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Calculation of a formal moment generating function by using a differential operator

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Abstract

A differential form in a formal moment generating function is given by the decomposition of powers in terms of the Hermite polynomials. This paper shows that this differential form for calculating the expectation of normal and χ^2 distributions has the benefit of avoiding divergence for Edgeworth type approximations from the viewpoint of a formal power series ring. A symbolic computational algorithm is also discussed, within the distribution theory of statistics.
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1. Introduction

Attempts to obtain asymptotic expansions for the distributions of random variables involve algebraically complicated calculation. A computer algebra system (*CA system*) is useful for avoiding the complication. A brief survey of techniques without the help of CA systems can be found in Barndorff-Nielsen and Cox (1989) and Chapter 6 of Stuart and Ord (1994). On studies with CA systems in the distribution theory of multivariate analysis, Niki and Konishi (1984) have derived higher order asymptotic expansions for the distribution of Fisher's transformation of the sample correlation coefficient. Nakagawa and Niki (1992) and Nakagawa et al. (1998) have given computer algorithms for obtaining moments of multivariate statistics with a *symmetric property*. Their key technique is using a change of bases of the module of symmetric polynomials.

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In this paper, the decomposition of powers in terms of the Hermite polynomials, by using a differential operator, is adopted to calculate formal generating functions of statistics. A similar method without a CA system has been given by Iwashita (1997). He has derived a differential formula for getting asymptotic distributions for the expectation of a function of a sample mean and a sample covariance matrix under the elliptical distribution. This differential formula is partially implemented in the *Mathematica* package by Inoue et al. (2005). Before realizing such a formula for multivariate cases like Inoue et al. (2005), the univariate case needs to be summarized in detail.

2. Hermite inversion formula

Let $H_n(x)$ denote the Hermite polynomial of degree n $(n \geq 0)$ defined by

$$H_n(x) = (-1)^n e^{\frac{1}{2}x^2} \frac{d^n}{dx^n} e^{-\frac{1}{2}x^2} = (-1)^n e^{\frac{1}{2}x^2} D_x^n e^{-\frac{1}{2}x^2} \tag{1}$$

where $D_x = \frac{d}{dx}$ and $D_x^0 = 1$. The set of Hermite polynomials constitutes an orthogonal basis; therefore the power x^n can be expressed as a linear combination of the Hermite polynomials. The explicit expression is described in Ex 13.1.8 on Page 733 in Arfken and Weber (1995). This linear combination for x^n can also be rewritten using the above differentiation rule (1) as follows:

$$x^{2n} e^{-\frac{1}{2}x^2} = \sum_{j=0}^{n} \begin{bmatrix} 2n \\ 2j \end{bmatrix} D_x^{2j} e^{-\frac{1}{2}x^2}, \quad x^{2n+1} e^{-\frac{1}{2}x^2} = -\sum_{j=0}^{n} \begin{bmatrix} 2n+1 \\ 2j+1 \end{bmatrix} D_x^{2j+1} e^{-\frac{1}{2}x^2}. \tag{2}$$

Here $n!!$ denotes the double factorial of n and

$$\begin{bmatrix} j \\ k \end{bmatrix} = \binom{j}{k} (j-k-1)!!. \tag{3}$$

3. Calculation of the formal moment generating function

Let $\mathbb{C}[[x]]$ be the power series ring in x and $Q(x)$ denote a family of functions

$$Q(x) = \left\{ p(x)\, e^{-\frac{1}{2}x^2} \;\middle|\; p(x) \in \mathbb{C}[[x]] \right\}. \tag{4}$$

Consider a distribution whose probability density function (*p.d.f.*), cumulative distribution function (*c.d.f.*) and characteristic function (*c.f.*) are $f(x)$, $F(x)$ and $\psi(t)$, respectively. And we suppose the case where (i) only $\psi(t)$ is known and (ii) $\psi(t) \in Q(t)$. The Edgeworth expansion is a typical example for the assumption (ii).

The moment generating function (*m.g.f.*) $\eta(s)$ of a random variable $T(X)$ having a Taylor expansion in x from the population $F(x)$ may be obtained by:

(1) Inverting the *c.f.* to obtain the *p.d.f.*:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-itx} \psi(t) dt, \tag{5}$$

(2) Taking the expectation of $e^{sT(X)}$ to give the *m.g.f.*:

$$\eta(s) = \int_{-\infty}^{\infty} e^{sT(x)} f(x) dx. \tag{6}$$

In most cases, however, it is not easy to get the two definite integrals (5) and (6). On the other hand, the following lemma is clearly obtained from the Eq. (2) and bears Algorithm 2 for getting the symbolic computation of $\mathrm{E}\left[\mathrm{e}^{sT(X)}\right]$.

Lemma 1. *There uniquely exists* $\tilde{p}(D_x)\,\mathrm{e}^{-\frac{1}{2}x^2}$ *for any* $p(x)\,\mathrm{e}^{-\frac{1}{2}x^2} \in Q(x)$.

Algorithm 2 (*Calculation of the Formal Moment Generating Function*). (1) The *c.f.* $\psi(t) = p(t)\,\mathrm{e}^{-\frac{1}{2}t^2} \in Q(t)$ can be rewritten, by using Lemma 1, in the form

$$\psi(t) = \tilde{p}(D_t)\,\mathrm{e}^{-\frac{1}{2}t^2}. \tag{7}$$

(2) The identity equation

$$D_t^n \mathrm{e}^{-\frac{1}{2}t^2}\Big|_{t=-it} = i^n D_t^n \mathrm{e}^{\frac{1}{2}t^2} \quad (n = 0,\ 1,\ 2,\ \ldots) \tag{8}$$

gives the *m.g.f.* $m(t)$ of $F(x)$ as

$$m(t) = \psi(-it) = \tilde{p}(iD_t)\,\mathrm{e}^{\frac{1}{2}t^2}. \tag{9}$$

(3) The *m.g.f.* $\eta(s)$ is obtained from

$$\eta(s) = \mathrm{E}\left[\mathrm{e}^{sT(X)}\right] = \mathrm{e}^{sT(D_t)}\,\tilde{p}(iD_t)\,\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}. \tag{10}$$

(4) Finally, the expansion of $\mathrm{e}^{sT(D_t)}\,\tilde{p}(iD_t)$ into a series $\hat{p}(s, D_t) \in \mathbb{R}[[s, D_t]]$ gives

$$\eta(s) = \hat{p}(s, D_t)\,\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}. \tag{11}$$

The fact that $\mathrm{e}^{\frac{1}{2}t^2}$ is the *m.g.f.* of the standard normal distribution; that is, for any non-negative integer n,

$$D_t^{2n}\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} = (2n-1)!!, \qquad D_t^{2n+1}\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} = 0; \tag{12}$$

may suffice to complete the task concerned.

4. Application to computational statistics

Assume that $F(x)$ has a known parameter N and tends to the standard normal distribution as the parameter N tends to infinity. The most common form of the *c.f.*'s in such a case is

$$\psi(t) = \left\{1 + \frac{1}{\sqrt{N}}\,k_1(t) + \frac{1}{N}\,k_2(t) + \cdots\right\}\mathrm{e}^{-\frac{1}{2}t^2}, \quad k_j(t) \in \mathbb{C}[t]\ (j = 1,\ 2,\ \ldots) \tag{13}$$

and, from Lemma 1, the corresponding $m(t) = \psi(-it)$ can be supposed to be

$$m(t) = \left\{1 + \frac{1}{\sqrt{N}}\,h_1(D_t) + \frac{1}{N}\,h_2(D_t) + \cdots\right\}\mathrm{e}^{\frac{1}{2}t^2}, \tag{14}$$

where $h_j(D_t) \in \mathbb{R}[D_t]$ $(j = 1,\ 2,\ \ldots)$. The discussion of the function $T(x)$ concerns the following two cases:

(1) the expansion of $T(x)$ is of order x:

$$T(x) = x + \frac{1}{\sqrt{N}}\,u_1(x) + \frac{1}{N}\,u_2(x) + \cdots; \tag{15}$$

(2) the expansion of $T(x)$ is of order x^2:

$$T(x) = x^2 + \frac{1}{\sqrt{N}}\, u_1(x) + \frac{1}{N}\, u_2(x) + \cdots; \tag{16}$$

where $u_j(x) \in \mathbb{R}[x]$ $(j = 1, 2, \ldots)$. When $T(x)$ is seen as a series in $\frac{1}{\sqrt{N}}$, unfortunately the convolution $\exp(sT(x))$ does not converge in the series of $\frac{1}{\sqrt{N}}$ from the viewpoint of the theory of the power series ring, because $T(x)$ includes the constant term x or x^2. Lemmas 3 and 5 below are required for obtaining fruitful results for avoiding the divergence.

Lemma 3. *For any $g(s, x) \in \mathbb{R}[[s, x]]$, it holds formally that*

$$\mathrm{e}^{sD_t}\, g(s, D_t)\, \mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} = \mathrm{e}^{\frac{1}{2}s^2}\, g(s, s + D_t)\, \mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}. \tag{17}$$

Eq. (17) means that the exponential function e^{sD_t} acts on $g(s, D_t)$ as the shift operator.

Proof. By formal operations, it holds that

$$\begin{aligned}
\mathrm{e}^{sD_t}\, g(s, D_t)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} &= \int_{-\infty}^{\infty} \mathrm{e}^{sx}\, g(s, x)\, \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}x^2} \mathrm{d}x \\
&= \int_{-\infty}^{\infty} g(s, x)\, \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x-s)^2 + \frac{1}{2}s^2\right\} \mathrm{d}x \\
&= \int_{-\infty}^{\infty} g(s, x+s)\, \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}x^2 + \frac{1}{2}s^2\right\} \mathrm{d}x \\
&= \mathrm{e}^{\frac{1}{2}s^2} \int_{-\infty}^{\infty} g(s, x+s)\, \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}x^2} \mathrm{d}x \\
&= \mathrm{e}^{\frac{1}{2}s^2}\, g(s, s + D_t)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0},
\end{aligned}$$

which proves the lemma. □

Let V_j be the set of partitions of degree j, that is,

$$V_j = \left\{ (1^{m_1}\, 2^{m_2}\, \ldots\, j^{m_j}) \;\middle|\; \sum_{k=1}^{j} k\, m_k = j,\; m_k \geq 0 \right\}. \tag{18}$$

Theorem 4. *Let X be a random variable with m.g.f. $m(t)$ defined by (14) and let $T(x)$ be the function of x defined by (15). Then the m.g.f. $\eta(s)$ of $T(X)$ is obtained as*

$$\eta(s) = \mathrm{E}\left[\mathrm{e}^{sT(X)}\right] = \mathrm{e}^{\frac{1}{2}s^2} \left\{ 1 + \frac{1}{\sqrt{N}}\, \bar{v}_1(s) + \frac{1}{N}\, \bar{v}_2(s) + \cdots \right\}, \tag{19}$$

where

$$\bar{v}_j(s) = \hat{v}_j(s, s + D_t)\, \mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} \in \mathbb{R}[s], \quad j = (1, 2, \ldots), \tag{20}$$

$$\hat{v}_j(s, x) = \sum_{\substack{k \geq 0,\, l \geq 0, \\ k+l=j}} q_k(s, x)\, h_l(x) \in \mathbb{R}[s][x], \tag{21}$$

$$q_j(s,x) = \sum_{(1^{m_1}\,2^{m_2}\,\ldots\,j^{m_j})\in V_j} \prod_{k=1}^{j} \frac{u_k(x)^{m_k}}{m_k!}\, s^{m_k} \in \mathbb{R}[s][x], \tag{22}$$

providing $q_0(s,x) = h_0(x) = 1$.

Proof.

$$\begin{aligned}
\eta(s) = \mathrm{E}\left[\mathrm{e}^{sT(X)}\right] &= \exp\left(sD_t + \sum_{k=1}^{\infty} \frac{su_k(D_t)}{N^{\frac{k}{2}}}\right)\left(\sum_{k=0}^{\infty}\frac{h_k(D_t)}{N^{\frac{k}{2}}}\right)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}\\
&= \mathrm{e}^{sD_t}\left\{\sum_{k=0}^{\infty}\frac{q_k(s,D_t)}{N^{\frac{k}{2}}}\right\}\left(\sum_{k=0}^{\infty}\frac{h_k(D_t)}{N^{\frac{k}{2}}}\right)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}\\
&= \mathrm{e}^{sD_t}\left\{1 + \frac{1}{\sqrt{N}}\,\hat{v}_1(s,D_t) + \frac{1}{N}\,\hat{v}_2(s,D_t) + \cdots\right\}\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}\\
&= \mathrm{e}^{\frac{1}{2}s^2}\left\{1 + \frac{1}{\sqrt{N}}\,\hat{v}_1(s,s+D_t) + \frac{1}{N}\,\hat{v}_2(s,s+D_t) + \cdots\right\}\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}\\
&= \mathrm{e}^{\frac{1}{2}s^2}\left\{1 + \frac{1}{\sqrt{N}}\,\bar{v}_1(s) + \frac{1}{N}\,\bar{v}_2(s) + \cdots\right\}. \quad \square
\end{aligned}$$

Lemma 5. *For any* $g(s,x) \in \mathbb{R}[[s,x]]$, *it holds formally that*

$$\mathrm{e}^{sD_t^2} g(s,D_t)\,\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} = \frac{1}{\sqrt{1-2s}}\, g\left(s, \frac{D_t}{\sqrt{1-2s}}\right)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0}. \tag{23}$$

Proof. Like in the proof for Lemma 3, by formal operations, it holds that

$$\begin{aligned}
\mathrm{e}^{sD_t^2} g(s,D_t)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} &= \int_{-\infty}^{\infty} \mathrm{e}^{sx^2} g(s,x)\,\frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-\frac{1}{2}x^2}\mathrm{d}x\\
&= \int_{-\infty}^{\infty} g(s,x)\,\frac{1}{\sqrt{2\pi}}\exp\left\{-\frac{1}{2}(1-2s)x^2\right\}\mathrm{d}x\\
&= \frac{1}{\sqrt{1-2s}}\int_{-\infty}^{\infty} g\left(s,\frac{x}{\sqrt{1-2s}}\right)\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{1}{2}x^2}\,\mathrm{d}x\\
&= \frac{1}{\sqrt{1-2s}}\, g\left(s,\frac{D_t}{\sqrt{1-2s}}\right)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0},
\end{aligned}$$

which proves the lemma. $\square$

Theorem 6. *Let X be a random variable with m.g.f. $m(t)$ defined by (14) and let $T(x)$ be the function of x defined by (16). Then the m.g.f. $\eta(s)$ of $T(X)$ is obtained as*

$$\eta(s) = \frac{1}{\sqrt{1-2s}}\left\{1 + \frac{1}{\sqrt{N}}\,\bar{w}_1(s) + \frac{1}{N}\,\bar{w}_2(s) + \cdots\right\}, \tag{24}$$

where $\hat{v}_j(s,x)$ and $q_j(s,x)$ are given by (21) and (22), respectively, and

$$\bar{w}_j(s) = \hat{v}_j\left(s,\frac{D_t}{\sqrt{1-2s}}\right)\mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} \in \mathbb{R}\left[\left[\frac{1}{\sqrt{1-2s}}\right]\right] \quad (j = 1, 2, \ldots).$$

Eq. (24) indicates that the limiting distribution of $T(X)$ is the χ^2 distribution with 1 degree of freedom.

5. Simple example

A set of term-rewriting rules written in *Mathematica* language is designed as a help to algebraic computation in our proposed methods. The following calculations including expansions, substitutions, differentiations, and the Hermite inversion formula are conducted in the *Mathematica* system.

A simple case may be a statistic as a function of the sample mean. Let $X_1, X_2, \ldots, X_N$ be mutually independent and identically distributed random variables, with cumulants $\kappa_1 = 0, \kappa_2 = 1, \kappa_3, \kappa_4$ and

$$\bar{X} = N^{-1}\sum_{i=1}^{N} X_i,\ X = \sqrt{N}\,\bar{X} \ \text{ and } \ T(X) = \sqrt{N}\,g(\bar{X}),$$

where g may be supposed to a continuous and differentiable function at the origin, providing $g(0) = 0$, $g'(0) = 1$ without loss of generality. The *c.f.* of X is in the form

$$\psi(t) = \left\{1 + \frac{\kappa_3}{6\sqrt{N}}(it)^3 + \frac{\kappa_4}{24\,N}(it)^4 + \frac{\kappa_3^2}{72\,N}(it)^6 + O(N^{-\frac{3}{2}})\right\} \mathrm{e}^{-\frac{1}{2}t^2},$$

and the *m.g.f.* is in the formally differential form

$$m(t) = \left\{1 + \frac{1}{\sqrt{N}}h_1(D_t) + \frac{1}{N}h_2(D_t) + O(N^{-\frac{3}{2}})\right\} \mathrm{e}^{\frac{1}{2}t^2}$$

by Eq. (2), where

$$h_1(D_t) = \frac{\kappa_3\,D_t^3}{6} - \frac{\kappa_3\,D_t}{2},$$

$$h_2(D_t) = -\frac{5\,\kappa_3^2}{24} + \frac{5\,\kappa_3^2\,D_t^2}{8} - \frac{5\,\kappa_3^2\,D_t^4}{24} + \frac{\kappa_3^2\,D_t^6}{72} + \frac{\kappa_4}{8} - \frac{\kappa_4\,D_t^2}{4} + \frac{\kappa_4\,D_t^4}{24}$$

Taylor expansion gives

$$T(X) = X + \frac{c_2}{2\sqrt{N}}X^2 + \frac{c_3}{6\,N}X^3 + O(N^{-\frac{3}{2}})$$

where $c_i = g^{(i)}(0)$. Then

$$\begin{aligned}
\mathrm{E}[sT(X)] &= \mathrm{E}\left[\exp(s\,X)\,\exp\left(\frac{s\,c_2}{2\sqrt{N}}X^2 + \frac{s\,c_3}{6\,N}X^3 + O(N^{-\frac{3}{2}})\right)\right] \\
&= \mathrm{e}^{sD_t}\left\{1 + \frac{s\,c_2}{2\sqrt{N}}(D_t)^2 + \frac{s\,c_3}{6\,N}(D_t)^3 + \frac{s^2\,c_2^2}{8\,N}(D_t)^4 + O(N^{-\frac{3}{2}})\right\} \\
&\quad \times \left\{1 + \frac{1}{\sqrt{N}}h_1(D_t) + \frac{1}{N}h_2(D_t) + O(N^{-\frac{3}{2}})\right\} \mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} \\
&= \mathrm{e}^{\frac{1}{2}s^2}\left\{1 + \frac{s\,c_2}{2\sqrt{N}}(s + D_t)^2 + \frac{s\,c_3}{6\,N}(s + D_t)^3 + \frac{s^2\,c_2^2}{4\,N}(s + D_t)^4 + O(N^{-\frac{3}{2}})\right\} \\
&\quad \times \left\{1 + \frac{1}{\sqrt{N}}h_1(s + D_t) + \frac{1}{N}h_2(s + D_t) + O(N^{-\frac{3}{2}})\right\} \mathrm{e}^{\frac{1}{2}t^2}\Big|_{t=0} \\
&\sim \mathrm{e}^{\frac{1}{2}s^2}\left(1 + a_1 s + \frac{a_2}{2}s^2 + \frac{a_3}{6}s^3 + \frac{a_4}{24}s^4\right)
\end{aligned}$$

which yields the ith moment a_i ($i = 1\ldots, 4$) of $T(X)$ as follows:

$$a_1 = \frac{c_2}{2\sqrt{N}} + O(N^{-\frac{3}{2}}), \quad a_2 = 1 + \frac{3\,c_2^2}{4\,N} + \frac{c_3}{N} + \frac{c_2\,\kappa_3}{N} + O(N^{-\frac{3}{2}}),$$

$$a_3 = \frac{9\,c_2}{2\sqrt{N}} + \frac{\kappa_3}{\sqrt{N}} + O(N^{-\frac{3}{2}}), \quad a_4 = 3 + \frac{45\,c_2^2}{2\,N} + \frac{10c_3}{N} + \frac{20\,c_2\,\kappa_3}{N} + \frac{\kappa_4}{N} + O(N^{-\frac{3}{2}}).$$

These results $a_1, \ldots, a_4$ are well known and can check the correctness of Algorithm 2.

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