Characterization of Threshold for Single Tone Maximum Likelihood Frequency Estimation

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***Abstract*—This paper presents a simple and direct approach to understanding the threshold effect associated with maximum likelihood estimation of 'he frequency of a single complex tone. Motivation for the approach, stemming from known results in the field of phase locked loops, is given. It is shown both theoretically and experimentally that the onset of threshold can be directly characterized by a single, easily computed parameter, namely the Cramer-Rao bound on the phase estimation error variance.**

I. Introduction

The problem of estimating the frequency, phase, and amplitude of a single sinusoidal tone measured in noise is one of considerable interest. This paper considers the maximum likelihood (ML) approach to the problem, first espoused in [1], and is concerned with characterizing the onset of the so-called *threshold effect* experienced by the ML estimator (MLE) at low signal-to-noise ratios (SNR's). The threshold effect is the name given to that phenomenon caused by the nonlinear nature of the frequency estimation problem: when SNR decreases below a certain critical SNR, the estimation performance (as measured by the estimation error variance) exhibits a rapid deterioration.

There appear to be two ways of gaining an understanding of the threshold effect. The approach of [1] sought to expose the mechanism underlying the threshold effect by an intimate consideration of the properties of the ML algorithm. More specifically, it related the onset of threshold to an increased probability of frequency estimates far removed from the true frequency (or *outliers*) below a certain SNR. As such, it provided an *internal* type description of the phenomenon. This paper considers an alternative approach motivated by well-known results in the phase acquisition and tracking literature. It is well known that a phase locked loop (PLL) (a device used to track the phase and/or frequency of a sinusoid in the presence of noise) also experiences a threshold phenomenon that may be associated with a certain value of phase error variance [2], [3]. In other words, the PLL can tolerate a certain level of phase error before a sudden deterioration in tracking performance is observed. This idea permits recognition of *symptoms* rather than *causes* of threshold. (Another major reason for adopting this approach is the difficulty in applying the internal-style analysis, so successful in the single tone case, to the multiharmonic case, as evidenced in [4].) In this paper, we demonstrate that a similar approach is possible for the ML estimation algorithm.

In Section II, a discrete time formulation of the estimation problem and a detailed description of the approach are given. Section III is concerned with the definition of a certain approximate ML estimator and the calculation of its error variances. This supplies the key to our characterization of threshold. Finally, Section IV demonstrates the rapprochement of the theoretical results of Section III with the experimental results of [1].

Manuscript received December 14, 1991; revised October 28, 1993. This work was supported by the Defense Science and Technology Organization, the Australian Telecommunications and Electronics Research Board, Fujitsu Corporation, the ANU Center for Information Science Research, and the Cooperative Research Center for Robust and Adpative Systems. The associate editor coordinating the review of this paper and approving it for publication was Prof. Don H. Johnson.

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IEEE Log Number 9409784.

II. Problem Formulation

As in [1], we consider the following underlying real signal

$$s(t) = b_0 \cos(\omega_0 t + \theta_0) \tag{II.1}$$

and its quadrature counterpart

$$\check{s}(t) = b_0 \sin(\omega_0 t + \theta_0). \tag{II.2}$$

The parameters b_0, ω_0, and θ_0 are assumed constant but unknown. Suppose that a set of N discrete noisy measurements are taken at intervals of T s beginning at time t_0 s

$$X_n = s(t_0 + nT) + w(t_0 + nT) \tag{II.3a}$$

and

$$Y_n = \check{s}(t_0 + nT) + \check{w}(t_0 + nT) \tag{II.3b}$$

where $0 \le n \le N-1$. The sequences w and $\check{w}$ define zero-mean, white, and independent Gaussian noise processes, each of variance σ^2.

A. ML Estimation of ω_0 and θ_0

The ML estimates of the frequency ω_0 and the phase θ_0 based on the measurements $X_n + jY_n, n = 0, 1, \cdots, N-1$ are given by (whether b_0 is known or not—see [1])

$$\hat{\omega} \triangleq \arg\max |A(\omega)| \tag{II.4a}$$

and

$$\hat{\theta} \triangleq \angle A(\hat{\omega}) \tag{II.4b}$$

where

$$A(\omega) \triangleq \frac{1}{N}\sum_{n=0}^{N-1}(X_n + jY_n)\exp(-nj\omega T). \tag{II.5}$$

(Note that $A(\omega)$ is simply the discrete fourier transform (DFT) of the measurement data.) For simplicity's sake (and without significant loss of generality), b_0 is assumed known, and t_0 is assumed zero.

Associated with the ML estimates are the Cramer-Rao (CR) bounds. These are lower bounds on the ML estimation error variances (and in general on the estimation error variances of *any* unbiased estimator applied to the problem). For fixed SNR and sufficiently large N or, equivalently, fixed N and sufficiently high SNR, the actual ML estimation error variances are given approximately by the CR bounds. The region of values of SNR (for a given N) for which this holds is referred to as the *linear region*. The CR bounds for the case where both frequency and phase are unknown are given below. (These expressions are valid only for large N; see [1].)

$$\mathrm{var}(\hat{\omega}) \geq \frac{12\sigma^2}{T^2 b_0^2 N^3} \tag{II.6a}$$

$$\mathrm{var}(\hat{\theta}) \geq \frac{4\sigma^2}{b_0^2 N}. \tag{II.6b}$$

In general, $|A(\omega)|$ is a multimodal function of ω, with the result that at low values of SNR, its global maximum, with high probability, lies distant from the true frequency ω_0. Frequency estimates corresponding to such maxima are termed *outliers* and are the cause of the threshold effect, in as much as the large size of the resultant estimation error coupled with the relatively high probability of their occurrence at low SNR's leads to a steep increase in the error variance. A theoretical expression for the probability of an outlier may be derived, given prior knowledge of the statistics of the measurement noise. Performance curves may then be calculated that predict the existence of a threshold. This approach is taken in [1].

The approach of this paper is fundamentally different in that no attention is paid to the internal cause of the threshold effect (i.e., outliers). Instead, a characterization of threshold is sought in terms of the behavior of the frequency and phase estimation performance curves (i.e., the plot of mean square estimation errors versus SNR). Consider the case of frequency for which performance curves are given in Fig. 1 for various values of N. Suppose that for a fixed N, the mean square frequency estimation error is approximated by the corresponding CR bound over all values of SNR. Then define the threshold point to be that value of SNR for which the magnitude of the approximation error becomes large, as would happen in the vicinity of the familiar "knee" of the performance curve. We seek a means of knowing *when* the said approximation is poor. To achieve this, we define an estimator (albeit physically nonimplementable) that generates estimates closely approximating the ML frequency and phase estimates, provided that a certain key parameter is sufficiently small and whose error variances are *identically* (i.e., for *all* values of SNR) equal to the CR bounds. We then argue that the *variances* of the approximate estimator (the CR bounds) approximate the *variances* of the ML estimator, provided that the *mean square value* of the key parameter is small. This route is taken in the next section.

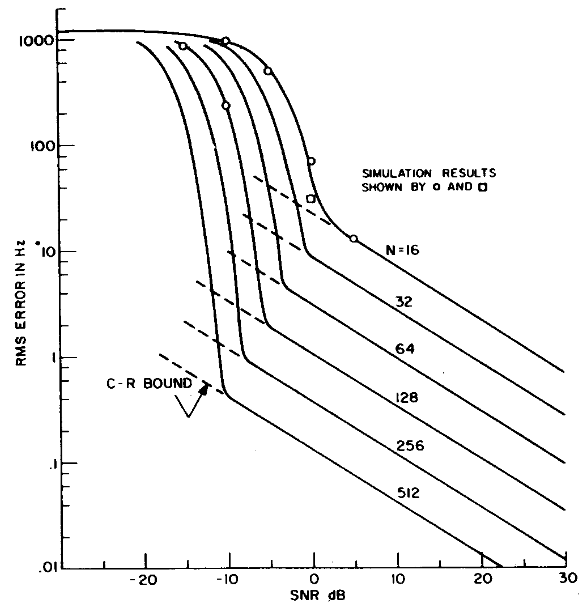

Fig. 1. ML frequency estimation performance [1].

III. Approximate ML Estimator

In this section, we derive an approximate ML estimator whose error variances are identically the CR bounds of (II.6a)–(II.6b) for all values of SNR. The calculations involved are lengthy, and, for reasons of space and continuity, are given in outline only in the Appendix. We shall be content here with a summary of the approximation procedure and its assumptions.

The first step in the procedure is to express $A(\omega)$ as a function of δ (with slight abuse of notation, $A(\delta)$) where

$$\delta \triangleq (\omega_0 - \omega)\frac{T}{2} \tag{III.1}$$

is a normalized frequency error. From this, we note that if $\hat{\delta}$ (i.e., the value of δ corresponding to the ML estimate $\hat{\omega}$ of ω_0) maximizes $|A(\delta)|$, then $4/T^2 E(\hat{\delta})^2$ is the frequency estimation error variance (where E denotes mathematical expectation). The second step in the procedure leads to an approximation δ^* for $\hat{\delta}$ by approximating $|A(\delta)|^2$ with a quadratic polynomial obtained by truncating a series expansion (about the point $\delta = 0$), to give

$$|A(\delta)|^2 \approx \alpha_0 + \alpha_1\delta + \alpha_2\delta^2 \tag{III.2}$$

where α_1 and α_2 are defined in (A.5a)–(A.5b).[1] (It is more convenient to work with $|A(\cdot)|^2$ than $|A(\cdot)|$. Clearly, their maxima occur at the same locations.) The value of δ maximizing the RHS of (III.2) (and, hence, approximately the value

[1] It turns out that α_0 is irrelevant to calculating δ^*. It *is* relevant to the estimation of b_0 if the latter is unknown.

of $\hat{\delta}$) is given by

$$\delta^* \triangleq \frac{-\alpha_1}{2\alpha_2}. \tag{III.3}$$

Remarks:

- Since ω_0 is unknown, it is not possible to implement an estimator that generates δ^*, given the measurement data (II.3a)–(II.3b).
- It transpires that the quadratic approximation defined in (III.2) will have small error, provided $N\delta$ is sufficiently close to zero (see the Appendix).
- The coefficients α_0, α_1, and α_2 are random variables as a result of the dependence of $A(\delta)$ on the measurement noise (see (II.5)).

Since the RHS of (III.2) constitutes a good approximation to $|A(\delta)|^2$ if $N\delta$ is small, we conclude that δ^* will be a good approximation to $\hat{\delta}$ if $N\delta^*$ is small. Similarly, we argue that $E(\delta^*)^2$ will be a good approximation to $E(\hat{\delta})^2$ if $E(N\delta^*)^2$ is small. The quantity $4/T^2 E(\delta^*)^2$ is therefore an approximation (the validity of which is governed by the magnitude of $E(N\delta^*)^2$) to the ML frequency estimation error variance. In line with the discussion at the end of Section II, we need to show that this approximation is equal to the CR bound given by (II.6a). To this end, the coefficients α_1 and α_2 are approximated in a mean square sense to give

$$\alpha_1 \approx \hat{\alpha}_1 \triangleq \frac{2b_0}{N} \sum_{n=0}^{N-1} (N-1-2n) u(nT) \sin(\phi_n - \theta_0) \tag{III.4a}$$

and

$$\alpha_2 \approx \hat{\alpha}_2 \triangleq \frac{-b_0^2 N^2}{3}. \tag{III.4b}$$

The error so incurred may be made arbitrarily small by choosing N sufficiently large (see (A.6)). The expressions $u(nT)$ and ϕ_n define independent, white random sequences with samples that are respectively Rayleigh distributed and uniformly distributed (on $[0, 2\pi]$), such that $u(nT)\sin(\phi_n - \theta_0)$ is a zero-mean, white, Gaussian noise sequence of variance σ^2. From (III.3), (III.4a), and (III.4b), there holds

$$\delta^* = \frac{3}{b_0 N^3} \sum_{n=0}^{N-1} (N-1-2n) u(nT) \sin(\phi_n - \theta_0). \tag{III.5}$$

From this, it follows that

$$E(\delta^*)^2 = \frac{9}{b_0^2 N^6} \sigma^2 \sum_{n=0}^{N-1} (N-1-2n)^2 \tag{III.6}$$

whence, for large N, some algebra reveals that

$$E(\delta^*)^2 = \frac{3\sigma^2}{b_0^2 N^3} \tag{III.7}$$

so that

$$E(\hat{\omega} - \omega_0)^2 \approx \frac{4}{T^2} E(\delta^*)^2 = \frac{12\sigma^2}{T^2 b_0^2 N^3} \tag{III.8}$$

which agrees with the CR bound for frequency estimation given in (II.6a). The corresponding expression for the phase error variance may be obtained by setting (after (II.4b))

$$\theta^* \triangleq \angle A(\delta^*). \tag{III.9}$$

Using the expression for $A(\delta)$ in (A.1), a lengthy calculation results in the following expression for the phase error

$$\theta^* - \theta_0 \approx (N-1)\delta^* + \frac{1}{b_0 N} \sum_{n=0}^{N-1} u(nT) \sin(\phi_n - \theta_0) \tag{III.10}$$

from which (and after substitution for δ^* from (III.5)) the following expression (again valid only for large N) identical to the CR bound (II.6b) may be calculated for the phase error variance

$$E(\hat{\theta} - \theta_0)^2 \approx E(\theta^* - \theta_0)^2 = \frac{4\sigma^2}{b_0^2 N}. \tag{III.11}$$

Note that (III.10)) is obtained, as in the frequency case, by the mean square approximation of coefficients appearing in truncated series expansions.

A. Threshold Indicator Quantity

Thus far, we have defined a physically nonimplementable estimator (nonimplementable since it requires knowledge of ω_0), whose error variances (given large enough N) are identical to the CR bounds *for all SNR*. We know under what circumstance the estimates produced by this approximate estimator are close to the ML estimates, namely, that $N\delta^*$ is sufficiently small. From this, we claim that the circumstance under which the variances of the approximate estimator (i.e., the CR bounds) are close to those of the ML estimator is simply that $E(N\delta^*)^2$ is small. Hence, the quantity $E(N\delta^*)^2$ acts as an *indicator* of threshold in the sense that when threshold occurs (i.e., when the CR bounds are no longer close to the ML variances), then $E(N\delta^*)^2$ is no longer small (i.e., it exceeds a value determined by the particular approximation error for which threshold is defined). From (III.7), the indicator quantity is calculated to be

$$E(N\delta^*)^2 = \frac{3\sigma^2}{b_0^2 N} \tag{III.12}$$

which is proportional to the CR bound on the phase error variance (II.6b). In the next section, experimental evidence is presented in support of this conclusion.

IV. Agreement with Simulation Data

The theoretical argument of the last section has answered the following question: under what condition are the CR bounds good approximations to the actual ML estimation error variances? The conclusion was that the approximations are good, provided the CR bound on the phase error variance is sufficiently small. In other words, a certain level of phase error is tolerable before a dramatic deterioration in frequency estimation performance (the threshold effect) is exhibited by the ML algorithm. We now present supporting experimental evidence.

TABLE I
SNR AND FREQUENCY ERROR VARIANCE AT THRESHOLD [1]

N	SNR (dB)	$E(\hat{\omega}-\omega_0)^2$ (Hz)^2
512	−11	$(0.4)^2$
256	−8.25	$(0.9)^2$
128	−5.5	2^2
64	−2.75	5^2
32	0.0	10^2

Reproduced in Fig. 1 are the experimental performance curves plus CR bound presented in [1] for ML estimation of the frequency of a single complex tone for various values of N. The SNR (in decibels) for this figure is defined to be SNR $= 10\log(b_0^2/2\sigma^2)$. The threshold point for each value of N is defined to be the "knee" of the associated performance curve. Obtained from Fig. 1 and collated in Table I are approximate values of SNR and mean square frequency error at threshold for each value of N. The following conclusions concerning the experimental data are possible:

1) The curves show that threshold occurs approximately at the same fixed value of phase error variance and is hence associated with the failure of a certain approximation.

Proof: Mean square (m.s.) phase error $= E(\tilde{\theta})^2 = 4\sigma^2/b_0^2N$. Doubling N and halving the SNR leaves the m.s. phase error unchanged. Doubling N ensures that threshold ensues at half the SNR. This is borne out by Table I. Therefore, threshold occurs at roughly the same value of m.s. phase error for different values of N. The CR bounds are close to the actual variances provided the m.s. value of $(N\delta^*)$ is small. Recall that

$$E(N\delta^*)^2 = \frac{3\sigma^2}{b_0^2N} = \frac{3}{4} \times m.s.\,phase\,error. \tag{IV.1}$$

Hence, threshold is associated with a roughly fixed m.s. value of $(N\delta^*)$ for different values of N. At values of SNR lower than that associated with the threshold point (for a fixed value of N), the m.s value of $(N\delta^*)$ is greater than that at threshold. From Fig. 1, we see that for such values of SNR, the CR bound no longer agrees with the actual frequency error variance.

2) The m.s. phase error associated with threshold is roughly 0.0625 rad^2. To see this, consider $N = 32$. Then, threshold occurs at roughly 0 dB. Therefore, the m.s. phase error $= 2 \times \frac{1}{32} = 0.0625$ rad^2.

3) The m.s. frequency error is consistent with that predicted by the approximate formula of (III.8).

Proof: From (III.8) and (III.11), there holds

$$m.s.\,frequency\,error = \frac{3}{T^2N^2} \times m.s.\,phase\,error. \tag{IV.2}$$

For $N = 512$, the rms frequency error is given by Table I to be 2.5 rad $\cdot$ s^{-1}. ($T = \frac{1}{4000}$ s.) From (IV.2) and point 2, the formula gives, at threshold

$$rms\,frequency\,error = \frac{4000}{4 \times 512} \approx 2\,rad \cdot s^{-1}. \tag{IV.3}$$

V. CONCLUSIONS

This paper has considered a novel approach to the understanding of the threshold effect associated with ML frequency estimation. It has demonstrated that threshold is characterized by the phase estimation error variance attaining a critical level, beyond which a certain approximate method of calculating the ML estimation performance is no longer accurate. The approach offers alternative insight into the threshold phenomenon to that provided by the outlier theory of [1] and appears closely related to known results concerning the threshold effect for PLL's. For example, in [3] it is stated that for a PLL applied to a sinusoid with a particular type of frequency variation, thresholding behavior is observed upon the phase error variance reaching 0.25 rad^2.

As a means of characterizing the threshold effect for a more general estimation problem (namely, the ML estimation of the fundamental frequency and harmonic phases of a multiharmonic signal), the approach has proved very fruitful and is the subject of ongoing research.

APPENDIX
SUMMARY OF CALCULATIONS

We are forced by limited space to be as brief as possible. Recall the definition of δ in (III.1). Then, there holds from (II.3a), (II.3b), and (II.5)

$$\begin{aligned} A(\omega) &= \frac{1}{N}\sum_{n=0}^{N-1}[s(nT) + j\check{s}(nT)]\exp(-nj\omega T) \\ &\quad + \frac{1}{N}\sum_{n=0}^{N-1}[w(nT) + j\check{w}(nT)]\exp(-nj\omega T) \\ &= b_0\exp[j(N-1)\delta + j\theta_0]\frac{\sin N\delta}{N\sin\delta} \\ &\quad + \frac{1}{N}\sum_{n=0}^{N-1}[w(nT) + j\check{w}(nT)] \\ &\quad \cdot\exp(-nj\omega_0T)\exp(2nj\delta) \\ &= A_0(\delta) + N_0(\delta) \end{aligned} \tag{A.1}$$

where $A_0(\delta)$ arises from the deterministic part of the measured signal and $N_0(\delta)$ from the stochastic part. Notice that $A(\delta)$ is simply the well-known expression for the DFT of a sinusoid of amplitude b_0, frequency ω_0, and phase θ_0. The expression for $N(\delta)$ can be further simplified via the standard result [5]

$$u(nT)\exp(j\phi_n) = [w(nT) + j\check{w}(nT)]\exp(-nj\omega_0T) \tag{A.2}$$

where $u(\cdot)$ is an independent random sequence with samples that are Rayleigh distributed, and ϕ_n is an independent random process with samples that are uniformly distributed on $[0, 2\pi]$. This follows directly from the easily checked fact that the real and imaginary parts of the RHS of (A.2) are independent, white, zero mean, Gaussian random sequences of identical variance σ^2.

From (A.1), it follows that

$$|A(\delta)|^2 = |A_0(\delta)|^2 + 2\text{Re}[A_0(\delta)\overline{N}_0(\delta)] + |N_0(\delta)|^2 \tag{A.3}$$

where the overbar $\overline{(\cdot)}$ denotes complex conjugation. Using the Maclaurin series for sine and cosine and the expansion

$$\frac{\sin(N\delta)}{N\sin\delta} = 1 - \left(\frac{N^2-1}{3!}\right)\delta^2 + \left(\frac{N^4}{5!} - \frac{N^2}{36} - \frac{1}{5!} + \frac{1}{36}\right)\delta^4 + \cdots \tag{A.4}$$

each summand of (A.3) may, after tedious calculation, be expressed to second order in δ. The key step as far as quality of approximation is concerned is the truncation of the RHS of (A.4) needed to give the required second-order approximations to $|A_0(\delta)|^2$ and $2\mathrm{Re}[A_0(\delta)\overline{N}_0(\delta)]$. The resulting error in approximation will be small if $N\delta$ is small. Combination of these second-order approximations to the summands leads to the expression in (III.2), with

$$\begin{aligned}\alpha_1 = &\frac{2b_0}{N}\sum_{n=0}^{N-1}(N-1-2n)u(nT)\sin(\phi_n-\theta_0)\\ &-\frac{4}{N^2}\sum_{0\le k<l\le N-1} u(kT)u(lT)\\ &\cdot\sin(\phi_k-\phi_l)(k-l)\end{aligned} \tag{A.5a}$$

and

$$\begin{aligned}\alpha_2 = &-\frac{b_0^2N^2}{3} - \frac{2b_0(N^2-1)}{3N}\sum_{n=0}^{N-1}u(nT)\cos(\phi_n-\theta_0)\\ &-\frac{b_0}{N}\sum_{n=0}^{N-1}u(nT)\cos(\phi_n-\theta_0)(N-1-2n)^2\\ &-\frac{2}{N^2}\sum_{0\le k<l\le N-1}u(kT)u(lT)\\ &\cdot\cos(\phi_k-\phi_l)(k-l)^2.\end{aligned} \tag{A.5b}$$

The above expressions are too unwieldy for continued analysis. Considerable simplification is afforded via a mean square approximation procedure that neglects those terms on the RHS of each of the expressions in (A.5a)–(A.5b), whose m.s. value is much less than the m.s. value of the remainder. This leaves only the first term on the right of each of the two equations, and the resulting approximations $\hat{\alpha}_i, i = 1, 2$ are given in (III.4a)–(III.4b). This can be done if N is sufficiently large. In fact, it is possible to show from the previous definitions of $u(nT)$ and ϕ_n that

$$\lim_{N\to\infty}\frac{E(\alpha_i-\hat{\alpha}_i)^2}{E(\hat{\alpha}_i)^2} = 0, \qquad i = 1, 2. \tag{A.6}$$

The proof of (A.6) will not be given.

Starting with (A.1), a similar strategy of series truncation followed by mean square approximation leads to the expression for the phase error given in (III.10). Again, truncation of the series (A.4) is the key step, with the result that the approximation in (III.10) is good, provided $N\delta$ is small. The steps in the calculation are not presented here.

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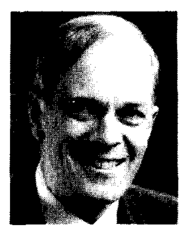

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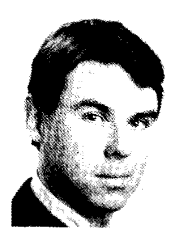

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