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ASYMPTOTIC EXPANSIONS OF SOME MATRIX ARGUMENT HYPERGEOMETRIC FUNCTIONS, WITH APPLICATIONS TO MACROMOLECULES*

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Abstract. We have studied the asymptotics of two special two-matrix hypergeometric functions. The validity of the asymptotic expressions for these functions is seen in several selected numerical comparisons between the exact and asymptotic results. These hypergeometric functions find applications in configuration statistics of macromolecules as well as multivariate statistics.

Key words and phrases: Asymptotics, hypergeometric functions of matrix argument, Wishart distribution, macromolecule size and shape distribution functions.

1. Introduction

Hypergeometric functions of matrix argument have found wide applications in expressing certain probability density functions of the principal components of some chosen positive definite symmetric matrices. Two areas where principal component analysis is used are multivariate statistics and configuration statistics of macromolecules. In the former, a classical example is the joint distribution of the latent roots of a sample covariance matrix (James (1964), Muirhead (1982)). In the field of macromolecular configuration statistics, it has been found (Eichinger (1977, 1985), Wei (1990*a*)) that both size and shape distribution functions for Gaussian macromolecules can be expressed in terms of hypergeometric functions of matrix argument. As in the case of multivariate statistics (see, for example, Muirhead (1978)), a study of the asymptotics of the hypergeometric functions appearing in these distribution functions can provide much insight into the nature of the extended configurations of macromolecules, an understanding of which is essential

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in the theory of rubber elasticity (Eichinger (1983), Eichinger *et al.* (1989)) and the reptation dynamics of DNA (see Zimm (1988) for instance).

In this paper, we first review the mathematical analysis that leads to asymptotic results for two special two-matrix hypergeometric functions. Numerical comparisons between the asymptotic results and the exact evaluations in the asymptotic regions of the functions then follow. Finally, several conclusions are drawn from these comparisons.

2. Analysis

We consider here a single macromolecule (Flory (1953, 1969), deGennes (1979), Doi and Edwards (1986)) imbedded in a k-dimensional space. The molecule is pictured as a molecular graph with each of its n vertices corresponding to a selected atom along the backbone, and each edge representing a submolecule or segment consisting of a number of chemical bonds. This approximate representation of the configuration of a molecule becomes increasingly accurate as the size of the molecule increases. For simplicity, the mass of each vertex or bead, as it is often called in polymer theory, is taken to be the same fixed number, and all segments have the same length.

This model of a polymer molecule has a potential energy function that is quadratic in the coordinates of the beads, and is often called a Gaussian model (for details and the development of the model, see Fixman (1962), Coriell and Jackson (1967), Fujita and Norisuye (1970), Yamakawa (1971), Šolc and Stockmayer (1971), Šolc (1971, 1972), Eichinger (1972, 1977, 1980, 1985), Šolc and Gobush (1974), Stockmayer (1974), Martin and Eichinger (1978), Shy and Eichinger (1986), Wei (1989, 1990*a*), Wei and Eichinger (1989, 1990*a*, 1990*b*, 1990*c*, 1991)). The Boltzmann factor for the system, which is proportional to the probability density for finding the system in a particular equilibrium configuration, takes a form that is frequently encountered in multivariate statistics.

Define a non-negative definite symmetric matrix, called the gyration tensor, as the product of a $k \times n$ matrix and its transpose, the matrix elements of which are the Cartesian coordinates of the n beads relative to the center of mass of the molecular system (see for example Eichinger (1985)). This matrix is simply related to the inertial tensor for the mechanical system that the masses represent, and it is further similar to the covariance matrix found in multivariate statistics. Here the matrix measures the shape of the molecule. The distribution function of this matrix may then be formulated from the fundamental principles of statistical mechanics. We note that the gyration tensor does not, in general, have the well-known Wishart distribution except for the $k = n - 1$ case, where a macromolecule, when imbedded in a 3-dimensional space, can only have 4 beads.

Let $\tilde{\boldsymbol{S}}_d = \mathrm{diag}(\tilde{S}_1, \tilde{S}_2, \ldots, \tilde{S}_k)$ denote the k eigenvalues (latent roots or principal components) of the gyration tensor for a Gaussian macromolecule of n beads imbedded in a k-dimensional space. The trace of the matrix $\tilde{\boldsymbol{S}}_d$, $\mathrm{tr}(\tilde{\boldsymbol{S}}_d)$, is the radius of gyration $\tilde{s}^2$, which is a measure of the size of the molecule. For nondegenerate $\tilde{\boldsymbol{S}}_d$, i.e., all the principal components are distinct, the shape distribution function or the joint density function of the principal components $P(\tilde{\boldsymbol{S}}_d)$ is given

by Eichinger (1985).

$$P(\tilde{\boldsymbol{S}}_d) = \pi^{k/2}|\tilde{\boldsymbol{\Lambda}}|^{k/2}\left\{\prod_{\alpha=1}^{k}\frac{\Gamma(\alpha/2)}{\Gamma[(n-\alpha)/2]}\right\}\prod_{\alpha<\beta}^{k}|\tilde{S}_\alpha - \tilde{S}_\beta| \times |\tilde{\boldsymbol{S}}_d|^{(n-k-2)/2}{}_0F_0^{(n-1)}(\tilde{\boldsymbol{\Lambda}}, -\tilde{\boldsymbol{S}}_{n-1}) \tag{2.1}$$

where $k \leq n-1$, $\tilde{\boldsymbol{S}}_{n-1} = (\tilde{\boldsymbol{S}}_d, \boldsymbol{0})$ is a $(n-1)\times(n-1)$ diagonal matrix, $\tilde{\boldsymbol{\Lambda}} = \operatorname{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_{n-1})$ denotes the nonzero eigenvalues of the symmetric Kirchhoff matrix that describes the architecture of the molecule, $|\tilde{\boldsymbol{\Lambda}}|$ is the determinant of $\tilde{\boldsymbol{\Lambda}}$, and ${}_0F_0$ is the well-known hypergeometric function of matrix argument. The size distribution function $P(\tilde{s}^2)$ takes the form (Eichinger (1977), Wei (1990*a*, 1990*b*))

$$P(\tilde{s}^2) = \frac{|\boldsymbol{A}_m|^{1/2}}{\Gamma(m/2)}(\tilde{s}^2)^{m/2-1}{}_0F_0(\boldsymbol{A}_m, -\tilde{s}^2) \tag{2.2}$$

where $m = k(n-1)$ and $\boldsymbol{A}_m = \boldsymbol{1}_k \otimes \tilde{\boldsymbol{\Lambda}}$ is the direct product of a $k\times k$ unit matrix and $\tilde{\boldsymbol{\Lambda}}$. Note that ${}_0F_0(\boldsymbol{A}_m, -\tilde{s}^2)$ in (2.2) is the notation of James (1964) for ${}_0F_0^{(m)}(\boldsymbol{A}_m, -\tilde{s}^2\boldsymbol{I}_1)$ where $\boldsymbol{I}_1 = \operatorname{diag}(1,0,0,0,\ldots,0)$ is m by m.

We now study the asymptotics of the two hypergeometric functions in (2.1) and (2.2) for large values of the principal components. We first make use of the following integral representations (Eichinger (1977, 1985), Wei (1990*a*, 1990*b*)):

$$\begin{aligned}{}_0F_0(\boldsymbol{A}_m, -\tilde{s}^2) &= \frac{\Gamma(m/2)}{2\pi}|\boldsymbol{A}_m|^{-1/2}(\tilde{s}^2)^{-(m/2-1)}\int_{-\infty}^{\infty} e^{i\tilde{s}^2x}|\boldsymbol{1} + ix\boldsymbol{A}_m^{-1}|^{-1/2}dx \\ &= (4\pi)^{-k/2}\prod_{\alpha=1}^{k}\frac{\Gamma[(n-\alpha)/2]}{\Gamma(\alpha/2)}|\tilde{\boldsymbol{\Lambda}}|^{-k/2}|\tilde{\boldsymbol{S}}_d|^{-(n-k-2)/2} \\ &\quad\times\int|\boldsymbol{1} + i\boldsymbol{x}\otimes\tilde{\boldsymbol{\Lambda}}^{-1}|^{-1/2}{}_0F_0^{(k)}(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x})\prod_{\alpha<\beta}^{k}|x_\alpha - x_\beta|\prod_{\alpha=1}^{k}dx_\alpha\end{aligned} \tag{2.3, 2.4}$$

and

where $\boldsymbol{x} = \operatorname{diag}(x_1, x_2, \ldots, x_k)$ with $-\infty \leq x_k \leq \cdots \leq x_1 \leq \infty$. To take into account any degeneracy of the $n-1$ eigenvalues of $\tilde{\boldsymbol{\Lambda}}$, i.e., multiplicity of roots of $\tilde{\boldsymbol{\Lambda}}$, we write

$$|\tilde{\boldsymbol{\Lambda}}| = \prod_{j=1}^{p}\kappa_j^{\omega_j} \tag{2.5}$$

with $0 < \kappa_1 < \kappa_2 < \cdots < \kappa_p$ and ω_j being the degeneracy of the j-th distinct eigenvalue κ_j of $\tilde{\boldsymbol{\Lambda}}$. From (2.3), it is found (Wei (1989)) that

$${}_0F_0(\boldsymbol{A}_m, -\tilde{s}^2) \sim \frac{\Gamma(m/2)}{\Gamma(k\omega_1/2)}B_1^{k/2}|\boldsymbol{A}_m|^{-1/2}(\tilde{s}^2)^{-(m-k\omega_1)/2}e^{-\kappa_1\tilde{s}^2} \tag{2.6}$$

for large $\tilde{s}^2$, where B_j is defined as

$$B_j = \kappa_j^{\omega_j} \prod_{l \neq j}^{p} (1 - \kappa_j/\kappa_l)^{-\omega_l}. \tag{2.7}$$

For large values of the principal components, the integral in (2.4) may be evaluated approximately with use of the multidimensional saddle-point method—a multivariate extension of Laplace's method for integrals developed by Hsu (1948) (see also Muirhead (1982) and Wei and Eichinger (1990*a*)). This proceeds as follows. First write

$$\begin{aligned} &\int |\mathbf{1} + i\boldsymbol{x} \otimes \tilde{\boldsymbol{\Lambda}}^{-1}|^{-1/2} {}_0F_0^{(k)}(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x}) \prod_{\alpha<\beta}^{k} |x_\alpha - x_\beta| \prod_{\alpha=1}^{k} dx_\alpha \\ &\qquad = \int \exp[f(\boldsymbol{x})] \prod_{\alpha=1}^{k} dx_\alpha. \end{aligned} \tag{2.8}$$

Next, make use of the identity (Bingham (1974))

$${}_0F_0^{(k)}(\boldsymbol{a}, \boldsymbol{b}) = \operatorname{etr}(\boldsymbol{a}\boldsymbol{b} - \tilde{\boldsymbol{a}}\tilde{\boldsymbol{b}}) {}_0F_0^{(k)}(\tilde{\boldsymbol{a}}, \tilde{\boldsymbol{b}}) \tag{2.9}$$

where $\operatorname{etr}(\cdot) = \exp[\operatorname{tr}(\cdot)]$ and $\tilde{\boldsymbol{a}} = \boldsymbol{a} - a_0\mathbf{1}_k$ and $\tilde{\boldsymbol{b}} = \boldsymbol{b} - b_0\mathbf{1}_k$ with a_0 and b_0 being any numbers, and write

$${}_0F_0^{(k)}(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x}) = \operatorname{etr}(i\tilde{\boldsymbol{S}}_d\boldsymbol{x}) W(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x}) \tag{2.10}$$

where the W-function is chosen according to (2.9). We have from (2.8)

$$\begin{aligned} f(\boldsymbol{x}) = i \operatorname{tr}(\tilde{\boldsymbol{S}}_d\boldsymbol{x}) - \frac{1}{2} \sum_{\alpha=1}^{k} \sum_{j=1}^{p} \omega_j \ln(1 + i x_\alpha/\kappa_j) \\ + \sum_{\alpha<\beta}^{k} \ln(x_\alpha - x_\beta) + \ln[W(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x})]. \end{aligned} \tag{2.11}$$

Solving $\partial f(\boldsymbol{x})/\partial \boldsymbol{x} = \mathbf{0}$, we find that $f(\boldsymbol{x})$ is maximized when $ix_\alpha = -\kappa_\alpha + \omega_\alpha/2\tilde{S}_\alpha$ for large $\tilde{S}_\alpha$. We further notice that the product $\prod_{\alpha=2}^{k} \prod_{\beta=1}^{\alpha-1} [i(1 - \kappa_\alpha/\kappa_\beta)^{\omega_\beta/2}]$ must be real to ensure a real-valued asymptotic expression (see also Wei and Eichinger (1990*a*, 1990*b*, 1991) and Wei (1990*a*)). The multidimensional saddle-point method finally gives (see Wei (1990*a*))

$$\begin{aligned} &{}_0F_0^{(n-1)}(\tilde{\boldsymbol{\Lambda}}, -\tilde{\boldsymbol{S}}_{n-1}) \\ &\quad \sim (2\pi)^{-k/2} |\tilde{\boldsymbol{\Lambda}}|^{-k/2} |\tilde{\boldsymbol{S}}_d|^{-(n-k-2)/2} \\ &\qquad \times \prod_{\alpha<\beta}^{k} \left\{ \frac{|(\kappa_\alpha - \kappa_\beta)(\tilde{S}_\alpha^{-1} - \tilde{S}_\beta^{-1})|^{1/2}}{|\tilde{S}_\alpha - \tilde{S}_\beta|} \right\} \\ &\qquad \times \prod_{\alpha=1}^{k} \left\{ \frac{\Gamma[(n-\alpha)/2]}{|eB_\alpha|^{-1/2}} \left(\frac{2e\tilde{S}_\alpha}{\omega_\alpha} \right)^{(\omega_\alpha - 1)/2} e^{-\kappa_\alpha \tilde{S}_\alpha} \right\} \end{aligned} \tag{2.12}$$

where the asymptotic expression (see Muirhead (1982)) for ${}_0F_0^{(k)}(\tilde{\boldsymbol{S}}_d, i\boldsymbol{x})$ at the saddle point has been used. Note that for nondegenerate $\tilde{\boldsymbol{\Lambda}}$, i.e., $\omega_\alpha = 1$ for all values of α, the result given in (2.12), apart from an insignificant constant factor resulting from the lower-order approximation to the exact saddle-point, reduces to that of James (1969). Substitution of (2.12) in (2.1) yields the following asymptotic expansion of $P(\tilde{\boldsymbol{S}}_d)$ (Wei (1990*a*), Wei and Eichinger (1991)):

$$P(\tilde{\boldsymbol{S}}_d) \sim 2^{-k/2} \left\{ \prod_{\alpha<\beta}^{k} |(\kappa_\alpha - \kappa_\beta)(\tilde{S}_\alpha^{-1} - \tilde{S}_\beta^{-1})|^{1/2} \right\} \times \prod_{\alpha=1}^{k} \left\{ \frac{|eB_\alpha|^{1/2}}{\Gamma(\alpha/2)} \left(\frac{2e\tilde{S}_\alpha}{\omega_\alpha} \right)^{(\omega_\alpha - 1)/2} e^{-\kappa_\alpha \tilde{S}_\alpha} \right\}. \tag{2.13}$$

It is gratifying to see here that asymptotic expansions of the matrix hypergeometric function ${}_0F_0$ with both of its argument matrices having degenerate eigenvalues can be obtained from easily produced results for the nondegenerate case. Although the interesting asymptotics case where only one argument matrix has equal eigenvalues has been thoroughly studied in the statistical literature, we have seen, to date, no attempt at obtaining asymptotic expansions for the general case where both argument matrices may have multiple sets of equal eigenvalues. Our results (see (2.12)) thus represent the first such attempt, though it is still limited to the cases that interest polymer theorists.

3. Numerical comparisons

The exact numerical values of $P(\tilde{s}^2)$ computed according to (2.2) and (2.3) (Wei (1989, 1990*a*)) are compared with $P(\tilde{s}^2)$ calculated from (2.2) and (2.6) for two types of macromolecules—linear (nondegenerate $\tilde{\boldsymbol{\Lambda}}$) and odd-$n$ circular (doubly-degenerate $\tilde{\boldsymbol{\Lambda}}$) chains of two different values of n imbedded in 3-dimensional space. The relative error ϵ is defined as

$$\epsilon = |P_{\text{asymp.}}/P_{\text{exact}} - 1| = |{}_0F_{0\text{asymp.}}/{}_0F_{0\text{exact}} - 1|, \tag{3.1}$$

and the results are plotted in Fig. 1. As can be seen, ϵ decreases monotonically as $\tilde{s}^2$ increases in both cases, with very weak dependence of ϵ on n. For linear chains with $n = 99$, the range $[0.40, \infty)$ of $\tilde{s}^2$, may be regarded as the asymptotic region with $\epsilon \leq 0.04$. Note that the most probable radius of gyration $*\tilde{s}^2$ for a 99-bead linear chain is less than 0.40. In general, the asymptotic region lies beyond $*\tilde{s}^2$ for a given type of molecules. From Fig. 2, it is seen that the monotonic decay of ϵ with increasing $\tilde{s}^2$ depends strongly on k. In all cases, we have found that ϵ goes to zero as $\tilde{s}^2 \to \infty$.

Similar numerical comparison between $P(\tilde{\boldsymbol{S}}_d)$ computed from (2.1) and (2.4) (Wei and Eichinger (1990*b*)) and that from (2.1) and (2.12) for a 29-bead linear chain in three dimensions has been carried out. We have seen a monotonic decay of the relative error with any one of the three principal components when the

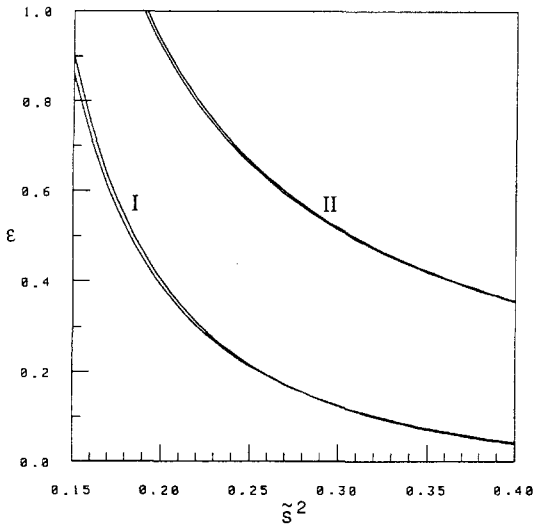
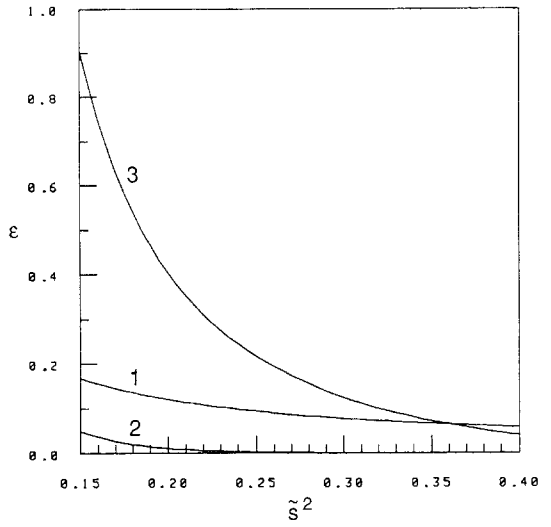


Fig. 1. Relative error ϵ as a function of $\tilde{s}^2$ for linear (I) and circular (II) macromolecules with $n = 11$ (lower curve) and 99 (upper curve).

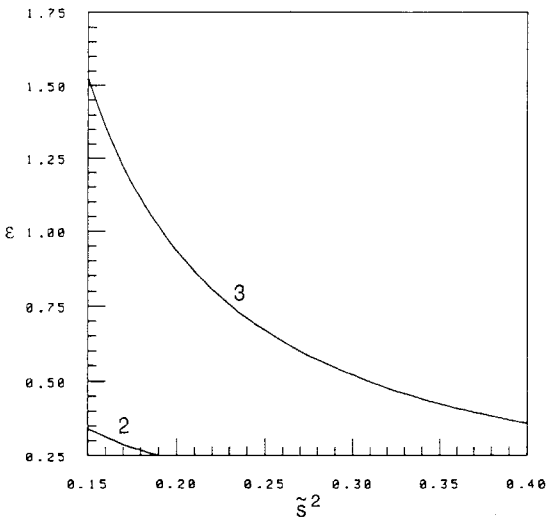
other two are fixed in the asymptotic region. In this case, the asymptotic region is identified as the part of the variable domain $0 < \tilde{S}_3 < \tilde{S}_2 < \tilde{S}_1 < \infty$ with $\tilde{S}_1 \in [*\tilde{S}_1, \infty)$, $\tilde{S}_2 \in [*\tilde{S}_2, \infty)$ and $\tilde{S}_3 \in [*\tilde{S}_3, \infty)$, where the $*\tilde{S}_\alpha$ denote the most probable principal components. For $\tilde{S}_2 = 0.15$ and $\tilde{S}_3 = 0.06$, for example, it is found that the relative error decreases monotonically to zero as $\tilde{S}_1$ increases from $0.20(= *\tilde{S}_1)$ to ∞. It is further seen that the relative error decreases considerably as the spacing between any pair of the principal components increases in the asymptotic region.

4. Conclusion

The asymptotics of two special hypergeometric functions of matrix arguments have been studied, based on their new representations as single or multiple integrals in Fourier space. Several selected numerical comparisons between the exact and asymptotic results of the size and shape distribution functions which involve these hypergeometric functions show that the analytic asymptotic expressions of the hypergeometric functions of matrix arguments are indeed very good representations of the functions in the asymptotic regions. The asymptotics study presented here has important applications in several areas of statistical mathematics, including the asymptotic distribution of the trace of the Wishart matrix, and polymer theory.



(a)



(b)

Fig. 2. (a) Plots of ϵ vs. $\tilde{s}^2$ for a 99-bead linear macromolecule in one, two, and three dimensions. The numerical value numbering each curve denotes the dimensionality of the space in which the molecule is imbedded. (b) Same as (a) for two and three dimensions except that the molecule is circular. The curve corresponding to $k = 1$ disappears into the far left of Curve 2.

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