EXTENDING THE FOURIER TRANSFORM - THE POSITIVITY CONSTRAINT

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1. INTRODUCTION

In radio astronomy it is often necessary to estimate a brightness distribution from a limited number of samples of its Fourier transform. The manifest requirement that the brightness distribution be everywhere positive imposes definite constraints on its Fourier transform which yield information about unmeasured Fourier components. Here we discuss the question: given the first n+1 values, ρ_0, ρ_1 ... ρ_n, of a uniformly sampled Fourier transform of a real positive function, what can we say about Fourier terms of higher order?

We first show that ρ_{n+1} must lie within a circle in the complex plane, whose radius and centre can be calculated from ρ_0, ρ_1, ... ρ_n. For a value of ρ_{n+1} outside this circle there is no positive function whose Fourier transform passes through the values ρ_0, ρ_1, ... ρ_{n+1}.

The known values ρ_0, ρ_1, ... ρ_n constrain higher-order terms to successively larger, calculable, areas in the complex plane. If these areas are small enough, we may decide that ρ_{n+1}, ... ρ_{n+m} are determined to sufficient accuracy and it is therefore unnecessary to measure them.

Now in view of the residual uncertainty in each ρ_{n+m} ($m \geqslant 1$), how do we select a value for each within its "allowable" range? It is shown in Section 3 that any choice of ρ_{n+1} places additional constraints on all higher-order terms but if we estimate ρ_{n+1} by selecting the centre of its "circle of constraint" this imposes the minimal additional constraint on ρ_{n+m} ($m \geqslant 2$). The value of ρ_{n+2} then lies within a calculable circle, and if we select the centre of this circle as our estimate of ρ_{n+2}, once again the additional constraints on higher terms are minimized. The process can be iterated indefinitely. This prescription provides the greatest likelihood that a measurement of ρ_{n+m} (where m is an arbitrarily chosen integer $\geqslant 2$) will fit with the terms of lower order to form an acceptable auto-correlation sequence. The procedure is illustrated numerically in Section 4. In Section 5 it is shown that choosing the centre of the circle of constraint for each successive higher-order term leads to the maximum entropy solution.

C. van Schooneveld (ed.), Image Formation from Coherence Functions in Astronomy, 241-247.

2. THE FOURIER TRANSFORM OF A POSITIVE FUNCTION

If F(x) is a real positive function we may write

$$F(x) = f(x) \cdot f^*(x) \equiv |f(x)|^2 .$$

Then the Fourier transform of F is the auto-correlation of g, the Fourier transform of f. If we are interested in F(x) for only those values of x within the range $-x_0/2 \leqslant x \leqslant x_0/2$ the auto-correlation function need be specified only at discrete intervals yielding an auto-correlation sequence with mth term

$$\rho_m = \sum_{k=-\infty}^{\infty} g_k \, g^*_{k-m}$$

where g_ℓ is the discrete Fourier transform of f(x). This expression can be regarded as the scalar product of two complex vectors. Consider a set of unit vectors such that the jth vector, $\overline{V}_j$, has as its ℓth component $g_{j+\ell}$. It can be shown that the mth term of the auto-correlation sequence may be written as the scalar product of the jth and (j-m)th vectors

$$\rho_m = \overline{V}_j \cdot \overline{V}^*_{j-m} . \tag{1}$$

Since the vectors $\overline{V}_j$ are unit vectors, $\rho_0 = 1$. In fact it may be shown that the numbers $\rho_0, \rho_1, \ldots \rho_n$ are successive members of a normalized auto-correlation sequence if and only if a set of n+1 unit vectors exists such that (1) is satisfied for all j and m.

Without loss of generality we may write

$$\overline{V}_j = \sum_{k=1}^{n} \alpha_{k,n} \, \overline{V}_{j-k} + \beta_n \, \overline{\varepsilon}_0 , \tag{2}$$

where β_n and the $\alpha_{k,n}$ are constants and the unit vector $\overline{\varepsilon}_0$ is such that

$$\overline{\varepsilon}_0 \cdot \overline{V}^*_{j-p} = 0 , \quad 1 \leqslant p \leqslant n . \tag{3}$$

It then follows that

$$\overline{V}_j \cdot \overline{V}^*_{j-p} = \sum_{k=1}^{n} \alpha_{k,n} \, \overline{V}_{j-k} \cdot \overline{V}^*_{j-p} + \beta_n^2 \, \delta_{p,0} , \quad 0 \leqslant p \leqslant n .$$

In view of equation (1) these may be written

$$\rho_p - \sum_{k=1}^{n} \alpha_{k,n} \, \rho_{p-k} = \beta_n^2 \, \delta_{p,0} , \quad 0 \leqslant p \leqslant n . \tag{4}$$

Knowing the values of $\rho_0 (\equiv 1), \rho_1, \rho_2 \ldots \rho_n$, we may solve the n+1 equations represented by (4) for the n+1 unknowns β_n^2, and $\alpha_{k,n}$, $(1 \leqslant k \leqslant n)$, yielding values which are independent of j. Accordingly, in place of equations (2) and (3), we may write

$$\overline{V}_{j+1} - \sum_{k=1}^{n} \alpha_{k,n} \, \overline{V}_{j+1-k} = \beta_n \, \overline{\varepsilon}_1 , \tag{5}$$

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where

$$\bar{\varepsilon}_1' \cdot \bar{V}^*_{j+1-p} = 0 \ , \quad 1 \leqslant p \leqslant n \ . \tag{6}$$

The unit vector $\bar{\varepsilon}_1'$ may be written quite generally

$$\bar{\varepsilon}_1' = \lambda_{1,1}\, \bar{\eta} + \lambda_{1,2}\, \bar{\varepsilon}_1 \ , \tag{7}$$

where the unit vector $\bar{\eta}$ is a linear combination of the unit vectors $\bar{V}_j, \bar{V}_{j-1} \ldots \bar{V}_{j-n}$, such that

$$\bar{\eta} \cdot \bar{V}^*_{j+1-k} = 0 \ , \quad 1 \leqslant k \leqslant n \ .$$

This defines $\bar{\eta}$ uniquely with

$$\bar{\eta} = \left\{ \bar{V}_{j-n} - \sum_{k=1}^{n} \alpha^*_{k,n}\, \bar{V}_{j-n+k} \right\} \beta_n^{-1} \ . \tag{8}$$

The unit vector $\bar{\varepsilon}_1$ satisfies the relation

$$\bar{\varepsilon}_1 \cdot \bar{V}^*_{j+1-q} = 0 \ , \quad 1 \leqslant q \leqslant n+1 \ ;$$

and the numbers $\lambda_{1,1}$ and $\lambda_{1,2}$ satisfy $|\lambda_{1,1}|^2 + |\lambda_{1,2}|^2 = 1$. From equations (5), (7) and (8)

$$\bar{V}_{j+1} - \sum_{k=1}^{n} \alpha_{k,n}\, \bar{V}_{j+1-k} = \lambda_{1,1} \left\{ \bar{V}_{j-n} - \sum_{k=1}^{n} \alpha^*_{k,n}\, \bar{V}_{j-n+k} \right\} + \lambda_{1,2}\, \beta_n\, \bar{\varepsilon}_1 \ . \tag{9}$$

Taking the scalar product of (9) with $\bar{V}^*_{j-n}$, we obtain

$$\rho_{n+1} - \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+1-k} = \lambda_{1,1}\, \beta_n^2 \ . \tag{10}$$

An essentially identical argument yields

$$\rho_{n+2} - \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+2-k} - \lambda_{1,1} \left\{ \rho_1 - \sum_{k=1}^{n} \alpha^*_{k,n}\, \rho_k \right\}$$

$$= \lambda_{2,1}(1-|\lambda_{1,1}|^2)\, \beta_n^2 \ , \quad |\lambda_{2,1}| \leqslant 1 \ . \tag{11}$$

Equations (10) and (11) define the constraints imposed on ρ_{n+1} and ρ_{n+2} by the known values of $\rho_0, \rho_1 \ldots \rho_n$. Any value of $\lambda_{1,1}$ (such that $|\lambda_{1,1}| \leqslant 1$) substituted into (10) yields an "acceptable" value of ρ_{n+1}, and any combination of $\lambda_{1,1}$ and $\lambda_{2,1}$ such that $|\lambda_{1,1}| \leqslant 1$ and $|\lambda_{2,1}| \leqslant 1$ yields an "acceptable" value of ρ_{n+2} when substituted into (11).

3. EXTRAPOLATING THE FOURIER TRANSFORM

The foregoing argument has shown that, given $\rho_0, \rho_1 \ldots \rho_n$, and hence $\alpha_{k,n}$ and β_n^2 from equation (4), we can write

$$\rho_{n+1} = \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+1-k} + \lambda_{1,1}\, \beta_n^2 \tag{12}$$

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$$\rho_{n+2} = \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+2-k} + \lambda_{1,1}(\rho_1 - \sum_{k=1}^{n} \alpha^*_{k,n}\, \rho_{k+1}) + \lambda_{2,1}(1-|\lambda_{1,1}|^2)\, \beta_n^2 \; ; \quad |\lambda_{1,1}| \text{ and } |\lambda_{2,1}| \leqslant 1 \; . \tag{13}$$

Equation (12) tells us that ρ_{n+1} lies somewhere within a circle in the complex plane, the centre of the circle being at $R_{n+1}(\equiv \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+1-k})$ and its radius being β_n^2. The value of β_n^2 depends of course on the nature of the power spectrum, and it may be shown that β_n^2 either decreases or remains constant as n increases. Clearly the smaller β_n^2 the more accurately we know ρ_{n+1}.

In the absence of further information we have no reason to prefer any one point within the circle as representing the "true" value of ρ_{n+1}. However, consider the result of assigning to ρ_{n+1} its extreme value - i.e. consider the result of setting $|\lambda_{1,1}| = 1$, with the phase of $\lambda_{1,1}$ fixed. This constrains ρ_{n+1} to a particular, but arbitrary, value as can be seen from equation (12). Furthermore, from (13), ρ_{n+2} is then also determined as are all terms of higher order. If we had some independent way of determining the value of ρ_{n+10} (say) we have no reason to expect agreement with the value obtained by extrapolating from n with $|\lambda_{1,1}| = 1$.

On the other hand, if we set $\lambda_{1,1} = 0$, ρ_{n+2} is no longer completely constrained and ranges within values determined from equation (13). The range of values within which ρ_{n+2} can lie is largest when $\lambda_{1,1} = 0$. Similarly it can be shown that if $\lambda_{1,1} = 0$, and also $\lambda_{2,1} = 0$, the range of values within which ρ_{n+3} can lie is greatest. Thus: sequentially setting each term to the middle of its permitted range maximizes the possible range of all higher-order terms. If we had some independent method of determining ρ_{n+10} (say) this procedure provides our best chance that its value will lie within the range permitted by the lower terms.

Setting $\lambda_{1,1} = 0$ leads to the iterative algorithm

$$\rho_{n+m} = \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+m-k} \; . \tag{14}$$

In Section 4 this procedure is illustrated.

In general, the constraints on ρ_{n+m} weaken as m increases. Thus it can be shown (Komesaroff and Lerche, 1978) that

$$\rho_{n+m} - \sum_{k=1}^{n} \alpha_{k,n}\, \rho_{n+m-k} = |\beta_n|^2\, S_{n+m} \; , \quad m \geqslant 1 \; , \tag{15a}$$

where S_{n+m} satisfies

$$S_{n+m} = \bar{\varepsilon}^*_n \cdot \varepsilon_m + \sum_{k=1}^{n} \alpha^*_{k,n}\, S_{n+m+k} \; , \quad m \geqslant 1 \; , \tag{15b}$$

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where $\bar{\varepsilon}_n$ is an arbitrary complex unit vector. It can also be shown that

$$\rho_{n+m} - \sum_{k=1}^{n} \alpha^*_{k,n}\, \rho_{n+m+k} = |\beta_n|^2\, P_{n+m}\ , \quad m \geqslant 1\ , \tag{16a}$$

where P_{n+m} satisfies

$$P_{n+m} = \bar{\varepsilon}^*_n \cdot \bar{\varepsilon}_m + \sum_{k=1}^{n} \alpha_{k,n}\, P_{n+m-k}\ , \quad m \geqslant 1\ . \tag{16b}$$

Equations (15) and (16) can be solved (Komesaroff and Lerche, 1978) leading to expressions for S_{n+m} and P_{n+m} in terms of sums of the $\alpha_{k,n}$ and products of two ε factors. But see Komesaroff and Lerche (1978) for the general constraint conditions on ρ_{n+m}. Here we note that equations (15) and (16) can be used as the basis for recursive algorithms expressing the uncertainty in ρ_{n+m} in terms of the ρ_{n+m-k} $(n+m > k \geqslant 1)$. This point has already been anticipated by the illustration involving ρ_{n+1} and ρ_{n+2}.

4. A NUMERICAL EXAMPLE

An application of the procedure is illustrated in Figure 1. A non-negative function, sampled at 512 points, is illustrated in Figure 1(a). The Fourier transform has been calculated for $\rho_0 \ldots \rho_{32}$ by the usual Fourier inversion technique and the values of $\rho_{33} \ldots \rho_{512}$ estimated by the extrapolation method just outlined. Transforming the result yields Figure 1(b). In the case of Figure 1(c) the usual Fourier inversion technique has been used to calculate $\rho_0 \ldots \rho_{32}$ and, in addition, ρ_{64}, ρ_{96}, ρ_{128}, ρ_{160}, ρ_{192}, ρ_{224}, ρ_{256}. The missing values have been estimated from the extrapolation method. For comparison, the effects of merely truncating the transform to the values indicated above are shown in Figures 1(d) and 1(e).

5. RELATION TO MAXIMUM ENTROPY

If we knew the ρ_m (all m) <u>exactly</u> then $Q(x)\left(\equiv \sum_{m=-\infty}^{+\infty} \rho_m \exp(2\pi i m x/x_0)\right)$ is, of course, just proportional to $F(x)$. But if we use relation (14) to <u>estimate</u> ρ_{m+n} $(m \geqslant 1)$, the resulting estimate for $Q(x)$ is equivalent to the maximum entropy spectral estimate. We show this as follows. Equation (14) is equivalent to demanding

$$\bar{\varepsilon}'_m \cdot \bar{\varepsilon}^*_0 = \delta_{m,0}\, \beta_n^2\ , \tag{17}$$

where

$$\bar{\varepsilon}'_m = \bar{V}_{j+m} - \sum_{k=1}^{n} \alpha_{k,n}\, \bar{V}_{j+m-k}\ . \tag{18}$$

Introduce the following change in nomenclature

$$\gamma_k = \delta_{k,0} - \alpha_{k,n}(1-\delta_{k,0}), \quad 0 \leqslant k \leqslant n\ . \tag{19}$$

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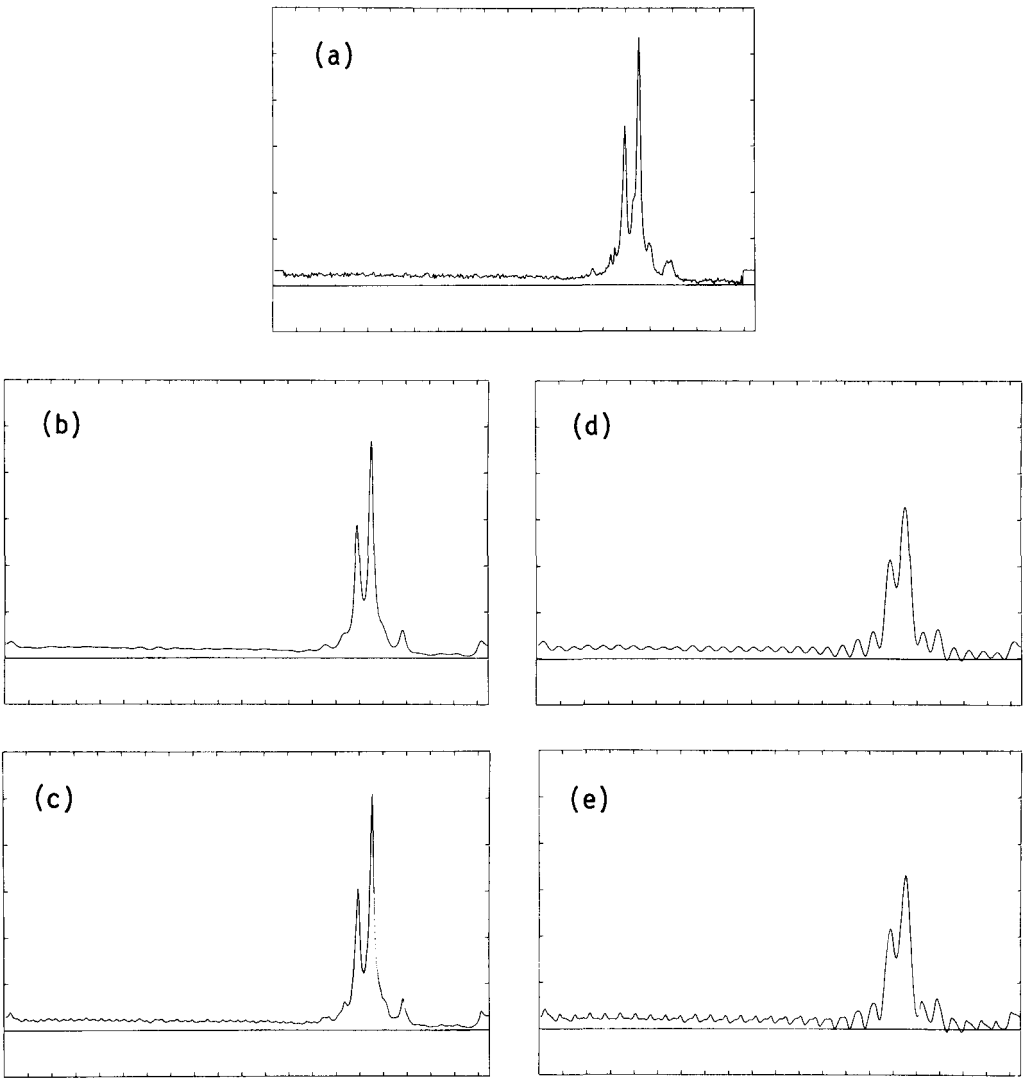

Fig. 1(a) - A 512-point H_2O spectrum measured at Parkes.

(b) - For the data of Figure 1(a) Fourier components ρ_0 ... ρ_{32} were calculated by Fourier inversion, and the missing higher-order terms were estimated by the method outlined in the text. The result was then retransformed.

(c) - Fourier components ρ_0 ... ρ_{32} and also ρ_{64}, ρ_{96}, ρ_{128}, ρ_{160}, ρ_{192}, ρ_{224}, ρ_{256} were calculated by Fourier inversion and the missing terms were estimated as in Figure 1(b).

(d) & (e) - Fourier transform truncated as for Figures 1(b) and (c) respectively and the missing terms set to zero.

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Then
$$\sum_{k=0}^{n} \gamma_k \, \overline{V}_{j+m-k} = \beta_n \, \overline{\varepsilon}'_m \, , \tag{20}$$
and thus from (17) and (18)
$$\sum_{m=-\infty}^{+\infty} \sum_{k=0}^{n} \gamma_k \sum_{\ell=0}^{n} \gamma^*_\ell \, \rho_{m-k+\ell} \exp(2\pi i m x/x_0) = \beta_n^2 \, . \tag{21}$$
With the replacement M = m-k+ℓ we have
$$\sum_{M=-\infty}^{+\infty} \rho_M \exp(2\pi i M x/x_0) = \beta_n^2 \left| \sum_{k=0}^{n} \gamma_k \exp(2\pi i k x/x_0) \right|^{-2} \tag{22}$$
which result is formally identical with the maximum entropy algorithm.

Many authors have written on the subject of maximum entropy. In particular Burg (1967) and Van den Bos (1971) have discussed its connection with the positivity constraint. The papers of Ables (1974) and Newman (1977) are oriented towards its radio astronomy application.

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