Statistics of the MLE and Approximate Upper and Lower Bounds – Part 1: Application to TOA Estimation

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Abstract—In nonlinear deterministic parameter estimation, the maximum likelihood estimator (MLE) is unable to attain the Cramer-Rao lower bound at low and medium signal-to-noise ratios (SNR) due to the threshold and ambiguity phenomena. In order to evaluate the achieved mean-squared-error (MSE) at those SNR levels, we propose new MSE approximations (MSEA) and an approximate upper bound by using the method of interval estimation (MIE). The mean and the distribution of the MLE are approximated as well. The MIE consists in splitting the a priori domain of the unknown parameter into intervals and computing the statistics of the estimator in each interval. Also, we derive an approximate lower bound (ALB) based on the Taylor series expansion of noise and an ALB family by employing the binary detection principle. The accuracies of the proposed MSEA and the tightness of the derived approximate bound 1 are validated by considering the example of time-of-arrival estimation.

Index Terms—Nonlinear estimation, threshold and ambiguity phenomena, maximum likelihood estimator, mean-squared-error, upper and lowers bounds, time-of-arrival.

I. INTRODUCTION

NONLINEAR estimation of deterministic parameters suffers from the threshold effect [2][11]. This effect means that for a signal-to-noise ratio (SNR) above a given threshold, estimation can achieve the Cramer-Rao lower bound (CRLB), whereas for SNRs lower than that threshold, estimation deteriorates drastically until the estimate becomes uniformly distributed in the a priori domain of the unknown parameter.

As depicted in Fig. 1(a), the SNR axis can be split into three regions according to the achieved mean-squared-error (MSE):

1) A priori region: Region in which the estimate is uniformly distributed in the a priori domain of the unknown parameter (region of low SNRs).

2) Threshold region: Region of transition between the a priori and asymptotic regions (region of medium SNRs).

3) Asymptotic region: Region in which the CRLB is achieved (region of high SNRs).

In addition, if the autocorrelation (ACR) of the signal carrying the information about the unknown parameter is oscillating, then estimation will be affected by the ambiguity phenomenon [12, pp. 119] and a new region will appear so the SNR axis can be split, as shown Fig. 1(b), into five regions:

1) A priori region.

2) A priori-ambiguity transition region.

3) Ambiguity region.

4) Ambiguity-asymptotic transition region.

5) Asymptotic region.

The MLE achieved in the ambiguity region is determined by the envelope of the ACR. In Figs. 1(a) and 1(b), we denote by $\rho_{pr}$, $\rho_{am1}$, $\rho_{am2}$ and $\rho_{as}$ the a priori, begin-ambiguity, end-ambiguity and asymptotic thresholds delimiting the different regions. Note that the CRLB is achieved at high SNRs with asymptotically efficient estimators, such as the maximum likelihood estimator (MLE), only. Otherwise, the estimator achieves its own asymptotic MSE (e.g. MLE with random signals and finite snapshots [13][14]. Capon algorithm [15]).

The exact evaluation of the statistics, in the threshold region, of some estimators such as the MLE has been considered as a prohibitive task. Many lower bounds (LB) have been derived for both deterministic and Bayesian (when the unknown parameter follows a given a priori distribution)
parameters in order to be used as benchmarks and to describe the behavior of the MSE in the threshold region \[16\]. Some upper bounds (UB) have also been derived like the Seidman UB \[17\]. It will suffice to mention here \[16, 18\] the Cramer-Rao, Bhattacharyya, Chapman-Robbins, Barankin and Abel deterministic LBs, the Cramer-Rao, Bhattacharyya, Bobrovsky-MayerWolf-Zakai, Bobrovsky-Zakai, and Weiss-Weinstein Bayesian LBs, the Ziv-Zakai Bayesian LB (ZZLB) \[2\] with its improved versions; Bellini-Tartara \[4\], Chazan-Ziv-Zakai \[19\], Weinstein \[21\] (approximation of Bellini-Tartara), and Bell-Steinberg-Ephraim-VanTrees \[21\] (generalization of Ziv-Zakai and Bellini-Tartara); and the Reuven-Messmer LB \[22\] for problems of simultaneously deterministic and Bayesian parameters.

The CRLB \[23\] gives the minimum MSE achievable by an unbiased estimator. However, it is very optimistic for low and moderate SNRs and does not indicate the presence of the threshold and ambiguity regions. The Barankin LB (BLB) \[24\] gives the greatest LB of an unbiased estimator. However, its general form is not easy to compute for most interesting problems. A useful form of this bound, which is much tighter than the CRLB, is derived in \[25\] and generalized to vector cases in \[26\]. The bound in \[25\] detects the asymptotic region much below the true one. Some applications of the BLB can be found in \[10–12, 29–35\].

The Bayesian ZZLB family \[2, 4, 19, 21\] is based on the minimum probability of error of a binary detection problem. The ZZLBs are very tight; they detect the ambiguity region roughly and the asymptotic region accurately. Some applications of the ZZLBs, discussions and comparison to other bounds can be found in \[10–12, 29–35\].

In \[36\] pp. 627-637], Wozencraft considered time-of-arrival (TOA) estimation with cardinal sine waveforms and employed the method of interval estimation (MIE) to approximate the MSE of the MLE. The MIE \[18\] pp. 58-62\] consists in splitting the a priori domain of the unknown parameter into intervals and computing the probability that the estimate falls in a given interval, and the estimator mean and variance in each interval. According to \[18\] \[37\], the MIE was first used in \[38, 39\] before Wozencraft \[36\] and others introduced some modifications later. The approach in \[36\] is imitated in \[18, 37, 40, 41\] for frequency estimation and in \[42\] for angle-of-arrival (AOA) estimation. The ACRs in \[15, 18, 36, 37, 40, 42\] have the special shape of a cardinal sine (oscillating baseband with the mainlobe twice wider than the sidelobes); this limitation makes their approach inapplicable on other shapes. In \[1\], McAulay considered TOA estimation with carrier-modulated pulses (oscillating passband ACRs) and used the MIE to derive an approximate UB (AUB); the approach of McAulay can be applied to any oscillating ACR. Indeed, it is followed (independently apparently) in \[15, 43, 44\] for AOA estimation and in \[41\] (for frequency estimation as mentioned above) where it is compared to Wozencraft’s approach. The ACR considered in \[43, 44\] has an arbitrary oscillating baseband shape (due to the use of non-regular arrays), meaning that it looks like a cardinal sine but with some strong sidelobes arbitrarily located. The MSEAs based on Wozencraft’s approach are very accurate and the AUBs using McAulay’s approach are very tight in the asymptotic and threshold regions. Both approaches can be used to determine accurately the asymptotic region. Various estimators are considered in the aforementioned references. More technical details about the MIE are given in Sec. \[V\].

We consider the estimation of a scalar deterministic parameter. We employ the MIE to propose new approximations (rather than AUBs) of the MSE achieved by the MLE, which are highly accurate, and a very tight AUB. The MLE mean and probability density function (PDF) are approximated as well. More details about our contributions with regards to the MIE are given in Secs. \[IV\] and \[V\]. We derive an approximate LB (ALB) tighter than the CRLB based on the second order Taylor series expansion of noise. Also, we utilize the binary detection principle to derive some ALBs; the obtained bounds are very tight. The theoretical results presented in this paper are applicable to any estimation problem satisfying the system model introduced in Sec. \[II\]. In order to illustrate the accurateness of the proposed MSEAs and the tightness of the derived bounds, we consider the example of TOA estimation with baseband and passband pulses.

The materials presented in this paper compose the first part of our work divided in two parts \[45, 46\].

The rest of the paper is organized as follows. In Sec. \[II\] we introduce our system model. In Sec. \[III\] we describe the threshold and ambiguity phenomena. In Sec. \[IV\] we deal with the MIE. In Sec. \[V\] we propose an AUB and an MSEA. In Sec. \[VI\] we derive some ALBs. In Sec. \[VII\] we consider the example of TOA estimation and discuss the obtained numerical results.

II. SYSTEM MODEL

In this section we consider the general estimation problem of a deterministic scalar parameter (Sec. \[II-A\]) and the particular case of TOA estimation (Sec. \[II-B\]).

A. Deterministic scalar parameter estimation

Let \(\Theta\) be a deterministic unknown parameter with \(D_\Theta = [\Theta_1, \Theta_2]\) denoting its a priori domain. We can write the \(i\)th, \((i = 1, \cdots, I)\) observation as:

\[
r_i(t) = \alpha s_i(t; \Theta) + \tilde{w}_i(t) \tag{1}
\]

where \(s_i(t; \Theta)\) is the \(i\)th useful signal carrying the information on \(\Theta\), \(\alpha\) is a known positive gain, and \(\tilde{w}_i(t)\) is an additive white Gaussian noise (AWGN) with two-sided power spectral density (PSD) of \(\frac{\sigma^2}{2}\); \(\tilde{w}_1(t), \cdots, \tilde{w}_I(t)\) are independent.

Denote by \(E_x(\theta) = \sum_{i=1}^I \int_{-\infty}^{+\infty} x_i^2(t; \theta)dt\) the sum of the energies of \(x_1(t; \theta), \cdots, x_I(t; \theta)\), by \(\dot{x}\) and \(\ddot{x}\) the first and second derivatives of \(x\) w.r.t. \(\theta\), and by \(E, \Re, \P\) the expectation, real part and probability operators respectively. From (1) we can write the log-likelihood function of \(\Theta\) as:

\[
\Lambda(\theta) = -\frac{1}{N_0} \left[ E_x + \alpha^2 E_x - 2\alpha X_{s,r}(\theta) \right] \tag{2}
\]

where \(\theta \in D_\Theta\) denotes a variable associated with \(\Theta\), and

\[
X_{s,r}(\theta) = \sum_{i=1}^I \int_{-\infty}^{+\infty} s_i(t; \theta)r_i(t)dt = \alpha R_x(\theta, \Theta) + w(\theta) \tag{3}
\]
is the crosscorrelation (CCR) with respect to (w.r.t.) \( \theta \), with
\[
R_s(\theta, \theta') = \sum_{i=1}^{I} \int_{-\infty}^{+\infty} s_i(t; \theta)s_i(t; \theta') \, dt
\]
denoting the ACR w.r.t. \((\theta, \theta')\) and
\[
w(\theta) = \sum_{i=1}^{I} \int_{-\infty}^{+\infty} s_i(t; \theta) \tilde{w}_i(t) \, dt
\]
being a colored zero-mean Gaussian noise of covariance
\[
C_w(\theta, \theta') = \sum_{i=1}^{I} \mathbb{E} \{ w_i(\theta)w_i(\theta') \} = \frac{N_0}{2} R_s(\theta, \theta').
\]  
1) MLE, CRLB and envelope CRLB: By assuming \( E_s(\theta) = E_s \) in (\( ? \)), that is, \( E_s(\theta) \) is independent of \( \theta \), we can respectively write the MLE and the CRLB of \( \Theta \) as [23, pp. 39]:
\[
\hat{\Theta} = \arg\max_{\theta \in \Phi} X_{s,r}(\theta)
\]
\[
c(\Theta) = \frac{-1}{\mathbb{E}\{ \Lambda(\theta) \mid \theta = \Theta \}} = \frac{-N_0/2}{\alpha^2 R_s(\Theta, \Theta)} = \frac{1}{\rho \beta^2_s(\Theta)}
\]
where
\[
\rho = \frac{\alpha^2 E_s}{N_0/2}
\]
\[
\beta^2_s(\Theta) = -\frac{\dot{R}_s(\Theta, \Theta)}{E_s}
\]  
Now, we define the ECRLB as:
\[
c_{e}(\Theta) = -\frac{N_0/2}{\alpha^2 \mathbb{E}\{ \dot{e}_{R_s}(\Theta, \Theta) \}} = \frac{1}{\rho \beta^2_s(\Theta)}
\]  
where
\[
\beta^2_s(\Theta) = -\frac{\mathbb{E}\{ \dot{e}_{R_s}(\Theta, \Theta) \}}{E_s}
\]  
2) BLB: The BLB can be written as [25]:
\[
c_B = (\Theta - \Theta)^T D^{-1} (\Theta - \Theta)
\]
with $\theta_1, \ldots, \theta_N \ (n_1 \leq 0, n_0 > 0, \theta_0 = \Theta)$ denoting \( N \) testpoints in the \( a \ priori \) domain of \( \Theta \), and
\[
d_{0,0} = \frac{\alpha^2 E_s(\theta)}{N_0/2} = \frac{1}{c(\Theta)}
\]
where $\mu_U = \frac{\theta_{1,0} + \Theta}{2}$ and $\sigma^2_U = \frac{\theta_{2,0} - \Theta}{2}$ is achieved when the estimator becomes uniformly distributed in $\Phi$.  

The system model considered in this subsection is satisfied for various estimation problems such as TOA, AOA, phase, frequency and velocity estimation. Therefore, the theoretical results presented in this paper are valid for the different mentioned parameters. TOA is just considered as an example to validate the accurateness and the tightness of our MSEAs and upper and lower bounds.

B. Example: TOA estimation

With TOA estimation based on one observation \((I = 1)\), \( s_1(t; \Theta) = s(t - \Theta) \) where \( s(t) \) denotes the transmitted signal and \( \Theta \) represents the delay introduced by the channel. Accordingly, we can write the ACR in (\( ? \)) as \( R_s(\theta, \theta') = R_s(\theta - \theta') \) where \( R_s(\theta) = \int_{-\infty}^{+\infty} s(t + \theta) s(t) \, dt \), and the CCR in (\( ? \)) as:
\[
X_{s,r}(\theta) = \alpha R_s(\theta - \Theta) + w(\theta).
\]  
The CRLB \( c_{e}(\Theta) \) in (\( 8 \)), ECRLB \( c_{e}(\Theta) \) in (\( ? \)), mean frequency \( f_s(\Theta) \) in (\( 12 \)), normalized curvatures \( \beta^2_2(\Theta) \) in (\( 10 \)) and \( \beta^2_2(\Theta) \) in (\( 16 \)) become now all independent of \( \Theta \). Furthermore, \( \beta^2_2(\Theta) \) and \( \beta^2_2(\Theta) \) denote now the mean quadratic bandwidth (MQBW) and the envelope MQBW (EMQBW) of \( s(t) \) respectively.

The CRLB in (\( 8 \)) is much smaller than the ECRLB in (\( ? \)) because the MQBW in (\( ? \)) is much larger than the EMQBW.
In fact, for a signal occupying the whole band from 3.1 to 10.6 GHz \( (f_c = 6.85 \text{ GHz}, \text{ bandwidth} B = 7.5 \text{ GHz}) \), we obtain \( \beta = 2\pi B^2 \approx 185 \text{ GHz}^2, 4\pi^2 f_c^2 \approx 10\beta_c^2, \beta_c^2 \approx 11\beta_c^2 \text{ and } c \approx \frac{\beta}{11}. \) Therefore, the estimation performance seriously deteriorates at relatively low SNRs when the ECRLB is achieved instead of the CRLB due to ambiguity.

III. THRESHOLD AND AMBIGUITY PHENOMENA

In this section we explain the physical origin of the threshold and ambiguity phenomena by considering TOA estimation with UWB pulses as an example. The transmitted signal

\[
s(t) = 2\sqrt{r \frac{E_s}{T_w}} e^{-\pi \frac{t^2}{T_w^2}} \cos(2\pi f_c t)
\]

is a Gaussian pulse of width \( T_w \) modulated by a carrier \( f_c \). We consider three values of \( f_c \) (\( f_c = 0, 4 \text{ and } 8 \text{ GHz} \)) and three values of the SNR (\( \rho = 10, 15 \text{ and } 20 \text{ dB} \)) per considered \( f_c \). We take \( \Theta = 0, T_w = 0.6 \text{ ns}, \text{ and } D_\Theta = [-1.5, 1.5]T_w. \)

In Figs. 2(a)–2(c) we show the normalized ACR \( R(\theta - \Theta) = \frac{R(\theta - \Theta)}{R_s} \) for \( f_c = 0 \) (baseband pulse), 4 and 8 GHz (passband pulses) respectively, and 1000 realizations per SNR of the maximum \( M(\hat{\Theta}, X(\hat{\Theta})) \) of the normalized CCR \( X(\Theta) = X_s(\Theta). \) Denote by \( N_0, (n = n_1, \ldots, n_N), (N \text{ is the number of local maxima in } D_\Theta), (n_1 < 0, n_N > 0), (n = 0 \text{ corresponds to the global maximum}) \) the number of samples of \( M \) falling around the \( n \)th local maximum (i.e. between the two local minima adjacent to that maximum) of \( R(\theta - \Theta). \) In Table II we show w.r.t. \( f_c \) and \( \rho \) the number of samples falling around the maxima number 0 and 1, the CRLB square root (SQRT) \( \sqrt{c} \) of \( \Theta \), the root MSE (RMSE) \( \sqrt{\text{CRLB}} \) obtained by simulation and the RMSE to CRLB SQRT ratio \( \frac{\sqrt{\text{CRLB}}}{\sqrt{c}} \).

Consider first the baseband pulse. We can see in Fig. 2(a) that the samples of \( M \) are very close to the maximum of \( R(\theta - \Theta) \) for \( \rho = 20 \text{ dB} \), and they start to spread progressively along \( R(\theta - \Theta) \) for \( \rho = 15 \text{ and } 10 \text{ dB} \). Table II shows that the CRLB is approximately achieved for \( \rho = 20 \text{ and } 15 \text{ dB} \), but not for \( \rho = 10 \text{ dB} \). Based on this observation, we can describe the threshold phenomenon as follows. For sufficiently high SNRs (resp. relatively low SNRs), the maximum of the CCR falls in the vicinity of the maximum of the ACR (resp. spreads along the ACR) so the CRLB is (resp. not) achieved.

Consider now the pulse with \( f_c = 4 \text{ GHz} \). Fig. 2(b) and Table II show that for \( \rho = 20 \text{ dB} \) all the samples of \( M \) fall around the global maximum of \( R(\theta - \Theta) \) and the CRLB is achieved, whereas for \( \rho = 15 \text{ and } 10 \text{ dB} \) they spread along the local maxima of \( R(\theta - \Theta) \) and the achieved MSE is much larger than the CRLB. Based on this observation, we can describe the ambiguity phenomenon as follows. For sufficiently high SNRs (resp. relatively low SNRs) the noise component \( w(t) \) in the CCR \( X_{s,r}(\Theta) \) in (21) is (resp. is) sufficiently high to fill the gap between the global maximum and the local maxima of the ACR. Consequently, for sufficiently high SNRs (resp. relatively low SNRs) the maximum of the CCR always falls around the global maximum (resp. spreads along the local maxima) of the ACR so the CRLB is (resp. is not) achieved. Obviously, the ambiguity phenomenon affects the threshold phenomenon because the SNR required to achieve the CRLB depends on the gap between the global and the local maxima.

Let us now examine the RMSE achieved at \( \rho = 20 \text{ dB} \).
for $f_c = 4$ and 8 GHz; it is 3.5 times smaller with $f_c = 4$ GHz than with $f_c = 8$ GHz whereas the CRLB SQRT is 2 times smaller with the latter. In fact, the samples of $M$ do not fall all around the global maximum for $f_c = 8$ GHz. This amazing result (observed in [50] from experimental results) exhibits the significant loss in terms of accuracy if the CRLB is not achieved due to ambiguity. It also shows the necessity to design our system such that the CRLB be attained.

IV. MIE-BASED MLE STATISTICS APPROXIMATION

We have seen in Sec. III that the threshold phenomenon is due to the spreading of the estimates along the ACR. To characterize this phenomenon we split the a priori domain $D_\Theta$ into $N$ intervals $D_n = [d_n, d_{n+1}), (n = n_1, \cdots, n_N)$, $(n_1 \leq 0, n_N \geq 0)$ and write the PDF, mean and MSE of $\Theta$ as

$$p(\theta) = \sum_{n=n_1}^{n_N} P_n p_n(\theta)$$

$$\mu = \int_{\Theta} \theta p(\theta) d\theta = \sum_{n=n_1}^{n_N} P_n \mu_n$$

$$e = \int_{\Theta} (\theta - \mu)^2 p(\theta) d\theta = \sum_{n=n_1}^{n_N} P_n \left( (\Theta - \mu_n)^2 + \sigma_n^2 \right)$$

where

$$P_n = P\{\hat{\Theta} \in D_n\}$$

$$= P\{\exists \xi \in D_n : X_{s,r}(\xi) > X_{s,r}(\theta), \forall \theta \in \cup_{n' \neq n} D_{n'}\}$$

denotes the interval probability (i.e. probability that $\hat{\Theta}$ falls in $D_n$). and $p_n(\theta)$, $\mu_n = E(\hat{\Theta}_n)$ and $\sigma_n^2 = E\{(\hat{\Theta}_n - \mu_n)^2\}$ represent, respectively, the PDF, mean and variance of the interval MLE ($\hat{\Theta}$ given $\hat{\Theta} \in D_n$)

$$\hat{\Theta}_n = \hat{\Theta}|\hat{\Theta} \in D_n.$$ (24)

Denote by $\theta_n$ a testpoint selected in $D_n$ and let $X_n = X_{s,r}(\theta_n) = \alpha R_n + w_n$ with $R_n = R_s(\theta_n, \Theta)$ and $w_n = w(\theta_n)$. Using (??), $P_n$ in (??) can be approximated by

$$P_n = P\{X_n > X_{n'}, \forall n' \neq n\} = \int_{-\infty}^{+\infty} dx_n \int_{-\infty}^{x_n} dx_{n+1} \cdots \int_{-\infty}^{x_n} dx_{n-1} \int_{-\infty}^{x_n} dx_n \cdots p_X(x) dx_N$$

where

$$p_X(x) = \frac{1}{(2\pi)^{\frac{3}{2}} |C_X|^\frac{1}{2}} e^{-\frac{(x - \mu^T X)}{2 |C_X|^{-1}(x - \mu^T X)^T}}$$

represents the PDF of $X = (X_{n_1} \cdots X_{n_N})^T$ with $\mu_X = (\mu_{X_{n_1}} \cdots \mu_{X_{n_N}})^T = \alpha (R_n \cdots R_N)^T$ being its mean and $C_X = \Sigma^{-1}(R_s(\theta_n, \theta_n))_{n,n'}|_{n_1,\cdots,n_N}$ its covariance matrix.

The accuracy of the approximation in (??) depends on the choice of the intervals and the testpoints. For an oscillating ACR we consider an interval around each local maximum and choose the abscissa of the local maximum as a testpoint. For both oscillating and non-oscillating ACRs, $D_0$ contains the global maximum and $\theta_0$ is equal to $\Theta$.

The testpoints are chosen as the roots of the ACR (except for $\theta_0 = \Theta$ in [18, 36, 37, 41, 42], as the local extrema abscissa in [1], and as the local maxima abscissa in [15, 31, 43, 44].

A. Computation of the interval probability

We consider here the computation of the approximate interval probability $\hat{P}_n$ in (??).

1) Numerical approximation: To the best of our knowledge there is no closed form expression for the integral in (??) for correlated $X_n$. However, it can be computed numerically using for example the MATLAB function QSCMVNV (written by Genz based on [51, 53]) that computes the multivariate normal probability with integration region specified by a set of linear inequalities in the form $b_1 < B(X - \mu_X) < b_2$. Using QSCMVNV, $\hat{P}_n$ can be approximated by:

$$P_n^{(1)} = \text{QSCMVNV}(N_p, C_X, b_1, B, b_2)$$

where $N_p$ is the number of points used by the algorithm (e.g. $N_p = 3000$), $b_1 = (-\infty \cdots - \infty)^T$ and $b_2 = \mu_X - (\mu_{X_{n_1}} \cdots \mu_{X_{n_N}})^T$ two $(N-1)$-column vectors, and $B = \begin{bmatrix} B_1 & B_2 & B_3 & B_4 & B_5 \end{bmatrix}$ an $(N-1) \times N$ matrix with $B_1 = I(n - n_1)$, $B_2 = \text{zeros}(N + n_1 - n - 1, n - n_1)$, $B_3 = \text{zeros}(N - n - 1, n - n_1)$, $B_4 = \text{zeros}(N - N + n + 1, n - n_1)$ and $B_5 = I(n - n - 1)$. [6]

2) Analytic approximation: Denote by $Q(y) = \frac{1}{\sqrt{2\pi}} \int_{y}^{\infty} e^{-\frac{x^2}{2}} dx$ the Q function. As $P\{A_1 \cap A_2\} \leq P\{A_1\}$, we can upper bound $\hat{P}_n$ in (??) by:

$$P_n^{(2)} = \begin{cases} P(\theta_n, \theta_1) & n = 0 \\ P(\theta_n, \theta_0) & n \neq 0 \end{cases}$$

where

$$P(\theta, \theta') = P\{X_{s,r}(\theta) > X_{s,r}(\theta')\} = \sqrt{2} \left( \frac{R(\theta', \Theta) - R(\theta, \Theta)}{\sqrt{1 - R(\theta, \theta')}} \right)$$

with $R(\theta, \Theta) = \frac{R_s(\theta, \Theta)}{E}\frac{R_s(\theta, \Theta)}{E}$ denoting the normalized ACR. $P(\theta, \theta')$ is obtained (??) from (??) and (??) by noticing that $X_{s,r}(\Theta) - X_{s,r}(\theta) \sim N(\alpha[R_s(\theta, \Theta) - R_s(\theta, \Theta)], N_0[E_s - R_s(\theta, \Theta)])$ [7]. If $N$ approaches infinity, then both $\sum_{n=n_1}^{n_N} P_n^{(2)}$ and the MSE in (??) will approach infinity.

Using (??), we propose the following approximation:

$$P_n^{(3)} = \frac{P_n^{(2)}}{\sum_{n=n_1}^{n_N} P_n^{(2)}}.$$

In this subsection we have seen that the interval probability $\hat{P}_n$ in (??) can be approximated by $P_n^{(1)}$ in (??) or $P_n^{(3)}$ in (??), and upper bounded by $P_n^{(2)}$ in (??).

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6 We denote by $I(k)$ the identity matrix of rank $k$ and $\text{zeros}(k_1, k_2)$ and ones($k_1, k_2$) the zero and one matrices of dimension $k_1 \times k_2$.

7 $N(m, v)$ stands for the normal distribution of mean $m$ and variance $v$. 
The UB $P_n^{(2)}$ is adopted in [1, 13, 41, 43, 44] with minor modifications; in fact, $P_0$ is approximated by one in [1] and by $1 - \sum_{n \neq 0} P_n^{(2)}$ in [13, 41, 43, 44]. In the special case where $X_1, \ldots, X_n$ are independent and identically distributed such as in [18, 36, 37, 40–42] thanks to the cardinal sine ACR, then $P_n = P_n^{(2)}$, $\forall n \neq 0$, and $P_0 = 1 - P_A$ ($P_A$ is the approximate probability of ambiguity); consequently, the MSEA in (30) can be written as the sum of two terms: $e \approx P_A e_U + P_0 c(\theta)$; $P_0$ can be calculated by performing one-dimensional integration. If $X_n \sim N(\alpha E_n, \Sigma_{E_n})$ and $X_n \sim N(0, \frac{\sigma^2}{n} E_n)$, $\forall n \neq 0$, like in [18, 36, 43, 44] then $P_A$ can be upper bounded using the union bound [36].

As an example, to evaluate the accurateness of $P_n^{(1)}$ in (38) and to compare them to $P_n^{(2)}$ in (39), we consider the pulse in (27) with $f_c = 6.85$ GHz, $T_w = 2$ ns, $\Theta = 0$ and $D_\Theta = [-2, 1.5]T_w$. In Fig. 3 we show for $n = 0$ and 1, the interval probability $P_n^{(S)}$ obtained by simulation based on 10000 trials, $P_n^{(1)}$, $P_n^{(2)}$ and $P_n^{(S)}$, all versus the SNR. We can see that $P_n^{(S)}$ converges to $\frac{1}{2}$ at low SNRs for all intervals; however, it converges to 1 at high SNRs ($P_n^{(S)} = 0.99$ for $\rho \approx 30$ dB) for $\rho = 0$ (probability of non-ambiguity) and to 0 for $\rho \neq 0$. Both $P_n^{(1)}$ and $P_n^{(3)}$ are very accurate and closely follow $P_n^{(S)}$. The UB $P_n^{(2)}$ is not tight at low SNRs; it converges to 0.5 $\forall n$ instead of $\frac{1}{2}$ due to (39). However, it converges to 1 (resp. 0) for $n = 0$ (resp. $n \neq 0$) at high SNRs simultaneously with $P_n^{(S)}$ so it can be used to determine accurately the asymptotic region.

**B. Statistics of the interval MLE**

We approximate here the statistics of the interval MLE $\hat{\Theta}_n$ in (39). We have already mentioned in Sec. IV that for an oscillating (resp. a non-oscillating) ACR we consider an interval around each local maximum (resp. split the a priori domain into equal intervals); the global maximum is always contained in $D_n$. Accordingly, the ACR inside a given interval is either increasing then decreasing or monotone (i.e. increasing, decreasing or constant).

As the distribution of $\theta_n$ should follow the shape of the ACR in the considered interval, the interval variance is upper bounded by the variance of uniform distribution in $D_n = [d_n, d_{n+1}]$. Therefore, the interval mean $\mu_n$ and variance $\sigma^2_n$ can be approximated by

$$\mu_n, \sigma_n \approx \frac{d_n + d_{n+1}}{2}$$

For intervals with local minima (not considered here), the ACR decreases then increases so $\sigma_n^2$ is upper bounded by the variance of a Bernoulli distribution of two equiprobable atoms:

$$\sigma_n^2 \leq \frac{(d_{n+1} - d_n)^2}{4}$$

In [1], it is assumed that $\sigma_n^2$ is upper bounded by $\sigma_n^2$ in [31] even for intervals with local minima. See [35, 56] for further information on the maximum variance.

The CCR $X_{s,r}(\theta)$ in (33) can be approximated inside $D_n$ by its Taylor series expansion about $\theta_n$ limited to second order:

$$X_{s,r}(\theta) = \theta R_s(\theta, \Theta) + w(\theta) \approx (\alpha R_n + w_n) + (\alpha R_n + w_n)(\theta - \theta_n)$$

with

$$\sigma^2_w = \frac{N_0}{2} \int_{-\infty}^{\infty} s^2(t; \theta_n) dt$$

Let us first consider an interval with monotone ACR. By neglecting $\hat{w}_n$ and $R_n$ in (39) (linear approximation), we can approximate the interval MLE by:

$$\hat{\Theta}_n = \arg\max_{\theta \in D_n} \{ X_{s,r}(\theta) \}$$

As $P\{\alpha R_n + w_n = 0\} = 0$, the latter approximation follows a two atoms Bernoulli distribution with probability, mean and variance given from (39, 34) and (40) by:

$$\mu_{n, B} = d_n P\{d_n\} + d_{n+1} P\{d_{n+1}\}$$

$$\sigma^2_{n, B} = \frac{d_n P\{d_n\} + d_{n+1} P\{d_{n+1}\}}{(d_n + d_{n+1} - d_n)^2}$$

$$\sigma^2_{n, B} = \frac{d_n P\{d_n\} + d_{n+1} P\{d_{n+1}\}}{(d_n + d_{n+1} - d_n)^2}$$

Figure 3. Simulated interval probability $P_n^{(S)}$, the approximations $P_n^{(1)}$ and $P_n^{(3)}$, and the AUB $P_n^{(2)}$ for $n = 0, 1$ w.r.t. the SNR.
where $\sigma_{n,B}^2$ is upper bounded by $\sigma_{n,\text{max}}^2$ in (42) and reaches it for $\mathbb{P}\{d_n\} = 0.5$; $\mathbb{P}\{d_n\} = 0.5$ just means that $\hat{\Theta}_n$ is uniformly distributed in $D_n$ (because $\Theta_n$ can fall anywhere inside $D_n$); therefore, $\mu_n$ and $\sigma_n^2$ can be approximated by:

$$
\mu_{n,1,c} = \mu_{n,B}
$$

(41)

$$
\sigma_{n,1,c}^2 = \min\{\sigma_{n,U}^2, \sigma_{n,B}^2\}
$$

(42)

By neglecting $\bar{w}_n$ in (43) and (47) (because $\sigma_n^2 \ll (\Theta - \mu_n)^2$ for $n \neq 0$, see (48)) we obtain the following approximation:

$$
\mu_{n,2,c} = \left\{ \begin{array}{ll}
d_n & \hat{R}_n < 0 \\
\frac{d_{n+1} - d_{n+1} + d_{n+2}}{2} & \hat{R}_n = 0 \\
\frac{d_n}{d_n + d_{n+1}} & \hat{R}_n > 0 \end{array} \right.
$$

(43)

$$
\sigma_{n,2,c}^2 = 0.
$$

(44)

Consider now an interval with a local maximum. By neglecting $\bar{w}_n$ in (43), and taking into account that $\hat{R}_n = 0$ (local maximum), $\Theta_n$ can be approximated by:

$$
\hat{\Theta}_n = \arg \max_{\theta \in D_n} \{X_s, r(\theta)\} \approx \theta_n - \frac{\bar{w}_n}{\alpha R_n}
$$

(45)

which follows a normal distribution whose PDF, mean and variance can be obtained from (8), (34), (36) and (48):

$$
p_{n,N}(\theta) = \frac{1}{2\pi \sigma_{n,N}} e^{-\frac{(\theta - \mu_n)^2}{2\sigma_{n,N}^2}}
$$

(46)

$$
\mu_{n,N} = \theta_n
$$

(47)

$$
\sigma_{n,N}^2 = \frac{\alpha^2 R_n^2}{N E_z(\theta_n)}
$$

(48)

For $n = 0$, $\sigma_{n,N}^2$ is equal to the CRLB in (8) since $\tilde{\hat{R}}_0 = E_z(\theta_0)$. To take into account that $D_n$ is finite, we propose from (46), (47) and (48) the following approximation:

$$
\mu_{n,1,o} = \int_{d_n}^{d_{n+1}} \mathbb{P}_{n,1,o}(\theta) d\theta \approx \theta_n
$$

(49)

$$
\sigma_{n,1,o}^2 = \int_{d_n}^{d_{n+1}} (\theta - \mu_{n,1,o})^2 \mathbb{P}_{n,1,o}(\theta) d\theta
$$

(50)

where $\mathbb{P}_{n,1,o}(\theta) = \frac{p_{n,N}(\theta)}{\int_{d_n}^{d_{n+1}} p_{n,N}(\theta) d\theta}$. By neglecting $w(\theta)$ in (48) and (49), we obtain the following approximation:

$$
\mu_{n,2,o} = \theta_n
$$

(51)

$$
\sigma_{n,2,o}^2 = 0.
$$

(52)

For both oscillating and non-oscillating ACRs, $D_0$ contains the global maximum. To guarantee the convergence of the MSEA in (40) to the CRLB, $\mu_0$ and $\sigma_0^2$ should always be approximated using (49) and (50) by:

$$
\mu_{0,0} = \Theta
$$

(53)

$$
\sigma_{0,0}^2 = \min\{c, \sigma_{0,U}^2\}.
$$

(54)

For TOA estimation, we can write [40] and [43] as $\mathbb{P}\{d_n\} = Q\left(\sqrt{\frac{R_n}{E_z}}\right)$ and $\sigma_{n,N}^2 = \frac{R_n^2}{R^2}$.

We have seen in this subsection that the interval mean and variance can be approximated by

- $\mu_{0,0}$ in (53) and $\sigma_{0,0}^2$ in (54) for $n = 0$.
- $\mu_{n,U}$ in (45) and $\sigma_{n,U}^2$ in (46), $\mu_{n,1,c}$ in (41) and $\sigma_{n,1,c}^2$ in (42), or $\mu_{n,2,c}$ in (43) and $\sigma_{n,2,c}^2$ in (44) for intervals with monotone ACR.
- $\mu_{n,U}$ and $\sigma_{n,U}^2$, $\mu_{n,1,o}$ and $\sigma_{n,1,o}^2$, in (51) and $\sigma_{n,2,o}^2$ in (52) for intervals with local maxima.

In Fig. 4 we show the approximate interval standard deviations (STD) $\sigma_{n,U}$ and $\sigma_{n,1,o}$ w.r.t. the interval number $n = -6, \cdots, 6$ for $\rho = 10$ dB.

![Figure 4. Simulated interval STD $\sigma_{n,S}$ and approximations $\sigma_{n,U}$ and $\sigma_{n,1,o}$ in Fig. 4](image)

- $\mu_{0,0}$ in (53) and $\sigma_{0,0}^2$ in (54) for $n = 0$.
- $\mu_{n,U}$ in (45) and $\sigma_{n,U}^2$ in (46), $\mu_{n,1,c}$ in (41) and $\sigma_{n,1,c}^2$ in (42), or $\mu_{n,2,c}$ in (43) and $\sigma_{n,2,c}^2$ in (44) for intervals with monotone ACR.
- $\mu_{n,U}$ and $\sigma_{n,U}^2$, $\mu_{n,1,o}$ and $\sigma_{n,1,o}^2$, in (51) and $\sigma_{n,2,o}^2$ in (52) for intervals with local maxima.

In Fig. 4 we show the approximate interval standard deviations (STD) $\sigma_{n,U}$ and $\sigma_{n,1,o}$ w.r.t. the interval number $n = -6, \cdots, 6$ for $\rho = 10$ dB. We have shown in Fig. 3 how our approximations are accurate. To the best of our knowledge all previous authors adopt the McAulay probability UB (except for the case where $X_{n_1, \cdots, X_{n_N}}$ are independent thanks to the cardinal sine ACR). We have proposed two new approximations for the interval mean and variance, one for intervals with monotone ACRs and one for intervals with local maxima. We have seen in Fig. 4 how our approximations are accurate. To the best of our knowledge all previous authors either upper bound the interval variance or neglect it. Thanks to the proposed probability approximations our MSEs (e.g. $e_{1,1,c}$ in Fig. 4) are highly accurate and outperform the MSE UB of McAulay ($e_{2,U}$ in Fig. 5) and thanks to the proposed interval variance approximations the MSEA is improved ($e_{1,U}$ and $e_{1,2,c}$ outperform $e_{1,1,c}$ in Fig. 6). We have applied the MIE to non-oscillating ACRs. To the best of our knowledge this case is...
not considered before.

V. AN AUB AND AN MSEA BASED ON THE INTERVAL PROBABILITY

In this section we propose an AUB (Sec. V-A) and an MSEA (Sec. V-B), both based on the interval probability approximation $P_n^{(3)}$ in (??).

A. An AUB

As $P_n^{(3)}$ approximates the probability that $\hat{\Theta}$ falls in $D_0$, the PDF of $\hat{\Theta}$ can be approximated by the limit of $P_n^{(3)}$ as $N$ (number of intervals) approaches infinity (so that the width of $D_n$ approaches zero). Accordingly we can write the approximate PDF, mean and MSE of $\Theta$ as

$$p_M(\theta) = \lim_{N \to \infty} P_n^{(3)} = \frac{P(\theta, \Theta)}{\int_{\Theta}^\Theta P(\theta, \Theta)d\theta} \quad (55)$$

$$\mu_M = \int_{\Theta}^\Theta \theta p_M(\theta)d\theta \quad (56)$$

$$e_M = \int_{\Theta}^\Theta (\theta - \Theta)^2 p_M(\theta)d\theta. \quad (57)$$

We will see in Sec. VII that $e_M$ acts as an UB and also converges to a multiple of the CRLB. In fact, $p_M(\theta)$ overestimates the true PDF of $\Theta$ in the vicinity of $\Theta$ because it is obtained from $P_n^{(3)}$ which is in turn obtained from the interval probability UB $P_n^{(2)}$ in (??).

B. An MSEA

To guarantee the convergence of the MSEA to the CRLB, we approximate the PDF of $\Theta$ inside $D_0 \approx [\Theta - \theta - \theta_0, \Theta + \theta + \theta_0]$ by $p_{0,n}(\theta)$ in (??) (the mean of $\hat{\Theta}$ is the ME) and outside $D_0$ by $p_M(\theta) = P(\theta, \Theta)/\int_{D_0} P(\theta, \Theta)d\theta$ (the corresponding mean and MSE are $\mu_M = \int_{D_0} \theta p_M(\theta)d\theta$ and $e_M = \int_{D_0} (\theta - \Theta)^2 p_M(\theta)d\theta$), and propose the following approximation:

$$p_{MN}(\theta) = (1 - \hat{\theta}) p_{0,n}(\theta) + \hat{\theta} p_{AP_M}(\theta) \quad (58)$$

$$\mu_{MN} = (1 - \hat{\theta}) \Theta + \hat{\theta} \mu'_{AP_M} \quad (59)$$

$$\sigma^2_{MN} = (1 - \hat{\theta}) \sigma^2 + \hat{\theta} \sigma^2' \quad (60)$$

where $\hat{\theta} = 2P(\theta_1, \Theta)$ approximates the probability that $\hat{\Theta}$ falls outside $D_0$. With oscillating ACRs, $\theta_1$ is the abscissa of the first local maximum after the global one; thus, $\theta_1 \approx \Theta + 1/\sqrt{\sigma(\Theta)}$. With non-oscillating ACRs, the vicinity of the maximum is not clearly marked off; so, we empirically take $\theta_1 = \Theta + 2\sigma(\Theta)$.

The first contribution in this section is the AUB $e_M$ which is very tight (as will be seen in Figs. 7 and 9) and also very easy to compute. The second one is the highly accurate MSEA $e_{MN}$ (as will be seen in Figs. 6 and 8): to the best of our knowledge, this is the first approximation expressed as the sum of two terms when $X_{n_1}, \cdots, X_{n_N}$ are correlated (see 11 55 41 43 44).

VI. ALBS

In this section we derive an ALB based on the Taylor series expansion of the noise limited to second order (Sec. VI-A) and a family of ALBs by employing the principle of binary detection which is first used by Ziv and Zakai [2] to derive LBs for Bayesian parameters (Sec. VI-B).

A. An ALB based on the second order Taylor series expansion of noise

From (??), the MLE of $\Theta$ can be approximated by:

$$\hat{\Theta} = \arg\max_{\theta} \{X_s, r(\theta)\} \approx \hat{\Theta}_C = \Theta - \frac{\bar{\eta}_0}{\alpha R_0 + \bar{\eta}_0} \quad (61)$$

where $\bar{\eta}_0/(\alpha R_0 + \bar{\eta}_0)$ is a ratio of two normal variables. Statistics of normal variable ratios are studied in [57-59].

Let $\delta(\xi) = 1$ (resp. $-1$) for $\xi \geq 0$ (resp. $\xi < 0$), $\delta^4(\theta) = E_s(\theta)/E_s$, $h = \frac{\gamma(\sigma_0)\sigma_\delta\sqrt{1 - \nu_0^2}}{\nu_0^2 + \sigma_\delta^2}$, $a_1 = \nu_0\sigma_\delta/\sigma_\theta$, $a_2 = \sigma_\delta/h$, $a_3 = \alpha R_0 a_1/h$, $a_4 = -\alpha R_0/\sigma_\theta$, $\delta(\xi) = (a_3\xi + a_4)/\sqrt{1 + \xi^2}$. We can show from (68) that $\hat{\Theta}_C$ in (??) is distributed as:

$$\hat{\Theta}_C \sim \Theta + a_1 + \frac{\chi}{a_2} \quad (62)$$

where the PDF of $\chi$ is given by:

$$p_\chi(\xi) = \frac{e^{-\frac{x^2 + \xi^2}{2}}}{\pi(1 + \xi^2)} \left\{1 + \sqrt{2\pi q(\xi)} e^{\frac{\xi^2}{2}} \left(\frac{1}{2} - Q[q(\xi)]\right)\right\}. \quad (63)$$

From (??) we can approximate the PDF, mean, variance and MSE of $\hat{\Theta}_C$ by

$$p_C(\theta) = \text{sign}(\nu_0) a_2 p_X(\theta - \Theta - a_1) \quad (64)$$

$$\mu_C = \int_{\Theta}^\Theta \theta p_C(\theta)d\theta \quad (65)$$

$$\sigma^2_C = \int_{\Theta}^\Theta (\theta - \mu_C)^2 p_C(\theta)d\theta. \quad (66)$$

$$e_C = (\mu_C - \Theta)^2 + \sigma^2_C. \quad (67)$$

Note that the moments $\int_{-\infty}^{\infty} q(\xi) p_X(\xi)d\xi, i = 1, 2, \cdots$ (infinite domain) are infinite like with Cauchy distribution [58]. We will see in Sec. VII that $e_C$ behaves as an LB; this result can be expected from the approximation in (??) where the expansion of the noise is limited to second order.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{Decision problem with two equiprobable hypotheses: $H_1: \Theta = \theta_0$ and $H_2: \Theta = \theta_0 + \xi$.}
\end{figure}
B. Binary detection based ALBs

Let $\hat{\Theta}$ be an estimator of $\Theta$, $\epsilon|\Theta = \hat{\Theta} - \Theta$ the estimation error given $\Theta = \theta$, $p(\epsilon|\theta, \xi)$ the PDF of $|\epsilon|$, and $P_{||}\epsilon|\xi|\theta$ the probability that $|\epsilon| > \xi$. For $\Theta = \theta_0$, the MSE of $\hat{\Theta}$ can be written as [66]:

$$e|\theta_0 = \int_0^{e_{\text{max}}} \xi^2 p_{|\epsilon|}(\xi) d\xi = 2 \int_0^{e_{\text{max}}} \xi^2 P_{|\epsilon|>\xi|\theta_0} d\xi$$

$$- \{\xi^2 P_{|\epsilon|>\xi|\theta_0}\}_{e_{\text{max}}} = 1 \int_0^{e_{\text{max}}} \xi^2 P_{|\epsilon|>\xi|\theta_0} d\xi$$

where $e_{\text{max}} = \max\{\Theta_2 - \theta_0, 0, -\Theta_1\}$. By assuming $P_{|\epsilon|>\xi|\theta}$ and $P_{|\epsilon|<\xi|\theta}$ constant $\forall \theta \in D_0$, we can write [67]:

$$P_{|\epsilon|>\xi|\theta_0} = 2 \left[ \frac{1}{2} P_{|\epsilon|>\xi|\theta_0} + \frac{1}{2} P_{|\epsilon|<\xi|\theta_0} \right]$$

$$\approx 2 \left\{ \begin{array}{ll} P_{e_1} & = \frac{1}{2} P_{|\epsilon|>\xi|\theta_0} - \frac{1}{2} P_{|\epsilon|<\xi|\theta_0} \\ P_{e_2} & = \frac{1}{2} P_{|\epsilon|>\xi|\theta_0} + \frac{1}{2} P_{|\epsilon|<\xi|\theta_0} \end{array} \right\}$$

$$\geq 2 \left\{ \begin{array}{ll} P_{\min}(\theta_0 - \xi, \theta_0) & \rho \approx 2 \xi P_{\min}(\theta_0, \theta_0 + \xi) \end{array} \right\}$$

where $P_{e_1}$ and $P_{e_2}$ denote the probabilities of error of the nearest decision rule

$$\bar{H} = \left\{ \begin{array}{ll} H_1 & \text{if } \{\hat{\Theta} - (\Theta|H_1)\} \leq \{\hat{\Theta} - (\Theta|H_2)\} \\ H_2 & \text{otherwise} \end{array} \right\}$$

of the two-hypothesis decision problems (the decision problem in [73] is illustrated in Fig. 5):

$$H = \left\{ \begin{array}{ll} H_1 & : \Theta = \theta_0 - \xi \quad \text{Pr}_{H_1} = 0.5 \\ H_2 & : \Theta = \theta_0 \quad \text{Pr}_{H_2} = 0.5 \end{array} \right\}$$

and $P_{\min}(\theta_0 - \xi, \theta_0)$ and $P_{\min}(\theta_0, \theta_0 + \xi)$ the minimum probabilities of error obtained by the optimum decision rule based on the likelihood ratio test [66, pp. 30]:

$$\bar{H} = \left\{ \begin{array}{ll} H_1 & \text{if } \Lambda(\Theta|H_1) - \Lambda(\Theta|H_2) \geq \ln \frac{P_{H_2}}{P_{H_1}} \end{array} \right\}$$

with $\Lambda(\theta)$ denoting the log-likelihood function in (?). The probability of error of an arbitrary detector $\hat{H}$ is given by

$$P_e = P_{H_1} P_{\Theta = \theta_0 - \xi} + P_{H_2} P_{\Theta = \theta_0}$$

From (?) and (?) we obtain the following ALBs:

$$z_1 = \int_0^{e_1} \xi P_{\min}(\theta_0 - \xi, \theta_0) d\xi$$

$$z_2 = \int_0^{e_2} \xi P_{\min}(\theta_0, \theta_0 + \xi) d\xi$$

where $e_1 = \min\{\theta_0 - \Theta_1, 2(\Theta_2 - \theta_0)\}$ and $e_2 = \min\{\Theta_2 - \theta_0, 2(\theta_0 - \Theta_1)\}$. The integration limits are set to $e_1$ and $e_2$ to make the two hypotheses in [72] and [73] fall inside $D_0$. As $P_{|\epsilon|>\xi|\theta_0}$ is a decreasing function, tighter bounds can be obtained by filling the valleys of $P_{\min}(\theta_0 - \xi, \theta_0)$ and $P_{\min}(\theta_0, \theta_0 + \xi)$ (as proposed by Bellini and Tartara in [4]):

$$b_1 = \int_0^{e_1} \xi V\{P_{\min}(\theta_0 - \xi, \theta_0)\} d\xi$$

$$b_2 = \int_0^{e_2} \xi V\{P_{\min}(\theta_0, \theta_0 + \xi)\} d\xi$$

where $V\{f(\xi)\} = \max\{f(\xi) \geq \xi\}$ denotes the valley-filling function. When $P_{\min}(\theta, \theta')$ is a function of $\theta' - \theta$ (e.g., TOA estimation) we can write the bounds in (76–79) as ($i = 1, 2$):

$$z_i = \int_0^{e_i} \xi V\{\min(\xi)\} d\xi$$

$$b_i = \int_0^{e_i} \xi V\{\min(\xi)\} d\xi$$

If $\theta_0 - \Theta_1 > \Theta_2 - \theta_0$, then $e_1 > e_2$; hence, $z_1$ and $b_1$ become tighter than $z_2$ and $b_2$, respectively. From (?) and (?) and (?) we can write the minimum probability of error as

$$P_{\min}(\theta, \theta') = 0.5 [P_{\Lambda(\theta') > \Lambda(\theta)}|\Theta = \theta + P_{\Lambda(\theta) > \Lambda(\theta')}|\Theta = \theta']$$

$$= 0.5 [P_{\theta', \theta}|\Theta = \theta' + P_{\theta', \theta}|\Theta = \theta']$$

$$= Q\left( \frac{\sqrt{1 - \rho|\theta, \theta'|}}{2} \right)$$

There are two main differences between our bounds (deterministic) and the Bayesian ones: i) with the former we integrate along the error only whereas with the latter we integrate along the error and the a priori distribution of $\Theta$ (e.g, see (14) in [21]); ii) all hypotheses (e.g, $\Theta = \theta_0$ and $\Theta = \theta_0 + \xi$ in [73]) are possible in the Bayesian case thanks to the a priori distribution whereas only one hypothesis ($\Theta = \theta_0$) is possible in the deterministic case. So in order to utilize the minimum probability of error we have approximated $P_{|\epsilon|>\xi|\theta_0}$ in (??) by $P_{|\epsilon|>\xi|\theta_0}$ (see Fig. 5).

In this section we have two main contributions. The first one is the ALB $e_c$ whereas the second one is the deterministic ZLBB family. These bounds can from now on be used as benchmarks in deterministic parameter estimation (like the CRLB) where it is not rigorous to use Bayesian bounds. Even though the derivation of $e_c$ was a bit complex, the final expression is now ready to be utilized.

VII. NUMERICAL RESULTS AND DISCUSSION

In this section we discuss some numerical results about the obtained MSEs, AUB, and ALBs. We consider TOA estimation using baseband and passband pulses. Let $T_w = 2$ ns, $f_c = 6.85$ GHz, $\Theta = 0$ and $D_0 = [-2, 1.5]T_w$. With the baseband pulse we consider 9 equal duration intervals. Let

$$e_{i,j,x} = P_{i,j,x}^{(\theta)} \sigma_{0,0}^{2} + \sum_{n=-N}^{N} P_{i}^{(n)} \left[ (\theta - \mu_{n,j,x})^2 + \sigma_{n,j,x}^2 \right]$$

be the MSE based on (?) and using the interval probability approximation $P_{i,j,x}^{(\theta)} (i \in \{1, 2, 3\}, \theta, (?)$, (?) and interval mean and variance approximations $\mu_{n,j,x}$ and $\sigma_{n,j,x}^2$)
A. Baseband pulse

Consider first the baseband pulse. In Fig. 6 we show the SQRTs of the maximum MSE \( e_U \), the CRLB \( c \), the MSEAs \( e_{1,1,c}, e_{1,2,c}, e_{3,1,c} \) and \( e_{\text{MN}} \), and the simulated MSE \( e_S \), w.r.t. the SNR. In Fig. 7 we show the SQRTs of five MSEAs:\( \rho \text{dB and } e_{\text{MN}} \), because a non-oscillating ACR, and \( e_A \). Baseband pulse of non-ambiguity \([15, 37]\) (for simplicity reasons).

We can see from \( e_S \) that, as cleared up in Sec. I, the SNR axis can be divided into three regions: 1) the \textit{a priori} region where \( e_U \) is achieved, 2) the threshold region and 3) the asymptotic region where \( c \) is achieved. We define the \textit{a priori} and asymptotic thresholds by \([6]\):

\[ \rho_{\text{pr}} = \rho : e(\rho) = \alpha_{\text{pr}} e_U \]
\[ \rho_{\text{as}} = \rho : e(\rho) = \alpha_{\text{as}} c. \]

We take \( \alpha_{\text{pr}} = 0.5 \) and \( \alpha_{\text{pr}} = 1.1 \). From \( e_S \), we have \( \rho_{\text{pr}} = 4 \) dB and \( \rho_{\text{as}} = 16 \) dB. Thresholds are defined in literature w.r.t. two magnitudes at least: i) the achieved MSE \([3, 9, 21]\) like in our case (which is the most reliable because the main concern in estimation is to minimize the MSE) and ii) the probability of non-ambiguity \([15, 37]\) (for simplicity reasons).

The MSEAs \( e_{1,1,c}, e_{1,2,c}, e_{3,1,c} \) obtained from the MIE (Sec. V) are very accurate and follow \( e_S \) closely; \( e_{1,1,c} \) more accurately than \( e_{3,1,c} \) which slightly overestimates \( e_S \) because \( e_{1,1,c} \) uses the probability approximation \( P_n^{(1)} \) in (\ref{eq:approx1}) that considers all testpoints during the computation of the probability, whereas \( e_{3,1,c} \) uses the approximation \( P_n^{(3)} \) in (\ref{eq:approx3}) based on the probability UB \( P_n^{(2)} \) in (\ref{eq:ub1}) that only considers the 0th and the \( n \)th testpoints; \( e_{1,1,c} \) is more accurate than \( e_{1,2,c} \) which slightly overestimates \( e_S \) and than \( e_{1,2,c} \) which slightly underestimates it, because \( e_{1,1,c} \) uses the variance approximation \( \sigma_n^{2,1,c} \) in (\ref{eq:var1}) obtained from the first order Taylor series expansion of noise, whereas \( e_{1,2,c} \) uses \( \sigma_n^{2,1,2} \) in (\ref{eq:var3}) assuming the MLE uniformly distributed in \( D_n \) (overestimation of the noise), and \( e_{1,2,c} \) uses \( \sigma_n^{2,1,2} \) in (\ref{eq:var4}) neglecting the noise. The MSEA \( e_{\text{MN}} \) proposed in Sec. V-A based on our probability approximation \( P_n^{(3)} \) is very accurate as well.

The AUB \( e_{2,U} \) proposed in (\ref{eq:aul}) is very tight and converges to the asymptotic region simultaneously with \( e_S \). However, it is less tight in the \textit{a priori} and threshold regions because it uses the probability UB \( P_n^{(2)} \) which is not very tight in these regions (see Fig. 7). Moreover, \( e_{2,U} \rightarrow \infty \) when \( N \rightarrow \infty \). The AUB \( e_M \) (Sec. V-A) is very tight. However, it converges to 2.68 times the CRLB at high SNRs. This fact was discussed in Sec. V-A and also solved in Sec. V-B by proposing \( e_{\text{MN}} \) (examined above). Nevertheless, \( e_M \) can be used to compute the asymptotic threshold accurately because it converges to its own asymptotic regime simultaneously with \( e_S \).

Both the BLB \( e_B \) and the ALB \( e_C \) (Sec. VI-A) outperform the CRLB. Unlike the passband case considered below, \( e_C \) outperforms the BLB. The ALB \( e_C \) (Sec. VI-B) is very tight and converges to the CRLB simultaneously with \( e_S \).

B. Passband pulse

Consider now the passband pulse. In Fig. 8 we show the SQRTs of the maximum MSE \( e_U \), the CRLB \( c \), the ECRBL \( c_b \) in (\ref{eq:ubp}) (equal to CRLB of the baseband pulse), three MSEAs:\( e_{1,1,o}, e_{1,2,o}, e_{3,1,o} \) in (\ref{eq:approx2}) and \( e_{\text{MN}} \) in (\ref{eq:approx3}), and the MSEs obtained by simulation for both the passband \( e_S \) and the baseband \( e_{S,BB} \) pulses. In Fig. 9 we show the SQRTs of \( e_U \), two AUBs:\( e_{2,U} \) in (\ref{eq:aul}) and \( e_M \) in (\ref{eq:aul}), \( c \), \( e_c \), the BLB \( e_B \), three ALBs:\( e_C \) in (\ref{eq:alb}), \( z_1 \) in (\ref{eq:alb}) and \( b_1 \) in (\ref{eq:alb}), and the simulated MSE \( e_S \).

By observing \( e_S \), we identify five regions: 1) the \textit{a priori} region, 2) the \textit{a priori}-ambiguity transition region, 3) the ambiguity region where the ECRBL is achieved, 4) the ambiguity-asymptotic transition region and 5) the asymptotic region. We define the begin-ambiguity and end-ambiguity thresholds.
marking the ambiguity region by [7]

\[ \rho_{am1} = \rho : e(\rho) = \alpha_{am1} e \]

\[ \rho_{am2} = \rho : e(\rho) = \alpha_{am2} e, \]

We take \( \alpha_{am1} = 2 \) and \( \alpha_{am2} = 0.5 \). From \( e_S \) we have \( \rho_{pr} = 7 \) dB, \( \rho_{am1} = 15 \) dB, \( \rho_{am2} = 28 \) dB and \( \rho_{as} = 33 \) dB.

The MSEs \( e_{1,1,o} \), \( e_{3,1,o} \) (Sec. [V]) and \( e_{MN} \) (Sec. [V-B]) are very tight. However, it converges to 1.75 times the CRLB in the asymptotic region.

The BLB \( e_C \) detects the ambiguity and asymptotic regions much below the true ones; consequently, it does not determine accurately the thresholds \( \rho_{am1} = 5 \) dB, \( \rho_{am2} = 20 \) dB and \( \rho_{as} = 26 \) dB instead of 15, 28 and 33 dB). The ALB \( e_C \) (Sec. [VI-A]) outperforms the CRLB, but is outperformed by the BLB (unlike the baseband case). The ALB \( z_1 \) (Sec. [VI-B]) is very tight, but \( b_1 \) (Sec. [VI-B]) is tighter thanks to the valley-filling function. They both can calculate accurately the asymptotic threshold and to detect roughly the ambiguity region.

Let us compare the MSEs \( e_{S,BB} \) and \( e_S \) achieved by the baseband and passband pulses (Fig. 8). Both pulses approximately achieve the same MSE below the end-ambiguity threshold of the passband pulse \( \rho_{am2} = 28 \) dB) and achieve the ECRLB between the begin-ambiguity and end-ambiguity thresholds. The MSE achieved with the baseband pulse is slightly smaller than that achieved with the passband pulse because with the former the estimates spread in continuous manner along the ACR whereas with the latter they spread around the local maxima. The asymptotic threshold of the baseband pulse (16 dB) is approximately equal to the begin-ambiguity threshold of the passband pulse (15 dB). Above the end-ambiguity threshold, the MSE of the passband pulse rapidly converges to the CRLB while that of the baseband one remains equal to the ECRLB.

To summarize we can say that for a given nonlinear estimation problem with an oscillating ACR, the MSE achieved by the ACR below the end-ambiguity threshold is the same as that achieved by its envelope. Between the begin-ambiguity and end-ambiguity thresholds, the achieved MSE is equal to the ECRLB. Above the latter threshold, the MSE achieved by the ACR converges to the CRLB whereas that achieved by its envelope remains equal to the ECRLB.

VIII. CONCLUSION

We have considered nonlinear estimation of scalar deterministic parameters and investigated the threshold and ambiguity phenomena. The MLE is employed to approximate the statistics of the MLE. The obtained MSEs are highly accurate and follow the true MSE closely. A very tight AUB is proposed as well. An ALB tighter than the CRLB is derived using the second order Taylor series expansion of noise. The principle of binary detection is utilized to compute some ALBs which are very tight.

APPENDIX A

CURVATURES OF THE ACR AND OF ITS ENVELOPE

In this appendix we prove (31). From (11) and (13) we can write the FT of the complex envelope \( e_{R_s}(\theta, \Theta) \) as

\[ F_{e_R_s}(f) = 2 F_{e_c}^+(f + f_c(\Theta)) \]

where \( x^+(f) = \left\{ \begin{array}{ll} x(f) & \text{if } f > 0 \\ 0 & \text{if } f \leq 0 \end{array} \right. \). Form (13) we can write

\[ \hat{R}_{s}(\theta, \Theta) = \Re \left\{ e^{j2\pi(\theta - \Theta)} f_s(\Theta) \left[ j4\pi f_c(\Theta) \hat{e}_{R_s}(\theta, \Theta) + \hat{e}_{R_s}(\theta, \Theta) - 4\pi^2 f_c^2(\Theta) e_{R_s}(\theta, \Theta) \right] \right\} \]

As from (13) \( \Re \{ e_{R_s}(\Theta, \Theta) \} = R_s(\Theta, \Theta) = E_s, (31) \) gives

\[ \hat{R}_{s}(\Theta, \Theta) = \Re \left\{ \hat{e}_{R_s}(\Theta, \Theta) - 4\pi^2 f_c^2(\Theta) E_s + 4\pi f_c(\Theta) \Re \{ j\hat{e}_{R_s}(\Theta, \Theta) \} \right\}. \]
To prove (22) from (21) we must prove that \( \Re\{j\hat{e}_{R_c}(\Theta, \Theta)\} \) is null. Using (19) and the inverse FT, we can write

\[
\hat{e}_{R_c}(\Theta, \Theta) = \int_{-\infty}^{+\infty} j2\pi f \mathcal{F}_{R_c}(f) e^{j2\pi f(\Theta-\Theta)} df
\]

\[
= \int_{-\infty}^{+\infty} j4\pi f \mathcal{F}_{R_c}^+(f + f_c(\Theta)) e^{j2\pi f(\Theta-\Theta)} df
\]

\[
= \int_{-\infty}^{+\infty} j4\pi f \mathcal{F}_{R_c}^+(f) e^{j2\pi f(\Theta-\Theta)} df
\]

\[
= \int_{0}^{+\infty} j4\pi f \mathcal{F}_{R_c}^+(f) e^{j2\pi f(\Theta-\Theta)} df
\]

so \( \hat{e}_{R_c}(\Theta, \Theta) \) becomes

\[
\Re\{j\hat{e}_{R_c}(\Theta, \Theta)\} = -\int_{0}^{+\infty} 4\pi [f - f_c(\Theta)] \Re\{\mathcal{F}_{R_c}(f)\} df = 0.
\]

Hence, (21) is proved.

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