boldsymbol{\kappa}}$ can be expressed in terms of the normalized Davis polynomials $d_{\boldsymbol{\kappa}}$ as follows:

$$\mu_{\boldsymbol{\kappa}} = 2^k \boldsymbol{\kappa}! d_{\boldsymbol{\kappa}}(A_1, \ldots, A_r),$$

and the results in Section 2.3 give both long and short recursions for their computation.

For both the central and noncentral normal case, Kan (2008) presents an efficient method for computing $\mu_{\boldsymbol{\kappa}}$. Proposition 4 of Kan (2008) shows that

$$\mu_{\boldsymbol{\kappa}} = \frac{1}{k!} \sum_{\mathbf{0} \leq \boldsymbol{\nu} \leq \boldsymbol{\kappa}} (-1)^{|\boldsymbol{\nu}|} \binom{\boldsymbol{\kappa}}{\boldsymbol{\nu}} E[(z' B_{\boldsymbol{\nu}} z)^k], \tag{35}$$

where $B_{\boldsymbol{\nu}} = \sum_{i=1}^r \left(\frac{k_i}{2} - \nu_i\right) A_i$, $k = |\boldsymbol{\kappa}|$, and

$$\binom{\boldsymbol{\kappa}}{\boldsymbol{\nu}} = \frac{\boldsymbol{\kappa}!}{\boldsymbol{\nu}!(\boldsymbol{\kappa} - \boldsymbol{\nu})!}.$$

As noted in Kan (2008), half of the terms on the right hand side of (35) are repeated, so one can compute $\mu_{\boldsymbol{\kappa}}$ by computing the k-th moments of $\lfloor \prod_{i=1}^r (k_i + 1)/2 \rfloor$ different quadratic forms in z, where $\lfloor x \rfloor$ stands for the integral part of x. Kan (2008) suggests using the recurrence relation (22) to compute $E[(z' B_{\boldsymbol{\nu}} z)^k]$. With the super-short recurrence algorithm given in (28)–(30), we can now significantly improve the computation speed of $E[(z' B_{\boldsymbol{\nu}} z)^k]$, especially when k is large. Although, with the super-short recurrence relation on $E[(z' B_{\boldsymbol{\nu}} z)^k]$, (35) is quite efficient, there are circumstances where we still prefer to use a recurrence relation on $\mu_{\boldsymbol{\kappa}}$. This is particularly so if we need to compute not just a single $\mu_{\boldsymbol{\kappa}}$ but all $\mu_{\boldsymbol{\nu}}$ with $\mathbf{0} \leq \boldsymbol{\nu} \leq \boldsymbol{\kappa}$.

4.1 Long and Short Recursions for the Noncentral Case

The joint MGF of $(q_1, \ldots, q_r)$ is given by:

$$M_{q_1,\ldots,q_r}(\boldsymbol{\tau}) = |I_n - 2A(\boldsymbol{\tau})|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - 2A(\boldsymbol{\tau}))^{-1}\mu}{2} - \frac{\mu'\mu}{2}\right) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} \frac{\mu_{\boldsymbol{\kappa}}}{\boldsymbol{\kappa}!} \boldsymbol{\tau}^{\boldsymbol{\kappa}},$$

where $A(\boldsymbol{\tau}) = \tau_1 A_1 + \cdots + \tau_r A_r$ (see, e.g., Phillips, 1980, eqn. (30)).

Let

$$\tilde{D}(\boldsymbol{t}) = |I_n - A(\boldsymbol{t})|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - A(\boldsymbol{t}))^{-1}\mu}{2} - \frac{\mu'\mu}{2}\right) = \sum_{k=0}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} \tilde{d}_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{36}$$

where $A(\boldsymbol{t}) = t_1 A_1 + \cdots + t_r A_r$. The product moments themselves are given by:

$$\mu_{\boldsymbol{\kappa}} = \mathbb{E}[q_1^{k_1} q_2^{k_2} \cdots q_r^{k_r}] = 2^{|\boldsymbol{\kappa}|} \boldsymbol{\kappa}! \tilde{d}_{\boldsymbol{\kappa}}.$$

Defining $\tilde{P}(\boldsymbol{t})$ as in (9), we have

$$\tilde{P}(\boldsymbol{t}) = \frac{1}{2} \sum_{k=1}^{\infty} [\mathrm{tr}(A(\boldsymbol{t})^k) + k\mu' A(\boldsymbol{t})^k \mu] = \sum_{k=1}^{\infty} \sum_{|\boldsymbol{\kappa}|=k} \tilde{p}_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{37}$$

where, for $k = |\boldsymbol{\kappa}|$,

$$\tilde{p}_{\boldsymbol{\kappa}} = \frac{1}{2} [\boldsymbol{t}^{\boldsymbol{\kappa}}][\mathrm{tr}(A(\boldsymbol{t})^k) + k\mu' A(\boldsymbol{t})^k \mu].$$

We can also write $\tilde{P}(\boldsymbol{t})$ in the form

$$\tilde{P}(\boldsymbol{t}) = \frac{1}{2}\mathrm{tr}(A(\boldsymbol{t})(I_n - A(\boldsymbol{t}))^{-1}) + \frac{1}{2}\mu'(I_n - A(\boldsymbol{t}))^{-1} A(\boldsymbol{t})(I_n - A(\boldsymbol{t}))^{-1}\mu,$$

so it is clear that this satisfies the hypotheses of Lemma 2, with $m = 2n$. Defining

$$\tilde{E}(\boldsymbol{t}) = |I_n - A(\boldsymbol{t})|^2 = \sum_{k=0}^{2n} \sum_{|\boldsymbol{\kappa}|=k} \tilde{e}_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}}, \tag{38}$$

we see that both $\tilde{E}(\boldsymbol{t})$ and

$$\tilde{G}(\boldsymbol{t}) = \tilde{E}(\boldsymbol{t})\tilde{P}(\boldsymbol{t}) = \sum_{k=1}^{2n} \sum_{|\boldsymbol{\kappa}|=k} \tilde{g}_{\boldsymbol{\kappa}} \boldsymbol{t}^{\boldsymbol{\kappa}} \tag{39}$$

are polynomials of degree $2n$ in $\boldsymbol{t}$.

In view of the results in Section 2.3, we can use (11), (12), and (14) to obtain the following three apparently new recurrence relations for the functions $\tilde{d}_{\boldsymbol{\kappa}}$ defined by (36).

THEOREM 2. *Using $\tilde{p}_{\boldsymbol{\kappa}}$, $\tilde{e}_{\boldsymbol{\kappa}}$ and $\tilde{g}_{\boldsymbol{\kappa}}$ as defined by (37), (38) and (39), the $\tilde{d}_{\boldsymbol{\kappa}}$ in (36) can be* *recursively obtained from any of the following recurrence relations:*

$$\tilde{d}_{\boldsymbol{\kappa}} = \frac{1}{k}\sum_{j=1}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}}\tilde{p}_{\boldsymbol{\nu}}\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{40}$$

$$\tilde{d}_{\boldsymbol{\kappa}} = \frac{1}{k_l}\sum_{j=1}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}}\frac{\nu_l}{j}\tilde{p}_{\boldsymbol{\nu}}\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}} \quad \text{when } k_l > 0, \tag{41}$$

$$\tilde{d}_{\boldsymbol{\kappa}} = \sum_{j=1}^{\min[k,2n]}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}}\left(\frac{c_{\boldsymbol{\nu}}}{k}-\tilde{e}_{\boldsymbol{\nu}}\right)\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{42}$$

where $c_{\boldsymbol{\nu}} = |\boldsymbol{\nu}|\tilde{e}_{\boldsymbol{\nu}} + \tilde{g}_{\boldsymbol{\nu}}$*, and we have the initial condition* $\tilde{d}_{\mathbf{0}} = 1$*.*

Remark 5. *(41) can also be obtained by using the recurrence relation between moments and cumulants for multivariate distributions (see, for example, Smith (1995, Eq.10)). Bao and Ullah (2010) use a different method to obtain a recurrence relation on* $\mu_{\boldsymbol{\kappa}}$*, and their formula can also be obtained by using (41).*

To use the above recursive algorithms to compute $\tilde{d}_{\boldsymbol{\kappa}}$, we need to first obtain the coefficients $\tilde{p}_{\boldsymbol{\kappa}}$ and $\tilde{e}_{\boldsymbol{\kappa}}$. When n is very small, we can use a symbolic mathematics program to compute $\tilde{p}_{\boldsymbol{\kappa}}$ and $\tilde{e}_{\boldsymbol{\kappa}}$. 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 $\tilde{p}_{\boldsymbol{\kappa}}$ and $\tilde{e}_{\boldsymbol{\kappa}}$. HKW provide an efficient method for computing the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ in the expansion of $\mathrm{tr}(A(\boldsymbol{t})^{|\boldsymbol{\kappa}|})$, which then allows us to easily obtain the $\tilde{e}_{\boldsymbol{\kappa}}$. In addition, their algorithm can be extended in a straightforward manner to compute the coefficients of $\boldsymbol{t}^{\boldsymbol{\kappa}}$ in the expansion of $\mu' A(\boldsymbol{t})^{|\boldsymbol{\kappa}|}\mu$. Therefore, both the $\tilde{e}_{\boldsymbol{\kappa}}$ and $\tilde{p}_{\boldsymbol{\kappa}}$ can be efficiently computed by the methods described in HKW.[5]

Compared with the long recurrence relations (40) and (41) which are in terms of the $\tilde{p}_{\boldsymbol{\kappa}}$, the short recurrence relation (42) only involves the $\tilde{e}_{\boldsymbol{\kappa}}$ and $\tilde{g}_{\boldsymbol{\kappa}}$, and these vanish for $|\boldsymbol{\kappa}| > 2n$. Regardless of the value of $\boldsymbol{\kappa}$, (42) suggests that $\tilde{d}_{\boldsymbol{\kappa}}$ can be expressed as a linear combination of at most $(2n+r)!/[(2n)!r!]-1$ other $\tilde{d}_{\boldsymbol{\nu}}$'s with $\boldsymbol{\nu} < \boldsymbol{\kappa}$. Therefore, (42) can provide a significant improvement over (40) and (41) when k_i's are large.

4.2 Super-short Recursion

Similar to the univariate case, the short recursion is numerically unstable for computing $\tilde{d}_{\boldsymbol{\kappa}}$ even though it is efficient. This is because the coefficients $c_{\boldsymbol{\nu}}/k - \tilde{e}_{\boldsymbol{\nu}}$ in (42) generally take different signs, leading to cancellation error. In contrast, the following Lemma shows that when A_1 to A_r are positive semi-definite, then $\tilde{p}_{\boldsymbol{\nu}}$ for the long recursions in (40) and (41) are nonnegative, and hence the long recursions are numerically stable.

LEMMA 4. *Suppose A_1 to A_r are positive semi-definite. We have*

$$\tilde{p}_{\boldsymbol{\kappa}} = \frac{1}{2}[\boldsymbol{t}^{\boldsymbol{\kappa}}][\mathrm{tr}(A(\boldsymbol{t})^k) + k\mu' A(\boldsymbol{t})^k \mu] \geq 0.$$

The proof of Lemma 4 is given in the Appendix.

To overcome the numerical stability issue, we provide a multivariate generalization of the super-short recursion of $\tilde{d}_k$ in Section 3.2 for $\tilde{d}_{\boldsymbol{\kappa}}$. We first introduce a matrix $G_{\boldsymbol{\kappa}}$ and a vector $h_{\boldsymbol{\kappa}}$, defined as

$$G_{\boldsymbol{\kappa}} = \sum_{j=1}^{k} \sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} [\boldsymbol{t}^{\boldsymbol{\nu}}] A(\boldsymbol{t})^j d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}, \tag{43}$$

$$h_{\boldsymbol{\kappa}} = \left(\sum_{j=1}^{k} j \sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} [\boldsymbol{t}^{\boldsymbol{\nu}}] A(\boldsymbol{t})^j d_{\boldsymbol{\kappa}-\boldsymbol{\nu}} \right) \mu. \tag{44}$$

With $G_{\boldsymbol{\kappa}}$ and $h_{\boldsymbol{\kappa}}$ defined, we can now write (40) as

$$\tilde{d}_{\boldsymbol{\kappa}} = \frac{1}{k} \sum_{j=1}^{k} \sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} \tilde{p}_{\boldsymbol{\nu}} \tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}} = \frac{1}{2k}[\mathrm{tr}(G_{\boldsymbol{\kappa}}) + \mu' h_{\boldsymbol{\kappa}}]. \tag{45}$$

The key is to derive super-short recursions for $G_{\boldsymbol{\kappa}}$ and $h_{\boldsymbol{\kappa}}$. For $G_{\boldsymbol{\kappa}}$, we break it into two terms:

$$G_{\boldsymbol{\kappa}} = \sum_{\substack{|\boldsymbol{\nu}|=1,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} [\boldsymbol{t}^{\boldsymbol{\nu}}] A(\boldsymbol{t}) \tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}} + \sum_{j=2}^{k} \sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} [\boldsymbol{t}^{\boldsymbol{\nu}}] A(\boldsymbol{t})^j \tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}}. \tag{46}$$

Writing $\boldsymbol{\kappa}_{(i)} = [k_1, \ldots, k_{i-1},\ k_i - 1,\ k_{i+1}, \ldots, k_r]$, the first term can be written as

$$\sum_{\substack{|\boldsymbol{\nu}|=1,\\ \boldsymbol{\nu}\leq\boldsymbol{\kappa}}} [\boldsymbol{t}^{\boldsymbol{\nu}}] A(\boldsymbol{t}) \tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}} = \sum_{\substack{1\leq i\leq r,\\ k_i>0}} A_i \tilde{d}_{\boldsymbol{\kappa}_{(i)}},$$

and the second term can be written as

$$\begin{aligned}
\sum_{j=2}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j}\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}} &= \sum_{j=1}^{k-1}\sum_{\substack{|\boldsymbol{\nu}|=j+1,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j+1}\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}}\\
&= \sum_{\substack{1\le i\le r,\\ k_i>0}} A_i \sum_{j=1}^{k-1}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}_{(i)}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j}\tilde{d}_{\boldsymbol{\kappa}_{(i)}-\boldsymbol{\nu}}\\
&= \sum_{\substack{1\le i\le r,\\ k_i>0}} A_i G_{\boldsymbol{\kappa}_{(i)}}.
\end{aligned}$$

Combining the two terms, we have the following super-short recursion for $G_{\boldsymbol{\kappa}}$:

$$G_{\boldsymbol{\kappa}} = \sum_{\substack{1\le i\le r,\\ k_i>0}} A_i[\tilde{d}_{\boldsymbol{\kappa}_{(i)}} I_n + G_{\boldsymbol{\kappa}_{(i)}}], \tag{47}$$

with the initial condition of $G_{\mathbf{0}} = 0_{n\times n}$. Similarly, a super-short recursion for $h_{\boldsymbol{\kappa}}$ can be obtained as follows:

$$\begin{aligned}
h_{\boldsymbol{\kappa}} &= \left(\sum_{j=1}^{k}\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j}d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}\right)\mu + \left(\sum_{j=2}^{k}(j-1)\sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j}d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}\right)\mu\\
&= G_{\boldsymbol{\kappa}}\mu + \left(\sum_{j=1}^{k-1} j \sum_{\substack{|\boldsymbol{\nu}|=j+1,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j+1}d_{\boldsymbol{\kappa}-\boldsymbol{\nu}}\right)\mu\\
&= G_{\boldsymbol{\kappa}}\mu + \sum_{\substack{1\le i\le r,\\ k_i>0}} A_i \left(\sum_{j=1}^{k-1} j \sum_{\substack{|\boldsymbol{\nu}|=j,\\ \boldsymbol{\nu}\le\boldsymbol{\kappa}_{(i)}}}[\boldsymbol{t}^{\boldsymbol{\nu}}]A(\boldsymbol{t})^{j}d_{\boldsymbol{\kappa}_{(i)}-\boldsymbol{\nu}}\right)\mu\\
&= G_{\boldsymbol{\kappa}}\mu + \sum_{\substack{1\le i\le r,\\ k_i>0}} A_i h_{\boldsymbol{\kappa}_{(i)}},
\end{aligned} \tag{48}$$

with the initial condition of $h_{\mathbf{0}} = 0_n$. Since (45), (47), and (48) allow us to compute $d_{\boldsymbol{\kappa}}$ from $d_{\boldsymbol{\kappa}_{(i)}}$, $i = 1, \dots, r$, and the length of recursion only depends on r but not n or $|\boldsymbol{\kappa}|$, we call this the super-short recursion for $\tilde{d}_{\boldsymbol{\kappa}}$.[6]

Note that regardless of $\boldsymbol{\kappa}$, the super-short recursion requires only at most r matrix-matrix multiplications and $r+1$ matrix-vector multiplications to compute $\tilde{d}_{\boldsymbol{\kappa}}$ from $d_{\boldsymbol{\kappa}_{(i)}}$. Therefore, it takes $rn^3 + O(n^2)$ arithmetic operations for the super-short recursion to compute a new $\tilde{d}_{\boldsymbol{\kappa}}$. In contrast, the short recursion typically requires $4(2n+r)!/[r!(2n)!]$ arithmetic operations to compute a new $\tilde{d}_{\boldsymbol{\kappa}}$. When $r \geq 3$, the super-short recursion is far more efficient than the short recursion. Even for $r = 2$, the short recursion tends to be less efficient than the super-short recursion because we need to pre-compute $\tilde{p}_{\boldsymbol{\nu}}$ and $\tilde{g}_{\boldsymbol{\nu}}$ for $|\boldsymbol{\nu}| \leq 2n$ for the short recursion to start, and this can be very time consuming. In terms of memory space, the super-short recursion requires storing $G_{\boldsymbol{\nu}}$, $h_{\boldsymbol{\nu}}$ and $\tilde{d}_{\boldsymbol{\nu}}$ for $|\boldsymbol{\nu}| = k-1$ in order to compute $\tilde{d}_{\boldsymbol{\kappa}}$ with $|\boldsymbol{\kappa}| = k$. In contrast, the short recursion only requires storing $c_{\boldsymbol{\nu}}$, $\tilde{e}_{\boldsymbol{\nu}}$ and $\tilde{d}_{\boldsymbol{\kappa}-\boldsymbol{\nu}}$ for $|\boldsymbol{\nu}| \leq 2n$, and it can have an advantage over the super-short recursion, especially when $|\boldsymbol{\kappa}|$ is large. However, the memory space requirement for the super-short recursion can be substantially reduced in many situations. For example, if we wish to compute $\tilde{d}_{5,100}$, then we only need to have six G matrices and six h vectors for the recursion to finish.[7] There is no need to have 106 G's and 106 h's unless we need to compute all $\tilde{d}_{i,j}$'s with $i+j = 105$. Finally, in terms of numerical stability, we can easily show that when A_1 to A_r are positive semi-definite, $G_{\boldsymbol{\kappa}}$ and the matrix in $h_{\boldsymbol{\kappa}}$ are also positive semi-definite. As a result, there is no cancellation error in the super-short recursion and it is numerically just as stable as the long recursion. In summary, the super-short recursion may require more memory space than the short recursion in the multivariate case, but for numerical stability and efficiency, we still recommend its use for the computation of $\tilde{d}_{\boldsymbol{\kappa}}$.

5. FINAL APPLICATION: RATIOS OF POWERS OF QUADRATIC FORMS

In this section we give results for the more complicated problem of evaluating expectations of the form

$$\mu_s^r = \mathbb{E}\left[\frac{(z'Az)^r}{(z'Bz)^s}\right], \tag{49}$$

where A is a symmetric $n \times n$ matrix, B is a positive definite $n \times n$ matrix, $z \sim N(\mu, I_n)$, r is a nonnegative integer and s is a positive real number. We shall assume throughout that the largest eigenvalue of A is positive (i.e., A is not negative definite). If A is negative definite the results to follow can be applied to $(-1)^r\mu_s^r$, rather than μ_s^r itself. It is easy to show that the expectation in (49) exists if and only if $\frac{n}{2} + r > s$, and we shall assume that this condition is satisfied throughout this section.

Many estimators in statistics take the form of ratio of quadratic form in normal random variables. As a result, the problem of computing expectations of the form given in (49) has attracted the attention of many researchers. Most of the results in this literature are based on a lemma due to Sawa (1972), and present formulae that take the form of a one-dimensional integral that must be evaluated numerically.[8] For the development of this type of formula, see the excellent papers of Magnus (1986) and Meng (2005) and the references therein. We shall briefly describe the result here before presenting our own results.

Let $B = P\Lambda P'$, where Λ is a diagonal matrix of the eigenvalues of B, and P is a matrix of the corresponding eigenvectors. By combining the results of Theorem 6 of Magnus (1986) and Lemma 1 of Meng (2005), we obtain

$$\mu_s^r = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} |\Delta| \exp\left(\frac{\mu' P[(I_n + 2t\Lambda)^{-1} - I_n] P'\mu}{2} \right) E[(w'Rw)^r] \mathrm{d}t, \tag{50}$$

where $\Delta = (I_n + 2t\Lambda)^{-\frac{1}{2}}$, $R = \Delta P' A P \Delta$, and $w \sim N(\Delta P'\mu, I_n)$. Currently, this is the only practical method that can be used for numerical evaluation of μ_s^r. However, there are two problems associated with the use of this formula. The first is in the computation of $\mathbb{E}[(w'Rw)^r]$, which we have discussed in Section 3.1 above. As we have seen, both explicit formulae for this term, and efficient recursions for evaluating it, are available. However, because R is a function of t, this expectation must be evaluated many times. The second problem is that it is difficult to control the accuracy of the numerical integration: there is no general result in the literature that allows us to analyze and control the errors in the numerical integration of (50). For these reasons, we seek here a more efficient method for evaluating the μ_s^r based on the results in Section 2. Before doing so, we briefly describe the exact formulae that are available.

5.1 Explicit Formulae

Smith (1989) provides a very different expression for the μ_s^r. He shows that μ_s^r can be expressed as a doubly infinite series involving the top-order invariant polynomials $d_{\boldsymbol{\kappa}}$. In our notation, his expression is:

$$\mu_s^r = \frac{2^{r-s}\beta^s r! \Gamma\left(\frac{n}{2} + r - s\right) e^{-\frac{\delta}{2}}}{\Gamma\left(\frac{n}{2} + r\right)} \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{(s)_j \left(\frac{n}{2} + r - s\right)_k}{2^k \left(\frac{1}{2}\right)_k \left(\frac{n}{2} + r\right)_{j+k}} d_{r,j,k}\left(A, I_n - \beta B, \mu\mu'\right), \tag{51}$$

reducing to

$$\mu_s^r = \frac{2^{r-s}\beta^s r! \Gamma\left(\frac{n}{2} + r - s\right)}{\Gamma\left(\frac{n}{2} + r\right)} \sum_{j=0}^\infty \frac{(s)_j}{\left(\frac{n}{2} + r\right)_j} d_{r,j}\left(A, I_n - \beta B\right), \tag{52}$$

when $\mu = 0_n$. Here, $\delta = \mu'\mu$, and β is a constant that satisfies $0 < \beta < 2/b_{\max}$, with $b_{\max}$ the largest eigenvalue of B.[9] When $B = I_n$ we may choose $\beta = 1$, so that the sum on j in (51) vanishes, and we have the simpler result

$$\mu_s^r = \frac{2^{r-s} r! \Gamma\left(\frac{n}{2} + r - s\right) e^{-\frac{\delta}{2}}}{\Gamma\left(\frac{n}{2} + r\right)} \sum_{k=0}^{\infty} \frac{\left(\frac{n}{2} + r - s\right)_k}{2^k \left(\frac{1}{2}\right)_k \left(\frac{n}{2} + r\right)_k} d_{r,k}\left(A, \mu\mu'\right). \tag{53}$$

Finally, when both $B = I_n$ and $\mu = 0_n$ we have

$$\mu_s^r = \frac{2^{r-s} r! \Gamma(\frac{n}{2} + r - s)}{\Gamma(\frac{n}{2} + r)} d_r\left(A\right),$$

a multiple of the corresponding moment of q dealt with in Section 3.1 above. Smith (1993) makes an attempt to use these formulae to compute the moments for the case $r = 1$, and with either $\mu = 0_n$ or $B = I_n$, but there has been great difficulty in using (51) for the general case.

Recently, HKW have given an efficient recursive algorithm for computing the top-order invariant polynomials. In principle, their algorithm can be used to compute the $d_{r,j,k}(A, I_n - \beta B, \mu\mu')$, and the moments approximated by truncating the double series in (51) at some suitable point. However, this process is extremely inefficient. As a result, HKW focus only on the simpler special case of $\mu = 0_n$, when only a singly infinite series of top-order invariant polynomials with two matrix arguments is involved. In addition, for the case $\mu = 0_n$, HKW give an upper bound on the approximation error when truncating the infinite series at $j = M$. For the general case of $\mu \neq 0_n$, it is a significant challenge to bound this truncation error.

5.2 New Formula for μ_s^r

To address these difficulties, in this section we provide a new formula that greatly simplifies the evaluation of the μ_s^r for the general case when $\mu \neq 0_n$. Unlike Smith's formula, our new expression involves only a singly infinite series, and the coefficients are easily obtained using various recurrence relations. In addition, we also provide error control, so we can compute the expectation up to any desired level of accuracy.

The results we develop are based on the following formal representation for μ_s^r — which is also the basis of the formula (50) (see Sawa (1972) or Cressie, Davis, Folks, and Policello (1981)):

$$\mu_s^r = \frac{r![t^r]}{\Gamma(s)} \int_0^{\infty} x^{s-1} M_{q_1,q_2}(t, -x) \mathrm{d}x,$$

where $M_{q_1,q_2}(t_1,t_2)$ is the joint moment generating function of $q_1 = z'Az$ and $q_2 = z'Bz$ when $z \sim N(\mu, I_n)$, i.e.,

$$M_{q_1,q_2}(t_1,t_2) = |I_n - 2t_1 A - 2t_2 B|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - 2t_1 A - 2t_2 B)^{-1}\mu}{2} - \frac{\delta}{2}\right),$$

where $\delta = \mu'\mu$. Our starting point is thus the following integral expression for μ_s^r:

$$\mu_s^r = \frac{r![t^r]}{\Gamma(s)} \int_0^\infty x^{s-1} |I_n - 2tA + 2xB|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - 2tA + 2xB)^{-1}\mu}{2} - \frac{\delta}{2}\right) \mathrm{d}x.$$

We discuss the existence of the integral as necessary below. For convenience later we transform to $y = x/\beta$ in the integral, with β a positive constant to be chosen. This leads to the following expression for μ_s^r:

$$\mu_s^r = \frac{\beta^s r![t^r]}{\Gamma(s)} \int_0^\infty y^{s-1} |I_n - 2tA + 2y\beta B|^{-\frac{1}{2}} \exp\left(\frac{\mu'(I_n - 2tA + 2y\beta B)^{-1}\mu}{2} - \frac{\delta}{2}\right) \mathrm{d}y. \tag{54}$$

Our results are obtained by rewriting the matrix $I_n - 2tA + 2y\beta B$ as:

$$I_n - 2tA + 2y\beta B = (1+2y)\left(I_n - \frac{2t}{1+2y}A - \frac{2y}{1+2y}\tilde{B}\right), \tag{55}$$

where $\tilde{B} = I_n - \beta B$. Define, for fixed μ, functions $h_{i,j}(A_1, A_2)$ by the generating function[10]

$$\begin{aligned} H_{A_1,A_2}(t_1,t_2) &= |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} \exp\left(\frac{(1-t_2)\mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu}{2} - \frac{\mu'\mu}{2}\right) \\ &= \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} h_{i,j}(A_1,A_2) t_1^i t_2^j, \end{aligned} \tag{56}$$

Transforming now to $b = 2y/(1+2y)$ in (55), the integrand in (54) has the form

$$2^{-s} b^{s-1} (1-b)^{\frac{n}{2}-s-1} \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} [2t(1-b)]^i b^j h_{i,j}(A, \tilde{B}),$$

so that the coefficient of t^r in the expansion of the integrand is

$$2^{r-s} b^{s-1} (1-b)^{\frac{n}{2}+r-s-1} \sum_{j=0}^{\infty} b^j h_{r,j}(A, \tilde{B}).$$

We show in the Appendix that term-by-term integration can be justified when $\frac{n}{2} + r > s$ and $0 < \beta < 2/b_{\max}$. We may therefore state the result that follows.

THEOREM 3. *For (r,s) satisfying $\frac{n}{2}+r>s$, and any choice of β satisfying $0<\beta<2/b_{\max}$, where $b_{\max}$ is the largest eigenvalue of B, we have the following expression for the moments μ_s^r :*

$$\mu_s^r = \frac{2^{r-s}\beta^s r!\Gamma\left(\frac{n}{2}+r-s\right)}{\Gamma\left(\frac{n}{2}+r\right)} \sum_{j=0}^{\infty} \frac{(s)_j}{\left(\frac{n}{2}+r\right)_j} h_{r,j}(A, I_n - \beta B). \tag{57}$$

Note that when $\mu = 0_n$, $h_{r,j}(A, I_n - \beta B) = d_{r,j}(A, I_n - \beta B)$, and (57) specializes to (52).

The expression for μ_s^r given in Theorem 3 seems superficially similar to Smith's expression (51) given above. However, there are two important simplifications that make (57) much more efficient for computation purposes than is (51). The first is simply that these new expressions involve only a singly infinite series, rather than the doubly infinite series present in (51). The second, and more important, aspect of the results is that the generating function $H_{A_1,A_2}(t_1,t_2)$ satisfies the hypotheses of Lemma 2, so that a short recursion is available for the $h_{r,j}$. In addition, a super-short recursion can also be derived for $h_{r,j}$. We describe these in more detail below, but first give some additional results for the special case in which $B = I_n$, when the above results simplify considerably.

5.3 The Special Case: $B = I_n$

The moments μ_s^r simplify considerably when $B = I_n$. Clearly, like the moments μ_k of $q = z'Az$, they depend only upon the matrices A and $\mu\mu'$, and in fact, like the μ_k, they can be concisely expressed in terms of the functions $a_{r,l}$ introduced in Section 3.1. To obtain this result we make use of the following independently useful Lemma:

LEMMA 5. *With the functions $a_{r,l}$ as defined by (24),*

$$d_{r,k}(A, \mu\mu') = \frac{\left(\frac{1}{2}\right)_k}{k!} \sum_{l=0}^{k} \binom{k}{l} \delta^{k-l} a_{r,l},$$

where $\delta = \eta_0 = \mu'\mu$.

The proof of Lemma 5 is given in the Appendix. Inserting this result into (53) we obtain

$$\begin{aligned}
\mu_s^r &= \frac{2^{r-s} r!\Gamma\left(\frac{n}{2}+r-s\right) e^{-\frac{\delta}{2}}}{\Gamma\left(\frac{n}{2}+r\right)} \sum_{k=0}^{\infty} \frac{\left(\frac{n}{2}+r-s\right)_k}{2^k k! \left(\frac{n}{2}+r\right)_k} \sum_{l=0}^{k} \binom{k}{l} \delta^{k-l} a_{r,l} \\
&= \frac{2^{r-s} r!\Gamma\left(\frac{n}{2}+r-s\right) e^{-\frac{\delta}{2}}}{\Gamma\left(\frac{n}{2}+r\right)} \sum_{l=0}^{\infty} \sum_{k=0}^{\infty} \frac{\left(\frac{n}{2}+r-s\right)_{k+l} \delta^k}{2^{k+l} k! l! \left(\frac{n}{2}+r\right)_{k+l}} a_{r,l}
\end{aligned}$$

$$= \frac{2^{r-s}r!\Gamma\left(\frac{n}{2}+r-s\right)e^{-\frac{\delta}{2}}}{\Gamma\left(\frac{n}{2}+r\right)}\sum_{l=0}^{r}\frac{\left(\frac{n}{2}+r-s\right)_l}{2^l l!\left(\frac{n}{2}+r\right)_l}{}_1F_1\left(\frac{n}{2}+r-s+l,\frac{n}{2}+r+l;\frac{\delta}{2}\right)a_{r,l}$$

$$= 2^{r-s}r!\sum_{l=0}^{r}\frac{\Gamma\left(\frac{n}{2}+r-s+l\right)}{2^l l!\Gamma\left(\frac{n}{2}+r+l\right)}{}_1F_1\left(s,\frac{n}{2}+r+l;-\frac{\delta}{2}\right)a_{r,l},$$

where the third equality follows from the fact that $a_{r,l}=0$ for $l>r$, and the last step follows from the Kummer formula for the confluent hypergeometric function: $e^{-z}{}_1F_1(a,c;z)={}_1F_1(c-a,c;-z)$. We may therefore state the theorem that follows.

THEOREM 4. *When $B=I_n$,*

$$\mu_s^r = 2^{r-s}r!\sum_{l=0}^{r}\frac{\Gamma\left(\frac{n}{2}+r-s+l\right)}{2^l l!\Gamma\left(\frac{n}{2}+r+l\right)}{}_1F_1\left(s,\frac{n}{2}+r+l;-\frac{\delta}{2}\right)a_{r,l}, \qquad (58)$$

where the functions $a_{r,l}$ are defined by (24), and satisfy the recursion (26) or (31)–(32).

Remark 6. *For $r=0$, (58) is the inverse moment of a noncentral chi-squared distribution (see Krishnan, 1967). For $r=1$, Smith (1993) uses a different approach to obtain the same expression as ours. For the case that $r=s$, Ghazal (1994) presents the results for $r=1$ to 4. Our results are more general in that s can be an arbitrary positive real number and r can be any nonnegative integer.*

Although it is straightforward to evaluate the $a_{r,l}$ numerically, we present the explicit expressions of $a_{r,l}$ for $r=1$ to 4 here for easy reference. Setting $\tau_i=\mathrm{tr}(A^i)$ and $\eta_i=\mu' A^i\mu$, we have:

Table 1: The $a_{r,l}$ for $1\le r\le 4$

l \ r	1	2	3	4
0	$\frac{\tau_1}{2}$	$\frac{\tau_1^2}{8}+\frac{\tau_2}{4}$	$\frac{\tau_1^3}{48}+\frac{\tau_1\tau_2}{8}+\frac{\tau_3}{6}$	$\frac{\tau_1^4}{384}+\frac{\tau_1^2\tau_2}{32}+\frac{\tau_2^2}{32}+\frac{\tau_1\tau_3}{12}+\frac{\tau_4}{8}$
1	η_1	$\frac{\tau_1\eta_1}{2}+\eta_2$	$\frac{\tau_1^2\eta_1}{8}+\frac{\tau_2\eta_1}{4}+\frac{\tau_1\eta_2}{2}+\eta_3$	$\frac{\tau_1^3\eta_1}{48}+\frac{\tau_1\tau_2\eta_1}{8}+\frac{\tau_1^2\eta_2}{8}+\frac{\tau_3\eta_1}{6}+\frac{\tau_2\eta_2}{4}+\frac{\tau_1\eta_3}{2}+\eta_4$
2	·	η_1^2	$\frac{\tau_1\eta_1^2}{2}+2\eta_1\eta_2$	$\frac{\tau_1^2\eta_1^2}{8}+\frac{\tau_2\eta_1^2}{4}+\tau_1\eta_1\eta_2+\eta_2^2+2\eta_1\eta_3$
3	·	·	η_1^3	$\frac{\tau_1\eta_1^3}{2}+3\eta_1^2\eta_2$
4	·	·	·	η_1^4

5.4 Recursions for the $h_{r,j}$

We now show that the results in Section 2.3 provide both long and short recursions for the functions $h_{r,j}$ and give the details for implementing these. Defining $\tilde{P}(t_1,t_2)$ as

$$\begin{aligned}\tilde{P}(t_1,t_2) &= t_1\frac{\partial \ln H(t_1,t_2)}{\partial t_1}+t_2\frac{\partial \ln H(t_1,t_2)}{\partial t_2}\\ &= \frac{1}{2}P(\boldsymbol{t})+\frac{1}{2}(1-t_2)\mu'(I_n-t_1A_1-t_2A_2)^{-2}\mu-\frac{1}{2}\mu'(I_n-t_1A_1-t_2A_2)^{-1}\mu,\end{aligned}$$

where

$$P(\boldsymbol{t})=\operatorname{tr}\left((t_1A_1+t_2A_2)(I_n-t_1A_1-t_2A_2)^{-1}\right)=\sum_{\substack{j=0\\ j+k>0}}^{\infty}\sum_{k=0}^{\infty}p_{j,k}t_1^jt_2^k.$$

This clearly satisfies the hypotheses of Lemma 2, with

$$\tilde{E}(\boldsymbol{t})=|I_n-t_1A_1-t_2A_2|^2=\sum_{i=0}^{2n}\sum_{j=0}^{2n-i}\tilde{e}_{i,j}t_1^it_2^j, \tag{59}$$

and $\tilde{G}(\boldsymbol{t})$ both of degree $2n$. Now, for fixed μ, define functions $\eta_{j,k}$ of matrices A_1, A_2 by

$$\mu'(I_n-t_1A_1-t_2A_2)^{-1}\mu=\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\eta_{j,k}t_1^jt_2^k.$$

Then,

$$\tilde{p}_{j,k}=\frac{1}{2}p_{j,k}+\frac{1}{2}(j+k)(\eta_{j,k}-\eta_{j,k-1}). \tag{60}$$

We may therefore state the following result

THEOREM 5. *With the initial condition $h_{0,0}=1$, the functions $h_{i,j}$ defined by the generating function (56) may be generated by the long recursion given in (11), which has the form:*

$$h_{i,j}=\frac{1}{i+j}\sum_{\substack{k_1=0\\ k_1+k_2>0}}^{i}\sum_{k_2=0}^{j}\tilde{p}_{k_1,k_2}h_{i-k_1,j-k_2}, \tag{61}$$

where $\tilde{p}_{k_1,k_2}$ are as in (60). Or, they may be more efficiently generated using the short recursion given in Lemma 2, which has the form:

$$h_{i,j}=\sum_{\substack{k_1=0\\ 0<k_1+k_2\le 2n}}^{i}\sum_{k_2=0}^{j}\left(\frac{c_{k_1,k_2}}{i+j}-\tilde{e}_{k_1,k_2}\right)h_{i-k_1,j-k_2}, \tag{62}$$

with

$$c_{k_1,k_2} = (k_1 + k_2)\tilde{e}_{k_1,k_2} + \tilde{g}_{k_1,k_2},$$

and with the $\tilde{e}_{k_1,k_2}$ *as in (59) and the* $\tilde{g}_{k_1,k_2}$ *determined by*

$$\tilde{g}_{k_1,k_2} = \sum_{\substack{\nu_1=0 \\ \nu_1+\nu_2>0}}^{k_1} \sum_{\nu_2=0}^{k_2} \tilde{p}_{\nu_1,\nu_2} \tilde{e}_{k_1-\nu_1,k_2-\nu_2}.$$

To apply Theorem 5, we need to have an efficient method for computing $p_{i,j}$, $\tilde{e}_{i,j}$, and $\eta_{i,j}$. This can be easily accomplished by using the algorithm (with a slight modification) given in HKW.

Although the short recursion in Theorem 5 is efficient, it is not numerically stable. In contrast, the long recursion is inefficient but it is often numerically more stable than the short recursion (especially when $\tilde{p}_{k_1,k_2}$ are positive). To improve the efficiency of the long recursion, we provide a super-short recursion for $h_{r,j}$ by following the same approach as in Section 4.2.

THEOREM 6. *Let*

$$\begin{aligned} G_{i,j} &= \sum_{\nu_1=0}^{i} \sum_{\substack{\nu_2=0 \\ \nu_1+\nu_2>0}}^{j} [t_1^{\nu_1} t_2^{\nu_2}] A(\boldsymbol{t})^{\nu_1+\nu_2} h_{i-\nu_1,j-\nu_2}, \\ g_{i,j} &= \left[\sum_{\nu_1=0}^{i} \sum_{\substack{\nu_2=0 \\ \nu_1+\nu_2>0}}^{j} (\nu_1+\nu_2) \left([t_1^{\nu_1} t_2^{\nu_2}] A(\boldsymbol{t})^{\nu_1+\nu_2} - [t_1^{\nu_1} t_2^{\nu_2-1}] A(\boldsymbol{t})^{\nu_1+\nu_2-1} \right) h_{i-\nu_1,j-\nu_2} \right] \mu, \end{aligned}$$

where $A(\boldsymbol{t}) = t_1 A_1 + t_2 A_2$*, we have*

$$h_{i,j} = \frac{\mathrm{tr}(G_{i,j}) + \mu' g_{i,j}}{2(i+j)}.$$

Using the initial conditions of $G_{0,0} = 0_{n\times n}$*,* $g_{0,0} = 0_n$*, and* $h_{0,0} = 1$*, we can recursively obtain* $G_{i,j}$ *and* $g_{i,j}$ *using the following super-short recursions:*

$$\begin{aligned} G_{i,j} &= A_1(h_{i-1,j} I_n + G_{i-1,j}) + A_2(h_{i,j-1} I_n + G_{i,j-1}), \\ g_{i,j} &= G_{i,j}\mu - G_{i,j-1}\mu - h_{i,j-1}\mu + A_1 g_{i-1,j} + A_2 g_{i,j-1}. \end{aligned}$$

In the preceding equations, we adopt a convention that $G_{i,j} = 0_{n\times n}$*,* $g_{i,j} = 0_n$*, and* $h_{i,j} = 0$ *when either* i *or* j *is negative.*

5.5 Truncation Errors

When using (57) to evaluate μ_s^r, we must in practice truncate the infinite series at $j = M$ for some value of M. In order to control the accuracy of the computation, we need to obtain an upper bound on the truncation error. For the presentation of our error bounds, we introduce the following notation. Suppose A is a symmetric matrix. We define $A^+ = A$ when A is positive semidefinite or when r is even, and $A^+ = P\Lambda^+P'$ otherwise, where Λ^+ is a diagonal matrix of the absolute eigenvalues of A, and P is a matrix of the corresponding eigenvectors of A. With this notation, we now present an upper bound on the truncation error for (57).

THEOREM 7. *For any choice of β satisfying $0 < \beta \leq 1/b_{\max}$, where $b_{\max}$ is the largest eigenvalue of B, an upper bound on the approximation error of μ_s^r when truncating the infinite series in (57) at $j = M$ is given by*

$$\left|\mu_s^r - \frac{2^{r-s}\beta^s r!\Gamma\left(\frac{n}{2}+r-s\right)}{\Gamma\left(\frac{n}{2}+r\right)}\sum_{j=0}^{M}\frac{(s)_j}{\left(\frac{n}{2}+r\right)_j}h_{r,j}(A, I_n - \beta B)\right|$$
$$\leq \frac{2^{r-s}\beta^s r!\Gamma\left(\frac{n}{2}+r-s\right)}{\Gamma\left(\frac{n}{2}+r\right)}\frac{(s)_{M+1}}{\left(\frac{n}{2}+r\right)_{M+1}}\left[\frac{e^{\frac{\bar{\delta}-\delta}{2}}\tilde{d}_r(\bar{A},\bar{\mu})}{|\beta B|^{\frac{1}{2}}} - \sum_{j=0}^{M}\hat{h}_{r,j}(A^+, I_n - \beta B)\right],$$

where $\bar{\mu} = \sqrt{2}(\beta B)^{-\frac{1}{2}}\mu$, $\bar{\delta} = \bar{\mu}'\bar{\mu}$, $\bar{A} = B^{-\frac{1}{2}}A^+B^{-\frac{1}{2}}/\beta$, $\tilde{d}_r$ is defined as in (17), and the generating function of $\hat{h}_{i,j}(A_1, A_2)$ is given by

$$\hat{H}_{A_1,A_2}(t_1,t_2) = |I_n - t_1A_1 - t_2A_2|^{-\frac{1}{2}}\exp\left(\frac{(1+t_2)\mu'(I_n - t_1A_1 - t_2A_2)^{-1}\mu}{2} - \frac{\delta}{2}\right).$$

With the results in Theorem 7, we can now approximate μ_s^r to any desired level of accuracy.[11]

5.6 An Example

For illustrative purpose, we consider an example with $n = 20$, A a Toeplitz matrix with (i,j)th element given by $(|i-j|-1)/n^2$, B a diagonal matrix with i-th diagonal element $b_{ii} = i/n^2$, and μ is set to be a vector of $\mu_i = i/n$ for $i = 1,\dots,n$. Using the choice of $\beta = 1/b_{\max}$ for (57), Table 2 reports the value of μ_s^r for various combinations of r and s, with approximation errors less than 10^{-5}. The table also reports the number of required terms (M) to achieve the desired level of accuracy in parentheses.

Table 2: Expectation of Ratio of Quadratic Forms in Noncentral Normal Vectors

The table presents $\mathbb{E}[(z'Az)^r/(z'Bz)^s]$ for various values of r and s, where $z \sim N(\mu, I_n)$, $n = 20$, A is a Toeplitz matrix with its (i,j)th element as $a_{ij} = (|i-j|-1)/n^2$, B is a diagonal matrix with its ith diagonal element as $b_{ii} = i/n^2$ and $\mu_i = i/n$. 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.

	$s=1$	$s=2$	$s=3$	$s=4$	$s=5$	$s=10$
$r=0$	1.42721 (63)	2.36909 (91)	4.67693 (128)	11.30111 (176)	34.72798 (236)	n/a
$r=1$	1.40950 (69)	1.91118 (98)	2.96700 (135)	5.36157 (181)	11.50669 (239)	7638.94030 (726)
$r=2$	4.19497 (74)	5.18942 (102)	7.28829 (137)	11.80941 (179)	22.53012 (232)	27925.79115 (660)
$r=3$	13.34410 (86)	14.79819 (118)	18.34967 (156)	25.75133 (202)	41.50710 (256)	8655.50979 (678)
$r=4$	59.03048 (89)	60.36432 (118)	68.43545 (152)	86.92433 (192)	125.28018 (240)	10856.79180 (606)
$r=5$	295.93344 (108)	279.52112 (143)	290.15474 (183)	333.89538 (229)	430.35843 (282)	14607.30704 (668)
$r=10$	6425021.47108 (151)	4505458.62224 (185)	3383790.18983 (220)	2734240.84284 (258)	2389287.33517 (300)	5009200.42040 (579)

From Table 2, we can observe that for a fixed r, the number of required terms (M) increases with s, but even for $s = 10$, the computation of μ_s^r is very fast and efficient. Using a computer with an Intel i7-920 CPU, it takes less than 0.7 second for our Matlab program to generate the entire Table 2 using the super-short recursion.

6. CONCLUDING REMARKS

We have shown in this paper that, given a generating function for some objects of interest (moments, the coefficients in a series expansion, etc.), an associated generating function may be defined that induces a recurrence relation between the original objects of interest and a set of associated objects. This generalizes some known results relating moments and cumulants, and also results relating top-order zonal polynomials and power-sum symmetric functions. We then showed that, when the associated generating function is a ratio of two generating functions of finite order, more efficient recurrence relations of fixed length can be deduced.

These general results have been applied here to a number of problems involving quadratic forms in noncentral normal vectors, including the following much-studied problems: the moments of a single quadratic form, product-moments for several quadratic forms, and the expectation of a ratio of powers of two quadratic forms. For all these examples, we draw our inspiration from the work of Brown (1986) and introduce a new super-short recursive algorithm that is both numerically stable and efficient. In addition to their intrinsic interest, these examples show that the methodology is certainly useful for a number of different distribution-theoretic problems in statistics.

Many other distribution problems share many of the features present in the examples treated here. For example, the density and the distribution of a quadratic form of noncentral normal random variables have various series expansions (see Ruben, 1962; Shah and Khatri, 1961, 1963; and Kotz, Johnson, and Boyd, 1967), and the coefficients in these series expansions can be easily shown to have a short and super-short recurrence relations. In addition, many multivariate tests in statistics and econometrics (for example, the Wald statistic of testing linear restrictions on coefficients of multivariate linear model; see Phillips, 1986) have finite sample distributions that can be expressed as multiple infinite series involving the Davis-Chikuse invariant polynomials. It seems highly likely that our methodology will prove useful there, and we are confident many other new applications of the results will follow.

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Notes

[1]Note here that, for convenience, we define $E(t)$ in such a way that the e_k are the elementary symmetric functions of the eigenvalues of $-A$, rather than of A.

[2]Note that we treat $D(t)$ as a formal power series, without using any of the function-theoretic properties of the function that may be represented by the series, and without worrying about whether such a series converges or not.

[3]Note that the coefficients $\tilde{d}_k$ are functions of both A and μ, but we omit this dependence in the notation when A and μ are clear from the context.

[4]A two term recurrence relation for the moments of noncentral gamma distribution can be similarly derived.

[5]A set of Matlab programs for implementing various recursive algorithms discussed in the paper is available at `http://www.rotman.utoronto.ca/~kan/research.htm`.

[6]It can be easily shown that when $r = 1$, $\mathrm{tr}(G_{\boldsymbol{\kappa}}) = \sum_{i=1}^{n} u_{k,i}$ and $\mu' h_{\boldsymbol{\kappa}} = \sum_{i=1}^{n} v_{k,i}$, where $u_{k,i}$ and $v_{k,i}$ are defined in (29) and (30).

[7]This is because we can first compute $\tilde{d}_{i,0}$ for $i = 0, \ldots, 5$, and then compute $\tilde{d}_{i,1}$ for $i = 0, \ldots, 5$, and keep going until finally we compute $\tilde{d}_{i,200}$ for $i = 0, \ldots, 5$. Throughout this process, we only need to have six G's and six h's for the updating to continue.

[8]There are alternative formulae that express the moment of ratio of quadratic forms as integrals of the joint moment generating function of two quadratic forms (see, for instance, Williams (1941), White (1961), and Shenton and Johnson (1965)). However, these formulae either involve high dimensional integrals or work only for some special cases.

[9]This condition is needed to ensure that the expansion of $[1 - v'(I_n - \beta B)v]^{-s}$ as a power series in $v'(I_n - \beta B)v$ (from which (51) is derived) actually converges uniformly over the region of integration. This is so if and only if $|1 - \beta b_{\max}| < 1$, the condition stated.

[10]We include the term $\exp(-\mu'\mu/2)$ in the generating function to ensure that $h_{0,0}(A_1, A_2) = 1$.

[11]The recurrence relations for $\hat{h}_{r,j}$ are very similar to the ones for $h_{r,j}$, so we do not present these results separately.

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Appendix

Proof of Lemma 4. We first establish that if A and B are positive semi-definite matrices, then AB is also a positive semi-definite matrix. Suppose not, let $\lambda < 0$ be a negative eigenvalue of AB, and x be the corresponding eigenvector. We have

$$ABx = \lambda x.$$

Note that $y \equiv Bx \neq 0_n$ because otherwise the above equality cannot hold. Pre-multiplying both sides by $x'B'$, we obtain

$$y'Ay = x'B'ABx = \lambda x'B'x = \lambda x'Bx < 0.$$

Since A is a positive semi-definite matrix, we have $y'Ay \geq 0$ for all $y \neq 0_n$, so we have a contradiction. Therefore, AB must be a positive semi-definite matrix.

In order to show $\tilde{p}_{\boldsymbol{\kappa}} \geq 0$, it suffices to show that for any $x \neq 0_n$, we have $[\boldsymbol{t}^{\boldsymbol{\kappa}}]x'A(\boldsymbol{t})^k x \geq 0$, where $k = |\boldsymbol{\kappa}|$. This requires us to show that $\prod_{j=1}^{k} A_{i_j}$ is a positive semi-definite matrix, where $i_j \in \{1, \ldots, r\}$ for $j = 1, \ldots, k$. Since A_1 to A_r are positive semi-definite matrices, applying the above result repeatedly allows us to show that $\prod_{j=1}^{k} A_{i_j}$ is also a positive semi-definite matrix. ■

Proof of Lemma 5. From equation (16) we have that

$$\begin{aligned}
d_{r,k}(A, \mu\mu') &= [t_1^r t_2^k]|I_n - t_1 A - t_2 \mu\mu'|^{-\frac{1}{2}} \\
&= [t_1^r t_2^k]|I_n - t_1 A|^{-\frac{1}{2}}[1 - t_2 \mu'(I_n - t_1 A)^{-1}\mu]^{-\frac{1}{2}} \\
&= \frac{\left(\frac{1}{2}\right)_k}{k!}[t_1^r]|I_n - t_1 A|^{-\frac{1}{2}}[\mu'(I_n - t_1 A)^{-1}\mu]^k \\
&= \frac{\left(\frac{1}{2}\right)_k}{k!}[t_1^r]|I_n - t_1 A|^{-\frac{1}{2}}[\delta + \phi(t_1)]^k \\
&= \frac{\left(\frac{1}{2}\right)_k}{k!}\sum_{l=0}^{k}\binom{k}{l}\delta^{k-l}[t_1^r]|I_n - t_1 A|^{-\frac{1}{2}}\phi(t_1)^l \\
&= \frac{\left(\frac{1}{2}\right)_k}{k!}\sum_{l=0}^{k}\binom{k}{l}\delta^{k-l}a_{r,l},
\end{aligned}$$

by the definition of the $a_{r,l}$ in (24). ■

Proof of Convergence in (57). We shall show that, if β is chosen so that $0 < \beta < 2/b_{\max}$, the series in (57) converges, justifying the term-by-term integration. We shall make use here of the following two lemmas:

LEMMA 6. *The functions $h_{i,j}(A_1, A_2)$ defined by (56) can be expressed in terms of the invariant polynomials $d_{i,j,l}(A_1, A_2, \mu\mu')$ as follows:*

$$h_{i,j}(A_1, A_2) = e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \frac{1}{2^m m!} \sum_{l=0}^{j} \frac{(-1)^l}{2^l l!} \frac{(l+m)!}{\left(\frac{1}{2}\right)_{l+m}} d_{i,j-l,l+m}(A_1, A_2, \mu\mu').$$

Proof of Lemma 6. Since

$$\begin{aligned} H_{A_1,A_2}(t_1,t_2) &= e^{-\frac{\delta}{2}} |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} \sum_{m=0}^{\infty} \frac{(1-t_2)^m}{2^m m!} [\mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu]^m \\ &= e^{-\frac{\delta}{2}} |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} \sum_{l=0}^{\infty}\sum_{m=0}^{\infty} \frac{(-t_2)^l}{2^{m+l} l! m!} [\mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu]^{l+m}, \end{aligned}$$

we have

$$\begin{aligned} & h_{i,j}(A_1, A_2) \\ =\ & [t_1^i t_2^j] H_{A_1,A_2}(t_1,t_2) \\ =\ & e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \frac{1}{2^m m!} \sum_{l=0}^{j} \frac{(-1)^l}{2^l l!} [t_1^i t_2^{j-l}] |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} [\mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu]^{l+m} \\ =\ & e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \frac{1}{2^m m!} \sum_{l=0}^{j} \frac{(-1)^l}{2^l l!} \frac{(l+m)!}{\left(\frac{1}{2}\right)_{l+m}} d_{i,j-l,l+m}(A_1, A_2, \mu\mu'), \end{aligned}$$

where the last equality follows because

$$\begin{aligned} d_{i,j,k}(A_1, A_2, \mu\mu') &= [t_1^i t_2^j t_3^k] |I_n - t_1 A_1 - t_2 A_2 - t_3 \mu\mu'|^{-\frac{1}{2}} \\ &= [t_1^i t_2^j t_3^k] |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} [1 - t_3 \mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu]^{-\frac{1}{2}} \\ &= \frac{\left(\frac{1}{2}\right)_k}{k!} [t_1^i t_2^j] |I_n - t_1 A_1 - t_2 A_2|^{-\frac{1}{2}} \left[\mu'(I_n - t_1 A_1 - t_2 A_2)^{-1}\mu\right]^k. \end{aligned}$$

■

LEMMA 7. *If a_i is the largest absolute eigenvalue of A_i for each i, then*

$$|d_{\boldsymbol{\kappa}}(A_1, \ldots, A_r)| \le \frac{1}{\boldsymbol{\kappa}!} \left(\frac{n}{2}\right)_k \prod_{i=1}^{r} a_i^{k_i}.$$

Proof of Lemma 7. From equation (81) in HKW,

$$|d_{\boldsymbol{\kappa}}(A_1, \ldots, A_r)| = \frac{1}{\boldsymbol{\kappa}!} \left(\frac{n}{2}\right)_k \left| \int_{v'v=1} \left(\prod_{i=1}^{r} (v' A_i v)^{k_i} \right) (\mathrm{d}v) \right| \le \frac{1}{\boldsymbol{\kappa}!} \left(\frac{n}{2}\right)_k \int_{v'v=1} \prod_{i=1}^{r} |v' A_i v|^{k_i} (\mathrm{d}v).$$

But, it is well-known that

$$\sup_{v'v=1} |v'A_i v| = a_i.$$

This immediately yields the stated inequality. ■

Let a and $\tilde{b}$ be the largest absolute eigenvalue of A and $\tilde{B}$, respectively. Using Lemmas 6 and 7, we can bound $|h_{r,j}(A,\tilde{B})|$ by

$$\begin{aligned}
\left|h_{r,j}(A,\tilde{B})\right| &\leq e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \frac{1}{2^m m!} \sum_{l=0}^{j} \frac{(l+m)!}{2^l l! \left(\frac{1}{2}\right)_{l+m}} \left|d_{r,j-l,l+m}(A,\tilde{B},\mu\mu')\right| \\
&\leq e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \frac{1}{2^m m!} \sum_{l=0}^{j} \frac{(l+m)!}{2^l l! \left(\frac{1}{2}\right)_{l+m}} \frac{\left(\frac{n}{2}\right)_{r+j+m} a^r \tilde{b}^{j-l} \delta^{l+m}}{r!(j-l)!(l+m)!} \\
&= \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{r!} \sum_{m=0}^{\infty} \sum_{l=0}^{j} \frac{\left(\frac{n}{2}+r\right)_{j+m} \left(\frac{\delta}{2}\right)^{l+m} \tilde{b}^{j-l}}{m! l! (j-l)! \left(\frac{1}{2}\right)_{l+m}}.
\end{aligned}$$

Under the condition $0 < \beta < 2/b_{\max}$, we have $0 \leq \tilde{b} < 1$. Together with the condition $\frac{n}{2} + r > s$, we can bound the absolute value of the terms in the infinite series in (57) by

$$\begin{aligned}
\sum_{j=0}^{\infty} \frac{(s)_j}{\left(\frac{n}{2}+r\right)_j} |h_{r,j}(A,\tilde{B})| &\leq \sum_{j=0}^{\infty} |h_{r,j}(A,\tilde{B})| \\
&\leq \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{r!} \sum_{j=0}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{j} \frac{\left(\frac{n}{2}+r\right)_{j+m} \left(\frac{\delta}{2}\right)^{l+m} \tilde{b}^{j-l}}{m! l! (j-l)! \left(\frac{1}{2}\right)_{l+m}} \\
&= \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{r!} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \frac{\left(\frac{n}{2}+r\right)_{l+m} \left(\frac{\delta}{2}\right)^{l+m}}{m! l! \left(\frac{1}{2}\right)_{l+m}} \sum_{j=0}^{\infty} \frac{\left(\frac{n}{2}+r+l+m\right)_j \tilde{b}^j}{j!} \\
&= \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{(1-\tilde{b})^{\frac{n}{2}+r} r!} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \frac{\left(\frac{n}{2}+r\right)_{l+m} \left[\frac{\delta}{2(1-\tilde{b})}\right]^{l+m}}{m! l! \left(\frac{1}{2}\right)_{l+m}} \\
&= \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{(1-\tilde{b})^{\frac{n}{2}+r} r!} \sum_{k=0}^{\infty} \frac{\left(\frac{n}{2}+r\right)_k \left[\frac{\delta}{2(1-\tilde{b})}\right]^k 2^k}{\left(\frac{1}{2}\right)_k k!} \\
&= \frac{e^{-\frac{\delta}{2}} a^r \left(\frac{n}{2}\right)_r}{(1-\tilde{b})^{\frac{n}{2}+r} r!} {}_1F_1\left(\frac{n}{2}+r; \frac{1}{2}; \frac{\delta}{1-\tilde{b}}\right),
\end{aligned}$$

where the fourth line is obtained by using the identity

$$\sum_{j=0}^{\infty} \frac{\left(\frac{n}{2}+r+l+m\right)_j \tilde{b}^j}{j!} = (1-\tilde{b})^{-\frac{n}{2}-r-l-m}$$

when $0 \leq \tilde{b} < 1$, and the fifth line is obtained by using the identity $\sum_{l=0}^{k} \frac{k!}{l!(k-l)!} = 2^k$ and setting $k = l + m$. Since the ${}_1F_1$ converges uniformly for all values of its argument, this confirms the claim that term-by-term integration in (54) is justified. ■

Proof of Theorem 7. Following the proof of Lemma 6, we can show that

$$\hat{h}_{r,j}(A_1, A_2) = e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \sum_{l=0}^{j} \binom{l+m}{l} \frac{d_{r,j-l,l+m}(A_1, A_2, \mu\mu')}{2^{l+m} \left(\frac{1}{2}\right)_{l+m}}.$$

Under the assumption $0 < \beta \leq 1/b_{\max}$, $I_n - \beta B$ is positive semidefinite. Therefore, $d_{r,j,k}(A, I_n - \beta B, \mu\mu')$ is nonnegative when A is positive semidefinite or r is even. When A is not positive semidefinite and r is odd, we have $|z'Az| = |z'P\Lambda P'z| \leq z'P\Lambda^+ P'z = z'A^+z$. Using the fact that $z'(I_n - \beta B)z \geq 0$ and $z'\mu\mu'z \geq 0$, we have $|(z'Az)^r (z'(I_n - \beta B)z)^j (z'\mu\mu'z)^k| \leq (z'A^+z)^r (z'(I_n - \beta B)z)^j (z'\mu\mu'z)^k$, which implies

$$\left| d_{r,j,k}(A, I_n - \beta B, \mu\mu') \right| \leq d_{r,j,k}(A^+, I_n - \beta B, \mu\mu').$$

Using Lemma 6, we have

$$|h_{r,j}(A, I_n - \beta B)| \leq e^{-\frac{\delta}{2}} \sum_{m=0}^{\infty} \sum_{l=0}^{j} \binom{l+m}{l} \frac{|d_{r,j-l,l+m}(A, I_n - \beta B, \mu\mu')|}{2^{l+m} \left(\frac{1}{2}\right)_{l+m}} \leq \hat{h}_{r,j}(A^+, I_n - \beta B).$$

Using this result and the fact that $\frac{n}{2} + r > s$, we obtain

$$\begin{aligned}
\left| \sum_{j=M+1}^{\infty} \frac{(s)_j}{\left(\frac{n}{2} + r\right)_j} h_{r,j}(A, I_n - \beta B) \right| &\leq \sum_{j=M+1}^{\infty} \frac{(s)_j}{\left(\frac{n}{2} + r\right)_j} |h_{r,j}(A, I_n - \beta B)| \\
&\leq \sum_{j=M+1}^{\infty} \frac{(s)_j}{\left(\frac{n}{2} + r\right)_j} \hat{h}_{r,j}(A^+, I_n - \beta B) \\
&\leq \frac{(s)_{M+1}}{\left(\frac{n}{2} + r\right)_{M+1}} \left[\frac{e^{\frac{\bar{\delta} - \delta}{2}} \tilde{d}_r(\bar{A}, \bar{\mu})}{|\beta B|^{\frac{1}{2}}} - \sum_{j=0}^{M} \hat{h}_{r,j}(A^+, I_n - \beta B) \right].
\end{aligned}$$

The last inequality holds because

$$\begin{aligned}
& \sum_{j=0}^{\infty} \hat{h}_{r,j}(A^+, I_n - \beta B) \\
= \ & [t_1^r] \, |I_n - t_1 A^+ - (I_n - \beta B)|^{-\frac{1}{2}} \exp\left(\mu' \left[I_n - t_1 A^+ - (I_n - \beta B) \right]^{-1} \mu - \frac{\delta}{2} \right) \\
= \ & [t_1^r] |\beta B|^{-\frac{1}{2}} e^{-\frac{\delta}{2}} |I_n - t_1 \bar{A}|^{-\frac{1}{2}} \exp\left(\frac{\bar{\mu}'(I_n - t_1 \bar{A})^{-1} \bar{\mu}}{2} \right) \\
= \ & \frac{e^{\frac{\bar{\delta} - \delta}{2}}}{|\beta B|^{\frac{1}{2}}} \tilde{d}_r(\bar{A}, \bar{\mu}).
\end{aligned}$$

■