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An invariance property of marginal density and tail probability approximations for smooth functions

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Abstract: Asymptotic approximations of marginal densities and tail probabilities for smooth functions of a continuous random vector, developed by Tierney, Kass and Kadane (1989) and DiCiccio and Martin (1991), respectively, in general fail to be invariant under transformations of the underlying random vector. This lack of invariance raises the complex issue of which choice of variables yields the most accurate approximations. However, in this paper, we show that the density and tail probability approximations remain invariant under transformations of the underlying variables if the joint density of the transformed variables is specified appropriately. The invariance property allows approximations to be computed using a convenient choice of variables, thereby avoiding the need for explicit nonlinear transformation of the underlying joint density. The utility of the invariance property is illustrated in an example involving the Studentized mean.

Keywords: Asymptotic approximations, distribution function, Laplace approximation, non-linear transformation, normal approximation, saddlepoint methods, Studentized mean.

1. Introduction

Asymptotic approximations of marginal densities and marginal tail probabilities for smooth functions of a continuous random vector have been developed recently by Tierney, Kass and Kadane (1989) and DiCiccio and Martin (1991), respectively. These approximations have broad applicability to Bayesian and frequentist inference, as well as for approximating sampling distributions. Important features of the approximations are that they are easily computed and circumvent numerical integration in high dimensions. Moreover, both the density and the tail probability approximations have been shown to be very accurate in a wide range of problems.

Unfortunately, as Tierney, Kass and Kadane (1989) and DiCiccio and Martin (1991) observe, the approximations are generally not invariant under different choices of the underlying random vector. That is, if $X=(X^1,\ldots,X^p)$ and $Z=(Z^1,\ldots,Z^p)$ are distinct continuous random p-vectors, and we wish to estimate the density and tail probabilities of a real-valued random variable $Y=g(X)=\bar{g}(Z)$ for smooth functions g and $\bar{g}$, then the density and tail probability approximations for Y based on the variables X do not coincide, typically, with approximations constructed using the variables Z. In this paper we develop an approach to constructing the density and tail probability approximations so that results obtained for different choices of the underlying variables are identical.

The general lack of invariance raises the difficult question as to which choice of variables yields the most accurate approximations. Our result is significant because it implies that the most convenient choice of variables can be used to construct the approximations, and hence explicit nonlinear transformation of the underlying joint density is avoided.

Section 2 of the paper contains a development and proof of the invariance property. In Section 3, we provide an example of how the invariance property may be used to allow the construction of approximations to the density and tail probabilities of a Studentized mean under a convenient choice of variables.

2. Derivation of the invariance property

Consider a continuous random vector $X = (X^1, \ldots, X^p)$ having probability density function of the form

$$f_X(x) \propto b(x) \exp\{l(x)\}, \quad x = (x^1, \ldots, x^p). \tag{1}$$

Suppose that the function l takes its maximum value at $\hat{x} = (\hat{x}^1, \ldots, \hat{x}^p)$ and that $X_j - \hat{x}_j$ $(j = 1, \ldots, p)$ is $O_p(n^{-1/2})$ as some parameter n, usually sample size, increases to infinity. For each fixed x, assume that $l(x)$ and its partial derivatives are $O(n)$ and that $b(x)$ is $O(1)$. Suppose we are interested in estimating the density and distribution functions of a real-valued random variable $Y = g(X)$, where the function g is assumed to have continuous gradient that is non-zero at $\hat{x}$. Tierney, Kass and Kadane (1989) have given an asymptotic approximation to the true density $f_Y(y)$ of Y, and DiCiccio and Martin (1991) have derived an approximation to the distribution function of Y. An important feature of these approximations is that they do not require numerical integration.

To describe the approximations, let $\tilde{x} = \tilde{x}(y)$ be the value of x that maximizes $l(x)$ subject to the constraint $g(x) = y$. Let $l_i(x) = \partial l(x)/\partial x^i$, $l_{ij}(x) = \partial^2 l(x)/\partial x^i\, \partial x^j$, $g_i(x) = \partial g(x)/\partial x^i$, $g_{ij}(x) = \partial^2 g(x)/\partial x^i\, \partial x^j$, etc. $(i, j = 1, \ldots, p)$. Put

$$J_{ij}(y) = -l_{ij}\{\tilde{x}(y)\} + \frac{l_k\{\tilde{x}(y)\}}{g_k\{\tilde{x}(y)\}} g_{ij}\{\tilde{x}(y)\}, \quad i, j = 1, \ldots, p,$$

where k is any index for which $g_k\{\tilde{x}(y)\}$ is non-zero. Our assumptions about g guarantee the existence of such an index k. Define the $p \times p$ matrices $J(y) = \{J_{ij}(y)\}$ and $J(y)^{-1} = \{J^{ij}(y)\}$, and let

$$Q(y) = J^{ij}(y) g_i\{\tilde{x}(y)\} g_j\{\tilde{x}(y)\}, \qquad D(y) = \{Q(y)|J(y)|/|J(\hat{y})|\}^{-1/2}.$$

In the expression for the quadratic form $Q(y)$, and in forthcoming expressions, the notational convention is used whereby summation over the range $1, \ldots, p$ is understood for each index appearing as both a subscript and a superscript. Tierney, Kass and Kadane's (1989) asymptotic approximation to the marginal density of $Y = g(X)$ for $p \geqslant 1$ is

$$f_Y^*(y) \propto D(y) \frac{b\{\tilde{x}(y)\}}{b(\hat{x})} \exp[l\{\tilde{x}(y)\} - l(\hat{x})]. \tag{2}$$

See also Tierney, Kass and Kadane's (1991) correction note to their 1989 paper. A normalizing constant c may be computed so that $f_Y^*(y)$ integrates to $1 + O(n^{-3/2})$. Provided $y - \hat{y}$ is $O(n^{-1/2})$, the renormalized approximation has relative error of order $n^{-3/2}$; that is,

$$f_Y(y) = f_Y^*(y)\{1 + O(n^{-3/2})\}.$$

Leonard, Hsu and Tsui (1989) also describe the saddlepoint accuracy of $f_Y^*(y)$. The derivation of approximation (2) involves the application of a Laplace approximation to the joint density of $X^* = (Y, A^2, \ldots, A^p)$, where $A^j = A^j(X^1, \ldots, X^p)$ $(j = 2, \ldots, p)$, to obtain an approximation to the marginal density of $Y = g(X)$. Note that the transformation from X to X^* is not explicitly used in applying their approximation, except to the extent that the function g and its derivatives are required.

DiCiccio and Martin's (1991) approximation to the distribution function $F_Y(y) = P(Y \leqslant y)$ of Y is based on a standard normal approximation to the distribution of $R = r(Y)$, where

$$r(y) = \operatorname{sgn}(y - \hat{y})(2[l(\hat{x}) - l\{\tilde{x}(y)\}])^{1/2},$$

$\hat{y} = g(\hat{x})$, and the function $r(y)$ is assumed to be monotonically increasing. An initial approximation to the tail probability $P(Y \leqslant y)$, provided $y - \hat{y}$ is $O(n^{-1/2})$, is

$$P(Y \leqslant y) = \Phi(r) + O(n^{-1/2}),$$

where $r = r(y)$ and Φ is the standard normal distribution function. DiCiccio and Martin's (1991) improved approximation is

$$P(Y \leqslant y) = \Phi(r) + \phi(r)\left[\frac{1}{r} + D(y)\frac{b\{\tilde{x}(y)\}}{b(\hat{x})}\frac{g_k\{\tilde{x}(y)\}}{l_k\{\tilde{x}(y)\}}\right] + O(n^{-3/2}), \tag{3}$$

where ϕ is the standard normal density function and k is any index such that $g_k\{\tilde{x}(y)\}$ does not vanish. Expression (3) is derived by applying a tail probability approximation of DiCiccio, Field and Fraser (1990) to the Tierney, Kass and Kadane (1989) approximation of the density of a suitably chosen function of Y. See DiCiccio and Martin (1991) for details of this construction.

Tierney, Kass and Kadane note that their density approximation is generally not invariant under non-linear transformations of the density (1). DiCiccio and Martin also observe the same phenomenon for their tail probability approximation. More formally, let $Z = (Z^1, \ldots, Z^p)$ denote a continuous random vector that is a function of X, so that the probability density function of Z is

$$f_Z(z) \propto b(x)|\Delta(x)| \exp\{l(x)\},$$

where $x = x(z)$ and $\Delta(x) = \{x_i^a\}$ is the $p \times p$ matrix of partial derivatives $x_i^a = \partial x^a / \partial z^i$ $(a,\ i = 1, \ldots, p)$. Suppose $Y = \bar{g}(Z)$. To apply marginal density approximation (2) and tail probability approximation (3) in terms of Z, we write

$$f_Z(z) \propto \bar{b}(z) \exp\{\bar{l}(z)\},$$

with $\bar{b}(z)$ and $\bar{l}(z)$ to be specified. In general, the density approximation corresponding to (2) and the tail probability approximation corresponding to (3) constructed using Z yield different results to density and tail probability approximations constructed using X. For instance, if we choose $\bar{b}(z) = 1$ and $\bar{l}(z) = l(x) + \log|\Delta(x)|$, hence accounting for the Jacobian of the transformation from X to Z in the exponent, then the approximations corresponding to X and Z differ. In this note, we show that the approximations coincide if the joint density of Z is written so that

$$\bar{l}(z) = l(x) \tag{4}$$

and

$$\bar{b}(z) = b(x)|\Delta(x)|. \tag{5}$$

We now show that this specification of the density of Z results in invariance. Let $\hat{z}$ denote the value of z for which $\bar{l}$ is maximized and let $\tilde{z} = \tilde{z}(y)$ be the value of z which maximizes $\bar{l}$ subject to the constraint $\bar{g}(z) = y$. Define $\bar{l}_i(z) = \partial \bar{l}(z)/\partial z^i$, $\bar{l}_{ij}(z) = \partial^2 \bar{l}(z)/\partial z^i\, \partial z^j$, $\bar{g}_i(z) = \partial \bar{g}(z)/\partial z^i$ and $\bar{g}_{ij}(z) = \partial^2 \bar{g}(z)/\partial z^i\, \partial z^j$, $(i,\ j = 1, \ldots, p)$, etc. Denote versions of $J(y)$, $Q(y)$, $D(y)$ and $r(y)$, etc. computed using the variables Z by $\bar{J}(y)$, $\bar{Q}(y)$, $\bar{D}(y)$ and $\bar{r}(y)$, etc. Clearly, (4) implies $\bar{l}(\hat{z}) = l(\hat{x})$ and $\bar{l}\{\tilde{z}(y)\} = l\{\tilde{x}(y)\}$. In particular, observe that $\exp[\bar{l}\{\tilde{z}(y)\} - \bar{l}(\hat{z})] = \exp[l\{\tilde{x}(y)\} - l(\hat{x})]$. Moreover, since $\hat{y} = \bar{g}(\hat{z}) = g(\hat{x})$, it follows that $\bar{r}(y)=r(y)$, for each y. By differentiating the expression $\bar{g}(z)=g(x)$ and (4) with respect to $z^1,\ldots,z^p$, we obtain

$$\begin{aligned} \bar{l}_i(z) &= l_a(x)x_i^a, \\ \bar{g}_i\{\tilde{z}(y)\} &= g_a\{\tilde{x}(y)\}\tilde{x}_i^a, \end{aligned} \qquad i=1,\ldots,p, \tag{6}$$

where $x=x(z)$ and $\tilde{x}_i^a=\partial x^a/\partial z^i\,|_{z=\tilde{z}(y)}$. Similarly, further differentiation yields

$$\begin{aligned} \bar{l}_{ij}(z) &= l_{ab}x_i^a x_j^b + l_a(x)x_{ij}^a, \\ \bar{g}_{ij}\{\tilde{z}(y)\} &= g_{ab}\{\tilde{x}(y)\}\tilde{x}_i^a\tilde{x}_j^b + g_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a, \end{aligned} \qquad i,\ j=1,\ldots,p, \tag{7}$$

where $\tilde{x}_{ij}^a=\partial^2x^a/\partial z^i\,\partial z^j\,|_{z=\tilde{z}(y)}$.

A Lagrange multiplier argument for maximizing $\bar{l}(z)$ subject to the constraint $\bar{g}(z)=y$ involves solution of the system of equations

$$\bar{l}_i\{\tilde{z}(y)\} + \bar{\lambda}(y)\bar{g}_i\{\tilde{z}(y)\} = 0, \quad i=1,\ldots,p, \tag{8}$$

for $\tilde{z}(y)$. A similar argument for maximizing $l(x)$ subject to $g(x)=y$ involves solution of the system of equations

$$l_a\{\tilde{x}(y)\} + \lambda(y)g_a\{\tilde{x}(y)\} = 0, \quad a=1,\ldots,p, \tag{9}$$

for $\tilde{x}(y)$. It follows from (9) that

$$l_a\{\tilde{x}(y)\}\tilde{x}_i^a + \lambda(y)g_a\{\tilde{x}(y)\}\tilde{x}_i^a = 0, \quad i=1,\ldots,p, \tag{10}$$

and

$$l_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a + \lambda(y)g_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a = 0, \quad i,\ j=1,\ldots,p. \tag{11}$$

On combining (6) and (10), we see that

$$\bar{l}_i\{\tilde{z}(y)\} + \lambda(y)\bar{g}_i\{\tilde{z}(y)\} = 0, \quad i=1,\ldots,p,$$

and thus (8) yields

$$\lambda(y) = \bar{\lambda}(y) = -\frac{l_k\{\tilde{x}(y)\}}{g_k\{\tilde{x}(y)\}} = -\frac{\bar{l}_m\{\tilde{z}(y)\}}{\bar{g}_m\{\tilde{z}(y)\}}, \tag{12}$$

where k and m are any indices for which $g_k\{\tilde{x}(y)\}$ and $\bar{g}_m\{\tilde{z}(y)\}$ are non-zero. Hence, from (11) and (12),

$$l_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a - \frac{l_k\{\tilde{x}(y)\}}{g_k\{\tilde{x}(y)\}}g_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a = 0, \quad i,\ j=1,\ldots,p. \tag{13}$$

Equations (7) and (13) imply that

$$\begin{aligned} \bar{J}_{ij}(y) &= -\bar{l}_{ij}\{\tilde{z}(y)\} + \frac{\bar{l}_m\{\tilde{z}(y)\}}{\bar{g}_m\{\tilde{z}(y)\}}\bar{g}_{ij}\{\tilde{z}(y)\} \\ &= \left[-l_{ab}\{\tilde{x}(y)\} + \frac{l_k\{\tilde{x}(y)\}}{g_k\{\tilde{x}(y)\}}g_{ab}\{\tilde{x}(y)\}\right]\tilde{x}_i^a\tilde{x}_j^b \\ &\quad -\left[l_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a - \frac{l_k\{\tilde{x}(y)\}}{g_k\{\tilde{x}(y)\}}g_a\{\tilde{x}(y)\}\tilde{x}_{ij}^a\right] \\ &= J_{ab}(y)\tilde{x}_i^a\tilde{x}_j^b, \quad i,\ j=1,\ldots,p. \end{aligned} \tag{14}$$

Observe that $x^a = x^a\{z(x)\}$, so that $x_i^a z_b^i = \delta_b^a$, where $z_b^i = \partial z^i/\partial x^b$ and δ_b^a is Kronecker's delta. As a result, inversion of (14) yields $\bar{J}^{ij}(y) = J^{ab}(y)\tilde{z}_a^i \tilde{z}_b^j$, where $\tilde{z}_a^i = \partial z^i/\partial x^a|_{x=\tilde{x}(y)}$. Therefore,

$$\begin{aligned}\bar{Q}(y) &= \bar{J}^{ij}\bar{g}_i\{\tilde{z}(y)\}\bar{g}_j\{\tilde{z}(y)\}\\ &= J^{ab}(y)g_c\{\tilde{x}(y)\}g_d\{\tilde{x}(y)\}\tilde{x}_i^c\tilde{z}_a^i\tilde{x}_j^d\tilde{z}_b^j\\ &= J^{ab}(y)g_a\{\tilde{x}(y)\}g_b\{\tilde{x}(y)\}\\ &= Q(y).\end{aligned}$$

Thus,

$$\bar{D}(y) = \left\{\frac{\bar{Q}(y)|\bar{J}(y)|}{|\bar{J}(\hat{y})|}\right\}^{-1/2} = \left\{\frac{Q(y)|J(y)||\Delta\{\tilde{x}(y)\}|^2}{|J(\hat{y})||\Delta(\hat{x})|^2}\right\}^{-1/2} = D(y)\frac{|\Delta(\hat{x})|}{|\Delta\{\tilde{x}(y)\}|}. \tag{15}$$

By combining (5) and (15), we see that

$$\bar{D}(y)\frac{\bar{b}\{\tilde{z}(y)\}}{\bar{b}(\hat{z})} = D(y)\frac{b\{\tilde{x}(y)\}}{b(\hat{x})}. \tag{16}$$

It follows from (16) that approximation (2) is the same regardless of whether the variables X or Z are used in its construction. Moreover, noting (12) and recalling that $\bar{r}(y) = r(y)$ for each y, we see that approximation (3) is also invariant under the transformation from X to Z.

It should be stressed that our result does not address the important open question of how the functions b and l should be specified in (1) in order to achieve sufficiently accurate density and tail probability approximations for Y when the sample size n is small. Rather, our result guarantees that the density and tail probability approximations for Y obtained using a different choice of underlying variables Z will be identical to those corresponding to the variables X provided the joint density of the transformed variables Z is specified according to (4) and (5).

3. Example – the Studentized mean

The invariance property established in Section 2 can be used to demonstrate that density and tail probability approximations developed by Daniels and Young (1991) for a Studentized mean are equivalent to those obtained by applying approximations (2) and (3) directly to a saddlepoint approximation to the joint density of two means. Consider a random sample of n observations $V_1, \ldots, V_n$ of a continuous, real-valued random variable V and let $\bar{V} = n^{-1}\Sigma_1^n V_i$ and $S^2 = n^{-1}\Sigma_1^n(V_i - \bar{V})^2$. Interest centers on approximating the density and tail probabilities of the Studentized mean $T = \bar{V}/S$. Daniels and Young (1991) derive approximations to the density and distribution functions of T through the use of saddlepoint techniques. To briefly describe their approach, let $W = V^2$ and put $\bar{W} = n^{-1}\Sigma_1^n V_i^2$. Note that $T = \bar{V}/(\bar{W} - \bar{V}^2)^{1/2}$. The joint cumulant generating function of V and W is

$$K(U_1, U_2) = \log\{E(e^{U_1V + U_2W})\}.$$

The usual saddlepoint approximation to the joint density of $\bar{V}$ and $\bar{W}$ is

$$\hat{f}_n(\bar{v}, \bar{w}) = \frac{n}{2\pi}\exp[n\{K(\hat{U}_1, \hat{U}_2) - \hat{U}_1\bar{v} - \hat{U}_2\bar{w}\}]\Lambda(\hat{U}_1, \hat{U}_2), \tag{17}$$

where

$$K_{U_1}(\hat{U}_1, \hat{U}_2) = \bar{v}, \qquad K_{U_2}(\hat{U}_1, \hat{U}_2) = \bar{w},$$

$$\Lambda(U_1, U_2) = \left\{K_{U_1U_1}(U_1, U_2)K_{U_2U_2}(U_1, U_2) - K_{U_1U_2}(U_1, U_2)^2\right\}^{-1/2},$$

$K_{U_i}(U_1, U_2) = \partial K(U_1, U_2)/\partial U_i$, and $K_{U_iU_j}(U_1, U_2) = \partial^2 K(U_1, U_2)/\partial U_i\, \partial U_j$, $(i, j = 1, 2)$. For general reviews of saddlepoint methods, see Barndorff-Nielsen and Cox (1979) and Reid (1988). Daniels and Young then transform the approximate joint density (17) to an approximate joint density of T and S,

$$\tilde{f}_n(t, s) = \frac{n}{2\pi}\frac{\partial(\bar{v}, \bar{w})}{\partial(t, s)}\exp\left[n\left\{K(\hat{U}_1, \hat{U}_2) - \hat{U}_1 ts - \hat{U}_2 s^2(1+t^2)\right\}\right]\Lambda(\hat{U}_1, \hat{U}_2), \tag{18}$$

where

$$\frac{\partial(\bar{v}, \bar{w})}{\partial(t, s)} = \frac{\partial\bar{v}}{\partial t}\frac{\partial\bar{w}}{\partial s} - \frac{\partial\bar{v}}{\partial s}\frac{\partial\bar{w}}{\partial t} = 2s^2.$$

They obtained by direct Laplace approximation density and tail probability approximations for T, which it is easy to establish are the same as those obtained by applying (2) and (3) to the approximate joint density $\tilde{f}_n(t, s)$, using $Z = (T, S)$, $z = (t, s)$, $\tilde{b}(z) = 2s^2\Lambda(\hat{U}_1, \hat{U}_2)$, $\tilde{l}(z) = n\{K(\hat{U}_1, \hat{U}_2) - \hat{U}_1 ts - \hat{U}_2 s^2(1 + t^2)\}$, and $g(t, s) = t$.

A simpler approach, which does not require explicit transformation of the approximate joint density (17), involves the direct application of approximations (2) and (3) to $\hat{f}_n(\bar{v}, \bar{w})$, putting $X = (\bar{V}, \bar{W})$, $x = (\bar{v}, \bar{w})$, $b(x) = \Lambda(\hat{U}_1, \hat{U}_2)$, $l(x) = n\{K(\hat{U}_1, \hat{U}_2) - \hat{U}_1\bar{v} - \hat{U}_2\bar{w}\}$, and $g(\bar{v}, \bar{w}) = \bar{v}/(\bar{w} - \bar{v}^2)^{1/2}$. It is readily seen in this example that $\bar{v} = ts$, $\bar{w} = s^2(1 + t^2)$ and $|\Delta(x)| = 2s^2$. Therefore, (4) and (5) hold for the Daniels and Young approximations. Consequently, the invariance property established here implies that density and tail probability approximations constructed using X are identical to those obtained by Daniels and Young.

The approach of Daniels and Young can be generalized to more complicated functions of means, such as variances, ratios of means, and correlation coefficients. For such cases, a saddlepoint approximation to the joint density of several means is first transformed to an approximate joint density of a random vector Z, the first component of which is the statistic of interest. Density and tail probability approximations are then obtained by applying (2) and (3) to the approximate joint density of Z with $g(z) = z^1$. Although in the case of a Studentized mean the transformation of (17) to (18) is fairly simple, in more complex cases — for instance, when the statistic of interest is a sample correlation coefficient — the transformation required may be quite complicated. In particular, the Jacobian arising from the transformation of X to Z must be explicitly calculated to specify the approximate joint density of Z. The invariance property established in Section 2 guarantees that the simpler approach of applying (2) and (3) directly to the saddlepoint approximation of the joint density of the means can always be used to obtain identical results. This method is typically much easier to apply because it does not require use of the Jacobian of a non-linear transformation.

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