Threshold Effects in Multiharmonic Maximum Likelihood Frequency Estimation [1]

Robert C. Williamson [2] Ben James[3]
Brian D. O. Anderson [2] Peter J. Kootsookos[4]

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[2]Department of Systems Engineering, Research School of Physical Sciences and Engineering, Australian National University, Canberra, ACT 0200, Australia

[3]Industrial Systems Group, Department of Electrical and Electronic Engineering, Imperial College of Science, Technology and Medicine, Exhibition Road, London SW7 2BT, United Kingdom

[4]Cooperative Research Centre for Robust and Adaptive Systems, 89 Labs, DSTO, Salisbury, SA 5108, Australia

Abstract

This paper derives a general expression for the mean square error in estimating the fundamental frequency of a multiharmonic signal from a finite sequence of noisy measurements. The distinguishing feature of this expression is that it is applicable at values of signal-to-noise-ratio (SNR) *within the threshold region*, in contrast to earlier expressions (the Cramer Rao bounds) that are valid only at high SNR's. Theoretical performance curves are thereby calculated (mean square error versus SNR) that establish the existence of a threshold effect. Until now, the existence of a threshold effect was demonstrable only by simulation.

Examples are given comparing various multiharmonic estimation scenarios to the single tone case under comparable conditions. The theoretical performance curves in these examples are corroborated by Monte-Carlo simulation.

1 Introduction

The problem of estimating the frequency of a sine wave in noise is an old one, and many different solutions have been presented. The natural generalization of this problem whereby a harmonic signal is corrupted by noise and its fundamental frequency is estimated has not been considered to such an extent. Recently the maximum likelihood estimator (MLE) for this problem was derived in [1] and its performance in the high signal-to-noise-ratio (SNR) region analysed. Like the problem of estimating the frequency of a single tone, this *multiharmonic (MH) estimation problem* (as we will refer to it) exhibits a threshold effect. This manifests itself in a sudden degradation of performance as the SNR is lowered. We shall see that above this threshold point, the MH MLE attains a performance equal to the Cramer-Rao (CR) bound. It is the purpose of this paper to ascertain the performance at and below the threshold point.

Further motivation for a detailed analysis of the behaviour below the threshold point (and not just a determination of the point) comes from the observed successful application of a *tracking* estimator for sinusoidal signals based on Hidden Markov Models (see [2]). These estimators have been shown to work in remarkably low signal to noise ratio conditions, and in fact the MLE component of them is operating well below threshold. We aim eventually to extend the ML–HMM tandem estimator structure to the MH case. In order to be able to mathematically analyse the performance of the hybrid tracking estimator, it is necessary to have a good understanding of the behaviour of the MLE below threshold, in addition to the location of the threshold point.

One of the new features seen in operating the MH MLE below threshold is the phenomenon of rational harmonic locking. The effect has been observed in alternative MH estimators based on Coupled Phase-Locked Loops (see [3]). We provide a complete analysis of this effect for the MH MLE. We will also consider the effect of assuming there are more harmonics in the signal than there actually are.

An analysis of the threshold effect in single tone maximum likelihood frequency estimation has been carried out by Rife and Boorstyn in [4]. Their key idea was

to recognise that threshold is associated with an increasingly large probability of certain well-defined "outlier" events as the SNR is lowered. These outlier events correspond to the MLE procedure yielding estimates well away from, as opposed to in the vicinity of, the true frequency. The location of the threshold point may be determined theoretically (via performance curves) upon calculation of the outlier probabilities.

The purpose of this paper is to extend the analysis of Rife and Boorstyn to the multiharmonic case (with m harmonics present). The analysis follows the broad direction of Rife and Boorstyn, but is considerably more complex. The main reason for the extra difficulty is the possibility of rational harmonic locking (to be later precisely defined). The main result of the paper is contained in (58), a general expression for the mean square error, *applicable at SNR's within the threshold region*, in estimating the fundamental frequency of a multiharmonic signal from a finite number of measurements. The various parameters in (58) are defined in the body of the paper; thus (58) represents a complete determination of the performance of the MH-MLE. Some example calculations and a comparison with simulation results are presented in Section 5.

In the next section, by way of an introduction to outlier analysis of the multiharmonic MLE, the corresponding single tone analysis of [4] is briefly described.

2 Rife and Boorstyn outlier analysis – single tone MLE threshold

We consider the following underlying real signal

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

along with its *quadrature* counterpart

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

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 seconds beginning at time $t = 0$:

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

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

(where $0 \leq n \leq N-1$). The sequence w defines a zero-mean white, gaussian noise process of variance σ^2. The sequence $\check{w}$ is suitably defined in terms of the Hilbert Transform of w such that $\check{w}$ is also a zero-mean white, gaussian noise process of variance σ^2. As shown in [5] (see the discussion after lemma 1 in [5]) if the analytic signal $Z_n = S_n + jH(S_n)$ ($H(\cdot)$ the Hilbert transform operator) is downsampled by a factor of 2, Z_n will be white as long as S_n is white. Such downsampling is permissible since one only needs to sample a complex analytic signal of single sided bandwidth W at a rate W (rather than $2W$) in order to avoid aliasing. This point is discussed in more detail in [6]. We will ignore practical difficulties in generating the analytic signal, as they only arise when one has a single fixed block of data: if there is a continuous data stream arriving, then formation of the analytic signal is straightforward. Thus we can now assume we are given the *complex* valued time series $Z_n = X_n + jY_n$.

Given N noisy measurements of the complex tone $X_n + jY_n$, the ML estimates of the frequency ω_0 (assuming unknown phase) is given by

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

where

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

Note that $A(\omega)$ is just the discrete Fourier transform of the N samples of the complex tone. The formula for the ML frequency estimate holds whether the amplitude b_0 is known or not.

A variety of means may be employed to determine the ML estimate of the fre-

quency $\hat{\omega}$. In principle, it may be calculated to any desired degree of accuracy; the only constraints being those of a practical nature: computation time, wordlength etc. Rife and Boorstyn describe how such an algorithm is composed of two stages: a *coarse search* followed by a *fine search*. The coarse search is generally performed by passing the measurement data through an FFT (fast Fourier transform) routine. The coarse frequency estimate is then taken to be the frequency corresponding to the maximum of the magnitude of the output data. The fine search then uses the coarse frequency estimate as its initial condition.

The function $|A(\omega)|$ normally has a number of local maxima in addition to the global maximum corresponding to the ML frequency estimate $\hat{\omega}$. For high SNR, this global maximum occurs very near to the true frequency ω_0. However, as the measurement noise intensity increases (i.e., as the SNR decreases) the outlying maxima may increase in amplitude, with the result that the probability that the global maximum lies a "long way" from the true frequency increases rapidly. Such large (though rare) errors in the frequency estimate cause the frequency error variance to be much greater than the CR bound, in the threshold region.

The analysis of Rife and Boorstyn presented in [4] sought a means of computing the frequency error variance below threshold. This essentially reduces to the problem of determining the probability of an outlier; that is, a frequency estimate far removed from the true frequency. It is at the stage of the coarse search that outliers occur, since the fine search serves merely to provide a more accurate determination of the ML estimate in the immediate neighbourhood of the coarse frequency estimate. In other words, a grossly inaccurate frequency estimate will only happen when the coarse search fails. Hence consideration of a coarse search algorithm alone is sufficient for the purpose of computing the probability of an outlier and subsequently for computing the below threshold performance.

In the outlier analysis of Rife and Boorstyn, the coarse search is performed by evaluating $|A(\omega)|$ at the set of frequencies

$$\hat{\omega}_k = \frac{2\pi k}{NT} \; ; \; 0 \leq k \leq N-1 \tag{6}$$

with the assumption[1] that $\omega_0 = \pi/T$ (i.e., the true frequency is half the sampling frequency $\omega_s = 2\pi/T$). This is easily implemented via an FFT routine; in that case, N is always chosen to be a power of 2.

Given the assumption concerning the true frequency, the greatest element of the set $\{|A(\hat{\omega}_k)| : 0 \leq k \leq N-1\}$ should be $|A(\hat{\omega}_{N/2})|$. However, the presence of noise will ensure that sometimes $|A(\hat{\omega}_l)|$, for some $l \neq N/2$, will be the greatest. In this case, the coarse frequency estimate, $\hat{\omega}_l$, is called an outlier.

Hence we may identify two mutually exclusive events, one being the event that, given the measurement sequence, an outlier occurs in the coarse search, and the other being the event that no outlier occurs. The frequency error variance may then be expressed

$$\mathrm{E}(\hat{\omega} - \omega_0)^2 = (1-q)\mathrm{E}[(\hat{\omega} - \omega_0)^2 | \text{no outlier}] + q\mathrm{E}[(\hat{\omega} - \omega_0)^2 | \text{outlier}] \tag{7}$$

where $\hat{\omega}$ is the result of a fine search performed subsequent to the coarse search described above (and initialised by the coarse frequency estimate ω_k), and q is the probability of the occurrence of an outlier. For the case where no outlier occurs, $\mathrm{E}[(\hat{\omega} - \omega_0)^2 | \text{no outlier}]$ is approximated by the CR bound given on the frequency estimation error variance for the single tone problem given (from [4]) by

$$\mathrm{E}[(\hat{\omega} - \omega_0)^2 | \text{no outlier}] = \frac{12\sigma^2}{N(N^2-1)T^2 b_0^2} \ . \tag{8}$$

Where an outlier occurs, $\hat{\omega}$ is assumed to be uniformly distributed on the interval $[0, \omega_s]$, so that

$$\mathrm{E}[(\hat{\omega} - \omega_0)^2 | \text{outlier}] = \frac{\pi^2}{3T^2} \ . \tag{9}$$

Rife and Boorstyn derive analytical expressions for q by observing that $|A(\hat{\omega}_k)|$,

[1] This apparently restrictive assumption is made because the MLE is unbiased (i.e., $\mathrm{E}(\hat{\omega} - \omega_0) = 0$) only if $\omega_0 = \omega_s/2$ (see [4]). Large bias errors are introduced into the frequency estimate if ω_0 is close to 0 or ω_s. The outlier analysis is concerned only with errors caused by outliers, not bias, hence the choice of ω_0. Of course in practice, it is not possible to choose the sampling frequency ω_s so that $\omega_0 = \omega_s/2$ (if we could there would be no need to estimate ω_0!) Provided the sampling frequency is chosen so that bias errors are small, the analysis with $\omega_0 = \omega_s/2$ is strongly indicative of the resulting performance, as demonstrated by simulation.

for $0 \leq k \leq N-1$, defines a set of independent random variables that are Rayleigh distributed for $k \neq N/2$ and Rician otherwise. They were able to calculate theoretical performance curves that agree well with simulation results and clearly exhibit the existence of a threshold effect. In the next section we extend this basic approach to the multiharmonic case.

3 Outlier analysis of multiharmonic MLE threshold

This section presents new results relating to the multiharmonic MLE. The major result is the derivation of an approximate expression for the frequency estimation error (similar in form to (7)) that is applicable at SNR's above and below the threshold point. Also, the novel notion of *rational harmonic outliers* is introduced and explored in depth. These are entities unique to the multiharmonic case which greatly complicate the internal analysis.

To make the analysis tractable, we occasionally approximate or give bounds on the quantity of interest. The reasoning behind the approximations is given were necessary. The final justification for the approximations comes from the simulation results in Section 5 which corroborate the theoretically derived results.

We consider the following underlying real signal comprising a known number of harmonics, m

$$s(t) = \sum_{k=1}^{m} b_k \cos\left(k\omega_0 t + \theta_k\right) \tag{10}$$

with Hilbert Transform

$$\check{s}(t) = \sum_{k=1}^{m} b_k \sin\left(k\omega_0 t + \theta_k\right) . \tag{11}$$

The parameters $b_1, \ldots, b_m, \omega_0, \theta_1, \ldots, \theta_m$, are assumed constant but unknown. Suppose that a set of N discrete noisy measurements are taken at intervals of T seconds

beginning at time zero:

$$X_n = s(t_0 + nT) + w(t_0 + nT) \tag{12a}$$

$$Y_n = \check{s}(t_0 + nT) + \check{w}(t_0 + nT) \tag{12b}$$

(where $0 \leq n \leq N-1$). The sequence w defines a zero-mean white, gaussian noise process of variance σ^2. By downsampling (via the same argument as presented in section 2) the sequence $\check{w}$ is suitably defined in terms of the Hilbert Transform of w such that $w + j\check{w}$ is a complex zero-mean white, gaussian noise process of variance σ^2.

The ML estimate[2] , $\hat{\omega}$ of ω_0 is given, for the case where the amplitudes and phases are unknown, by

$$\hat{\omega} = \arg \max_{\omega} L(\omega) \tag{13}$$

where

$$L(\omega) \triangleq \sum_{l=1}^{m} |A(l\omega)|^2 \ . \tag{14}$$

Again, a numerical procedure is required to generate the ML estimates, given the measurement data. As before, it takes the form of a coarse search, followed by a fine search. Just as in the single tone case, the quantity to be maximised, $L(\omega)$, has a number of local maxima in addition to the global maximum corresponding to the ML frequency estimate, $\hat{\omega}$. Some of these local maxima are associated with the presence of harmonics in the measured signal. Of course, there is no analogue of this class of maxima in the single tone case; the presence of harmonics is the cause of much of the increase in difficulty associated with analyzing the threshold effect via outlier theory for the multiharmonic problem over that for the single tone problem.

There are, in fact, two classes of outliers in the multiharmonic case. The first is familiar to us from the single tone problem and comprises those outliers due solely to the measurement noise. The second is unique to the multiharmonic case, quite distinct in character from the first and potentially less damaging in nature,

[2] Equation (13) actually yields an *approximate* ML multiharmonic frequency estimator. However, asymptotically (as N increases) it is equivalent to the true ML estimator.

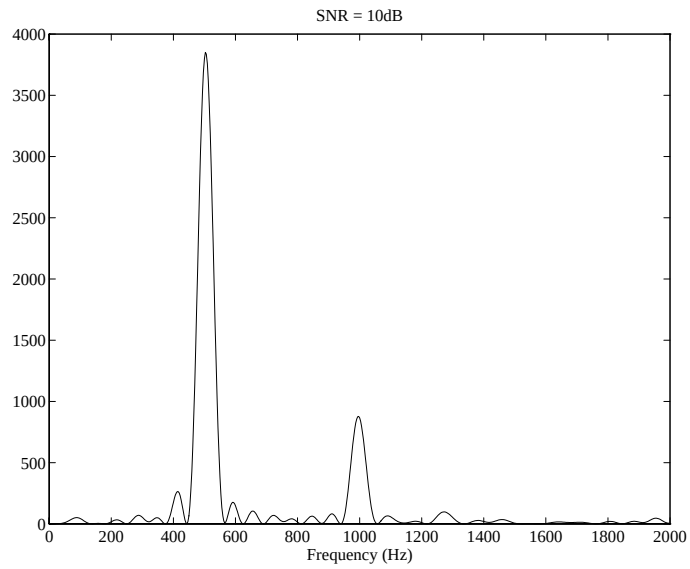

Figure 1: Typical $|A(\omega)|^2$ for SNR = 10dB; $\omega_0 \approx 500$

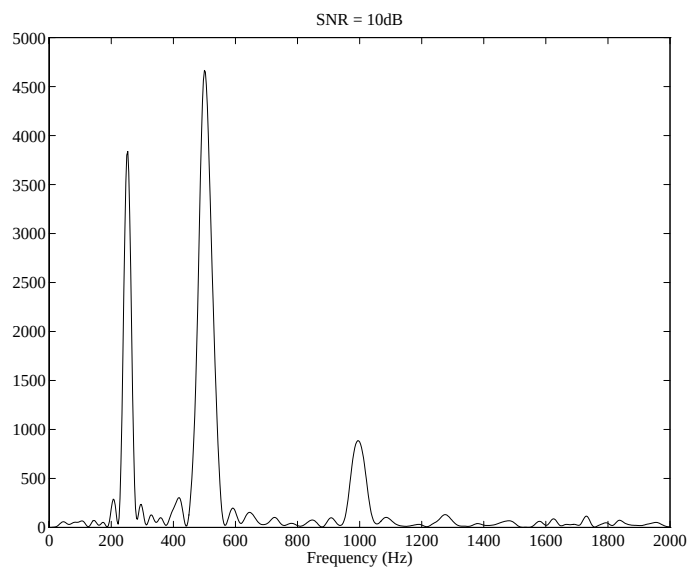

Figure 2: $L(\omega)$ corresponding to Figure 1

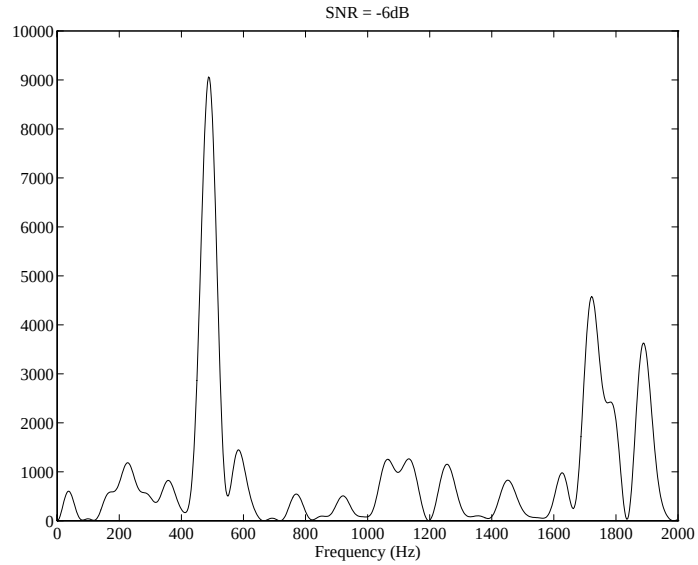

Figure 3: Typical $|A(\omega)|^2$ for SNR = -6dB (same signal as Figure 1)

for reasons that will be clear shortly. It comprises those outliers corresponding to global maxima of $L(\omega)$ occurring close to a frequency that is a *rational harmonic* of the fundamental frequency, ω_0. (We say that ω is a rational harmonic of ω_0 if $i\omega = j\omega_0$, where i and j are mutually prime positive integers. In other words, the ith harmonic of ω occurs at the same frequency as the jth harmonic of ω_0. If the multiharmonic signal with fundamental frequency ω_0 has a significant fraction of its energy in the jth harmonic, then incorrect identification of ω as the fundamental frequency is a distinct possibility.)

This type of outlier arises in a fashion exemplified by Figures 1–4. Figure 1 is a plot of the squared magnitude, $|A(\omega)|^2$, of the DFT (discrete Fourier transform) of a typical observed signal with two harmonics with fundamental frequency $\omega_0 = 500$Hz, for an SNR of 10dB. Figure 2 shows a graph of the corresponding likelihood function. The SNR is sufficiently high to ensure that no outlier of any kind occurs. Figure 3 is for the same deterministic signal as Figure 1 except that the effective SNR is now lowered to -6dB. In fact, it is sufficiently low that $L(\omega) = |A(\omega)|^2 + |A(2\omega)|^2$ attains its global maximum at $\omega \approx \omega_0/2$, as shown in Figure 4.

While clearly undesirable from the point of view of any practical multiharmonic

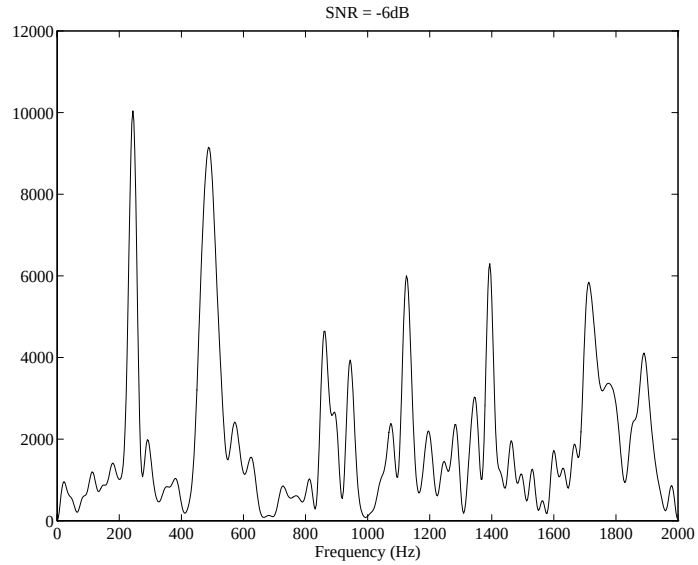

Figure 4: $L(\omega)$ corresponding to Figure 3

MLE, the outliers local to a rational harmonic frequency nevertheless have a clear relationship to the true frequency (i.e., via some rational multiplier). It would thus seem feasible to include an additional level of algorithm capable of recognizing rational harmonic outliers when they occur along with determining their relationship to the true frequency. In the absence of such an algorithm, the rational harmonic outliers are just as detrimental in their effect upon the performance of a practical MLE as those due to the measurement noise alone. However, we stress that the potential exists for their effect to be removed, and consequently that measures of performance of the MLE that include the detrimental effect of rational harmonic outliers are, in a significant sense, inappropriate.

As we discussed in Section 2, outliers are associated with the coarse search stage of the maximization procedure. In the analysis to follow, a particular coarse search algorithm that computes $L(\omega)$ at a finite set of frequencies (to be termed "bin" frequencies, after the FFT nomenclature) will be considered. As in the single tone case, a finite number of noise outliers then need only be considered, as opposed to a continuum of values. The number of rational harmonic outliers is also finite.

For parity with the single tone treatment, we assume that the coarse frequency estimate takes one of N values. To ensure this, mN measurements must be taken.

The likelihood function, $L(\omega)$, is computed at the bin frequencies

$$\hat{\omega}_k = \frac{k2\pi}{mNT} \ , \ 0 \leq k \leq N-1 \ . \tag{15}$$

We assume, just as for the single tone case, that the true frequency, ω_0, coincides with one of the bin frequencies, say $\hat{\omega}_r$ (see the remark below). As in the single tone case, the coarse frequency estimate is the bin frequency, $\hat{\omega}_l$, associated with the greatest element of the set

$$\mathcal{L} \triangleq \{L(\hat{\omega}_k) : 0 \leq k \leq N-1\} \ . \tag{16}$$

At least in a high SNR situation, this will usually be the true frequency $\hat{\omega}_l = \hat{\omega}_r = \omega_0$. However, the presence of noise will ensure that on some occasions $l \neq r$, in which case, an outlier, due either to noise or to a rational harmonic, has occurred.

Remark: The choice made for ω_0 is not critically important and is prompted by a desire for consistency with the single tone treatment where an argument based on the bias of the MLE was given. To the best of our knowledge, there has been no corresponding analysis of the multiharmonic MLE. One might conjecture on the basis of the single tone result, that such an analysis would specify the sampling frequency required for the multiharmonic MLE to be unbiased, and that this sampling frequency is such that ω_0 coincides with a bin frequency. If this were the case, the same supporting arguments given in relation to the choice of ω_0 for the single tone outlier analysis could be given here. If not (and if ω_0 did not coincide with a bin frequency), we could simply interpret a coarse frequency estimate given by $\hat{\omega}_r$ (where $\hat{\omega}_r$ is the bin frequency closest to ω_0) to be the coarse estimate corresponding to the true frequency ω_0.

Similarly to the single tone analysis, the frequency estimation error variance may be expressed in terms of the following mutually exclusive and collectively exhaustive events: the non-occurrence of an outlier, the occurrence of a rational harmonic outlier, and the occurrence of a noise outlier. In other words, the set of bin frequency

indices denoted by $\mathcal{Z}$, where

$$\mathcal{Z} \triangleq \{0, 1, \ldots, N-1\}, \tag{17}$$

may be decomposed into the union of three disjoint sets as follows,

$$\mathcal{Z} = \mathcal{S} \cup \mathcal{R} \cup \mathcal{N} \ . \tag{18}$$

The set $\mathcal{S}$ is defined by $\mathcal{S} \triangleq \{r\}$, where r is the bin frequency index corresponding to the true frequency ω_0. The set $\mathcal{R}$ is defined to contain those bin frequency indices corresponding to rational harmonic frequencies, and $\mathcal{N}$ contains the remainder, i.e., those indices corresponding to potential noise outliers.

We need to be more precise concerning the nature of the set $\mathcal{R}$, since it is clear that not all rational harmonic frequencies of ω_0 coincide with bin frequencies. As described earlier, a rational harmonic of ω_0 is a frequency, ω_ρ^{rh}, related to ω_0 via $\omega_\rho^{rh} = \rho\omega_0$; $\rho = i/j$, where i and j are mutually prime positive integers, with $i \leq m$, $j \leq m$, and $i \neq j$; (the case $i = j$ obviously does not correspond to an outlier). The quantity ρ is termed the *rational multiplier* of ω_ρ^{rh}. The set of possible rational multipliers for m harmonics is denoted $\Phi^{(m)}$ and is formally defined by

$$\Phi^{(m)} \triangleq \{\rho : \rho = \frac{i}{j}; 1 \leq i, j \leq m; i \neq j; i, j \text{ coprime}\} \tag{19}$$

(for example, $\Phi^{(4)} = \{\frac{1}{4}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \frac{3}{2}, \frac{4}{3}, 2, 3, 4\}$). The number of elements in $\Phi^{(m)}$ is given by the Lemma below. (The symbol # denotes "cardinality of".)

Lemma 3.1 *Let $\Phi^{(m)}$ be defined as in (19). Then*

$$\#\Phi^{(m)} = \nu(m) \triangleq 2\sum_{i=2}^{m} \phi(i) \tag{20}$$

where $\phi(i)$ is Euler's totient *function (see [7]) which denotes the number of integers less than i that are mutually prime to i.*

proof: See Appendix A.

A table of $\nu(m)$ is given below

m	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$\nu(m)$	0	2	6	10	18	22	34	42	54	62	82	90	114	126	142

As we mentioned before, the rational harmonics do not necessarily all coincide with the bin frequencies $\hat{\omega}_k$. (In other words, there may exist at least one $\rho \in \Phi^{(m)}$ such that $\rho\omega_0 \neq \hat{\omega}_k$, for all integers k such that $1 \leq k \leq N$.) However, each rational harmonic frequency will lie in a frequency interval of width $2\pi/mNT$ centred at a particular bin frequency. Such an interval is termed, perhaps obviously, the *frequency bin* corresponding to that particular bin frequency. Thus if the outcome of the coarse search is a bin frequency whose associated bin contains a rational harmonic frequency, then a rational harmonic outlier is said to have occurred. $\mathcal{R}$ is then defined to be the set of bin frequency indices whose associated bins contain rational harmonic frequencies, and so, the number of elements in $\mathcal{R}$ is given by $\nu(m)$, provided that there is no more than one rational harmonic frequency per frequency bin. This can be ensured by choosing N sufficiently large that $r/[m(m-1)] > 1$, where $r = \omega_0 mNT/2\pi$ is the index of ω_0, by an earlier definition. In this case, there exists a one-to-one relation between the elements of $\Phi^{(m)}$ and $\mathcal{R}$, e.g., ω_ρ^{rh} lies in the frequency bin corresponding to $\hat{\omega}_j$, $j \in \mathcal{R}$.

Having said this, we remark that a necessary and sufficient condition for all the rational harmonic frequencies to coincide with bin frequencies is that the *subharmonic* frequencies (i.e., those rational harmonic frequencies given by $\omega_\rho^{rh} = \rho\omega_0$, $\rho \in \Phi_{sub} \triangleq \{\rho : \ \rho = 1/k \ , \ 2 \leq k \leq m\}$) all coincide with bin frequencies. That the condition is sufficient is established straightforwardly as follows. Firstly observe (from the definition of $\Phi^{(m)}$ in (19)) that if $\rho \in \Phi^{(m)}$, then $\rho = i\rho_{sub}$ for some integer i, $1 \leq i \leq m^2$, and for some $\rho_{sub} \in \Phi_{sub}$. Since by assumption all the subharmonic frequencies coincide with bin frequencies, (i.e., for each $\rho_{sub} \in \Phi_{sub}$ there exists an integer k, $1 \leq k \leq N$ such that $\rho_{sub}\omega_0 = \hat{\omega}_k$) then the rational harmonic frequency

ω_ρ^{rh} can be written in the form

$$\begin{aligned} \omega_\rho^{rh} = \rho\omega_0 &= i(\rho_{sub}\omega_0) \\ &= i\hat{\omega}_k = \hat{\omega}_{(i\times k)} \end{aligned} \tag{21}$$

where i and ρ_{sub} are as earlier defined, and $\hat{\omega}_{(i\times k)}$ is a bin frequency. The necessity of the condition is trivial to establish, since $\Phi_{sub} \subset \Phi^{(m)}$. We also remark that it might well be easy, in practice, to satisfy the above condition by suitable choice of N and r. In this case, all the rational harmonic frequencies coincide with bin frequencies, with the result that $\mathcal{R}$ is given by the set $\{k:\ k = \rho r\ ,\ \rho \in \Phi^{(m)}\}$.

We return now to the discussion of the mutually exclusive outlier events. In order to define these precisely, let

$$D_k \stackrel{\Delta}{=} L(\hat{\omega}_k)\ ,\ 0 \le k \le N-1\ . \tag{22}$$

The events are then defined as follows.

Definition 3.1 *1. Let A denote the event that no outlier occurs.*

$$A: \quad arg\ \max_k D_k \in \mathcal{S} \tag{23}$$

2. Let B_j denote the event that an outlier at the bin frequency $\hat{\omega}_j$, $j \in \mathcal{R}$, corresponding to the rational harmonic frequency ω_ρ^{rh}, $\rho \in \Phi^{(m)}$ occurs.

$$B_j: \quad arg\ \max_k D_k = j \in \mathcal{R} \tag{24}$$

3. Let C denote the event that a noise outlier occurs

$$C: \quad arg\ \max_k D_k \in \mathcal{N} \tag{25}$$

The overall mean square frequency estimation error (MSE) is then given by the

weighted sum

$$\mathrm{E}(\hat{\omega}-\omega_0)^2 = \Pr(A)\mathrm{E}[(\hat{\omega}-\omega_0)^2|A] + \sum_{j\in\mathcal{R}} \Pr(B_j)\mathrm{E}[(\hat{\omega}-\omega_0)^2|B_j] + \Pr(C)\mathrm{E}[(\hat{\omega}-\omega_0)^2|C] \tag{26}$$

where

$$\Pr(A) + \sum_{j\in\mathcal{R}} \Pr(B_j) + \Pr(C) = 1 \ . \tag{27}$$

As before, $\hat{\omega}$ is the outcome of a fine search, the details of which are not important for this discussion. We should remark that (26) is not necessarily a fully adequate measure of error to the extent that it accounts for the possible occurrence of rational harmonic outliers. As we remarked earlier, such outliers are not necessarily damaging if their relationship to the true frequency (as determined by the associated rational multipliers) is known. One might envisage that their contribution to the error could be removed if additional means were available to determine that relationship. However, in the absence of such an extra level of algorithm, (26) stands as an accurate (if not in a practical sense adequate) representation of the error associated with the ML frequency estimates.

The task now is to calculate the various probabilities $\Pr(A)$, $\Pr(B_j)$ and $\Pr(C)$ appearing in (26). This proves to be singularly difficult (as opposed to the relatively straightforward nature of the single tone analysis); in most cases, only bounds on approximations to the probabilities are calculated.

3.1 Probability of an outlier due to noise alone – $\Pr(C)$

The quantities D_k, $k \in \mathcal{Z}$, due to the presence of measurement noise, are really random variables. Let us consider D_k for values of k in the set $\mathcal{N}$. These are simply the values of the likelihood function $L(\omega)$ at each of those bin frequencies that do *not* correspond to a rational harmonic frequency, or the true frequency. The cardinality of $\mathcal{N}$ is then easily seen to be $N - \nu(m) - 1$.

The random variable D_r (where r is the bin frequency index of the true fundamental frequency ω_0) is the value of $L(\omega)$ at ω_0. An outlier due to noise *alone* occurs if $\arg\ \max_k D_k \in \mathcal{N}$ (this is merely the definition of event C). We want to evaluate

the probability of this happening, namely $\Pr(C)$. Let $X_k(x)$ denote the event that $D_k < x$ and q^{noise} be an estimate of the desired probability, defined by

$$1 - q^{noise} = \Pr\{\bigcap_{k \in \mathcal{N}} X_k(D_r)\}.$$

The quantity q^{noise} is actually a conservative estimate of the probability $\Pr(C)$, in the sense that $q^{noise} > \Pr(C)$. This is because the event that $D_j > D_k > D_r$, for some $k \in \mathcal{N}$ and some $j \notin \mathcal{N}$, is possible, (if this were to happen, $\hat{\omega}_j$, a rational harmonic, would be the outlier, not $\hat{\omega}_k$), though highly improbable, at least for SNR's moderately far below the threshold point. This is supported by the results of example calculations, which indicate that for these SNR's, q^{noise} is generally a very small quantity, e.g. no greater than something of the order of 10^{-8}. We would therefore expect the probability of the event described above to be something roughly like the square of that number – a negligibly small amount.

Whether the conservative nature of the estimate q^{noise} of $\Pr(C)$ leads to the later overestimation of $\mathrm{E}(\hat{\omega} - \omega_0)^2$ (as defined in (26)) is difficult to say. This is because the interaction between the estimates of the various probabilities (some of which are yet to be defined) appearing on the RHS of (26) is not understood. However, simulation results in a later section suggest the estimate is not overly conservative. (Refer to the remark in Section 4 below.)

Conditioning on D_r:

$$1 - q^{noise} = \int_x \Pr\{\bigcap_{k \in \mathcal{N}} X_k(x)\} f_{D_r}(x) dx \tag{28}$$

where $f_{D_r}(x)$ is the probability density function (p.d.f.) of D_r. (The fact that $\hat{\omega}_k$ and $\hat{\omega}_r$ are not harmonically related is crucial for obtaining the second expression for $1 - q^{noise}$: it implies that D_k assumes a value based purely on the noise). Now

$$\Pr\{\bigcap_{k \in \mathcal{N}} X_k(x)\} = \Pr\{G < x\}$$

where

$$G \triangleq \max_{k \in \mathcal{N}} D_k. \tag{29}$$

A more convenient way of writing this is

$$\begin{aligned} q^{noise} &= \int_x \Pr\{G > x\} f_{D_r}(x) dx \\ &= \int_x \overline{F}_G(x) f_{D_r}(x) dx \end{aligned} \tag{30}$$

where $\overline{F}_G(x) = 1 - F_G(x)$ and $F_G(x)$ is the cumulative distribution function of G.

The difficulty now encountered is that (in contrast to the single tone case) the D_k, $k \in \mathcal{N}$, are not all independent, and so the determination of F_G is not trivial. (The non-independence of D_k, $k \in \mathcal{N}$, can be seen by writing $S_{i\times k} = |A(i\omega_k)|^2 = |A(\omega_{i\times k})|^2$. Thus $D_k = \sum_{i=1}^m S_{i\times k}$. Setting $m = 3$, D_6 and D_9 can both be seen to depend on S_3.)

In Appendix B, the following lemma is proven.

Lemma 3.2 *Let D_k be defined by (22), G by (29), and $\nu(m)$ by (20). Then*

$$[F_{D_k}(x)]^{\Pi(m,N)-m+1} \geq F_G(x) \geq [F_{D_k}(x)]^{N-\nu(m)-1}$$

(where F_{D_k} is the cumulative distribution function of D_k, $k \in \mathcal{N}$) or

$$1 - [F_{D_k}(x)]^{N-\nu(m)-1} \geq \overline{F}_G(x) \geq 1 - [F_{D_k}(x)]^{\Pi(m,N)-m+1}$$

where $\Pi(m,N) = \pi_{N-1} - \pi_m$ and π_n is the number of primes not exceeding n.

proof: See Appendix B.

Using this lemma and (30) we can write

$$\begin{aligned} &\int_{x=0}^{\infty} \left(1 - [F_{D_k}(x)]^{\Pi(m,N)-m+1}\right) f_{D_r}(x) dx \;\leq\; q^{noise} \;\leq \\ &\int_{x=0}^{\infty} \left(1 - [F_{D_k}(x)]^{N-\nu(m)-1}\right) f_{D_r}(x) dx. \end{aligned} \tag{31}$$

The functions F_{D_k} and f_{D_r} are derived in Appendix C and given by (87) and (89) respectively. Combining these with (31), there holds

$$\mathrm{L}(\Pi(m,N) - m + 1) \leq q^{noise} \leq \mathrm{L}(N - \nu(m) - 1) \tag{32}$$

where

$$\mathrm{L}(\alpha) = \int_{x=0}^{\infty} \left(1 - \left[\frac{\gamma(m, \psi x)}{\Gamma(m)}\right]^{\alpha}\right) \left(\frac{x}{\lambda}\right)^{\frac{m-1}{2}} \psi \exp\left[-\psi(\lambda + x)\right] I_{m-1}(2\psi\sqrt{\lambda x}) dx, \tag{33}$$

$\gamma(\cdot, \cdot)$ is the incomplete Gamma function defined in (86), I_k is the modified Bessel function of the first kind, of order k, and

$$\psi = \frac{N}{2\sigma^2} \tag{34a}$$

$$\lambda = \sum_{i=1}^{m} b_i^2 \ . \tag{34b}$$

An interesting feature of the above expressions is the appearance of the parameter $\lambda = \sum_{i=1}^{m} b_i^2$, as opposed to the effective signal power

$$\Lambda = \sum_{i=1}^{m} i^2 b_i^2 \tag{35}$$

that is so important in the expressions for the Cramer-Rao bounds derived in [8] and [1] and given in (55). A possible insight as to why this is so is given as follows. At high SNR's, the peaks of $|A(\omega)|$ corresponding to the harmonic and fundamental frequencies are tightly *synchronised* or *coherent*, in the sense that the frequencies at these peaks, to a very high order of approximation, obey a strict harmonic relationship. This is reflected by the form of the parameter of importance at these high SNR's, namely Λ, which is a sum of terms weighted by corresponding squared harmonic indices. As the SNR is lowered, the *coherence*, or *synchronism*, of the peaks is more or less maintained until the threshold point is reached (as evidenced by the agreement of the MLE performance with the CR bounds above threshold). Below the threshold point, coherence is, roughly speaking, lost. The parameters of importance in this region do not, then, include Λ, but those associated with outlier probabilities, one of which is $\sum_k b_k^2$. The multiharmonic frequency estimation problem is examined further in [9] and [3].

3.2 Probability of a rational harmonic outlier – $\Pr(B_j)$, $j \in \mathcal{R}$

As defined previously, ω_ρ^{rh}, for some $\rho \in \Phi^{(m)}$ denotes a frequency that is a rational harmonic of ω_0, with rational multiplier ρ, i.e., $\omega_\rho^{rh} = \rho\omega_0$. As already mentioned, each rational harmonic frequency is associated with a particular bin frequency. In the following analysis, we will ignore the fact that not all rational harmonic frequencies coincide exactly with bin centre frequencies. We assume either that N is chosen so that most of the rational harmonic frequencies of importance (i.e., those with rational multipliers $\rho = 1/k$, $1 \leq k \leq m$ – the so-called *subharmonics*) coincide with bin frequencies, or that N is sufficiently large to ensure that the distance between a rational harmonic frequency and its nearest bin frequency is essentially negligible (in the sense that the probabilities of coarse searches resulting in the two frequencies are virtually the same).

Once again, we seek an estimate of a probability, on this occasion, the probability that the outcome of the coarse search is the rational harmonic frequency ω_ρ^{rh}. More precisely, we seek an estimate of $\Pr(B_j)$, where B_j denotes the event that $\arg\ \max_k D_k = j$, $j \in \mathcal{R}$, and j is the frequency index corresponding to ρ.

It is expected (from empirical evidence) that rational harmonic outliers are more probable than noise outliers at intermediate noise levels. Therefore we make the assumption that if $D_j > D_r$, for some particular $j \in \mathcal{R}$, then it is very unlikely that $D_k > D_j,\ k \in \mathcal{N}$. In other words, if the value of $L(\omega)$ at $\hat{\omega}_j$ (D_j) is greater than that at the true frequency (D_r), then it is almost certain that no, greater, noise outlier will occur.

This does not account for the possibility of there being another highly likely rational harmonic outlier. We shall discuss this point further in Subsection 3.3 and an example for $m = 3$ is given in Section 5.

Therefore, as an estimate of the probability of an outlier corresponding to the rational harmonic frequency ω_ρ^{rh}, given that no other outlier has occurred, choose

$$q_\rho \triangleq \Pr\left\{\sum_{i=1}^{m} |A(i\omega_\rho^{rh})|^2 > \sum_{i=1}^{m} |A(i\omega_0)|^2\right\} . \tag{36}$$

Consider the RHS of the expression in (36). Note that the quantity in braces can be rewritten

$$\sum_{j \in H_\rho} |A(j\omega_0)|^2 > \sum_{k \in Z_m} |A(k\omega_0)|^2 \tag{37}$$

where

$$H_\rho \triangleq \{\rho, 2\rho, \ldots, m\rho\}. \tag{38}$$

and

$$Z_m \triangleq \{1, \ldots, m\} \ . \tag{39}$$

One can interpret an element of the set H_ρ as being the rational multiplier (with respect to ω_0) associated with a particular harmonic of an m harmonic signal with fundamental frequency ω_ρ^{rh}. The expression (37) can be further simplified with the aid of the following definitions

$$H_\rho^i \triangleq H_\rho \cap Z_m \tag{40}$$

$$H_\rho^s \triangleq Z_m \setminus H_\rho^i \tag{41}$$

$$H_\rho^r \triangleq H_\rho \setminus Z_m \ . \tag{42}$$

The set H_ρ^i corresponds to those harmonics of ω_ρ^{rh} that are also harmonics of ω_0; H_ρ^s to those harmonics of ω_0 that are *not* harmonics of ω_ρ^{rh} and finally H_ρ^r to those harmonics of ω_ρ^{rh} that are *not* harmonics of ω_0. The expression (36) may then be written

$$\begin{aligned} q_\rho &= \Pr\left\{ \sum_{j \in H_\rho} |A(j\omega_0)|^2 > \sum_{k \in Z_m} |A(k\omega)|^2 \right\} \\ &= \Pr\left\{ \sum_{j \in H_\rho^r} |A(j\omega_0)|^2 + \sum_{j \in H_\rho^i} |A(j\omega_0)|^2 > \sum_{k \in H_\rho^s} |A(k\omega_0)|^2 + \sum_{k \in H_\rho^i} |A(k\omega_0)|^2 \right\} \\ &= \Pr\left\{ \sum_{j \in H_\rho^r} |A(j\omega_0)|^2 > \sum_{k \in H_\rho^s} |A(k\omega_0)|^2 \right\}. \end{aligned} \tag{43}$$

For the sake of convenience, define $d_j \triangleq |A(j\omega_0)|^2$. Then, observe that, since $H_\rho^r \cap Z_m = \emptyset$, the term $\sum_{j \in H_\rho^r} d_j$ contains only noise terms, and since $H_\rho^s \subset Z_m$, the term $\sum_{k \in H_\rho^s} d_k$ contains only signal harmonic frequencies. Furthermore the fact that

$H_\rho^r \cap H_\rho^s = \emptyset$ means that the two terms are independent.

Thus we can use the p.d.f. of D_r and the c.d.f. of D_k for $k = r$ and $k \neq r$ (as derived in Appendix C) to calculate the distributions of

$$U_\rho^r \triangleq \sum_{j \in H_\rho^r} d_j \tag{44}$$

and

$$U_\rho^s \triangleq \sum_{k \in H_\rho^s} d_k. \tag{45}$$

Since U_ρ^r is made up of a sum of $l_r \triangleq \#H_\rho^r$ terms of the form $|A(\omega_k)|^2$, where all the frequencies ω_k do not correspond to any signal harmonics, we can see from (87) that $\left(\frac{NU_\rho^r}{\sigma^2}\right)$is distributed as χ^2 with $2l_r$ degrees of freedom. Thus

$$F_{U_\rho^r}(x) = \frac{1}{\Gamma(l_r)} \gamma(l_r, \psi x) \tag{46}$$

(with $\psi = \frac{N}{2\sigma^2}$ and γ is as defined in (86)).

Similarly we can see that U_ρ^s is a sum of $l_s \triangleq \#H_\rho^s$ terms $|A(\omega_k)|^2$ where all the frequencies ω_k correspond to some signal harmonic. Thus from (89), we can see that $\left(\frac{NU_\rho^s}{\sigma^2}\right)$ is distributed as non-central χ^2 with $2l_s$ degrees of freedom and non-centrality parameter $\lambda_\rho = \sum_{k \in H_\rho^s} b_k^2$. Hence the p.d.f. of U_ρ^s is

$$f_{U_\rho^s}(x) = \psi \left(\frac{x}{\lambda_\rho}\right)^{\frac{l_s - 1}{2}} \exp\left[-\psi(\lambda_\rho + x)\right] I_{l_s - 1}(2\psi\sqrt{\lambda_\rho x}) \tag{47}$$

where again $\psi = \frac{N}{2\sigma^2}$ and I_k is the modified Bessel function of the first kind, of order k.

Collecting (43), (47) and the analogue of (30) and using the fact that

$$\overline{F}_{U_\rho^r}(x) = 1 - F_{U_\rho^r}(x) = \frac{\Gamma(l_r, \psi x)}{\Gamma(l_r)}$$

(where $\Gamma(\cdot,\cdot)$ is the complementary incomplete gamma function:

$$\Gamma(a,x) = \int_{t=x}^{\infty} e^{-t} t^{a-1} dt = \Gamma(a) - \gamma(a,x),$$

and $\gamma(\cdot,\cdot)$ is as in (86)), we obtain

$$q_\rho = \int_{x=0}^{\infty} \frac{\Gamma(l_r, \psi x)}{\Gamma(l_r)} \psi \left(\frac{x}{\lambda_\rho}\right)^{\frac{l_s-1}{2}} \exp\left[-\psi(\lambda_\rho + x)\right] I_{l_s-1}(2\psi\sqrt{\lambda_\rho x}) dx \tag{48}$$

where $\psi = \frac{N}{2\sigma^2}$, $l_r = \#H_\rho^r$, $l_s = \#H_\rho^s$, $\lambda_\rho = \sum_{k \in H_\rho^s} b_k^2$.

3.3 Calculation of $\Pr(A)$

Having calculated estimates of $\Pr(B_j)$ and $\Pr(C)$, it remains to calculate an estimate of $\Pr(A)$. From (27) there holds

$$\Pr(A) = 1 - \Pr(B) - \Pr(C) \tag{49}$$

where

$$\Pr(B) \triangleq \sum_{j \in \mathcal{R}} \Pr(B_j) \tag{50}$$

is the probability of *any* rational harmonic outlier occurring.

The value of q_ρ is the probability of the rational harmonic outlier ρ, given that no other rational harmonic outlier has occurred. Recall that it has been assumed that the probability of a noise outlier is negligible at the intermediate SNR's of interest. The total rational harmonic outlier probability may be written therefore as

$$\Pr(B) = \sum_{\rho \in \Phi^{(m)}} q_\rho \Pr(D_j > \max_{i \in \mathcal{R} \setminus \{j\}} D_i) \tag{51}$$

where j is the index corresponding to $\rho\omega_0$, D_k is defined in (22) and r is the index of the frequency bin corresponding to the true frequency. It is generally difficult to get an estimate of

$$\Pr(D_j > \max_{i \in \mathcal{R} \setminus \{j\}} D_i)$$

for a given number of harmonics, m, however we give a specific example (for $m = 3$) where it is possible in Section 5.

An easily derived upper bound on $\Pr(B)$ is given simply by

$$\sum_{\rho \in \Phi^{(m)}} q_\rho \ . \tag{52}$$

The difficulty is that the events whose probabilities are given by q_ρ are not necessarily independent, so that (52) will be greater than $\Pr(B)$. Another upper bound on $\Pr(B)$ may be straightforwardly derived using the concept of *associated* random variables (as defined in Appendix B) and is stated below without proof,

$$\Pr(B) \ \leq \ 1 - \prod_{\rho \in \Phi^{(m)}} (1 - q_\rho) \ \triangleq \ \overline{q}_{\Phi^{(m)}} . \tag{53}$$

It is easy to see that this estimate is guaranteed to be less than unity, however it cannot in general be shown that the same guarantee holds for (52). Hence, using $\overline{q}_{\Phi^{(m)}}$ as an estimate of $\Pr(B)$ in (49), there holds

$$\Pr(A) \geq \prod_{\rho \in \Phi^{(m)}} (1 - q_\rho) - q^{noise} \ . \tag{54}$$

4 Evaluation of Mean Square Frequency Estimation Error

Having computed estimates of the various probabilities required for evaluation of the overall MSE in (26), the remaining task is to determine the individual contributions to the MSE by each of the mutually exclusive events, A, B_j, $j \in \mathcal{R}$ and C. This is particularly straightforward for the case where no outlier of any description has occurred (i.e., event A). The contribution to the total MSE, $\mathrm{E}(\hat{\omega} - \omega_0|A)^2$ is then simply the Cramer-Rao bound on the frequency estimation error variance for the multiharmonic problem given by (see [1])

$$\omega_e^2(\text{linear}) \triangleq \mathrm{E}(\hat{\omega} - \omega_0|A)^2 = \frac{12\sigma^2}{N(N^2-1)T^2 \sum_{k=1}^{m} k^2 b_k^2} \ . \tag{55}$$

(For high SNR's, this contribution completely dominates the expression for the overall MSE, i.e., $\Pr(A) \approx 1$, $\Pr(B) \approx 0$ and $\Pr(C) \approx 0$.)

The contribution due to a rational harmonic outlier at ω_ρ^{rh} (with associated bin frequency index $j \in \mathcal{R}$) is approximated as follows.

$$\omega_e^2(\rho) \triangleq \mathrm{E}[(\hat{\omega} - \omega_0)^2 | B_j] = \omega_0^2 (1-\rho)^2 \ . \tag{56}$$

The above expression is an approximation, since the rational harmonic outlier will not always fall exactly on the frequency $\rho\omega_0$, but in a small neighbourhood about it. However, the distance $|\omega_0 - \rho\omega_0|$ will be much greater than the size of the small random fluctuations about $\rho\omega_0$, and hence will be the dominant contributor to the MSE due to the rational harmonic outlier.

The final contribution to (26) is that due to the occurrence of an outlier caused by the measurement noise alone, (i.e., event C). Since the measurement noise is assumed white, it is equally likely that such an outlier can fall at any point within the interval $[0, \omega_s/2m]$. In other words, we assume that the noise outliers are uniformly distributed on that interval, ignoring the presence therein of a finite number of rational harmonic frequencies. The MSE contribution is then easily calculated as follows.

$$\begin{aligned} \omega_e^2(\text{noise}) &\triangleq \mathrm{E}(\hat{\omega} - \omega_0 | C)^2 \\ &= \frac{2m}{\omega_s} \int_{-\omega_0}^{\omega_s/2m - \omega_0} x^2 dx \\ &= \frac{\omega_s^2}{12m^2} - \frac{\omega_0 \omega_s}{2m} + \omega_0^2. \end{aligned} \tag{57}$$

The expression in (26) may now be fully evaluated to yield

$$\begin{aligned} \omega_e^2 \triangleq \mathrm{E}(\hat{\omega} - \omega_0)^2 \approx & \left[\prod_{\rho \in \Phi^{(m)}} (1 - q_\rho) - q^{noise} \right] \frac{12\sigma^2}{N(N^2-1)T^2 \sum_{k=1}^m k^2 b_k^2} \\ & + \omega_0^2 \sum_{\rho \in \Phi^{(m)}} q_\rho (1-\rho)^2 \\ & + q^{noise} \left[\frac{\omega_s^2}{12m^2} - \frac{\omega_0 \omega_s}{2m} + \omega_0^2 \right] \end{aligned} \tag{58}$$

where

$$\mathrm{L}(\Pi(m,N)-m+1) \leq q^{noise} \leq \mathrm{L}(N-\nu(m)-1), \tag{59}$$

$$\mathrm{L}(\alpha) = \int_{x=0}^{\infty} \left(1 - \left[\frac{\gamma(m,\psi x)}{\Gamma(m)}\right]^{\alpha}\right) \left(\frac{x}{\lambda}\right)^{\frac{m-1}{2}} \psi \exp\left[-\psi(\lambda+x)\right] I_{m-1}(2\psi\sqrt{\lambda x})dx, \tag{60}$$

$\gamma(\cdot,\cdot)$ is the incomplete Gamma function defined in (86), I_k is the modified Bessel function of the first kind, of order k, and

$$\psi = \frac{N}{2\sigma^2} \tag{61a}$$

$$\lambda = \sum_{i=1}^{m} b_i^2 \ . \tag{61b}$$

Also, from (48),

$$q_\rho = \int_{x=0}^{\infty} \frac{\Gamma(l_r,\psi x)}{\Gamma(l_r)} \psi \left(\frac{x}{\lambda_\rho}\right)^{\frac{l_s-1}{2}} \exp\left[-\psi(\lambda_\rho+x)\right] I_{l_s-1}(2\psi\sqrt{\lambda_\rho x})dx, \tag{62}$$

where $\psi = \frac{N}{2\sigma^2}$, $l_r = \#H_\rho^r$, $l_s = \#H_\rho^s$, $\lambda_\rho = \sum_{k\in H_\rho^s} b_k^2$.

Remark: As foreshadowed in Section 3.1, the question as to whether the use of estimates of the various probabilities in (26) (as shown in (58)) leads to the over or underestimation of ω_e^2 is difficult to answer. It is probably desirable for there to be an overestimation of ω_e^2 since this would give a "factor of safety" with respect to the threshold point. However, without an understanding of the interaction between the various estimates involved, we can draw no conclusion about the conservativeness or otherwise of the estimate of ω_e^2 in (58). The Monte Carlo simulations presented next give some guidance here.

5 Calculations and Simulations

In this section some example calculations using the above equations are presented, and these are compared with Monte-Carlo simulation results. The calculations were performed with the software package **Maple** [10]. An adaptive Newton-Coates algorithm was used to compute the key integral L of (33), a task of some numerical

difficulty because of the very small numbers involved.

In the examples which follow, three cases of interest have been chosen:

(i) Firstly, to aid comparison to previous work [4], performance curves for the case of estimating the frequency of a single-tone in noise are generated.

(ii) Secondly, to show how knowledge of the presence of one harmonic component alters the performance, we examine estimation of the fundamental frequency of a two-component multiharmonic signal.

(iii) Finally, to test the sensitivity of the multiharmonic frequency estimator to model inaccuracy, the presence of a third harmonic is falsely assumed when the signal of interest is truly a two-compnent signal.

In the theoretical calculations and simulations which follow, the *true* signal power (61b) is held constant. If the *effective* signal power of (35) was held constant, the single-tone and multiharmonic RMSE performance curves would coincide for small noise levels.

In all cases presented, the assumed sampling frequency is 4000Hz, for consistency with [4].

5.1 Root Mean Square Error Performance Curves

The root mean square error curves plotted in Figure 5, are calculated from (58) and demonstrate three cases:

Case (i) with $b_1 = 4.47$,

Case (ii) with $b_1 = 4$ and $b_2 = 2$, and

Case (iii) with $b_1 = 4$, $b_2 = 2$ and $b_3 = 0$.

Each signal has the same true power, namely $\lambda = 20$.

For case (i), the three solid curves plotted relate to whether the initial coarse search has been conducted over $[0, \omega_s]$ (curve A), $[0, \omega_s/2]$ (curve B) and $[0, \omega_s/3]$

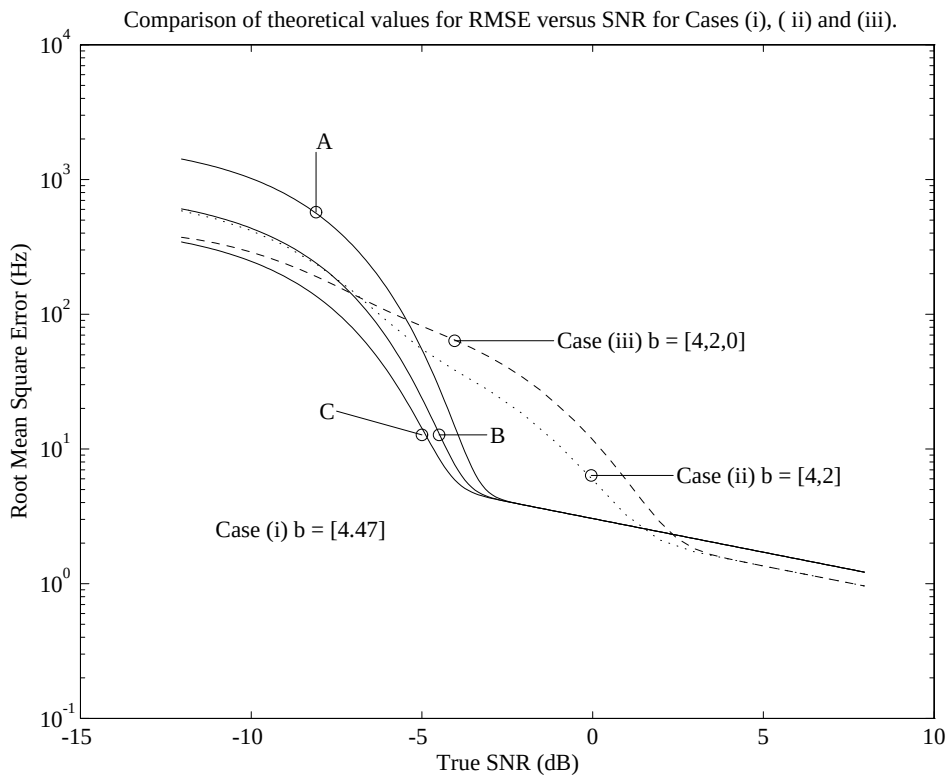

Figure 5: Plot of root mean square frequency estimation error versus SNR in dB for three different situations: (i) $b = 5.66$, (ii) $b = [4, 2]$, and (iii) $b = [4, 2, 0]$. In all cases, $N = 64$.

(curve C). The main effect of these different coarse search regions is to change the root MSE in the high-noise regions, see (57). In cases (ii) and (iii) the lower bound on q^{noise} given by (32) has been used.

For each curve, the SNRs at threshold are clear; thresholding occurs at -3dB for (i), 2dB for (ii) and 3dB for (iii).

The main points to note are:

- The presence of an extra harmonic improves the performance in the high SNR region.
- The performances of the MLE in relation to the two and three harmonic signals are identical at high SNR. This is simply because the *effective signal powers* of the signals, as defined by $\Lambda = \sum_k k^2 b_k$, and therefore the CR bound (see (55)), are identical. (Recall that the performance of the MLE meets the CR bound at high SNR.)
- The threshold performance is severely degraded (thresholding at least 5dB earlier that the single-tone case).
- When the third harmonic is incorrectly assumed to be present performance is further degraded: the estimator assuming only two harmonics performs better.

Comparison with Monte-Carlo Simulation Results

Figure 6 plots the results obtained by generating approximately 3000 realisations per SNR value of signals (i), (ii) and (iii) to which the multi-harmonic maximum likelihood estimator of frequency is then applied. The theoretical curves are also plotted, using both the lower and upper bounds of (32).

Note the close agreement between the theoretically calculated curves and those observed by simulation.

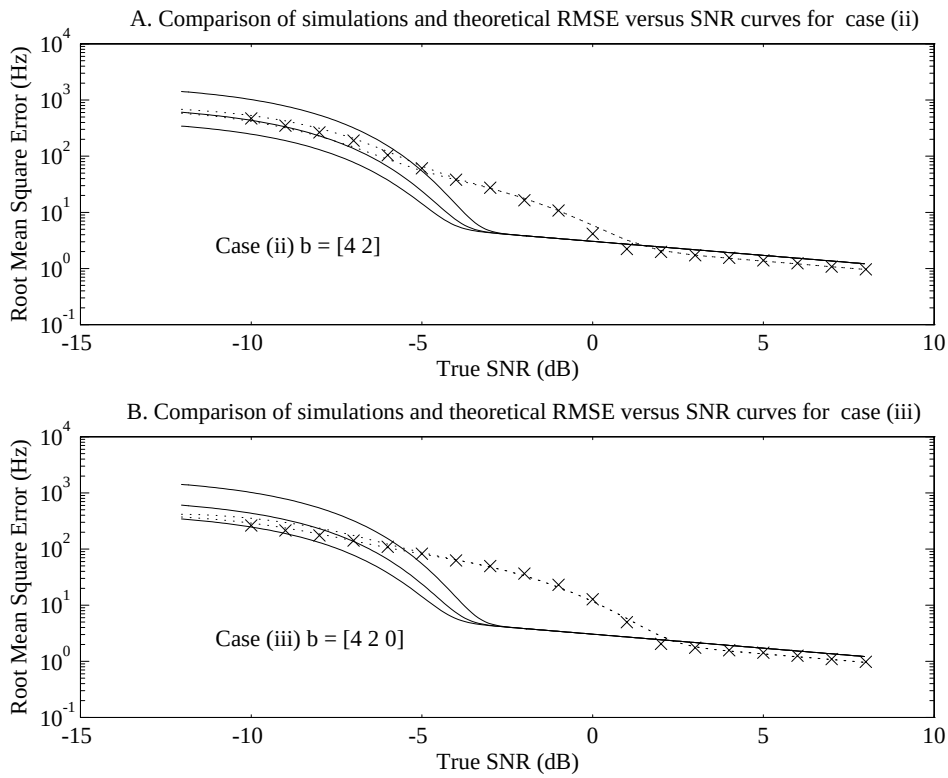

Figure 6: Plots of root mean square frequency estimation error versus SNR in dB displaying

— the theoretical performance of the single-tone case

····· theoretical bounds (both upper and lower) on the multiharmonic MLE performance calculated from (58) and subsequent equations and

x simulation results.

Graph A is case (ii) and graph B case (iii).

5.2 Outlier Probability Simulations

Comparison of the curves for signals (i) and (ii) in Figure 5 prompts the following interesting question. Suppose that (as previously discussed) an additional level of algorithm was incorporated into the MLE that was designed to detect rational harmonic outliers and derive accurate frequency estimates in their stead. Would this tend to equalise the respective threshold points in relation to (i) and (ii)? In other words, we are asking whether or not rational harmonic outliers are largely responsible for the higher SNR at threshold of (ii) in comparison with (i).

To compare our theoretically derived probability expressions with simulation results, we proceeded as follows.

For each effective SNR (35) from -10dB to 10dB in increments of 1dB, a number of realisations (100,000) of signal (ii) of length $N = 64$ with fundamental frequency $\omega = 3\pi/16$ were generated, and the likelihood functions, $L(\omega)$ calculated. From the results of a coarse search of these functions over the Fourier frequencies $\pi k/32$, $k = 0, 1, \ldots, N-1$, the number of events B (any rational harmonic outlier) and C (an outlier due to noise alone) were separately noted. These were then used to estimate $\Pr(B)$ and $\Pr(C)$. In order to save computing time, the full maximum likelihood estimator was not applied.

The resulting probability curves are plotted in Figure 7.

In Figure 8, the results of a similar procedure are displayed for case (iii), except that the number of realisations was 150,000.

For this $m = 3$ case (but the amplitude of the third harmonic is not necessarily zero), the set of rational harmonic outlier bins $\mathcal{R}$ splits into three disjoint subsets:

$$\mathcal{R}_1 = \left\{\frac{1}{2}r, \frac{1}{3}r\right\} \ ; \ \mathcal{R}_2 = \left\{\frac{2}{3}r, 2r\right\} \ ; \ \mathcal{R}_3 = \left\{\frac{3}{2}r, 3r\right\}$$

where r is the frequency bin corresponding to the true frequency, so that $\mathcal{R} = \mathcal{R}_1 \cup \mathcal{R}_2 \cup \mathcal{R}_3$. The probability of an outlier occurring at the bins in $\mathcal{R}_l$ ($l = 1, 2$ or 3) depends only on harmonic l (and the associated noise-only bins).

Due to this splitting of $\mathcal{R}$, we can assume that if $j \in \mathcal{R}_l$ with $l = 1, 2$ or 3 and

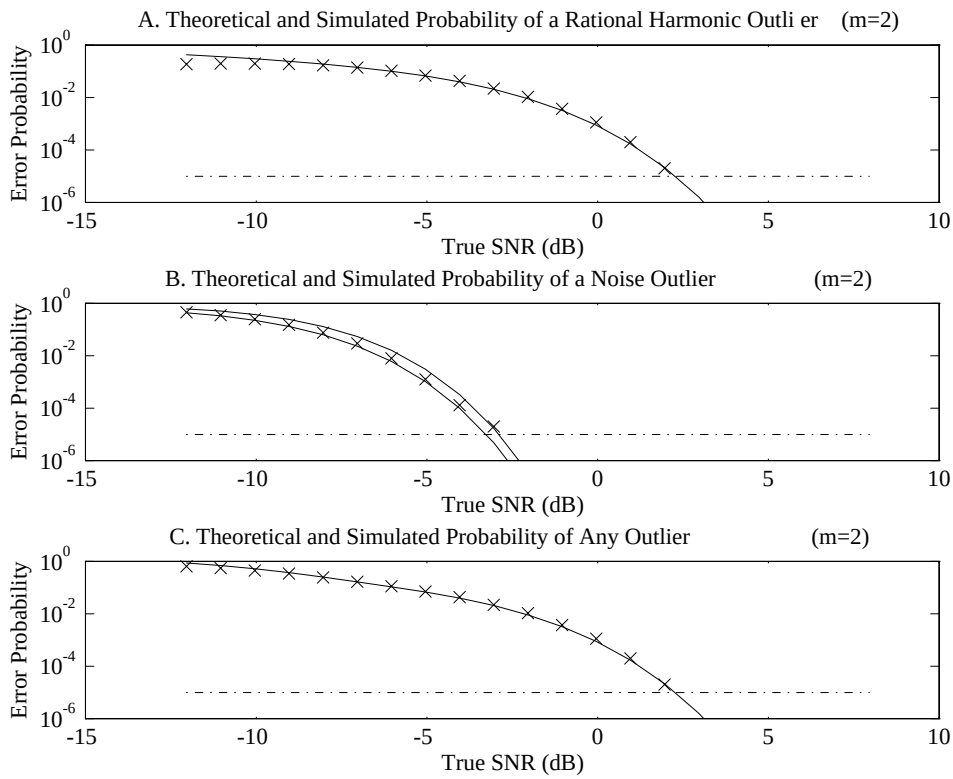

Figure 7: Simulation and theoretical outlier probabilities for case (ii) $b = [4, 2]$. The curves represent:

x the simulation results

— the theoretically derived results and

$- \cdot - \cdot -$ the inverse of the number of realisations (*i.e.* the smallest possible non-zero simulated probability).

$k \in \mathcal{R} \setminus \mathcal{R}_l$ then

$$\Pr(D_j > D_k) \approx 0.$$

This means, for example, the probability of an outlier occurring for $\rho = \frac{1}{2}$ if there is one for $\rho = 2$ is small. With this assumption, it is then trivial to show that if we now take $j \in \mathcal{R}_l$ and $k \in \mathcal{R}_l \setminus \{j\}$ then

$$\Pr(D_j > \max_{i \in \mathcal{R} \setminus \{j\}} D_i) \approx \Pr(D_j > D_k) = 0.5 \ .$$

We substitute this value into (51) to generate plots A. and C. in Figure 8.

For both case (ii) and case (iii), comparison of the top two graphs (A. and B.) in Figures 7 and 8 clearly show that it is the occurrence of rational harmonic outliers, rather than noise outliers, that is the major cause of thresholding at intermediate SNR's. (Observe that the probability of an outlier occurring at the threshold SNR is in fact very small. This is why it is advantageous to be able to calculate those probabilities rather than having to rely on very extensive simulations.)

Thus, the answer to our question is that a rational harmonic outlier detector would indeed equalise the threshold point of (i) with the thresholds of (ii) and (iii).

6 Conclusions

This paper has presented, in detail, the results of an analysis of the occurrence of outliers in the operation of the multiharmonic MLE. The major result of the paper is an approximate expression for the mean square frequency error that is applicable both above threshold and below. The significance of the result is that it enables the drawing of performance curves showing threshold, and studies of the effects of changing problem parameters by doing calculations, which although complicated, are nevertheless simpler and less time consuming than Monte Carlo simulation. (This can be paraphrased by saying that the result permits the threshold effect to be established *theoretically* as opposed to *experimentally*, via simulation.) We should point out that while the results of the internal analysis permit, in principle, the calculation of performance over the entire range of SNR, the nature of the

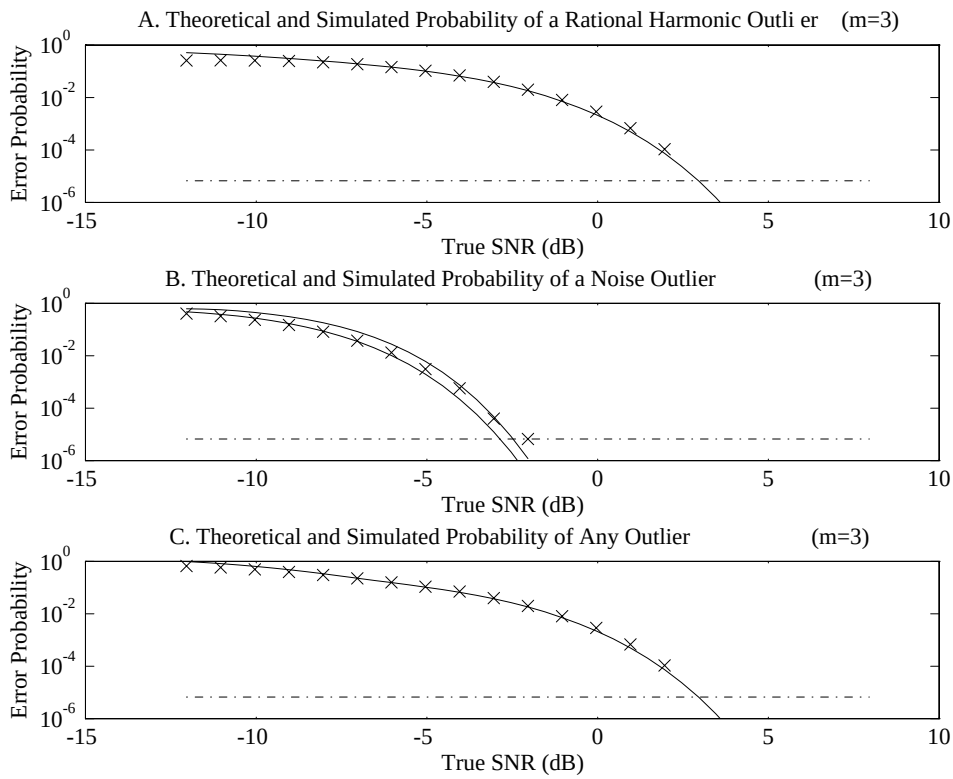

Figure 8: Simulation and theoretical outlier probabilities for case (iii) $b = [4, 2, 0]$. The curves represent:

x the simulation results

— the theoretically derived results and

$- \cdot - \cdot -$ the inverse of the number of realisations (*i.e.* the smallest possible non-zero simulated probability).

approximations used in this paper mean that performance may be calculated, with accuracy, only down to moderately low SNR's within the threshold region. This is, however, more than sufficient for establishing the existence of a threshold point, and calculating performance in its vicinity.

Some of the problems of the analysis include the fact that it does not provide insight into key quantities that might govern threshold, and that special numerical issues arise in the performance calculations due to the very small numbers involved in the evaluation of L (see the remarks at the beginning of Section 5). A different approach to threshold determination is pursued in [11] and [12] where insights into key quantities governing threshold are presented.

The issue of rational harmonic outliers was also raised, and it was noted that their inclusion in the measure of performance of the MLE is in some ways inappropriate. A means of recognizing these outliers is practically of great importance.

7 Acknowledgement

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8 Appendix A: Proof of Lemma 3.1

Let $\Phi_L^{(m)} = \{k : k \in \Phi^{(m)} \text{ and } k < 1\}$ and so $\Phi^{(m)} = \{k, \frac{1}{k} : k \in \Phi_L^{(m)}\}$ and $\#\Phi^{(m)} = 2\#\Phi_L^{(m)}$. Now observe that $\Phi_L^{(m)} = \Phi_L^{(m-1)} \cup \{\frac{k}{m} : \gcd(k, m) = 1\}$. Hence we have

$$\#\Phi_L^{(m)} = \#\Phi_L^{(m-1)} + \phi(m)$$

and the lemma follows by iteration of this relationship.

9 Appendix B: Proof of Lemma 3.2

In order to determine bounds on $F_G(x)$ we use the following results from [13].

Definition 9.1 *The random variables $T_1, \ldots, T_n$ are* associated *if*

$$cov[f(T_1, \ldots, T_n), g(T_1, \ldots, T_n)] \geq 0$$

for all functions f and g which are non-decreasing in each place, and for which $Ef(T_1, \ldots, T_n)$, $Eg(T_1, \ldots, T_n)$ and $Ef(T_1, \ldots, T_n)g(T_1, \ldots, T_n)$ exist.

The following two theorems are proven in [13].

Theorem 9.1

1. *Any subset of associated random variables is associated.*
2. *If two sets of associated random variables are independent of each other, then their union is a set of associated random variables.*
3. *The set consisting of a single random variable is associated.*
4. *Non-decreasing functions of associated random variables are associated.*
5. *Independent random variables are associated.*

Theorem 9.2 *Let $T_1, \ldots, T_n$ be associated random variables, $V_i \triangleq f_i(T_1, \ldots, T_n)$, and f_i non-decreasing $(i = 1, \ldots, k)$. Then*

$$\Pr[V_1 \leq s_1, \ldots, V_k \leq s_k] \geq \prod_{i=1}^{k} \Pr[V_i \leq s_i] \tag{63}$$

for all $s_1, \ldots, s_k$.

Lower (upper) bound on $F_G(x)$ ($\overline{F}_G(x)$)

The random variables defined by $|A(\hat{\omega}_k)|^2$ and $|A(\hat{\omega}_l)|^2$ are independent for $k \neq l$ (see [14], where it is shown that N samples of a length N DFT of white gaussian noise are independent). The elements of the set $\{|A(\hat{\omega}_k)|^2 : 1 \leq k \leq N\}$ are therefore associated random variables by point 5 of Theorem 9.1. From the definitions of D_k and $L(\omega)$ in (22) and (14), there holds

$$D_k = \sum_{i=1}^{m} |A(i\hat{\omega}_k)|^2 \ . \tag{64}$$

The set $\{D_k : 1 \leq k \leq N\}$ therefore defines a set of nondecreasing functions of the associated random variables $|A(\cdot)|^2$, which by point 4 of Theorem 9.1 are themselves associated. It follows trivially from point 1 of Theorem 9.1 that $\{D_k : k \in \mathcal{N}\}$ defines a set of associated random variables. This fact, and Theorem 9.2, enables determination of a lower bound on $F_G(x)$ as follows.

From the definition of $F_G(x)$ there holds

$$F_G(x) = \Pr(\max_{k \in \mathcal{N}} D_k < x) \ . \tag{65}$$

Application of Theorem 9.2 to the RHS of (65) gives

$$\begin{aligned} \Pr(\max_{k \in \mathcal{N}} D_k < x) &\geq \prod_{k \in \mathcal{N}} \Pr(D_k < x) \\ &= [F_{D_k}(x)]^{N - \nu(m) - 1} \end{aligned} \tag{66}$$

(since the D_k are identically distributed for $k \in \mathcal{N}$).

Therefore,

$$[F_{D_k}(x)]^{N-\nu(m)-1} \leq F_G(x) \tag{67}$$

and

$$\overline{F}_G(x) \leq 1 - [F_{D_k}(x)]^{N-\nu(m)-1} \ . \tag{68}$$

Upper (lower) bound on $F_G(x)$ ($\overline{F}_G(x)$)

Suppose that we find the largest $\mathcal{K} \subset \mathcal{N}$ with the property that the elements of the set $\{D_k : k \in \mathcal{K}\}$ are all mutually independent. Let $\mathrm{df}(X)$ denote the c.d.f. of the random variable X. Suppose X and Y are independent random variables, then (see [15])

$$\mathrm{df}[\max(X,Y)] = \mathrm{df}(X)\mathrm{df}(Y) \ . \tag{69}$$

Therefore,

$$\mathrm{df}(\max_{k\in\mathcal{K}} D_k) = \prod_{k\in\mathcal{K}} F_{D_k}(x) = [F_{D_k}(x)]^{\#\mathcal{K}} \tag{70}$$

since, by definition, the elements of $\{D_k : k \in \mathcal{K}\}$ are all independent.

Given the definition of G in (29) there holds

$$G = \max(X,Y) \tag{71}$$

where

$$X \triangleq \max_{k\in\mathcal{K}} D_k \tag{72a}$$

$$Y \triangleq \max_{k\in\mathcal{N}\setminus\mathcal{K}} D_k. \tag{72b}$$

We may then write

$$F_G(x) = \Pr(G < x) = \Pr(X < x, Y < x) = F_{XY}(x,x) \tag{73}$$

where $F_{XY}(x,x)$ is the joint c.d.f. of X and Y. It is easy to see that for *any* random variables X, Y, there holds

$$F_{XY}(x,x) \leq F_X(x) \tag{74}$$

where $F_X(x)$ is the c.d.f. of X. Therefore, for our particular X and Y,

$$F_G(x) = F_{XY}(x,x) \leq F_X(x), \tag{75}$$

where from (70)

$$F_X(x) = [F_{D_k}(x)]^{\#\mathcal{K}}, \tag{76}$$

with the result that

$$F_G(x) \leq [F_{D_k}(x)]^{\#\mathcal{K}}. \tag{77}$$

We now need to calculate the cardinality of $\mathcal{K}$, $\#\mathcal{K}$. The following result helps us to find the cardinality of a large $\mathcal{K} \subset \mathcal{N}$ with the property that the elements of the set $\{D_k : k \in \mathcal{K}\}$ are all independent, by first defining a certain set K^{Π}.

Lemma 9.1 *Let $K^{\Pi} \triangleq \{p_1, \ldots, p_v\}$ be the set of all primes p_i such that $m \leq p_i < N$. Then the set $D^{\Pi} \triangleq \{D_k : k \in K^{\Pi}\}$ contains only D_k which are mutually independent. Furthermore, $\#D^{\Pi} = \Pi(m,N) \triangleq \pi_{N-1} - \pi_m$ where π_n is the standard number theoretic function denoting the number of primes not exceeding n.*

Proof We need to show that for all $p_j, p_l \in K^{\Pi}$, there does not exist any $i, k \in \{1, \ldots, m\}$, $i \neq k$ such that

$$ip_j = kp_l.$$

This can be seen to be true since $p_j, p_l \geq m$ for all j, l. Let $\Pi(m,N)$ denote the number of primes p greater than or equal to m and less than N. Clearly $\Pi(m,N) = \#K^{\Pi}$ and $\Pi(m,N) = \pi_{N-1} - \pi_m$ where π_n is the number of primes not greater than n.

∎

Note that while there is no simple formula for π_n it can be calculated via enumeration for moderate n, and asymptotically using the prime number theorem (see [7]) ($\pi_n \sim$

$\frac{n}{\log n}$). A table of $\Pi(m, N)$ for $m = 5$ is given below.

N	32	64	128	256	512	1024	2048	4096	8192	16384	65356
$\Pi(5, N)$	9	16	29	52	95	170	307	562	1026	1898	6540

We will assume that m, N and r have been chosen so that the rational harmonic frequencies all coincide with bin frequencies. (See the comment after Lemma 3.1.) If we define

$$\mathcal{R}_{sub} \triangleq \{\rho r : \ \rho \in \Phi_{sub}\} \tag{78}$$

where Φ_{sub} is, as previously defined, the set $\{\rho : \ \rho = 1/k \ , \ 2 \leq k \leq m\}$, then it is easy to see (from the definition of $\Phi^{(m)}$) that the elements of $\mathcal{R} \setminus \mathcal{R}_{sub}$ are not prime (note that $\mathcal{R}_{sub} \subset \mathcal{R}$). Thus there can be at *most* $\#\mathcal{R}_{sub} = m - 1$ elements of K^{Π} that belong to $\mathcal{R}$ and which therefore do *not* belong to $\mathcal{N}$. Those elements are simply the subharmonic frequency indices that are *prime*. One way to derive a large set $\mathcal{K} \subset \mathcal{N}$ with the desired property, is simply to remove from K^{Π} those indices that do not belong to $\mathcal{N}$. Those indices can only be prime subharmonic indices, of which there are at most $m - 1$. Therefore define

$$\mathcal{K} \triangleq K^{\Pi} \setminus \mathcal{R}_{sub}. \tag{79}$$

There then holds

$$\#\mathcal{K} \geq \Pi(m, N) - m + 1 \ . \tag{80}$$

We remark that some further work might be able to establish just how many elements of $\mathcal{R}_{sub}$, given m, r and N, are prime. We feel that this effort is hardly justified in view of the observed insensitivity of calculations based on the above results with respect to small changes in the bound in (80).

Combination of (80) and (77) gives

$$F_G(x) \leq [F_{D_k}(x)]^{\Pi(m,N)-m+1} \tag{81}$$

and

$$\overline{F}_G(x) \geq 1 - [F_{D_k}(x)]^{\Pi(m,N)-m+1} \quad . \tag{82}$$

This concludes the proof of Lemma (3.2).

10 Appendix C: Derivation of F_{D_k}, $k \neq r$, and f_{D_r}

The c.d.f. of D_k, $k \neq r$

First consider D_k. We have

$$D_k = \sum_{i=1}^{m} |A(i\omega_k)|^2 = \sum_{i=1}^{m} C_k^2$$

where C_k is a quantity used by Rife and Boorstyn [4]. They give the p.d.f. of C_k as:

$$f_{C_k}(x) = \frac{Nx}{\sigma^2} \exp\left(\frac{-Nx^2}{2\sigma^2}\right) \tag{83}$$

for $x \geq 0$ and zero otherwise. We require $f_{C_k^2}(x)$. Given a random variable X, with p.d.f. f_X, then the p.d.f. of $Y = X^2$ is given by [15]

$$f_Y(y) = \frac{1}{2\sqrt{y}} \left(f_X(\sqrt{y}) + f_X(-\sqrt{y})\right). \tag{84}$$

Combining (83) and (84) gives

$$\begin{aligned} f_{C_k^2}(x) &= \frac{1}{2\sqrt{x}} f_{C_k}(\sqrt{x}) \\ &= \frac{N}{2\sigma^2} \exp\left(\frac{-Nx}{2\sigma^2}\right). \end{aligned}$$

Now observe that the p.d.f. of a χ^2 random variable with ν degrees of freedom is

$$f_{\chi^2}(x) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)} \exp\left(\frac{-x}{2}\right) x^{\frac{\nu}{2}-1}.$$

We can thus see that $\left(\frac{NC_k^2}{\sigma^2}\right)$ is χ^2 with 2 degrees of freedom.

Since $D_k = \sum_{j=1}^{m} C_j^2$, and all the C_j are i.i.d., $\left(\frac{ND_k}{\sigma^2}\right)$ is χ^2 with $2m$ degrees of freedom. Thus

$$f_{D_k}(x) = \frac{N}{\sigma^2}\frac{1}{2^m\Gamma(m)}\exp\left(\frac{-Nx}{2\sigma^2}\right)\left(\frac{Nx}{\sigma^2}\right)^{m-1} \qquad x \geq 0. \tag{85}$$

The cumulative distribution of a χ^2 random variable with ν degrees of freedom is

$$\begin{aligned} F(y) &= \int_0^y \frac{1}{2^{\nu/2}\Gamma(\nu/2)}\exp\left(\frac{-t}{2}\right)t^{\frac{\nu}{2}-1}dt \\ &= \frac{1}{\Gamma(\nu/2)}\gamma(\frac{\nu}{2},\frac{y}{2}), \end{aligned}$$

and $\gamma(\cdot,\cdot)$ is the incomplete gamma function

$$\gamma(a,x) = \int_0^x e^{-t}t^{a-1}dt. \tag{86}$$

Thus we can write the distribution function of D_k as

$$F_{D_k}(x) = \frac{1}{\Gamma(m)}\gamma(m,\frac{Nx}{2\sigma^2}) \tag{87}$$

The p.d.f. of D_r

We determine the distribution of D_r in terms of quantities defined by Rife and Boorstyn. We have

$$D_r = \sum_{i=1}^{m} C_{r,i}^2$$

and $C_{r,i}$ is distributed identically to Rife and Boorstyn's C_r (see equation (54), [4]). They give the p.d.f. of C_r (a Rician random variable) as:

$$f_{C_r}(x) = \frac{Nx}{\sigma^2}\exp\left[\frac{-N(x^2+b_0^2)}{2\sigma^2}\right]I_0\left(\frac{Nb_0x}{\sigma^2}\right),$$

where b_0 is the amplitude of the single tone and I_k is the modified Bessel function of the first kind, of order k. Again using the $Y = X^2$ transformation we obtain

$$f_{C_r^2}(y) = \frac{N}{2\sigma^2}\exp\left[\frac{-N(y+b_0^2)}{2\sigma^2}\right]I_0\left(\frac{Nb_0\sqrt{y}}{\sigma^2}\right).$$

This can be seen to be of the same form as a non-central χ^2 distribution. The p.d.f. of a non-central χ^2 random variable with ν degrees of freedom and non-centrality parameter λ is (see [16]):

$$f(x) = \frac{1}{2}\left(\frac{x}{\lambda}\right)^{\frac{1}{4}(\nu-2)} \exp\left[\frac{-1}{2}(\lambda + x)\right] I_{\frac{1}{2}(\nu-2)}(\sqrt{\lambda x}). \tag{88}$$

Comparison of these densities shows that $\left(\frac{NC_r^2}{\sigma^2}\right)$ is non-central χ^2 with 2 degrees of freedom and non-centrality parameter $\lambda = b_0^2$. Hence using the convolution properties of the non-central χ^2 distribution (from [16]) and the fact that all the $C_{r,i}$ are i.i.d., we can conclude that $\left(\frac{ND_r}{\sigma^2}\right)$ is non-central χ^2 with $2m$ degrees of freedom and non-centrality parameter $\lambda = \sum_{i=1}^{m} b_i^2$. Thus the p.d.f. of D_r is

$$f_{D_r}(x) = \frac{N}{2\sigma^2}\left(\frac{x}{\lambda}\right)^{\frac{m-1}{2}} \exp\left[\frac{-N}{2\sigma^2}(\lambda + x)\right] I_{m-1}(\frac{N}{\sigma^2}\sqrt{\lambda x}) \tag{89}$$

where $\lambda = \sum_{i=1}^{m} b_i^2$.