HIROSHIMA MATH. J.
22 (1992), 177–183

Saddlepoint approximation for the distribution function of the mean of random variables

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(Received January 8, 1991)

§1. Introduction

After Daniels [1] introduced a saddlepoint technique in statistics, this method is widely discussed for deriving an accurate approximation for the probability density function of the mean of a random sample. Reid [6] gave an excellent review in this field, and Davison and Hinkley [3] presented a non-parametric saddlepoint approximation. See also Jensen [4].

When we want to find an approximation for the distribution function, several saddlepoint methods are available. Most simple method is to integrate the approximated probability density function obtained by the saddlepoint method. However this integration may not be easily carried out. Another method is based on the inversion formula from the cumulant generating function to the distribution function. See Lugannani and Rice [5], and Daniels [2] for a review on the tail probability approximations.

Recall that the saddlepoint is defined by the solution T of the equation $\kappa'(T) = \bar{x}$, where $\kappa(T)$ is a cumulant generating function. The saddlepoint is useful for approximating the probability density function. In this article we consider the equation $\kappa'(T) = \bar{x} + 1/(nT)$ of T. Its solution will be called the quasi-saddlepoint. Using the quasi-saddlepoint, we propose an alternate approximation formula for the distribution function by evaluating the inversion formula (2.1).

§2. Approximation for the distribution function

Let X be a random variable with a distribution function $F(x)$. We denote its cumulant generating function by

$$\kappa(T) = \log \mathrm{E}\{\exp(TX)\} = \log\left(\int_{-\infty}^{\infty} \exp(Tx)\, dF(x)\right).$$

Suppose that $\kappa(T)$ is finite for $-a < T < b$, where a and b are positive constants. Our interest is to approximate the distribution function $\bar{F}^n(x)$ of the mean $\bar{X}_n$ of a sample of n independent observations from $F(x)$.

Put the integral

$$(2.1)\qquad I(c) = (2\pi i)^{-1} \int_{c-i\infty}^{c+i\infty} e^{n\{\kappa(T)-\bar{x}T\}}\, dT/T \qquad \text{for} \quad -a < c < b\,.$$

Then the inversion formula for the distribution function $\bar{F}^n(x)$ of $\bar{X}_n$ is given by

$$(2.2)\qquad \bar{F}^n(\bar{x}) = \begin{cases} 1 - I(c) & \text{if } c > 0\,, \\ \quad - I(c) & \text{if } c < 0\,. \end{cases}$$

The latter relation of (2.2) is derived by the residue theorem. The simple approach for evaluating $I(c)$ is given by (i) expanding $1/T$ around the saddlepoint $\hat{T}$ and (ii) integrating along the path $T = \hat{T} + iy$, where $\hat{T}$ is the unique solution of $\kappa'(T) = \bar{x}$. However, this aproximation breaks down at the neighborhood of the mean $\mu = \kappa'(0)$ because $\hat{T}$ is close to zero when $\bar{x}$ is near by μ.

We rewrite (2.1) as

$$(2.3)\quad 2\pi I(c) = \begin{cases} \displaystyle\int_{-\infty}^{\infty} \exp\{n\kappa(c+it) - n\bar{x}(c+it) - \log(c+it)\}\, dt & (c>0)\,, \\ \displaystyle -\int_{-\infty}^{\infty} \exp\{n\kappa(c+it) - n\bar{x}(c+it) - \log(-c-it)\}\, dt & (c<0)\,. \end{cases}$$

Our approach is based on the real solution $T = \hat{c}$ of the equation

$$(2.4)\qquad d\{\kappa(T) - \bar{x}T - (\log T)/n\}/dT = \kappa'(T) - \bar{x} - 1/(nT) = 0\,.$$

Now we may recall that a saddlepoint is the solution of $\kappa'(T) = \bar{x}$. Hence we say that $\hat{c}$ is a quasi-saddlepoint. Put $g(T) = \kappa'(T) - 1/(nT)$ for $-a < T < b$, $T \neq 0$. Then $g(T)$ is monotone increasing because $g'(T) = \kappa''(T) + 1/(nT^2)$ and $\kappa''(T)$ is a variance of a conjugate exponential family. Also $\lim_{T\to -0} g(T) = +\infty$ and $\lim_{T\to +0} g(T) = -\infty$ imply that (2.4) has at most two solutions. We denote the positive and negative solutions by $\hat{c}_+ = \hat{c}_+(\bar{x})$ and $\hat{c}_- = \hat{c}_-(\bar{x})$ respectively, if exist. Note that the saddlepoint $\hat{T}$ is independent of n. On the other hand the quasi-saddlepoints $\hat{c}_+$ and $\hat{c}_-$ depend on n. Further, putting $\mu = \mathrm{E}X = \kappa'(0)$, we have

LEMMA. *Suppose the equation* (2.4) *has positive and negative quasi-saddlepoints $\hat{c}_+$ and $\hat{c}_-$, respectively, for given $\bar{x}$. When $\bar{x} > \mu$ (i.e., $\hat{T} > 0$), then it holds that*

$$\hat{c}_- < 0 < \hat{T} < \hat{c}_+\,, \qquad \hat{c}_- = \mathrm{O}(n^{-1/2}) \quad \textit{and} \quad \hat{c}_+ = \hat{T} + \mathrm{O}(n^{-1/2})\,.$$

When $\bar{x} < \mu$ (i.e., $\hat{T} < 0$), then it holds that

$$\hat{c}_- < \hat{T} < 0 < \hat{c}_+\,, \qquad \hat{c}_- = \hat{T} + \mathrm{O}(n^{-1/2}) \quad \textit{and} \quad \hat{c}_+ = \mathrm{O}(n^{-1/2})\,.$$

Further $\hat{c}_+$ is a monotone decreasing function of n and $\hat{c}_-$ is a monotone increasing function of n.

To approximate $I(c)$ of (2.1), we employ the Taylor expansion of the exponent of (2.3). When $\bar{x} > \mu$, then take $\hat{c} = \hat{c}_+ = \hat{T} + O(n^{-1/2})$. Transforming t to $u = t/\hat{c}$, we have

$$
\begin{aligned}
&n\kappa(\hat{c} + \hat{c}iu) - n\bar{x}(\hat{c} + \hat{c}iu) - \log(1 + iu) \\
(2.5)\quad &= n\kappa(\hat{c}) - n\bar{x}\hat{c} - \alpha^2u^2/2 - \beta iu^3/6 + \gamma u^4/24 + \delta iu^5/120 - \varepsilon u^6/720 + o(u^6) \\
&= n\kappa(\hat{c}) - n\bar{x}\hat{c} - v^2/2 - \lambda_3 iv^3/6 + \lambda_4 v^4/24 + \lambda_5 iv^5/120 - \lambda_6 v^6/720 + o(n^{-2})
\end{aligned}
$$

where

$$
\begin{aligned}
&v = \alpha u\,, \qquad \alpha = \alpha(\hat{c}) = \{n\hat{c}^2\kappa''(\hat{c}) + 1\}^{1/2} = O(n^{1/2})\,, \\
&\beta = n\hat{c}^3\kappa^{(3)}(\hat{c}) - 2\,, \qquad \gamma = n\hat{c}^4\kappa^{(4)}(\hat{c}) + 6\,, \\
&\delta = n\hat{c}^5\kappa^{(5)}(\hat{c}) - 24\,, \qquad \varepsilon = n\hat{c}^6\kappa^{(6)}(\hat{c}) + 120\,, \\
(2.6)\quad &\lambda_3 = \lambda_3(\hat{c}) = \{n\hat{c}^3\kappa^{(3)}(\hat{c}) - 2\}\alpha^{-3} = O(n^{-1/2})\,, \\
&\lambda_4 = \lambda_4(\hat{c}) = \{n\hat{c}^4\kappa^{(4)}(\hat{c}) + 6\}\alpha^{-4} = O(n^{-1})\,, \\
&\lambda_5 = \lambda_5(\hat{c}) = \{n\hat{c}^5\kappa^{(5)}(\hat{c}) - 24\}\alpha^{-5} = O(n^{-3/2})\,, \\
&\lambda_6 = \lambda_6(\hat{c}) = \{n\hat{c}^6\kappa^{(6)}(\hat{c}) + 120\}\alpha^{-6} = O(n^{-2})\,.
\end{aligned}
$$

Thus we obtain the following formal expansion of $I(\hat{c})$ as

$$
\begin{aligned}
I(\hat{c}) &= \frac{e^{n\kappa(\hat{c}) - n\bar{x}\hat{c}}}{2\pi\hat{c}} \int_{-\infty}^{\infty} e^{-\alpha^2u^2/2 - \beta iu^3/6 + \gamma u^4/24 + \delta iu^5/5! - \varepsilon u^6/6! + \cdots}\, \hat{c}du \\
&= A_1\{(2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{-v^2/2} \cdot e^{-\lambda_3 iv^3/6 + \lambda_4 v^4/24 + \lambda_5 iv^5/5! - \lambda_6 v^6/6!}\, dv + o(n^{-2})\}\,,
\end{aligned}
$$

where

$$A_1 = \exp\{n\kappa(\hat{c}) - n\bar{x}\hat{c}\}/(2\pi\alpha^2)^{1/2}\,.$$

When $\bar{x} < \mu$, replacing $\hat{c}$ by $\hat{c}_-$ $(= \hat{T} + O(n^{-1/2}))$ and $A_1(\hat{c})$ by $-A_1(\hat{c}_-)$, we get the similar results. Further expanding the exponent and taking expectation we get

THEOREM. *Suppose that the equation* (2.4) *has the positive solution $\hat{c}_+$ and/or the negative solution $\hat{c}_-$. When $\bar{x} > \mu$, we get*

$$I(\hat{c}_+) = A_1(\hat{c}_+)\{1 + a_2(\hat{c}_+) + a_3(\hat{c}_+) + o(n^{-2})\}\,,$$

where

$$a_2(\hat{c}_+) = \frac{1}{8}\lambda_4 - \frac{5}{24}\lambda_3^2 = \mathrm{O}(n^{-1}),$$

and

$$a_3(\hat{c}_+) = \frac{385}{1152}\lambda_3^4 - \frac{35}{64}\lambda_3^2\lambda_4 + \frac{7}{48}\lambda_3\lambda_5 - \frac{1}{48}\lambda_6 + \frac{35}{384}\lambda_4^2 = \mathrm{O}(n^{-2}).$$

When $\bar{x} < \mu$, *we get*

$$I(\hat{c}_-) = -A_1(\hat{c}_-)\{1 + a_2(\hat{c}_-) + a_3(\hat{c}_-) + \mathrm{o}(n^{-2})\},$$

where a_2 *and* a_3 *are defined in the above, and* a_2, a_3 *and* λ_j *are evaluated at* $\hat{c}_-$.

We note that the coefficients of λ_j in a_2 and in a_3, defined in the above theorem, are the same when we approximate the density function by the saddlepoint $\hat{T}$. (At that time λ_j is defined by $\kappa^{(j)}(\hat{T})/\{\kappa''(\hat{T})\}^{j/2}$). When the equation (2.4) has two solutions $\hat{c}_+$ and $\hat{c}_-$, the distribution function of $\bar{X}_n$, expressed by (2.2), is approximated by the following two formulae as

$$\hat{F}_j^+(\bar{x}) = 1 - A_1(\hat{c}_+)\sum_{k=1}^{j} a_k(\hat{c}_+) \quad \text{and} \quad \hat{F}_j^-(\bar{x}) = A_1(\hat{c}_-)\sum_{k=1}^{j} a_k(\hat{c}_-)$$

for each $j = 1, 2, 3$, where $a_1(\cdot) \equiv 1$. From the lemma in the above we expect that $\hat{F}_j^+(\bar{x})$ provides a better approximation than $\hat{F}_j^-(\bar{x})$ does when $\bar{x} > \mu$. Conversely when $\bar{x} < \mu$, $\hat{F}_j^-(\bar{x})$ may be superior to $\hat{F}_j^+(\bar{x})$. Also when $\bar{x}$ is close to μ, then $\hat{T}$, $\hat{c}_+$ and $\hat{c}_-$ are close to zero. In deriving the relation (2.5), the magnitude of $\hat{c}$ is important. To improve the approximation around the mean μ, we combine two formulae smoothly in the following manner.

Let σ^2 be the variance $\kappa''(0)$ of X, and let $x = x_0$ be the solution of the equation

$$\hat{c}_+(x) = -\hat{c}_-(x). \tag{2.7}$$

From LEMMA following (2.4), the sign of $x - x_0$ determines whether $\hat{c}_+$ is greater than $|\hat{c}_-|$ or not when two solutions exist. If X follows a symmetric distribution with mean μ, x_0 coincides with μ. Thus we propose the approximation formulae:

$$\hat{F}_j(\bar{x}) = \begin{cases} \hat{F}_j^-(\bar{x}) & \text{if } \bar{x} \le x_0 - \sigma/(2n^{1/2}), \\ (1-t)\hat{F}_j^-(\bar{x}) + t\hat{F}_j^+(\bar{x}) & \text{if } \bar{x} = x_0 + (t - 1/2)\sigma n^{-1/2},\ 0 \le t \le 1, \\ \hat{F}_j^+(\bar{x}) & \text{if } \bar{x} \ge x_0 + \sigma/(2n^{1/2}), \end{cases} \tag{2.8}$$

for $j = 1, 2, 3$. The validity of this strategy will be shown in the examples listed in the section 4.

§ 3. Asymptotic properties

When $\bar{x} = \kappa'(0) = \mu$, quasi-saddlepoints are given by $\pm(n\sigma^2)^{-1/2} + o(n^{-1/2})$, where $\sigma^2 = \kappa''(0)$ is a variance of X. In this case λ_j of (2.6) is $O(1)$.

As n tends to infinity, by the central limit theorem most of the distribution lies in the region of $|\bar{x} - \mu| < \Delta n^{-1/2}$ where Δ is a positive constant. Therefore we need to consider the case $\bar{x} = \mu + \delta n^{-1/2}$ for fixed δ. Then the solution of $\kappa'(T) - (nT)^{-1} - (\mu + \delta n^{-1/2}) = 0$ is given by $\hat{c}_+$, $\hat{c}_- = \{\delta \pm (\delta^2 + 4\sigma^2)^{1/2}\}/\{2\sigma^2 n^{1/2}\} + o(n^{-1/2})$. Then $\lambda_j(\hat{c}_\pm) = O(1)$.

In the above two cases, $\lambda_j(\hat{c}_\pm)$ are $O(1)$. This implies that our approximation may not be good around μ. However in the tail area containing lower or upper 5% point, (2.8) works sufficiently well.

§ 4. Examples

To check our procedure we give two examples.

Example 1. A gamma distribution with density $f(x) = e^{-x}$ $(x > 0)$

Let X follow a gamma distribution with density $f(x) = e^{-x}$. Then its cumulant generating function $\kappa(T)$ is given by $-\log(1 - T)$, $T < 1$. For $\bar{x} > 0$, the saddlepoint and the quasi-saddlepoints are, respectively, given by $\hat{T} = 1 - 1/\bar{x}$ and $\hat{c}_+$, $\hat{c}_- = \{u \pm (u^2 + 4n\bar{x})^{1/2}\}/(2n\bar{x})$, where $u = n\bar{x} - n - 1$. Also the equation (2.7) has the unique solution $x_0 = 1 + 1/n$.

In the TABLE 1, we examine the behaviour of the approximation. EDGEWORTH denotes an edgeworth series with two terms, and $Q^{(2)}$ and Q^{LR} are calculated by Daniels [2]. The definitions of $Q^{(2)}$ and of Q^{LR} are, respectively, given by (3.11) and (4.9) of Daniels [2]. Our proposed formulae $\hat{F}_j(\bar{x})$ $(j = 1, 2, 3)$ are defined in (2.8).

Example 2. The standard normal distribution

Let X follow the standard normal distribution. Then $\kappa(T) = T^2/2$. Hence the saddlepoint is given by $\hat{T} = \bar{x}$. Further the quasi-saddlepoints are given by $\hat{c}_+$, $\hat{c}_- = \{n\bar{x} \pm (n^2\bar{x}^2 + 4n)^{1/2}\}/(2n)$. In this case (2.7) has the solution $x_0 = 0$. However when we put $\bar{x} = n^{-1/2}y$ for fixed y, $\hat{c}$ can be rewritten as $\{y \pm (y^2 + 4)^{1/2}\}/(2n^{1/2})$. Referring α and λ_k of (2.6), we know that our approximation for $\bar{F}^n(\bar{x}) = \Pr\{n^{1/2}\bar{X} \le n^{1/2}\bar{x} = y\} = \Phi(y)$ does not depend on n be-

TABLE 1. Approximation for the distribution function of the n-sample mean from the gamma distribution with density $f(x) = e^{-x}$ $(x > 0)$

$n\bar{x}$	EXACT	EDGEWORTH	$Q^{(2)}$	Q^{LR}	$\hat{F}_1(\bar{x})$	$\hat{F}_2(\bar{x})$	$\hat{F}_3(\bar{x})$
				$n = 1$			
0.5	.3935	.3983	.3923	.3957	.4091	.3934	.3932
1.0	.6321	.6325	.6330	.6330	.6537	.6325	.6329
3.0	.9502	.9384	.9490	.9500	.9503	.9489	.9508
5.0	$.9^2326$	.98031	$.9^2323$	$.9^2319$	$.9^2294$	$.9^2321$	$.9^2331$
7.0	$.9^3088$	.98931	$.9^3092$	$.9^3074$	$.9^3029$	$.9^3088$	$.9^3092$
9.0	$.9^3877$	.99205	$.9^3878$	$.9^3874$	$.9^3878$	$.9^3877$	$.9^3877$
				$n = 5$			
1	.00366	.00102	.00365	.00365	.00371	.00366	.00366
3	.1847	.1875	.1844	.1844	.1859	.1852	.1846
5	.5595	.5595	.5595	.5595	.5525	.5615	.5622
10	.9707	.9686	.9707	.9707	.9712	.9705	.9709
15	$.9^3143$	$.9^3682$	$.9^3143$	$.9^3142$	$.9^3142$	$.9^3141$	$.9^3144$
20	$.9^4831$	$.9^4999$	$.9^4831$	$.9^4831$	$.9^4829$	$.9^4830$	$.9^4831$
25	$.9^6733$	1.0000	$.9^6733$	$.9^6732$	$.9^6729$	$.9^6733$	$.9^6733$
				$n = 10$			
5	.0318	.0319	.0318	.0318	.0320	.0319	.0318
10	.5421	.5445	.5421	.5421	.5270	.5448	.5454
15	.9301	.9086	.9301	.9301	.9323	.9293	.9304
20	$.9^2500$	.97646	$.9^2500$	$.9^2500$	$.9^2503$	$.9^2499$	$.9^2501$
25	$.9^3779$	.98929	$.9^3778$	$.9^3778$	$.9^3778$	$.9^3778$	$.9^3779$
30	$.9^5288$	.99256	$.9^5288$	$.9^5287$	$.9^5284$	$.9^5288$	$.9^5288$

TABLE 2. Approximation for the standard normal distribution function

x	$\Phi(x)$	$\hat{F}_1(x)$	$\hat{F}_2(x)$	$\hat{F}_3(x)$
−3.0	.001350	.001344	.001351	.001350
−2.5	.006210	.006170	.006219	.006207
−2.0	.022750	.022815	.022815	.022726
−1.5	.066807	.065634	.067166	.066680
−1.0	.158655	.153982	.160095	.158313
−0.5	.308537	.293877	.312187	.309022
0.0	.500000	.500000	.500000	.500000
0.5	.691463	.706123	.687813	.690978
1.0	.841345	.846018	.839905	.841687
1.5	.933193	.934366	.932834	.933320
2.0	.977250	.977488	.977185	.977274
2.5	.993790	.993830	.993781	.993793
3.0	.998650	.998655	.998649	.998650

cause $\kappa''(T) \equiv 1$ and $\kappa^{(k)}(T) \equiv 0$ $(k = 3, 4, 5, \ldots)$. Also $\kappa(T)$ is an even function. Hence it holds $\hat{F}_j^+(x) - \Phi(x) = -\{\hat{F}_j^-(-x) - \Phi(-x)\}$.

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