CLOSED FORM FREQUENCY DOMAIN EXPRESSIONS FOR BEST ACHIEVABLE ACCURACY OF SPECTRAL DENSITY ESTIMATION

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ABSTRACT

This paper addresses the issue of quantifying the frequency domain accuracy of ARMA spectral estimates as dictated by the Cramér–Rao Lower Bound (CRLB). Classical work in this area has led to expressions that are asymptotically exact as both data length and model order tend to infinity, although they are commonly used in finite model order and finite data length settings as approximations. More recent work has established quantifications which, for AR models, are exact for finite model order. By employing new analysis methods based on rational orthonormal parameterisations, together with the ideas of reproducing kernel Hilbert spaces, this paper develops quantifications that extend this previous work by being exact for finite model order in all of the AR, MA and ARMA system cases. These quantifications, via their explicit dependence on poles and zeros of the underlying spectral factor, reveal certain fundamental aspects of the accuracy achievable by spectral estimates of ARMA processes.

1. INTRODUCTION

In a wide variety of applications including adaptive filtering, acoustics, econometrics, array processing, radar and speech processing it is necessary to estimate the correlation structure of a signal that can be modelled as a stationary stochastic process $\{y_t\}$.

This correlation structure is completely described by the spectral density $\Phi_y(\omega)$ of the process, and in turn this is often of interest in its own right. While there is a very large variety of methods available to estimate such a spectral density [1, 2, 3, 4], when it has a finite order rational form, the approach of using an ARMA model structure together with a Maximum–Likelihood criterion is well known to offer optimal accuracy, in the sense that the Cramér–Rao lower bound (CRLB) on parameter space variability is asymptotically achieved as the data length tends to infinity.

Via a first order Taylor series argument, this also implies that the associated estimate of the spectral density $\Phi_y(\omega)$ also asymptotically achieves its Cramér–Rao bound. This opens the question of quantifying what this bound on the estimate of $\Phi_y(\omega)$ is, both in order to inform what problem aspects might limit or enhance estimation accuracy, and also to actually quantify that accuracy.

Recognising this importance, several prior works (eg. [5, 6]) have sought to find expressions for it. A central motif of those contributions has been to simplify what appear to be quite complex expressions by a strategy of allowing the model order to tend to infinity, and then using the ensuing asymptotic in model order result as an approximate quantification applying for finite model order.

This paper progresses beyond this work by establishing quantifications that are exact for finite model order and hence a more accurate than pre-existing expressions which were only approximate for finite model order. In particular, the work here establishes that with $\Phi_y(\omega,\widehat{\theta}_N)$ denoting an estimate of the spectrum $\Phi_y(\omega)$ based on an intervening estimate $\widehat{\theta}_N$ of the ARMA parameters, then

$$\lim_{N\to\infty} N\mathrm{Var}\left\{\frac{\Phi_y(\omega,\widehat{\theta}_N)}{\Phi_y(\omega)}\right\} = 2\left[\sum_{k=0}^{2m-1}\frac{1-|\xi_k|^2}{|e^{j\omega}-\xi_k|^2}+ \mathrm{Re}\left\{\sum_{k=0}^{2m-1}\frac{1-\xi_k^2}{(e^{j\omega}-\xi_k)^2}\prod_{\ell=0}^{k-1}\left(\frac{1-\xi_\ell e^{j\omega}}{e^{j\omega}-\xi_\ell}\right)^2\right\}\right]. \quad (1)$$

Here N is the length of the data record used to generate the parameter estimate $\widehat{\theta}_N$, and $\{\xi_0,\cdots,\xi_{2m-1}\}$ are the poles and zeros of the m'th order ARMA representation which here (but not later) are assumed all real valued and also here (but not later) it has been assumed that the minimal one-step ahead prediction error variance σ^2 is known.

This establishes, for example, that the spectral estimate will be less accurate at frequencies close to any poles *or* zeros of the underlying ARMA process. As well, it establishes a 'waterbed' effect, in that since the integral of the right hand side of (1) over $\omega\in[-\pi,\pi]$ equals $8m\pi$, then any increase in relative spectral estimation error at certain frequencies (eg. near poles or zeros close to the unit circle) must be balanced by commensurate decreases at other frequencies.

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It should be emphasised that there is a fundamental difference between the concentration in this paper on the variability of *functions of* the parameter estimates and many well known previous works that have addressed the variability of the parameters themselves, and which are not the focus of this contribution.

For example [2, Appendix B.5], [1, pp293-296] detail how the CRLB on ARMA *parameter* estimates may be reliably computed, and then indicate how the CRLB of functions of the parameters may then be numerically evaluated via computation of certain quadratic forms.

The paper here extends this pre-existing work to show how *closed form* expressions for these quadratic forms may be derived. Apart from adding new insight into the parametric spectral estimation problem, the closed forms presented here also provides alternative means for reliably evaluating the associated CRLB.

2. PROBLEM FORMULATION AND BACKGROUND

Suppose that $\{y_t\}$ is a wide sense stationary and zero mean stochastic process with spectral density $\Phi_y(\omega)$ which is assumed to be bounded away from zero so that the Paley–Wiener condition is satisfied, and hence $\{y_t\}$ is a regular process that possesses a Wold decomposition devoid of deterministic component as follows

$$y_t = e_t + \sum_{n=1}^{\infty} h_n e_{t-n}. \tag{2}$$

Here $\{e_t\}$ is a zero mean i.i.d. process of variance $\mathbf{E}\left\{e_t^2\right\} = \sigma^2$ and the spectral factor

$$H(z) \quad = \quad 1 + \sum_{n=1}^{\infty} h_n z^{-n} \tag{3}$$

and its inverse $H^{-1}(z)$ are both analytic in $|z| \geq 1$. This permits an alternative expression for the power spectral density $\Phi_y(\omega)$ of $\{y_t\}$ in terms of this spectral factor $H(z)$ as

$$\Phi_y(\omega) = \sigma^2 |H(e^{j\omega})|^2.$$

Now, as mentioned in the introduction, it is often of interest to estimate this spectral density from observations of a realisation of $\{y_t\}$. Considering that the class of rational $|H(e^{j\omega})|^2$ are dense within the space of all continuous ones (with respect to the supremum norm) then a common strategy for estimating $\Phi_y(\omega)$ is to express (2) according to the so-called Auto-Regressive Moving Average (ARMA) model structure [7, 8, 9]

$$y_t = H(q,\theta) e_t = \frac{C(q,\theta)}{D(q,\theta)} e_t \tag{4}$$

where the numerator and denominator polynomials are of the form

$$D(q,\theta) \quad = \quad q^m + d_{m-1}q^{m-1} + \cdots + d_1 q + d_0, \tag{5}$$
$$C(q,\theta) \quad = \quad q^m + c_{m-1}q^{m-1} + \cdots + c_1 q + c_0 \tag{6}$$

and the parameter vector $\theta \in \mathbf{R}^n$ (with $n = 2m$) is defined as the vector of real valued co-efficients

$$\theta = [d_0, c_0, d_1, c_1, \cdots, d_{m-1}, c_{m-1}]^T.$$

There are two important sub-classes of this model structure; the Autoregressive (AR) and Moving Average (MA) cases which occur when (respectively) $C(q,\theta) = q^m$ and $D(q,\theta) = q^m$ are specified.

For all these AR, MA and ARMA cases, the mean-square optimal one-step ahead predictor $\widehat{y}_{t|t-1}(\theta)$ based on the model structure (4) is [7]

$$\widehat{y}_{t|t-1}(\theta) = \left[1 - H^{-1}(q,\theta)\right] y_t$$

with associated prediction error

$$\varepsilon_t(\theta) \triangleq y_t - \widehat{y}_{t|t-1}(\theta) = H^{-1}(q,\theta) y_t. \tag{7}$$

Therefore, if $\{e_t\}$ has a Gaussian distribution, then the Maximum Likelihood estimates $\widehat{\theta}_N$ and $\widehat{\sigma}^2_N$ of θ and σ^2 are given as

$$\widehat{\theta}_N \triangleq \arg\min_{\theta \in \mathbf{R}} \frac{1}{N} \sum_{t=1}^{N} \varepsilon_t^2(\theta), \qquad \widehat{\sigma}^2_N = \frac{1}{N} \sum_{t=1}^{N} \varepsilon_t^2(\widehat{\theta}_N). \tag{8}$$

This then leads to an estimate $H(z, \widehat{\theta}_N)$ of the spectral factor $H(z)$ in (3) and thereby also of the spectral density; viz.

$$\Phi_y(\omega, \widehat{\theta}_N) = \widehat{\sigma}^2_N \left| H(e^{j\omega}, \widehat{\theta}_N) \right|^2. \tag{9}$$

It is known that this Maximum–Likelihood approach leads to an estimate variability Var $\left\{\Phi_y(\omega, \widehat{\theta}_N)\right\}$ that asymptotically in the data length achieves the Cramér–Rao lower bound [7, 9, 8]. The focus of this paper is to provide an explicit formula for this bound, since it also quantifies the asymptotic variability of the spectral estimate (9) formed via (8) for cases in which $\{e_t\}$ is not Gaussian [10].

The importance of this evaluation of the CRLB was first recognised in [5] which established that for AR model structures

$$\lim_{m\to\infty} \lim_{N\to\infty} \frac{N}{m} \text{Var}\left\{\Phi_y(\omega, \widehat{\theta}_N)\right\} = 2\Phi_y^2(\omega), \qquad \omega \neq 0, \pi \tag{10}$$

which suggests the approximate quantification

$$\text{Var}\left\{\Phi_y(\omega, \widehat{\theta}_N)\right\} \approx \frac{2m}{N} \cdot \Phi_y^2(\omega), \qquad \omega \neq 0, \pi. \tag{11}$$

Later, the result (10) (and hence (11)) was shown to also be applicable in the case of ARMA modelling [6].

The motivation for allowing the model order to tend to infinity in (10) is to facilitate the derivation of a simple expression, such as the right hand side of (10). The clear drawback of this strategy is that it requires approximate convergence in (10) to have occurred in order for the ensuing quantification (11) to be accurate, and it is difficult to ensure that this convergence holds in practise.

The contribution of this paper is to present a new reproducing kernel based analysis method, which quantifies the CRLB on Var $\left\{\Phi_y(\omega,\widehat{\theta}_N)\right\}$ in closed form and without requiring that $m\to\infty$, while also addressing all of the parametric AR, MA and ARMA modelling cases.

3. MAIN RESULT

The main result of this paper is the following closed form quantification for the asymptotic (in data length N) variability of the parametric spectral density estimate (9).

Theorem 3.1. *Suppose that $\widehat{\theta}_N$ is calculated via (4)–(8) using the m'th order ARMA model structure (4), and that the data $\{y_t\}$ has true underlying spectral factor of $H(z) = C(z)/D(z)$ of minimal order equal to m. Suppose further that the zeros $\{\xi_k\}$ defined by*

$$C(z)D(z) = (z-\xi_0)(z-\xi_1)\cdots(z-\xi_{2m-1}) \qquad (12)$$

are all strictly within the open unit disk $\mathbf{D}$, and that $\{e_t\}$ satisfies the conditions

$$\boldsymbol{E}\left\{e_t^2\right\} = \sigma^2 < \infty, \qquad \boldsymbol{E}\left\{|e_t|^{4+\epsilon}\right\} < \infty \qquad (13)$$

for some $\epsilon > 0$. Then

$$\sqrt{N}\begin{bmatrix}\Phi_y(\omega,\widehat{\theta}_N)-\Phi_y(\omega)\\ \Phi_y(\lambda,\widehat{\theta}_N)-\Phi_y(\lambda)\end{bmatrix} \xrightarrow{\mathcal{D}} \mathcal{N}(0,\Sigma(\omega,\lambda))$$

as $N\to\infty$ where

$$\Sigma(\omega,\lambda) = \begin{bmatrix}|H(e^{j\omega})|^2 & 0\\ 0 & |H(e^{j\lambda})|^2\end{bmatrix}\times$$

$$\left[\mu I_2 + 2\sigma^4\Gamma(\omega,\lambda)\right]\begin{bmatrix}|H(e^{j\omega})|^2 & 0\\ 0 & |H(e^{j\lambda})|^2\end{bmatrix}$$

$$\Gamma(\omega,\lambda)\triangleq \mathit{Re}\left\{\begin{bmatrix}\varphi_m(\omega,\omega)+\psi_m(\omega,\omega) & \varphi_m(\lambda,\omega)+\psi_m(\lambda,\omega)\\ \varphi_m(\lambda,\omega)+\psi_m(\lambda,\omega) & \varphi_m(\lambda,\lambda)+\psi_m(\lambda,\lambda)\end{bmatrix}\right\}$$

where

$$\varphi_m(\lambda,\omega) = \sum_{k=0}^{2m-1}\frac{1-|\xi_k|^2}{(e^{j\lambda}-\xi_k)(e^{-j\omega}-\overline{\xi_k})}\times$$

$$\prod_{\ell=0}^{k-1}\left(\frac{1-e^{j\lambda}\overline{\xi_\ell}}{e^{j\lambda}-\xi_\ell}\right)\left(\frac{1-e^{-j\omega}\xi_\ell}{e^{-j\omega}-\overline{\xi_\ell}}\right) \qquad (14)$$

$$\psi_m(\lambda,\omega) = \varphi_{m-\rho}(\lambda,-\omega)+\sum_{\tau=0}^{\rho-1}\zeta_\tau(e^{j\lambda})\zeta_\tau(e^{j\omega}) \qquad (15)$$

with

$$\zeta_\tau(z)\triangleq\frac{\sqrt{1-|\xi_{r(\tau)}|^4}(z-\alpha)}{(z-\xi_{r(\tau)})(z-\overline{\xi_{r(\tau)}})}\prod_{\ell=0}^{r(\tau)-1}\left(\frac{1-\overline{\xi_\ell}z}{z-\xi_\ell}\right) \qquad (16)$$

$$r(\tau)\triangleq 2(m-\rho+\tau),\ \alpha\triangleq\frac{\xi_r(\tau)+\overline{\xi}_r(\tau)-\sqrt{(1-\xi^2_{r(\tau)})(1-\overline{\xi}^2_{r(\tau)})}}{1+|\xi_{r(\tau)}|^2}. \qquad (17)$$

In (15)– (17) it has been assumed (without loss of generality) that the zeros defined by (12) are arranged so that the first $2(m-\rho)$ of them are purely real valued, and the remaining 2ρ then occur in complex conjugate pairs.

The result also holds for the AR and MA cases with the following modifications:

1. *The model order m can be greater than an underlying true one ℓ;*
2. *The substitutions $C(z)=1$ and $D(z)=1$ in (12) are made for the AR or MA cases (respectively);*
3. *The zeros $\{\xi_{\ell+1},\cdots,\xi_m\}$ in (12) are set to zero.*

The most important consequence of this theorem is that it establishes the result

$$\lim_{N\to\infty} N\mathrm{Var}\left\{\frac{\Phi_y(\omega,\widehat{\theta}_N)}{\Phi_y(\omega)}\right\} = \frac{\mu}{\sigma^4}+2\mathrm{Re}\left\{\varphi_m(\omega,\omega)+\psi_m(\omega,\omega)\right\}. \qquad (18)$$

The first key point about (18) is that, via the formulae (14)-(15), it is a *closed form* expression for the asymptotic in N variability for all of the cases of AR, MA and ARMA parametric spectral estimates $\Phi_y(\omega,\widehat{\theta}_N)$.

The second key point about this closed form expression (18) is that, again in contrast to previous work such as [5, 7], it is *not* derived via an argument that is asymptotic in the model order m. Therefore, the approximation this paper now proposes for the practical case of finite data length N *and* finite model order settings of

$$\mathrm{Var}\left\{\frac{\Phi_y(\omega,\widehat{\theta}_N)}{\Phi_y(\omega)}\right\}\approx\frac{1}{N}\left[\frac{\mu}{\sigma^4}+2\mathrm{Re}\left\{\varphi_m(\omega,\omega)+\psi_m(\omega,\omega)\right\}\right] \qquad (19)$$

is likely to be far more accurate that ones such as (11) derived from previous results such as (10) which require $m\to\infty$. This is illustrated via simulation example in the following section.

The third key point is that the closed form expressions (18), (19) highlight that because all the denominators in (14), (15) are small when $e^{j\omega}$ is close to any of the $\{\xi_k\}$, then the relative estimation error is likely to be larger at those frequencies near both the poles *and* zeros of the underlying spectral factor $H(z)$. Furthermore, this relative estimation error is likely to be larger when those poles or zeros are very close to the unit circle, then when they are not.

Finally, returning to (18) which applies for any real or complex value of $\{\xi_k\}$, it can be used to establish that the average relative estimation error over all frequencies is given as

$$\lim_{N\to\infty} \frac{N}{2\pi}\int_{-\pi}^{\pi} \mathrm{Var}\left\{\frac{\Phi_y(\omega,\widehat{\theta}_N)}{\Phi_y(\omega)}\right\} \mathrm{d}\omega = \frac{\mu}{\sigma^4} + 4m. \quad (20)$$

This illustrates a "waterbed effect" in that, although as just discussed, the expression (18) indicates increased relative error near poles and zeros, with increased effect according to distance from the unit circle, these effects must be balanced by a commensurate *decrease* in relative error at other frequencies, since the average (over frequency) relative error depends only on the model order.

4. SIMULATION EXAMPLES

In order to provide concrete illustration of the results presented here, consider the case of a true ARMA system with spectral factor

$$H(z) = \frac{z^3 - 1.9235z^2 + 1.5910z - 0.5203}{z^3 - 1.9464z^2 + 1.5155z - 0.5368} \quad (21)$$

and suppose that the innovations driving this are Gaussian distributed with variance $\sigma^2 = 1$. Then according to (18), the variability of a Maximum–Likelihood estimate of the associated spectral density $\Phi_y(\omega)$ should be quantifiable via the CRLB for this estimation problem according to (19). This can be compared with the previous asymptotic results [5, 6], which are asymptotic in both data length N *and* model order m according to (10), and which have led to the pre-existing approximation

$$\mathrm{Var}\left\{\Phi_y(\omega,\widehat{\theta}_N)\right\} \approx \frac{1}{N}\Phi_y^2(\omega)\left[\frac{\mu}{\sigma^4} + 2m\right]. \quad (22)$$

Note that the first term within accounts for the possibility of estimating the value of σ^2, while previous work leading to (10) assumed this was known,

With this in mind, the new expression (19), whose accuracy does not depend on m is essentially different from (22) according to the φ_m and ψ_m terms, which are determined by the zeros of $C(z)$ and $D(z)$ in $H(z) = C(z)/D(z)$, which in this case are given as

$$\{\xi_k\} = \left\{0.7165, 0.9429, 0.852e^{\pm j0.784}, 0.7545e^{\pm j0.8433}\right\}. \quad (23)$$

The utility of the ensuing new quantification (19) is illustrated in figure 1, where it is profiled as a dashed line together with the 'true' variability $\mathrm{Var}\left\{\Phi_y(\omega,\widehat{\theta}_N)\right\}$ which is estimated in a Monte–Carlo fashion by computing the sample variance over 1000 simulation experiments, each of which involves $N = 10000$ data points. Clearly, the agreement is excellent, and certainly superior to the pre-existing quantification (22), which is shown as the dash-dot line.

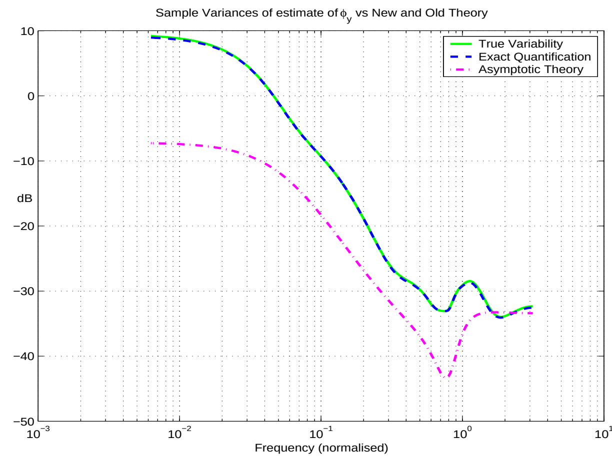

Fig. 1. *Variability of $\Phi_y(e^{j\omega},\widehat{\theta}_N)$. The solid line is the true variability, as estimated via averaging over Monte–Carlo trial, the dashed line exactly matching it is the new quantification (19) of this paper, while the dash-dot line is the pre-existing quantification (22) which depends on an asymptotic in model order argument.*

5. REFERENCES

[1] S. M. Kay, *Modern Spectral Estimation: Theory and Application*, Prentice Hall, 1987.

[2] Petre Stoica and Randolph Moses, *Introduction to Spectral Analysis*, Prentice Hall, 1997.

[3] David R. Brillinger, *Time Series: Data Analysis and Theory*, Holden-Day, 1981.

[4] M.B. Priestley, *Spectral Analysis and Time Series*, Academic Press, 1981.

[5] K. Berk, "Consistent autoregressive spectral estimates," *Annals of Statistics*, vol. 2, pp. 489–502, 1974.

[6] L.Ljung, "Asymptotic variance expressions for identified black-box transfer function models," *IEEE Transactions on Automatic Control*, vol. AC-30, no. 9, pp. 834–844, 1985.

[7] Lennart Ljung, *System Identification: Theory for the User, (2nd edition)*, Prentice-Hall, Inc., New Jersey, 1999.

[8] P.E. Caines, *Linear Stochastic Systems*, John Wiley and Sons, New York, 1988.

[9] T.Söderström and P.Stoica, *System Identification*, Prentice Hall, New York, 1989.

[10] L.Ljung and P.E.Caines, "Asymptotic Normality of prediction error estimators for approximate system models," *Stochastics*, vol. 3, pp. 29–46, 1979.