APPLICATION OF ARMA MODELING TO MULTICOMPONENT SIGNALS

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Abstract. This paper investigates the problem of estimating the parameters of a multicomponent signal observed in noise. The process is modeled as a special nonstationary autoregressive moving average (ARMA) process. The parameters of the multicomponent signal are determined from the spectral estimate of the ARMA model The spectral lines are closely spaced and the ARMA model must be determined from very short data records. Two high-resolution ARMA algorithms are developed for determining the spectral estimates. The first ARMA algorithm modifies the extended Prony method to account for the nonstationary aspects of noise in the model. For multicomponents signals with good signal to noise ratio (SNR) this algorithm provides excellent results, but for a lower SNR the performance degrades resulting in a loss in resolution. The second algorithm is based on the work of Cadzow. The algorithm presented overcomes the difficulties of Cadzow's and Kaye's algorithms and provides the coefficients for the complete model not just the spectral estimate. This algorithm performs well in resolving multicomponent signals when the SNR is low.

Keywords. Spectral Analysis; Discrete Systems; Modelling; Prediction; Parameter estimation.

INTRODUCTION

The problem of estimating highly spiked spectrums from short data records arises in all branches of Science and Engineering. Classical approaches to this problem have limited resolution because of their dependence on the data record length. More recently digital signal processing techniques using finite parameter modeling have been proposed as an alternative approach to spectral estimation. A comprehensive treatment of the topic is given by Kaye and Marple (1981). One of the major advantages of the so called modern approach is that since it is only necessary to estimate a relatively small number of parameters for the model very accurate high resolution spectra can often be obtained from short data records.

The most general finite parameter model has a feedback and moving average component and is called an autoregressive moving average (ARMA) model. A problem of particular interest which can be modelled with an ARMA model is the well known multicomponent signal (Cohn-Sfetcu, Smith and Nichols, 1975), formed by a superposition of components having the same location in time but different widths and amplitudes. These signals arise in nuclear magnetic resonance (Smith, Cohn-Stefcu and Buckmaster, 1976), compartmental analysis in physiology (Pizer and others, 1969), and pharmokinetics (Lin and Duh, 1974), to mention a few.

In this paper the multicomponent signal problem is converted to a spectral estimation problem, an ARMA model is formulated for the process and several new algorithms for determining the ARMA model are presented. Finally the algorithms are implemented and tested.

MULTICOMPONENT SIGNALS

Mathematically, the multicomponent continuous signal $s(\tau)$ formed by a superposition of components having the same location in time but different widths and amplitudes is given by

$$s(\tau) = \sum_{i=1}^{M} A_i p(\lambda_i \tau) + n(\tau) \quad (1)$$

where $\tau \varepsilon R^+$ and R^+ is the positive real line. The pulse shape $p(\tau)$ is known, while the unknown parameters M and $A_i, \lambda_i; i=1, \ldots, M$, are to be determined. For convenience the parameters λ_i are considered ordered so that $\lambda_1 < \lambda_2 \cdots < \lambda_M$. The additive noise is denoted $n(\tau)$. More generally the signal is given by the integral equation

$$s(\tau) = \int_0^{\infty} g(\lambda) p(\lambda\tau) d\lambda + n(\tau) \quad (2)$$

where the unknown function $g(\tau)$ is to be determined from the noisy observations $s(\tau)$. Equation

(1) is a particular case of the integral equation when $g(\tau)$ is given by the distribution

$$g(\tau) = \sum_{i=1}^{M} A_i\, \delta(\tau-\lambda_i), \tag{3}$$

where $\delta(\tau)$ is the dirac delta function. Smith and Cohn Sfetcu [4] showed the integral equation (2) can be mapped into a convolution integral equation. Their result is repeated here for completeness and extended slightly by multiplying by a factor of τ^a instead of τ.

Multiplying both sides of (2) by τ^a and introducing the log transformations $\tau = e^t$, $\lambda = e^{-t}$ gives the convolution integral

$$y(t) = \int_{-\infty}^{\infty} x(\lambda) h(t-\lambda) d\lambda + v(t) \tag{4}$$

for $-\infty < t < \infty$, where $y(t) = e^{at}\, s(e^t)$, $x(t) = e^{(a-1)t}\, g(e^{-t})$, $h(t) = e^{at}\, p(e^t)$ and $v(t) = e^{at}\, n(e^t)$. The input-output relationship (4) is a standard deconcolution problem when $x(t)$ is taken to be the unknown input, $h(t)$ the known impulse response of the system and $y(t)$ the noisy output observations is a standard deconvolution problem. For the multicomponent signal (1) the unknown input signal $x(t)$ is given by the distribution

$$x(t) = \sum_{i=1}^{M} B_i\, \delta(t + \ln\lambda_i) \tag{5}$$

where $B_i = A_i / \lambda_i^a$.

An estimate of the unknown signal $x(t)$ can be obtained by taking the Fourier transform of both sides of equation (4), dividing by $H(\omega)$, windowing the result and then inverse transforming to give

$$x(t) = F^{-1}\left[\frac{Y(\omega)\, W(\omega)}{H(\omega)}\right] .$$

where $W(\omega)$ is the window. Capitals are used to denote Fourier transforms. This estimate has been extensibely analyzed in the literature particularly since the advent of the FFT algorithm (Smith, Cohn-Stefcu and Buckmaster, 1976). The major advantages of such an approach to analyzing multicomponent signals are that no a-priori information on the parameters is required, all the parameters are determined simultaneously, and a reliable analysis of data could be performed by personnel unskilled in curve fitting.

The difficulties associated with this method have been detailed by a number of authors (Smith and Cohn-Stefcu, 1974, Smith and Nichols, 1983, kober, Gruble and Hillen, 1980, and Stockman, 1978). The major problems are the monotonically decreasing signal-to-noise ratio of the signals and the non-linear transformation of the experimental data $s(\tau)$ into the signal $y(t)$ used in the deconvolution equation Another problem is the resolution obtainable using linear deconvolution procedures is seriously limited by the high frequency noise introduced by deconvolution. This must be windowed off which restricts the resolution of the estimate. Roughly speaking the resolution will be limited to the reciprocal of the window width.

The use of this procedure on the analysis of true (non-simulated) experimental data from nmr analysis of tissue biopsy samples (Cohn-Stefcu and others, 1975), and activation reactions in radioactive decay (Stockman, 1978), have been reported. For experimental data the technique gave recognizable peaks, but the presence of noise required the application of filters that lead to a significant decrease in the resolution of the exponential components.

In recent years, several new digital processing techniques have become important and a wide variety of methods have been proposed for system modeling. A major advantage of the modeling technique is that since it is only necessary to estimate a relatively small number of parameters, very accurate results can often be obtained with short data records.

In the next section an ARMA model is derived for the multicomponent signal given by eqn(1).

MULTICOMPONENT ARMA MODEL

Transforming eqn. (4) and dividing by $H(\omega)$ gives the estimate

$$\tilde{X}(\omega) = \frac{Y(\omega)}{H(\omega)} = X(\omega) + N(\omega) , \tag{6}$$

where the noise

$$N(\omega) = V(\omega) / H(\omega) . \tag{7}$$

For the multicomponent signal (1), $X(\omega)$ is the Fourier transform of eqn. (5) and is a superposition of complex sinusoids given by

$$X(\omega) = \sum_{i=1}^{M} B_i e^{j\omega \ln\lambda_i} \tag{8}$$

In this case $\tilde{X}(\omega)$ is the sum of complex sinusoids in additive noise. Formulated as problem in spectral analysis $\tilde{X}(\omega)$ is the data signal while the desired spectral estimate corresponds to the distribution $x(t)$ given by eqn. (5).

To determine a finite parameter model, take uniformly spaced samples of eqn. (8) with frequency spacing $\Delta\omega$ giving

$$X_k = \sum_{i=1}^{M} B_i\, e^{j\Delta\omega \ln\lambda_i k} \tag{9}$$

for $k = 0, +=1, \ldots, +=\infty$. As $X(\omega)$ is strictly time limited with time width $\ln(\lambda_m / \lambda_1)$, for $\lambda_1 < \lambda_2 < \cdots < \lambda_M$, alaising is avoided provided $\Delta f\ ln(\lambda_M / \lambda_1) < 1$, where $\Delta\omega = 2\pi\Delta f$.

Taking the z-transform of equation (9) it is not difficult to show (Ulrych and Clayton 1976) that there is a set of M complex parameters $a_i : i = 1,2, \ldots, M$, such that the signal can be predicted exactly from M initial points using the autoregressive (AR) model

$$X_k + \sum_{i=1}^{M} a_i\, X_{k-i} = 0. \tag{10}$$

The prediction error filter

$$A(z) = 1 + \sum_{i=1}^{M} a_i z^{-i} \tag{11}$$

has roots on the unit circle given by

$$A(z) = \prod_{i=1}^{M} (1 - e^{j\Delta\omega \ln\lambda_i} z^{-1}) .$$

If the data is observed in additive noise then from equation (6) frequency samples of the estimate $\bar{X}(\omega)$ can be expressed by

$$\bar{X}_k = X_k + N_k \tag{12}$$

where N_k is due to the noise. Substituting into (10) gives the special autoregressive moving average (ARMA) model

$$\bar{X}_k + \sum_{i=1}^{M} a_i \bar{X}_{k-i} = N_k + \sum_{i=1}^{M} a_i N_{k-i} . \tag{13}$$

A similar expression is given in (Ulrych and Clayton 1976). There are however, several differences between the expression obtained by Ulrych and Clayton and equation (13). In equation (13) the signals are complex and the information signal is deterministic. Also through the original noise $n(\tau)$ is stationary, the noise samples $N_k = \frac{V_k}{H_k}$ of the deconvolved signal are nonstationary. The noise variance is given by $\sigma_N^2 = \sigma_k^2 / |H_k|^2$ where σ_k^2 denotes the variance of V_k. The noise usually increases substantially with increasing k because of the division by H_k.

In the next section two specialized algorithms are given which estimate the distribution (5).

TRANSIENT ERROR METHOD

A well known algorithm which can be used to estimate the distribution parameters $ln\lambda_i$ and B_i of eqn (5) when the noise is small, is the extended Prony method (Kay and Marple, 1981). This method is complicated for this problem because the AR model coefficients required are complex and it assumes stationary noise which is not the case. Further it is requires prior knowldege of the number of components M. Another approach called the Transient Error Method, avoids the computational difficulties of the extended Prony method and is described below.

Regard the sample values X_k, for $k \geq 0$, as the input to a discrete filter with transfer function $A(z)$. In the absence of noise the output of the filter, denoted E_k, satisfies the recursive equation

$$E_k = X_k + \sum_{i=1}^{M} a_i X_{k-i} \tag{14}$$

for $k \geq 0$. From equation (10) it follows that E_k will be zero for $k \geq M$. Because the input is taken to be zero for $k < 0$ the output transient $E_0, E_1, \ldots, E_{M-1}$ will be non-zero. Taking the z-transform of equation (14) and solving for $x(z)$ gives the ARMA model

$$x(z) = \frac{E(z)}{A(z)} . \tag{15}$$

The polynomial $A(z)$ is given by equation (11) and can be calculated once the AR model coefficients $a_1, a_2, \ldots, a_M$ are known. The polynominal $E(z)$ is calculated from

$$E(z) = \sum_{k=0}^{M-1} E_k z^{-k} ,$$

where $E_0, E_1, \ldots, E_{M-1}$ are determined from the M initial data values $X_0, X_1, \ldots, X_{M-1}$ using the equation (14). Once $A(z)$ and $E(z)$ are known equation (15) can be used to determine $x(z)$. Evaluating $x(z)$ on the unit circle gives an estimate of the distribution (5). Since the distribution has delta functions it may be necessary to move the poles of the polynominal $A(z)$ toward the origin slightly by exponentially weighting AR the model coefficients to permit calculation of the distribution. Equivalently $x(z)$ can be calculated on the circle $|z| = 1/r$ for $r < 1$.

In the presence of noise the filter output E_k will not be zero after the transient but if the AR fit gives a good model they will be small. The output transient depends on the initial data values which have much less noise than data values further from the origin because of the division by $H(\omega)$. So for the low noise equation (16) should provide a good estimate of the distribution.

Both the extended Prony method and the Transient Error method require as a first step, an algorithm to determine the AR coefficients. Two such algorithms are the well known Burg (1975) 1algorithm and Marple's (1980) least squares algorithm. Both these algorithms determine the AR coefficients based on the mean square of both the forward and backward prediction errors. Both are written for a complex data set. The use of forward and backward errors is based on the assumption that the data is weakly stationary. If the process is not weakly stationary the AR coefficients obtained from the forward prediction may be different than the AR coefficients obtained from the backward prediction. The Burg algorithm gives a minimum phase polynomial which insures a stable predictor but for short data lengths is known to biased estimates and can even result in line spitting. The LS algorithm does not insure a stable predictor but usually gives better estimates of the spectral peaks for short data lengths. The Marple LS algorithm is very sensitive to arithmetic errors and often does not converge. Another LS algorithm where the forward, backward and forward-backward predictions can be selected has been given by I. Barrodale and R.E. Errickson (1980). This algorithm was is not as efficient as the Marple algorithm but is less sensitive to arithmetic errors. This algorithm was written for real data but has been extended to complex data by the authors and is refered to as the complex least squares (CLS) algorithm. The CLS algorithm is used in this report to determine AR coefficients.

GENERAL ARMA ALGORITHM

In the previous section two special algorithms were given for determining the distribution of the multicomponent signal (1) when the noise is small. More generally if the multicomponent signal is given by the integral eqn.(2) or if the deconvolved data $X(\omega)$ is regarded as a process then it is desirable to fit $X(\omega)$ with a general ARMA model. For a process these models only give the spectral density of the signal. There are many algorithms available in the literature for determining the parameters of an ARMA model. The algorithm used in this paper is based on Cadzow's (1982) method and is referred to as the Improved Cadzow ARMA algorithm.

Cadzow's method provides high resolution estimates of the spectrum and does not produce spectral line splitting for short data records. It is computationally stable and uses Singular Value Decomposition (SVD) of the covariance matrix to obtain the order of the AR portion of the model. However, his method does not provide direct estimates of the order and parameters of the MA portion of the model and it can produce power spectral density estimates which are not positive real. An improved algorithm has been developed by the authors which overcomes the difficulties of Cadzow's method. The details of the improved algorithm are beyond the scope of the this paper but the steps involved are given below.

Improved Cadzow ARMA Algorithm

1) Select an initial guess for the AR and MA orders respectively.
2) Compute the covariance matrix of the data
3) Decompose the covariance matrix using SVD and determine the AR order from the effective rank of the matrix.
4) Calculate the AR coefficients using a pseudo inversion of the covariance matrix.
5) Compute Cadzow's modified MA coefficients and take the Fourier transform of these coefficients.
6) Check if the result obtained in 5) is positive definite. If not, the data is modified and step 5) is repeated.
7) Perform Cepstral analysis on the modified MA portion to estimate the MA coefficients and order.
8) Compute the ARMA estimate of the spectrum.

MULTICOMPONENT MODELING ALGORITHM

The steps involved in analyzing experimental multicomponent data are described below.

1) Log Transformation: The multicomponent integral equation is converted to a standard linear convolution integral by multiplying both sides of eqn.(2) by τ^{α} and then making a log transformation to get eqn.(4).

2) Discrete Time Deconvolution System: The continuous time deconvolution problem is converted into a discrete time deconvolution problem to facilitate digital analysis. This is achieved by multiplying both sides of eqn.(2) by τ^{α} and then taking log samples $\tau_n = e^{nT}$ or by uniformly sampling y(t) in eqn.(4) at a sampling rate 1/T. The sampling rate required depends on the bandwidth of the pulse. In practise one usually has uniformly spaced samples of $s(\tau)$ and it is necessary to interpolate the results to obtain the log samples. While the problem of interpolation is not investigated in this report good experimental results have been obtained using spline interpolators (Smith and Nichols, 1983).

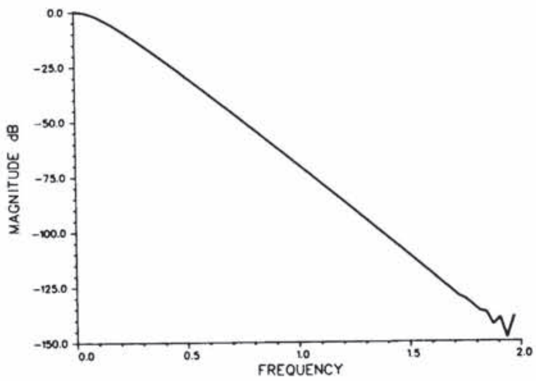

Fig. 1. Magnitude Spectrum

The class of pulses of interest are essentially time and frequency limited. For example: the exponential pulse $p(\tau) = e^{-\tau}$ maps to the pulse $h(t) = e^{(\alpha t)}e^{-e^t}$ and its magnitude spectrum is shown in Fig.1 for $\alpha = 1.0$.

In practise the noise $v(t)$ in eqn.(4) will be experimentally bandlimited to avoid aliasing effects on sampling. The previous paragraph demonstrated that the pulse h(t) can be taken to be strictly bandlimited with negligible aliasing. Denote the bandwidth by B Hz. Since the convolution integral (4) only depends on frequencies of the input signal x(t) in the same frequency range as h(t) it follows that x(t) is also effectively bandlimited to B Hz. Thus the convolution integral given by eqn.(4) can be written as the summation (Papoulis, 1977)

$$y(t) = T\sum_{-\infty}^{\infty} x(mT)h(t-mT) + v(t)$$

provided that 2BT>1. Sampling at a rate 1/T and letting x[n] = x(nT), h[n] = Th(nT), v[n] = v(nT) and y[n] = y(nT) gives the discrete time system

$$y[n] = \sum_{-\infty}^{\infty} x[m]h[n-m] + v[n]. \qquad (16)$$

3) Selection of the Data Values: The range of experimental data samples is of necessity finite and their selection is very important. The limits of the sample values for y[n] are given by $n_{MIN} < n < n_{MAX}$. The lower limit, denoted n_{MIN}, is restricted because the log spacing cannot become arbitrarily small. The upper limit, denoted n_{MAX}, best should be limited because of the monotonically decreasing signal to noise ratio of the signal. The selection of these limits requires some experimental testing. An alternative approach is to center the data between symmetrical limits, say $-n_0$ and n_0. For exponential pulses this can be achieved by multiplying the experimental data by e^{λ_0} with an appropriate selection of λ_0.

4) The Deconvolved Data Signal: The discrete time system (16) is deconvolved using an N point DFT as follows. The number of points N required for the DFT depends on range of the estimate of the distribution x[n] to avoid aliasing. For the multicomponent signal given by eqn.(1) the distribution range is $\ln(\lambda_M/\lambda_1)$ and so NT> $\ln(\lambda_M/\lambda_1)$. If N < $n_{MAX}-n_{MIN}+1$ then it is necessary to prealias the the data values y[n] and the pulse h[n] before taking their DFT's. The sample values $\bar{X}_k$ of the deconvolved data are then determined by

$$\bar{X}_k = \frac{DFT[y[n]]}{DFT[h[n]]}$$

for $-N/2 < k < N/2 - 1$, where y[n] and h[n] are aliased versions of y[n] and h[n] respectively. Because of the division by the DFT[h[n]] the estimate $\hat{X}_k$ becomes increasingly noisy and only the data values where the signal to noise ratio is high should used. Once the range of values is selected a model is fitted to the deconvolved data and the distribution is estimated.

5) Finite Parameter Model and Spectral Estimate of the Unknown Distribution: A finite parameter model is fitted to the deconvolved data values $\hat{X}_k$ for $-L < k < L$. The number of deconvolved data points is 2L+1 and L is selected to give values with good signal to noise ratios as described in step 4. Once the parameters of the selected model are determined an estimate of the unknown input distribution x(t) and hence $g(\tau)$ can both be calculated. Again it is noted that because of the way the deconvolved data is obtained, it is regarded as a frequency function while the desired distribution is its spectral estimate.

5.1) Transient Error method: For the multicomponent signal given by eqn.(1) the parameters of the unknown distribution can be estimated using the Prony method described earlier andis not used because of reasons mentioned. Another approach is to estimate the distribution x(t) using the Transient Error Method in the previous section. The steps in this method are recapped below for convience. The distribution is estimated using eqn.(15) via

$$x(z) = NT\frac{E(z)}{A(z)}$$

for $z = r^{-1}e^{-j2\pi t/NT}$, where $\Delta f = 1/NT$ and $r < 1$. The spectral estimate of the distribution is usually normalized and so the multicative factor is not required.

5.2) General Fitting Algorthms: In this paper the only general ARMA model considered is the improved Cadzow method. The method is decribed in the previous section.

SIMULATION RESULTS

To illustrate the algorithm developed in the report a multicomponent signal consisting of four exponential pulses is investigated. The purpose of this simulation is to illustrate the viability of the technique and not provide a detailed statistical study. The data signal is given by

$$s(\tau) = 0.5e^{-0.5\tau} + 2e^{-2\tau} + 5e^{-5\tau} + 10e^{-10\tau}$$

for $\tau \varepsilon R^{+}$.

Multiplying by τ^{a} and letting $\tau = e^{t}$ gives the linear deconvolution system described by eqn. (4). The distribution to be estimated is given by

$$x(t) = 0.5^{1-\alpha}\delta(t - ln 2) + 2^{1-\alpha}\delta(t + ln 2) + 5^{1-\alpha}\delta(t + ln 5)$$

$$+ 10^{1-\alpha}\delta(t + ln 10).$$

When $\alpha = 1$ all the delta functions have an equal weight of unity.

The distribution is estimated using the algorithm and described in the previous section. After the nonlinear log transformation the linear deconvolution system, given by the equation (4), is converted to a discrete time system by sampling at rate $1/T = 4.0Hz$, see Fig. 1. For $\alpha = 1$ the range of the sampled data was selected to be $n_{MIN} = -50$ and $n_{MAX} = 12$. These limits are determined by observing the sampled data. The selection of n_{MIN} is not critical but great care and usually some trail and error is required in selecting n_{MAX} since the noise is increasing exponentially. Once the range was determined, the data was transformed using a 64 point FFT algorithm and then deconvolved using equation (17). The useful range of the deconvolution data was selected to be $-16 \le k \le 16$. These limits again are critical and an initial estimate can be obtained by observing the deconvolved data. If the distribution components are widely spaced a visual selection is usually adequate, but for closely spaced impulses the deconvolution range was selected by recursively fitting the data and selecting the fit with the least normalized mean square error. The deconvolved data consists of samples of 4 complex sinusoidal signals in nonstationary noise with normalized frequencies 0.144 Hz., 0.101 Hz., 0.043 Hz. and -0.043 Hz. The associated spectrum (distribution) is estimated from 17 data points. Once the deconvolved signal is obtained the distribution can be estimated. Results for the algorithm given are shown below.

Fourier Transform Window Approach: The result obtained by windowing the deconvolved data with a Harris (1978) window to remove high frequency noise and then inverse transforming, rather than using the modelling technique described in this paper, is shown in Fig. 2 for $\alpha = 1$.

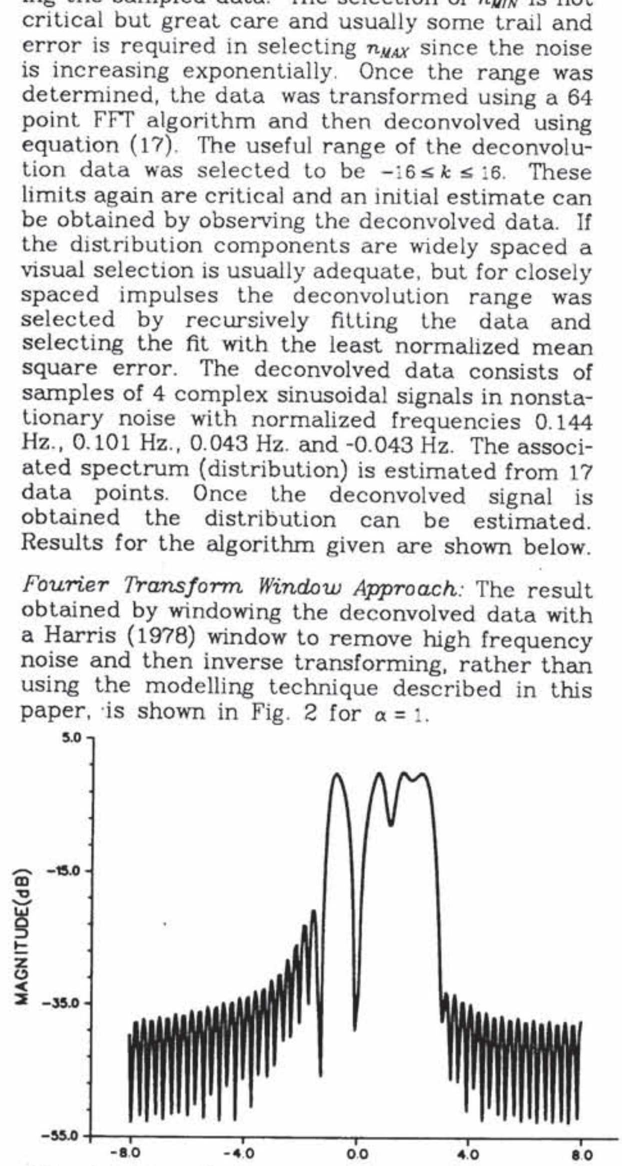

Fig. 2. Distribution Estimate using Window Method

Transient Error Method: The estimate of the distribution using the *transient error method* for the CLS algorithm is shown in Fig. 3 for $\alpha = 1$ and $\alpha = 1/2$. Both of these results was calculated for $z = 1/r \exp(2\pi jt/NT)$ with $r = 0.99$. This moves the poles away from the unit circle giving a better estimate of the peaks of the distribution. The magnitude of the results are expressed in dB and normalized to a maximum value of 0 dB. The actual peak value in both cases was 40 dB. The CLS gives very accurate location (hence an excellent estimate of λ_i) of the distribution impulses. The peaks of the distribution give a relative estimate of the amplitudes A_i/λ_i^{a}. The actual values can then be obtained by evaluating eqn. (1) for $\tau = 0.0$. For $\alpha = 1$ all the amplitudes are unity while for $\alpha = 1/2$ the amplitudes should increase as shown in Fig. 4. This method does not give as accurate an estimate of the amplitudes as it does of the impulse locations. This is expected because the poles are very close to the unit circle.

Burg's algorithm was also tested. It gave good results but the location of the peaks were slightly biased. It is well known that Burg's algorithm can give biased peak locations so the result was not unexpected. Marple's LS algorithm was also used but did not converge.

Improved Cadzow's ARMA Algorithm: The estimate of the distribution using the improved Cadzow's ARMA algorithm are shown in Fig. 4 for $\alpha = 1$ using a (4,4) ARMA model. The results of this method give excellent estimates of the peak locations but the amplitude are not as good as the previous methods. Arunachalm (1980) Burg's algorithm obtained reasonable estimates of the amplitudes by integrating. The ARMA algorithm was found to be computationally much more stable than any of the other algorithms. More importantly the *improved Cadzow ARMA algorithm* was found to give better estimate for lower SNR's.

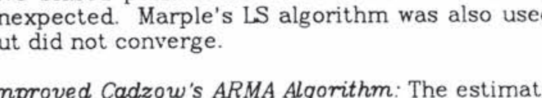

Fig. 3. Distribution Estimate using Transient Error Method

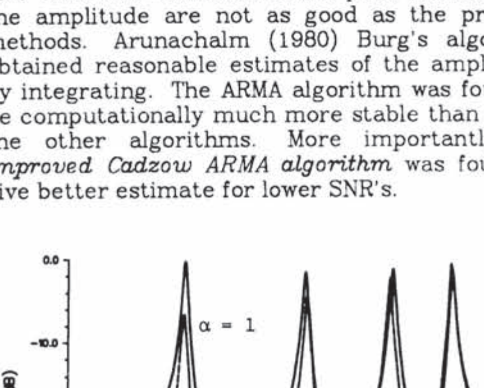

Fig. 4. Distribution using Improved Cadzow ARMA Algorithm

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