COMPUTING THE BARANKIN BOUND, BY SOLVING AN UNCONSTRAINED QUADRATIC OPTIMIZATION PROBLEM

Thomas L. Marzetta

Bell Labs, Mathematical Sciences Research Center
Lucent Technologies Murray Hill, NJ 07974-0636 USA
tlm@research.bell-labs.com

ABSTRACT

The Barankin bound is the greatest lower bound on the variance of any unbiased estimate for a nonrandom parameter. Computing this bound yields, as a byproduct, an unbiased estimator that is at least locally best in the following sense. The estimator formula contains a reference parameter; when the unknown parameter happens to be equal to the reference, the variance of the estimate achieves the Barankin bound. If the dependence of the Barankin estimate on the reference parameter vanishes, then the estimate is also uniformly minimum variance.

We obtain a simple derivation of the Barankin bound as the solution of an unconstrained convex quadratic optimization problem. In contrast the standard form of the Barankin bound involves the maximization of a ratio of quadratic quantities. For the case of PET inversion and natural gamma ray spectrometry, the Barankin estimate is only locally minimum variance, but it can be a viable alternative to the maximum likelihood estimate.

1. INTRODUCTION

Maximum likelihood (ML) estimation and the Cramer-Rao (CR) lower bound constitute the standard tools of nonrandom parameter estimation for statistical signal processing [1]. No unbiased estimate has variance that is smaller than the CR bound, and if any unbiased estimate everywhere has variance that is equal to the CR bound (an efficient estimate), it is the ML estimate. Moreover, under fairly general conditions, for high signal-to-noise ratios the ML estimate asymptotically is unbiased with variance equal to the CR bound. It is recognized widely, however, that the CR bound can be misleadingly optimistic.

In 1949, Barankin derived the greatest lower bound on the variance of any unbiased estimate [2] - [4]. The computation of the Barankin bound implicitly involves the construction of an unbiased estimate that is at least locally minimum variance, and that for some cases may be uniformly minimum variance. As engineers tackle progressively more difficult estimation problems the determination of the CR bound often is a major computational task. Since numerical calculations are required anyway, why not use the more powerful Barankin bound? An even more intriguing prospect is the possibility of replacing ML estimates with Barankin estimates. Two obstacles to this goal are the difficulty of computing the Barankin bound, and the absence of simple explanations of the theory.

The contribution of this paper is a simple derivation of the Barankin bound as the solution of an unconstrained convex quadratic optimization problem. In contrast the standard form of the Barankin bound involves the maximization of a ratio of quadratic quantities. We illustrate the theory with examples where efficient estimates do not exist, and where the Barankin bound is obtained analytically. For two cases the Barankin estimate is also uniformly minimum variance, while in the third case, associated with PET inversion and natural gamma ray spectrometry, the Barankin estimate is only locally minimum variance. However this locally minimum variance estimate happens to be a viable alternative to the ML estimate.

2. NEW DERIVATION OF BARANKIN BOUND

We observe a random vector, $\mathbf{r}$, whose probability density, $p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})$, depends on a vector of M nonrandom unknown parameters, $\mathbf{a}$, where $\mathbf{a}$ is contained in some parameter space, Θ. An estimator, $\hat{\mathbf{a}}(\mathbf{R})$, is an M-component vector-valued function of the observation. The estimate is unbiased if $E\{\hat{\mathbf{a}}(\mathbf{R})|\mathbf{A}\}=\mathbf{A}, \forall \mathbf{A}\in\Theta$.

We introduce an M-component random vector, $\mathbf{Z}$,

$$\mathbf{Z} = \int_{\mathbf{B}\in\beta} \mathbf{f}(\mathbf{B}) \frac{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{B})}{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})} d\mathbf{B}, \qquad (1)$$

where $\mathbf{f}(\mathbf{B})$ is an as-yet unspecified M-component function of an M-component vector, on a set β. The M×M correlation matrix of $\mathbf{Z}$ is

$$E\{\mathbf{Z}\mathbf{Z}^T|\mathbf{A}\} = \int_{\mathbf{B}\in\beta}\int_{\mathbf{C}\in\beta} k_{\mathbf{A}}(\mathbf{B},\mathbf{C})\mathbf{f}(\mathbf{B})\mathbf{f}^T(\mathbf{C})d\mathbf{B}d\mathbf{C}, \qquad (2)$$

where $k_{\mathbf{A}}(\mathbf{B},\mathbf{C})$ is a scalar-valued, symmetric, nonnegative-definite kernel,

$$k_{\mathbf{A}}(\mathbf{B},\mathbf{C}) = E\left\{ \frac{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{B})p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{C})}{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})} \,|\, \mathbf{A} \right\}. \qquad (3)$$

For any unbiased estimate, the M×M correlation matrix between the estimation error and $\mathbf{Z}$, for suitable β, is

$$E\{[\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}]\mathbf{Z}^T \mid \mathbf{A}\} = \int_{\mathbf{B}\in\beta} [\mathbf{B}-\mathbf{A}]\mathbf{f}^T(\mathbf{B})d\mathbf{B}. \quad (4)$$

Theorem 1 For any unbiased estimate, the error covariance matrix is lower-bounded as follows,

$$E\{[\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}][\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}]^T \mid \mathbf{A}\} \geq$$

$$\int_{\mathbf{B}\in\beta} ([\mathbf{B}-\mathbf{A}]\mathbf{f}_{\mathbf{A}}^T(\mathbf{B})+\mathbf{f}_{\mathbf{A}}(\mathbf{B})[\mathbf{B}-\mathbf{A}]^T)d\mathbf{B}$$

$$- \int_{\mathbf{B}\in\beta}\int_{\mathbf{C}\in\beta} k_{\mathbf{A}}(\mathbf{B},\mathbf{C})\mathbf{f}_{\mathbf{A}}(\mathbf{B})\mathbf{f}_{\mathbf{A}}^T(\mathbf{C})d\mathbf{B}d\mathbf{C}, \quad (5)$$

where $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$ is chosen to maximize the trace of the right-hand-side (r.h.s.). The bound is satisfied with equality, for some **A**, if and only if the unbiased estimate satisfies the following, with probability one,

$$\hat{\mathbf{a}}(\mathbf{R}) = \mathbf{A} + \int_{\mathbf{B}\in\beta} \mathbf{f}_{\mathbf{A}}(\mathbf{B})\frac{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{B})}{p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})}d\mathbf{B}. \quad (6)$$

An unbiased estimate that satisfies the Barankin bound with equality is unique. ◊

Proof The difference between the estimation error and **Z** is itself a random vector whose correlation matrix must be nonnegative-definite,

$$E\{[\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}-\mathbf{Z}][\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}-\mathbf{Z}]^T \mid \mathbf{A}\} \geq \mathbf{0}. \quad (7)$$

Expanding this correlation matrix, using (2) and (4), and rearranging the expression, gives a lower bound on the error covariance matrix of the form (5), that is valid for any $\mathbf{f}(\mathbf{B})$. We choose $\mathbf{f}(\mathbf{B})$ to maximize the trace of the bound. If the trace is unbounded there is no finite-variance unbiased estimate. If the trace is bounded, then we apply calculus of variations to obtain an integral equation for $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$,

$$\mathbf{0} = (\mathbf{B}-\mathbf{A}) - \int_{\mathbf{C}\in\beta} k_{\mathbf{A}}(\mathbf{B},\mathbf{C})\mathbf{f}_{\mathbf{A}}(\mathbf{C})d\mathbf{C}, \ \forall \mathbf{B}\in\beta. \quad (8)$$

For a particular value of **A**, if an unbiased estimate satisfies the bound (5) with equality, then (7) must hold with equality, so the error vector is equal to **Z** with probability one; this condition is equivalent to (6). Conversely if an unbiased estimate satisfies (6), where $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$ satisfies (8), then the covariance matrix for the difference of the l.h.s and r.h.s. of (6) is equal to zero. Expanding this expression implies that (5) is satisfied with equality.

Suppose that two distinct unbiased estimates satisfy the Barankin bound with equality for some parameter value, **A**. Then each estimate has the representation, (6), for a distinct $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$. Taking the mean-square difference of the two estimates using (2) and (3) gives zero, implying that the two estimates are equal with probability one. ◊

The relation (6) can be interpreted as a formula for an estimator, provided **A** is a user supplied reference parameter, rather than the unknown value of **a**; the point is that a legitimate estimate depends only on the observation, and not on the unknown value of **a**. This estimate is unbiased and at least locally minimum variance.

Theorem 2 Suppose that the trace of the right-hand side of (5) is bounded. Then the estimate, (6), is unbiased and locally minimum variance, i.e. when the value of the unknown parameter is equal to the reference parameter, the error covariance satisfies the Barankin bound with equality. Furthermore, if the dependence of the estimator formula (6) on the reference parameter vanishes, then the estimate is uniformly minimum variance. ◊

Proof Suppose that **A** is the reference parameter and that **C** is the actual value of the parameter. Taking the expectation of (6), conditioned on **C**, and using the fact that $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$ satisfies the integral equation (8), gives $E\{\hat{\mathbf{a}}(\mathbf{R})|\mathbf{C}\}=\mathbf{C}$, so the estimate is unbiased. If the unknown value of the parameter is equal to the reference parameter, i.e. $\mathbf{A}\leftarrow\mathbf{C}$, then we have an unbiased estimate that satisfies the condition (6), so Theorem 1 implies that the estimate satisfies the Barankin bound with equality, and it is locally minimum variance.

If the estimator formula (6) happens to be independent of the value of the reference parameter, then for any **C** we can change the reference parameter, $\mathbf{C}\leftarrow\mathbf{A}$, without changing the estimate; then condition (6) of Theorem 1 applies and we conclude that the estimate satisfies the Barankin bound with equality, so the estimate is uniformly minimum variance. ◊

Can a locally minimum variance unbiased estimate be useful? That depends on how close the unknown parameter is to the reference parameter, and how sensitive the estimate is the value of the reference parameter.

3. COMMENTS

The conventional form of the Barankin bound can be obtained from (5) by replacing $\mathbf{f}_{\mathbf{A}}(\mathbf{B})$ by $H\mathbf{g}(\mathbf{B})$, where H is an M×M matrix that is constant with respect to **B**, and $\mathbf{g}(\mathbf{B})$ is an M-component vector-valued function. Choosing H to maximize the trace of the r.h.s. of (5) gives the conventional form,

$$E\{[\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}][\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}]^T \mid \mathbf{A}\} \geq \left[\int_{\mathbf{B}\in\beta} [\mathbf{B}-\mathbf{A}]\mathbf{g}^T(\mathbf{B})d\mathbf{B}\right]$$

$$\cdot\left[\int_{\mathbf{B}\in\beta}\int_{\mathbf{C}\in\beta} k_{\mathbf{A}}(\mathbf{B},\mathbf{C})\mathbf{g}(\mathbf{B})\mathbf{g}^T(\mathbf{C})d\mathbf{B}d\mathbf{C}\right]^{-1}$$

$$\cdot\left[\int_{\mathbf{B}\in\beta} \mathbf{g}(\mathbf{B})[\mathbf{B}-\mathbf{A}]^T d\mathbf{B}\right], \quad (9)$$

where $\mathbf{g}(\mathbf{B})$ is chosen to maximize the trace of the r.h.s. of (9). The new form of the Barankin bound (5) is

simpler than the conventional form: a quadratic functional rather than a ratio of quadratic functionals, and the trace of (5) is separable with respect to the M components of $\mathbf{f}(\mathbf{B})$, while the trace of (9) is not separable with respect to the M components of $\mathbf{g}(\mathbf{B})$. The formulation of the Barankin bound as a simple maximization of a convex quadratic functional opens the problem of computing the bound to attack by modern numerical tools from functional optimization and integral equations, however such techniques have not yet been applied.

In some treatments, the Barankin bound has a still more complicated form than (9). In particular, setting $\mathbf{B}=\mathbf{A}$ in (8), and using the fact that $k_{\mathbf{A}}(\mathbf{A},\mathbf{C})=1$, we find that $\int_{\mathbf{B}\in\beta} \mathbf{f}_{\mathbf{A}}(\mathbf{B})d\mathbf{B}=\mathbf{0}$. Therefore if we enforce the equivalent constraint, $\int_{\mathbf{B}\in\beta} \mathbf{g}(\mathbf{B})d\mathbf{B}=\mathbf{0}$, we can remove the terms from (9) that contain products of $\mathbf{A}$ and $\mathbf{g}(\mathbf{B})$. However there appears to be no advantage in doing so.

4. EXAMPLES OF BARANKIN BOUND

We present three examples of the Barankin bound in this section, where efficient estimates do not exist, and where the integral equation (8) can be solved analytically. The test for the existence of an efficient estimate is to determine (by inspection) whether the $\mathbf{A}$-dependence vanishes in the expression, $[\mathbf{A} + J_{\mathbf{A}}^{-1}\nabla_{\mathbf{A}} \ln p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A})]$, where $J_{\mathbf{A}}$ is the Fisher information matrix [4].

Example 1 *Estimating the probability that a Poisson random variable is equal to zero* We observe N independent realizations of a discrete, Poisson random variable, $\{r_n,\ 1\le n\le N\}$, and the object is to estimate the probability that the random variable, r, is equal to zero: $a = \exp(-E\{r\})$. Although there is an efficient estimate for the mean of r, recall that efficiency does not commute with nonlinear transformations. The discrete probability for the observations is

$$p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|A) = \prod_{n=1}^{N} [(-\ln A)^{R_n} \cdot A/R_n!]. \qquad (10)$$

The kernel (3) is

$$k_A(B,C) = \left(\frac{BC}{A}\right)^N \cdot \exp\left(-\frac{N\cdot \ln B\cdot \ln C}{\ln A}\right), \qquad (11)$$

and for $\beta=(0,1)$, the solution to the integral equation (8) is

$$f_A(B) = A\cdot[\delta(B-A^{(N-1)/N}) - \delta(B-A)], \qquad (12)$$

where $\delta(\cdot)$ is the Dirac delta function. Substituting this solution into (5) gives the Barankin bound,

$$E\{[\hat{a}(\mathbf{R})-A]^2 \mid A\} \ge A^2\cdot(A^{-1/N} - 1). \qquad (13)$$

Substituting (12) into (6), and simplifying gives the locally minimum variance unbiased estimate,

$$\hat{a}(\mathbf{R}) = [(N-1)/N]^{\left(\sum_{n=1}^{N} R_n\right)}; \qquad (14)$$

since the A-dependence vanishes, this estimate is uniformly minimum variance. The estimator formula has previously been derived by means of Blackwell's technique, where one starts with a suboptimal unbiased estimate (e.g., the number of values of r that are equal to zero, divided by N) and then takes the expectation of the suboptimal estimate conditioned on a sufficient statistic [5]. ◊

Example 2 *Estimating the offset of an exponential random variable* We observe N independent realizations of an exponentially distributed random variable, $\{r_n,\ 1\le n\le N\}$, that is offset from the origin, and the object is to estimate the offset. The probability density function for the observations is

$$p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|A) = \prod_{n=1}^{N} [\gamma^{-1}\cdot e^{-(R_n-A)/\gamma}\cdot u_{-1}(R_n-A)], \qquad (15)$$

where $u_{-1}(\cdot)$ is the unit-step function. The kernel (3) is

$$k_A(B,C) = \exp\{N\cdot[\min(B,C) - A]/\gamma\},\quad B\ge A,\ C\ge A. \qquad (16)$$

For $\beta=[A,\infty)$, the solution to the integral equation (8) is

$$f_A(B) = \exp[-N(B-A)/\gamma] - \gamma\cdot\delta(B-A)/N,\quad B\ge A. \qquad (17)$$

Substituting this solution into (5) gives the Barankin bound,

$$E\{[\hat{a}(\mathbf{R})-A]^2 \mid A\} \ge (\gamma/N)^2. \qquad (18)$$

The A-dependence cancels in the estimator formula (6) giving the uniformly minimum variance unbiased estimate,

$$\hat{a}(\mathbf{R}) = \inf(\mathbf{R}) - \gamma/N, \qquad (19)$$

where $\inf(\mathbf{R})$ denotes the greatest lower bound on the N observations. This estimate was previously shown to satisfy the Barankin bound with equality [6]. ◊

Example 3 *PET inversion; natural gamma ray spectrometry* We observe N independent Poisson random variables, $\{r_n,\ 1\le n\le N\}$, and the object is to estimate a vector of M parameters, where the means of the observations are equal to linear combinations of the parameters,

$$E\{R_n \mid \mathbf{A}\} = \sum_{m=1}^{M} Q_{nm}A_m, \qquad (20)$$

and where the N×M matrix, Q, is known. We assume that $N\ge M$ and that Q is full-rank. For the PET (positron emission tomography) inversion problem [7], we wish to estimate a continuous density from a finite set of measurements, where the density is represented in terms of M basis functions. Natural gamma ray spectrometry [8],[9] is used in petroleum well logging; here the object is to estimate the concentrations of potassium, uranium, and thorium, from five measurements of gamma ray counts, each measurement having a different energy spectral response.

The log-likelihood of the observations is

$$\ln p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A}) = \sum_{n=1}^{N}\Big[R_n \cdot \ln\Big(\sum_{m=1}^{M} Q_{nm}A_m\Big) - \sum_{m=1}^{M} Q_{nm}A_m - \ln R_n!\Big]. \quad (21)$$

The gradient of the log-likelihood is

$$\nabla_{\mathbf{A}} \ln p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A}) = \mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}(\mathbf{R}-\mathbf{QA}), \quad (22)$$

where $\mathbf{D}_{\mathbf{QA}}$ is an N×N diagonal matrix,

$$[\mathbf{D}_{\mathbf{QA}}]_{nn} = \sum_{m=1}^{M} Q_{nm}A_m. \quad (23)$$

The M×M Fisher information matrix is

$$\mathbf{J}_{\mathbf{A}} = \mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{Q}. \quad (24)$$

To test whether or not there is an efficient estimate, we inspect the following expression for A-dependence,

$$\mathbf{A} + \mathbf{J}_{\mathbf{A}}^{-1}\nabla_{\mathbf{A}} \ln p_{\mathbf{r}|\mathbf{a}}(\mathbf{R}|\mathbf{A}) = (\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{Q})^{-1}\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{R}. \quad (25)$$

The A-dependence vanishes for two special cases: 1) M=1, and 2) N=M. For N>M>1, the expression depends on A, and 1) an efficient estimate does not exist; 2) there is no closed-form solution for the ML estimate (however the likelihood function is convex, and the maximum can be found reliably with the EM (expectation-maximization) algorithm [7]); 3) there are no closed-form expressions for the bias and the covariance of the ML estimate.

The kernel (3) is

$$k_{\mathbf{A}}(\mathbf{B},\mathbf{C}) = \exp\left\{\sum_{n=1}^{N}\left(\frac{[\mathbf{QB}]_n \cdot [\mathbf{QC}]_n}{[\mathbf{QA}]_n} - [\mathbf{QB}]_n - [\mathbf{QC}]_n + [\mathbf{QA}]_n\right)\right\}. \quad (26)$$

With the notation, $\delta(\mathbf{B}-\mathbf{A}) = \prod_{m=1}^{M}\delta(B_m - A_m)$, the solution to the integral equation (8) is

$$\mathbf{f}_{\mathbf{A}}(\mathbf{B}) = -(\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{Q})^{-1}\nabla_{\mathbf{B}}\delta(\mathbf{B}-\mathbf{A}). \quad (27)$$

Substituting this solution into (5) gives the Barankin bound

$$\mathrm{E}\{[\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}][\hat{\mathbf{a}}(\mathbf{R})-\mathbf{A}]^{\mathrm{T}}|\,\mathbf{A}\} \geq (\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{Q})^{-1}, \quad (28)$$

which is equal to the CR bound! Substituting the solution (27) into (6) gives the locally minimum variance unbiased estimate,

$$\hat{\mathbf{a}}(\mathbf{R}) = (\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{Q})^{-1}\mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\mathbf{QA}}^{-1}\mathbf{R}. \quad (29)$$

In short, there is no efficient estimate, but there is a locally minimum variance unbiased estimate - that is not ML - whose variance is (locally) equal to the CR bound.

In fact, natural gamma ray spectrometry, as used in well-logging, employs the locally minimum variance unbiased estimate [9]. Historically, this estimate was developed as follows: ignoring the Poisson distribution of the data, if one simply chooses A to minimize $(\mathbf{R}-\mathbf{QA})^{\mathrm{T}}\mathbf{W}(\mathbf{R}-\mathbf{QA})$, where W is a symmetric, positive-definite weight matrix, the resulting estimate,

$$\hat{\mathbf{a}}(\mathbf{R}) = (\mathbf{Q}^{\mathrm{T}}\mathbf{W}\mathbf{Q})^{-1}\mathbf{Q}^{\mathrm{T}}\mathbf{W}\mathbf{R}, \quad (30)$$

is unbiased. The error covariance depends on both the weight matrix and the unknown value of the parameters. Optimizing the weight matrix for nominal values of the parameters gives the locally minimum variance unbiased estimate, (29). Solutions to weighted least-squares problems are usually robust with respect to the weights, and in the case of natural gamma ray spectrometry where there is prior information about the parameters, the locally minimum variance estimate performs nearly optimally. ◊

4. CONCLUSIONS

The Barankin bound turns out to be rather simple to derive. The new formulation of the Barankin bound as the maximization of a convex quadratic functional opens the problem of computing the bound to attack by modern numerical tools from functional optimization and the solution of integral equations, however such techniques have not yet been applied. The question as to the utility of the locally minimum variance unbiased estimate - compared with that of the maximum likelihood estimate - is problem-dependent.

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