ON THE ATTAINMENT OF CRAMÉR-RAO AND BHATTACHARYYA BOUNDS FOR THE VARIANCE OF AN ESTIMATE

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Summary. If a variable X has density function $f(x, \theta)$, then in many cases the Cramér-Rao bound or the Bhattacharyya bounds may be used to show that a function d(x) is a uniformly minimum variance unbiased estimate of the real parameter θ .

In this paper it is shown that if $f(x, \theta)$ is a member of the family of densities of the Darmois-Koopman form, and if the variance of d(x) achieves the kth Bhattacharyya bound, but not the (k-1)th bound, then $f(x, \theta) = \exp[t(x)g(\theta) + g_0(\theta) + h(x)]$ and d(x) is a polynomial in t(x) of degree k. Further, the variance of any polynomial in t(x) of degree k will achieve the kth bound, so that if any such unbiased polynomial exists, it will necessarily be uniformly minimum variance unbiased. Some properties of these polynomial estimates are discussed.

Introduction. We will consider a one parameter family of density functions $f(x, \theta)$, $\theta \in \Omega$, such that

$$P\{X \in A\} = \int_A f(x,\theta) \ d\mu(x).$$

The variable X is possibly vector valued, as in the case where a random sample is observed, the set Ω is any set of real numbers, and μ is a measure independent of θ .

Conditions under which a Bhattacharyya bound is a valid lower bound for the variance of an estimate d(x) have been discussed in [1], [2], [4], and [5]. The conditions given by Wolfowitz [5] are for the sequential estimation problem. For the nonsequential case these can be written as

- (1) (a) Ω is the entire real line, or an open interval of the real line.
 - (b) d(x) has finite variance.
 - (c) Both $\int f(x, \theta) d\mu(x)$ and $\int d(x)f(x, \theta) d\mu(x)$ are differentiable under the integral sign with respect to θ . Specifically, if $\phi_i = [1/f(x, \theta)]$ $[\partial^i f(x, \theta)/\partial \theta^i]$, then, for almost all x, ϕ_i exists for all $\theta \in \Omega$, $i = 1, \dots, k$. The exceptional sets of x's do not depend on θ . Denote $E[d(X)\phi_i]$ by Λ_i .
- (d) The covariance matrix of ϕ_i exists and is non-singular for $\theta \in \Omega$. Then, if (1) is satisfied,

(2)
$$\sigma_{d}^{2} \geq - \begin{vmatrix} 0 & \Lambda_{1} & \cdots & \Lambda_{k} \\ \Lambda_{1} & E \phi_{1}^{2} & \cdots & E \phi_{1} & \phi_{k} \\ \vdots & & & & | E \phi_{i} & \phi_{j} | \\ \Lambda_{k} & E \phi_{k} & \phi_{1} & \cdots & E \phi_{k}^{2} \end{vmatrix}$$

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The right member of (2) is the kth Bhattacharyya bound. The Cramér-Rao bound is obtained by setting k = 1.

We will assume that the regularity conditions in (1) are satisfied, for some k, for all of the density functions considered here. However, it is worth noting that in many special cases (c) of (1) will follow from the fact that a Laplace transform may be differentiated under the integral sign, or, in other cases, from the fact that term by term differentiation is permitted whenever Ed(X) is a finite sum, as in the binomial distribution.

Results. Cramér [2] proved that if the equality in (2) holds for the case k = 1, then d(x) must be a linear function of ϕ_1 . Girshick and Savage [3] defined an exponential family of density functions and showed, under certain restrictions, the existence of a function whose variance achieves the Cramér-Rao bound The same exponential family is considered in the following theorem.

THEOREM 1. If the conditions in (1) are satisfied for $f(x, \theta)$ and d(x), and if $\sigma_d^2 > 0$ for all θ , then a necessary and sufficient condition that σ_d^2 achieve the Cramér-Rao bound is that $f(x, \theta) = \exp[d(x)g(\theta) + g_0(\theta) + h(x)]$, where $g'(\theta) \neq 0$.

If the maximum likelihood estimate $\hat{\theta}$ is given by the root of the equation $(\partial/\partial\theta)$ ln $f(x, \theta) = 0$, and if d(x) is an unbiased estimate of θ , then, in addition, $g'_0(\theta) = -\theta g'(\theta)$ and $d(x) = \hat{\theta}$.

Proof. We can, without loss of generality, write the density function of X in the form $f(x, \theta) = \exp[u(x, \theta)]$. Now, if the variance of d(x) achieves the Cramér-Rao lower bound, (2) becomes an equality, and this is a statement to the effect that the correlation coefficient of d(x) and ϕ_1 is unity. That is, d(x) is a linear function of ϕ_1 , except perhaps on a set of μ measure zero, and we can write

$$d(x) = a_0(\theta) + a_1(\theta)\phi_1$$

where

$$\phi_1 = \frac{\partial u(x,\theta)}{\partial \theta} = u'(x,\theta)$$
.

Since $\sigma_d^2 > 0$, it follows that d(x) is not a constant, so that $a_1(\theta) \neq 0$. Therefore, we can solve (3) for $u'(x, \theta)$ getting

$$u'(x, \theta) = d(x)a_1^{-1}(\theta) - a_0(\theta)a_1^{-1}(\theta)$$

and

$$u(x, \theta) = d(x)g(\theta) + g_0(\theta) + h(x).$$

To check sufficiency, we note that if $f(x, \theta) = \exp[d(x)g(\theta) + g_0(\theta) + h(x)]$, then $\phi_1 = d(x)g'(\theta) + g'_0(\theta)$ and ϕ_1 is the linear function of d(x) given by (3). That is, the correlation coefficient of d(x) and ϕ_1 is unity, and so the variance of d(x) achieves the Cramér-Rao bound.

Now, observing that $E\phi_1 = 0$, we get, from (3), $Ed(X) = a_0(\theta) + a_1(\theta)E\phi_1 = a_0(\theta)$. If d(x) is an unbiased estimate of θ , then $a_0(\theta) = \theta$ and, substituting these values in (3),

(4)
$$d(x) = \theta + a_1(\theta)[d(x)g'(\theta) + g'_0(\theta)].$$

Since d(x) does not contain θ , it follows that $a_1(\theta) = [g'(\theta)]^{-1}$ and $g'_0(\theta) = -\theta g'(\theta)$. To complete the proof of the theorem, we must consider the maximum likelihood estimate, $\hat{\theta}$. The coefficient of $a_1(\theta)$ in (4) is just the log of the likelihood function. Therefore, $d(x)g'(\hat{\theta}) + g'_0(\hat{\theta}) = 0$. But since the right member of (4) does not contain θ , we can substitute $\hat{\theta}$ for θ in (4) and obtain $d(x) = \hat{\theta}$. This completes the proof of the theorem.

Theorem 1 raises two important questions. First, we showed that if the variance of d(x) achieves the Cramér-Rao bound, then the density function is given by

(5)
$$f(x, \theta) = \exp \left[d(x)g(\theta) + g_0(\theta) + h(x) \right].$$

For such a function, we might now investigate the possibility that the variance of some function of d(x) might achieve one of the Bhattacharyya bounds, even though it does not achieve the Cramér-Rao bound. It also seems possible that if the exponent in (5) can be expressed as a polynomial in d(x), with coefficients depending only on θ , then some function of d(x) might achieve one of the higher bounds. This point is covered by Theorem 2.

A second question is concerned with maximum likelihood estimates. In Theorem 1 we showed that if the variance of an unbiased estimate d(x) achieves the Cramér-Rao bound, then d(x) is both minimum variance unbiased and maximum likelihood, and we might now ask if this result holds for the Bhattacharyya bounds. The answer is that it does not.

To illustrate this, suppose that the variance of the unbiased estimate d(x) achieves the second Bhattacharyya bound, but not the Cramér-Rao bound. In this case, (2) becomes an equality, and the multiple correlation coefficient of d(x) and ϕ_1 and ϕ_2 is unity. That is, we can write

(6)
$$d(x) = a_0(\theta) + a_1(\theta)\phi_1 + a_2(\theta)\phi_2.$$

Now for any k, $E\phi_k = 0$, so that in taking expected values of both sides of (6), we get $Ed(X) = a_0(\theta)$. If d(x) is unbiased, $a_0(\theta) = \theta$. Substituting the maximum likelihood estimate $\hat{\theta}$ for θ , as in the proof of Theorem 1, (6) becomes $d(x) = \hat{\theta} + a_2(\hat{\theta})\phi_2(\hat{\theta})$. In general, the term $a_2(\hat{\theta})\phi_2(\hat{\theta})$ will not vanish. That is, if $\hat{\theta}$ maximizes the likelihood function, then $\hat{\theta}$ will not be a solution of

$$\phi_2 = \frac{1}{f} \frac{\partial^2 f}{\partial \theta^2} = 0.$$

Hence, we would expect that the minimum variance unbiased estimate would not be the same as the maximum likelihood estimate.

If d(x) is a sufficient statistic, then the maximum likelihood estimate is necessarily a function of d(x), and the same thing may be said of any estimate whose variance achieves the kth Bhattacharyya bound. For such an estimate $d_1(x)$, (2) becomes an equality, and we write $d_1(x) = a_0(\theta) + \sum a_i(\theta)\phi_i$. The statement that $d_1(x)$ is a function of d(x) will be proved if we show that ϕ_i depends only on d(x) and θ .

Suppose that the density in question satisfies Neyman's criterion for sufficiency. That is, $f(x, \theta) = h[d(x), \theta]g(x)$. Then

$$\phi_i = \frac{1}{f} \frac{\partial^i f}{\partial \theta^i} = \frac{1g}{hg} \frac{\partial^i h}{\partial \theta^i} = \frac{1}{h} \frac{\partial^i h}{\partial \theta^i},$$

and ϕ_i is a function of the sufficient statistic d(x).

THEOREM 2. Consider a density function of the form

$$f(x,\theta) = \exp\left\{\sum_{i=0}^{n} [u(x)]^{\alpha_i} g_i(\theta) + v(x)\right\}$$

where the real numbers α_i , $i = 0 \cdots n$ satisfy the conditions $0 = \alpha_0 < \alpha_1 < \cdots < \alpha_n$, and $g'_n(\theta) \neq 0$. If the regularity conditions in (1) are satisfied for an estimate of θ , d(x), and the density $f(x, \theta)$, if $\sigma_d^2 > 0$ and σ_d^2 achieves the kth Bhattacharyya bound but not the (k-1)th bound, then the density may be expressed in the form $f(x, \theta) = \exp[t(x)g(\theta) + g_0(\theta) + h(x)]$ and d(x) is a polynomial in t(x) of degree k. Further, the variance of any polynomial in t(x) of degree k will achieve the kth bound.

Proof. In order to simplify notation, we define a general function

$$P_b[u(x)] = [u(x)]^b W_r(\theta) + \sum_{i=1}^{r-1} [u(x)^{b_i} W_i(\theta)],$$

where the real numbers b_i and b satisfy the conditions $0 \le b_i \le b$, $i = 1 \cdots (r-1)$. In the expression $P_b[u(x)]$, we will *not* be concerned with the particular values of r, or $W_i(\theta)$, $i = 1 \cdots r$. In fact, we do not exclude the possibility that $W_r(\theta) = 0$.

Notice that if the numbers b_i and b, $i = 1 \cdots (r-1)$ are integers, and if $W_r(\theta) \neq 0$, then $P_b[u(x)]$ is just a polynomial in u(x) of degree b, with coefficients depending on θ .

Now, for the density function $f(x, \theta) = \exp\{\sum_{i=0}^{n} [u(x)]^{\alpha_i} g_i(\theta) + v(x)\}$, we will show that

(7)
$$\phi_h = \left\{ \sum_{i=0}^n \left[u(x) \right]^{\alpha_i} g_i'(\theta) \right\}^h + P_{\alpha_n(h-1)} \left[u(x) \right].$$

For any integer value of $h, h \ge 1$,

$$\frac{\partial}{\partial \theta} \left[\frac{1}{f} \frac{\partial^{h-1} f}{\partial \theta^{h-1}} \right] = - \left[\frac{1}{f} \frac{\partial f}{\partial \theta} \right] \left[\frac{1}{f} \frac{\partial^{h-1} f}{\partial \theta^{h-1}} \right] + \frac{1}{f} \frac{\partial^h f}{\partial \theta^h}$$

and, using the definition of ϕ_i in (1), we get the recursion relation $\phi_h = \phi'_{h-1} + \phi_1 \phi_{h-1}$. Now,

$$\phi_2 = \phi_1^2 + \phi_1' = \left\{ \sum_{i=0}^n [u(x)]^{\alpha_i} g_i'(\theta) \right\}^2 + \sum_{i=0}^n [u(x)]^{\alpha_i} g_i''(\theta)$$

so that ϕ_2 is of the form given in (7).

Suppose next that ϕ_{h-1} is also given by (7). Then, using (7) and the recursion relation,

$$\begin{split} \phi_h &= (h-1) \left\{ \sum_{i=0}^n [u(x)]^{\alpha_i} g_i'(\theta) \right\}^{h-2} \left\{ \sum_{i=0}^n [u(x)]^{\alpha_i} g_i''(\theta) \right\} + \frac{\partial}{\partial \theta} P_{\alpha_n(h-2)}[u(x)] \\ &+ \left\{ \sum_{i=0}^n [u(x)]^{\alpha_i} g_i'(\theta) \right\} \left\{ \left(\sum_{i=0}^n [u(x)]^{\alpha_i} g_i'(\theta) \right)^{h-1} + P_{\alpha_n(h-2)}[u(x)] \right\} \\ &= \left\{ \sum_{i=0}^n [u(x)]^{\alpha_i} g_i'(\theta) \right\}^h + P_{\alpha_n(h-1)}[u(x)]. \end{split}$$

That is, ϕ_h is given by (7), and so (7) holds for all positive integral values of h.

If d(x) is an estimate such that $\sigma_d^2 > 0$ and σ_d^2 achieves the kth Bhattacharyya bound but not the (k-1)th bound, then, by the same reasoning that led to (4), we can write

(8)
$$d(x) = a_0(\theta) + \sum_{i=1}^k a_i(\theta) \phi_i,$$

where $a_k(\theta) \neq 0$.

Now, substituting (7) into (8) we get

(9)
$$d(x) = a_0(\theta) + \sum_{i=1}^k a_i(\theta) \left\{ \left(\sum_{j=0}^n [u(x)]^{\alpha_j} g'_j(\theta) \right)^i + P_{\alpha_n(i-1)}[u(x)] \right\}.$$

Notice that the right side of (9) can be expressed as a sum of terms, each term being a power of u(x) multiplied by a coefficient which does not depend on x. But d(x) itself is free of θ , so that the functions $a_i(\theta)$ must be chosen so that the coefficients in this series are free of θ .

Suppose now that (9) is expressed in descending powers of u(x). We will pay special attention to the expression

(10)
$$a_k(\theta) \left\{ \sum_{i=0}^n \left[u(x) \right]^{\alpha_i} g_i'(\theta) \right\}^k$$

because this contains the higher powers of u(x), and hence the first terms of the expansion in descending powers of u(x).

Recalling that $0 = \alpha_0 < \alpha_1 < \cdots < \alpha_n$, we observe that the first term in the expansion is

$$a_k(\theta)[u(x)]_{l}^{k\alpha_n}[g'_n(\theta)]^k.$$

Since the coefficient of $[u(x)]^{k\alpha_n}$ is independent of θ , it follows that $a_k(\theta) = C_n[g'_n(\theta)]^{-k}$, where C_n is a constant. Substitute this value of $a_k(\theta)$ into (10), and (10) becomes

(11)
$$C_n \left\{ \sum_{j=0}^n \left[u(x) \right]^{\alpha_j} \frac{g_j'(\theta)}{g_n'(\theta)} \right\}^k.$$

The next term in the expansion of (9) in descending powers of u(x), whose

coefficient might depend on θ , is obtained from (11). It is

$$C_n \frac{g'_{n-1}(\theta)}{g'_n(\theta)} [u(x)]^{\alpha_n(k-1)+\alpha_{n-1}}.$$

Again, the coefficient must be independent of θ , so that $g'_{n-1}(\theta) = C_{n-1}g'_n(\theta)$, where C_{n-1} is a constant.

Substituting this value in (11), we get

(12)
$$C_n \left\{ [u(x)]^{\alpha_n} + [u(x)]^{\alpha_{n-1}} C_{n-1} + [u(x)]^{\alpha_{n-2}} \frac{g'_{n-2}(\theta)}{g'_n(\theta)} + \cdots \right\}^k.$$

We see that the next term in the expansion whose coefficient might depend on θ is

$$\left\{ \operatorname{Constant} + C_n \frac{g'_{n-2}(\theta)}{g'_n(\theta)} \right\} [u(x)]^{\alpha_n(k-1) + \alpha_{n-2}}$$

and this implies that $g'_{n-2}(\theta) = C_{n-2}g'_{n}(\theta)$ where C_{n-2} is a constant.

Repeating this procedure on the remaining functions, it follows that

(13)
$$g'_{j}(\theta) = C_{j}g'_{n}(\theta), \quad j = 1, \dots, n-1.$$

But $\phi_1 = \sum_{j=0}^n [u(x)]^{\alpha_j} g'_j(\theta)$, and substituting (13) in this expression,

(14)
$$\phi_{1} = \sum_{j=1}^{n-1} [u(x)]^{\alpha_{j}} g'_{n}(\theta) C_{j} + [u(x)]^{\alpha_{n}} g'_{n}(\theta) + g'_{0}(\theta)$$
$$= g'_{n}(\theta) \left\{ \sum_{j=1}^{n-1} [u(x)]^{\alpha_{j}} C_{j} + [u(x)]^{\alpha_{n}} \right\} + g'_{0}(\theta).$$

In (14), let $t(x) = \sum_{j=1}^{n-1} [u(x)]^{\alpha_j} C_j + [u(x)]^{\alpha_n}$ and $g'_n(\theta) = g'(\theta)$, and we can say that $\phi_1 = t(x)g'(\theta) + g'_0(\theta)$. Since ϕ_1 is the derivative of the exponent of the density function stated in the theorem, we get

$$f(x, \theta) = \exp \left[t(x)g(\theta) + g_0(\theta) + h(x) \right]$$

and this concludes the proof of the first part of the theorem.

If $f(x, \theta)$ is of the above form, then (7) becomes $\phi_h = [t(x)g'(\theta) + g'_0(\theta)]^h + P_{h-1}[t(x)]$, where $P_{h-1}[t(x)]$ is a polynomial in t(x) of degree h-1 with coefficients depending only on θ .

Using this result and (8),

(15)
$$d(x) = a_0(\theta) + \sum_{i=1}^k a_i(\theta) \{ [t(x)g'(\theta) + g'_0(\theta)]^i + P_{i-1}[t(x)] \}$$

so that d(x) is a polynomial in t(x) of degree k.

Finally, we will show that if d(x) is any polynomial in t(x) of degree k, then the functions $a_i(\theta)$, $i = 1, \dots, k$ can be chosen so that (15) holds. To do this, let $P_{i-1}[t(x)] = \sum_{j=0}^{i-1} t^j(x) u_{ij}(\theta)$. As stated before, we will not be concerned

with the particular form of $u_{ij}(\theta)$. Substituting this expression in (15) we get

$$d(x) = a_{0}(\theta) + \sum_{i=1}^{k} a_{i}(\theta) \left\{ [tg' + g'_{0}]^{i} + \sum_{j=0}^{i-1} t^{j} u_{ij} \right\}$$

$$= a_{0}(\theta) + \sum_{i=1}^{k} a_{i}(\theta) \left\{ \sum_{j=0}^{i} \binom{i}{j} (tg')^{j} (g'_{0})^{i-j} + \sum_{j=0}^{i-1} t^{j} u_{ij} \right\}$$

$$= a_{0}(\theta) + \sum_{i=1}^{k} a_{i}(\theta) \left\{ (tg')^{i} + \sum_{j=0}^{i-1} t^{j} \left[\binom{i}{j} (g')^{j} (g'_{0})^{i-j} + u_{ij} \right] \right\}$$

$$= [tg']^{k} a_{k}(\theta) + \cdots$$

$$+ t^{n} \left\{ a_{n}(\theta) (g')^{n} + \sum_{i=n+1}^{k} a_{i}(\theta) \left[\binom{i}{n} (g')^{n} (g'_{0})^{i-n} + u_{in} \right] \right\} + \cdots$$

$$+ a_{0}(\theta) + \sum_{i=1}^{k} [(g'_{0})^{i} + u_{i0}] a_{i}(\theta).$$

Choose arbitrary constants, C_0 , C_1 , \cdots C_k , and let $a_k(\theta) = C_k[g'(\theta)]^{-k}$. For 0 < n < k, let

$$a_n(\theta) = \frac{C_n - \sum_{i=n+1}^k a_i(\theta) \left[\binom{i}{n} (g')^n (g'_0)^{i-n} + u_{in} \right]}{(g')^n}$$

and

$$a_0(\theta) = C_0 - \sum_{i=1}^k [(g'_0)^i + u_{i0}]a_i(\theta).$$

Using these functions in (15) we get $d(x) = \sum_{i=0}^{k} C_i t^i(x)$. Since the constants C_0, \dots, C_k are completely arbitrary, it follows that any polynomial in t(x) of degree k can be written in the form (15). This completes the proof of the last part of Theorem 2.

Theorem 2 provides a method for finding uniformly minimum variance unbiased estimates. That is, if $f(x, \theta)$ is of the form described in Theorem 2, then we look for an unbiased polynomial in t(x). If this polynomial is of degree k, then its variance achieves the kth Bhattacharyya bound and it is the best unbiased estimate.

On the other hand, we know that if the variance of d(x) achieves the kth bound, then d(x) is necessarily a polynomial in t(x). Therefore, if we find that no such polynomial is unbiased, there would seem to be no value in calculating any of the Bhattacharyya bounds if we are interested only in minimum variance unbiased estimates. The following examples illustrate uses of Theorems 1 and 2.

Example 1. Let X have density $\theta^{-(1/n)} \exp[-x\theta^{-(1/n)}]$, 0 < x, $0 < \theta$ where n is a positive integer, and suppose that an estimate is wanted for θ . We write the density as $\exp[-x\theta^{-(1/n)} - (1/n)\log\theta]$, and, in the notation of Theorem 2, t(x) = x, $g(\theta) = -\theta^{-(1/n)}$, and $g_0(\theta) = -(1/n)\log\theta$. If n = 1, then $g_0'(\theta) = -\theta g'(\theta)$, so that from Theorem 1, the estimate X is minimum variance unbiased.

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If n > 1, the estimate $x^n/n!$ is an unbiased estimate of θ , and, since it is a polynomial in x of degree n, it follows from Theorem 2 that the variance will achieve the nth Bhattacharyya bound. Hence, it is minimum variance unbiased.

By straightforward calculations we find that the maximum likelihood estimate is $\hat{\theta} = x^n$. If n = 1, $\hat{\theta}$ is unbiased, as stated in Theorem 1, but if n > 1, then $\hat{\theta}$ is a biased estimate.

Example 2. Let X have density $\theta^{-n} \exp[-x\theta^{-n}]$, 0 < x, $0 < \theta$, where n is an integer, n > 1, and an estimate is wanted for θ . Writing the density as in Theorem 2, $\exp[-x\theta^{-n} - n\log\theta]$. Now from Theorem 2, if the variance of an estimate d(x) achieves the kth bound, d(x) is a polynomial in x. But for this density we have, for any integer c, $EX^c = c!\theta^{nc}$. Therefore, no polynomial in x is an unbiased estimate of θ . This does not imply that no minimum variance unbiased estimate exists, but it does mean that the variance of any unbiased estimate will not achieve the kth bound.

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