JOSA COMMUNICATION

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Phase retrieval using boundary conditions

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It is shown that *a priori* knowledge of the edges of an object is not sufficient to ensure that it can be uniquely reconstructed from the modulus of its Fourier transform (or from its autocorrelation function). Furthermore, even in those cases for which the ultimate solution is unique, in intermediate steps in the solution by the recursive Hayes–Quatieri algorithm there can be ambiguities. An extension of the recursive algorithm that finds the solution (or solutions) is suggested, and it is shown that the recursive method can be applied to complex-valued objects.

INTRODUCTION

In a number of disciplines, including astronomy, x-ray crystallography, electron microscopy, and wave-front sensing, one encounters the phase-retrieval problem. One wishes to reconstruct $f(m, n)$, an object function, from $|F(p, q)|$, the modulus of its Fourier transform, where

$$F(p, q) = |F(p, q)|\exp[i\psi(p, q)] = \mathcal{F}[f(m, n)]$$

$$= \sum_{m=0}^{P-1}\sum_{n=0}^{Q-1} f(m, n)\exp[-i2\pi(mp/P + nq/Q)], \quad (1)$$

where $m, p = 0, 1, \ldots, P - 1$ and $n, q = 0, 1, \ldots, Q - 1$. The discrete transform is employed here since in practice one deals with sampled data in a computer. The problem of reconstructing the object from its Fourier modulus is equivalent to that of reconstructing the Fourier phase $\psi(p, q)$ from the Fourier modulus, since once one has the phase as well as the modulus, one can easily compute $f(m, n)$ by the inverse (discrete) Fourier transform (hence the name phase-retrieval problem). $r(m, n)$, the (aperiodic) autocorrelation of $f(m, n)$, is given by[1]

$$r(m, n) = \sum_{j=0}^{M-1}\sum_{k=0}^{N-1} f(j, k)f^*(j - m, k - n) \quad (2)$$

$$= \sum_{j=0}^{M-1}\sum_{k=0}^{N-1} f^*(j, k)f(j + m, k + n) \quad (3)$$

$$= \mathcal{F}^{-1}[|F(p, q)|^2], \quad (4)$$

where the asterisk denotes a complex conjugate and where it is assumed that $f(j, k) = 0$ for m outside $[0, M - 1]$ and for n outside $[0, N - 1]$. Note that, when simulating data, in order to avoid aliasing in the computation of $|F(p, q)|^2$ it is necessary that $M \leq P/2$ and $N \leq Q/2$. Since the autocorrelation function is easily computed from the Fourier modulus by Eq. (4), the phase-retrieval problem is equivalent to reconstructing an object from its autocorrelation function.

Several phase-retrieval algorithms have been demonstrated, all of them requiring some additional measurements or constraints on the solution. Examples include a reference point at least one object-diameter from the object[2] (giving rise to the holography condition[3]), a second intensity measurement in another plane[4,5] (in electron microscopy or wave-front sensing), nonnegativity and limited spatial extent[6,7] (in astronomy), just limited spatial extent,[8] atomic models[9] (in x-ray crystallography), objects consisting of collections of points having nonredundant spacings,[10] and objects having latent reference points[11] (not satisfying the holography condition). For some of these situations there is a proof of uniqueness of the solution that relies on the types of measurements made, on the *a priori* information available, or on the nature of the reconstruction algorithm itself.

Another proposed phase-retrieval algorithm is the Hayes–Quatieri (H-Q) recursive algorithm, which relies on *a priori* knowledge of the boundary conditions (i.e., the values of the edges of the object).[12,13] The purpose of this paper is to clarify the uniqueness questions pertaining to the H-Q recursive algorithm and to suggest a revised algorithm that finds the solution (or solutions) when the H-Q algorithm fails. The algorithm may also be applied to complex-valued objects. It is also pointed out that by the approach of using latent reference points,[11] special classes of objects can be shown to be unique for both real-valued and complex-valued objects.

AMBIGUITY USING BOUNDARY CONDITIONS

In Refs. 12 and 13 the H-Q recursive algorithm was put forward for reconstructing an object from the modulus of its Fourier transform, through the autocorrelation function, using boundary conditions, i.e., assuming knowledge of the edges of the object. A real-valued object, $f(m, n)$, was assumed to be zero outside the rectangular region of support $0 \leq m \leq M - 1$ and $0 \leq n \leq N - 1$. The top and bottom nonzero rows, $\beta(m) = f(m, N - 1)$ and $\alpha(m) = f(m, 0)$, respectively, and the leftmost and rightmost nonzero col-

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umns, $f(0, n)$ and $f(M-1, n)$, respectively, are assumed to be known *a priori*. Rows 1 and $N-2$ can then be determined by solving a system of $2M-1$ linear equations in $2M-4$ unknowns. From Eq. (3) we have, for $n = N-2$, the second from the top row of the autocorrelation:

$$
\begin{aligned}
r(m, N-2) &= \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} f^*(j,k) f(j+m, k+N-2) \\
&= \sum_{j=0}^{M-1} f^*(j,0) f(j+m, N-2) \\
&\quad + \sum_{j=0}^{M-1} f^*(j,1) f(j+m, N-1) \\
&= \sum_{j=0}^{M-1} \alpha^*(j) f(j+m, N-2) \\
&\quad + \sum_{j=0}^{M-1} f^*(j,1) \beta(j+m)
\end{aligned}
\tag{5}
$$

for $m = -M+1, \ldots, M-1$. These are $2M-1$ equations, one for each value of m, in $2M-4$ unknowns, $f(j, N-2)$ and $f(j, 1)$, for $j = 1, 2, \ldots, M-2$. Recall that $\alpha(j)$, $\beta(j)$, $f(0, N-2)$, $f(M-1, N-2)$, $f(0, 1)$, and $f(M-1, 1)$ are assumed to be known. After $f(j, N-2)$ and $f(j, 1)$ are determined by solving the system of equations given in Eqs. (5) above, then one can solve for $f(j, N-3)$ and $f(j, 2)$ using $r(m, N-3)$ in a similar manner. The remaining rows of the object are solved recursively in a similar manner.

The H-Q algorithm described above could work if the systems of equations had a unique solution for the unknowns. Restricting the solution to real-valued f's, a claim has been made that "It may be shown, however, that a sufficient condition for a unique solution ... to exist is that $\alpha(m)$ and $\beta(m)$ not be identically zero and that $\alpha(m)$ not be related to $\beta(M-1-m)$ by a constant scale factor."[12] However, no proof of that statement was provided. In what follows, three examples that clarify this situation are given. In the first, the underlying phase-retrieval problem is not unique, yet the two ambiguous solutions have the same boundary values that satisfy the conditions quoted above. Therefore we have the unexpected result that, although for two-dimensional (2-D) sampled objects the phase-retrieval problem is usually unique to begin with,[14] knowledge of the boundary values is *not* sufficient to guarantee uniqueness. In the second example, the underlying phase-retrieval problem is unique, and the boundary values of the object satisfy the conditions quoted above, yet the equations to be solved for the H-Q recursive method do not yield a unique solution, contrary to the claim quoted above. An extension of the method that finds the solutions for the first two examples is given. In the third example, the H-Q algorithm is shown to work for a complex-valued object although the method was originally limited to real-valued objects.[12]

Example 1

Figures 1(a) and 1(b) show two different sampled objects having the same boundaries, and for both objects $\alpha(m)$ is not proportional to $\beta(M-1-m)$, and yet they have the same Fourier modulus and the same autocorrelation function, which is shown in Fig. 1(c). Therefore knowledge of the boundaries is not necessarily sufficient information for a unique reconstruction even if the restrictive condition quoted above is satisfied.

2	3	3	3	1
3	7	4	4	2
3	6	5	4	2
1	2	2	2	1

(a)

2	3	3	3	1
3	3	6	6	2
3	4	5	6	2
1	2	2	2	1

(b)

2	7	13	19	21	17	11	5	1
7	27	52	77	88	73	48	23	5
13	52	100	153	179	147	97	48	11
15	63	123	188	230	188	123	63	15
11	48	97	147	179	153	100	52	13
5	23	48	73	88	77	52	27	7
1	5	11	17	21	19	13	7	2

(c)

Fig. 1. Example 1. Two different objects, (a) and (b), have the same boundary values and also have the same Fourier modulus (not shown) and the same autocorrelation (c).

An infinite number of ambiguous examples such as that shown in Fig. 1 can be generated. From the theory of Bruck and Sodin[14] it is known that the solution of the phase-retrieval problem [but not necessarily of Eqs. (5)] is unique unless the Fourier transform of the object is a factorable polynomial, which is unlikely to happen by chance for the 2-D case. Factorability of the Fourier transform is equivalent to the object's being expressible as a convolution of two functions, and so ambiguous cases can be constructed by forming an object by convolving (or cross correlating) two functions.[15] The object in Fig. 1(a) was fabricated by cross correlating the functions shown in Figs. 2(a) and 2(b). The ambiguous solution shown in Fig. 1(b) is the inverted convolution of the functions shown in Figs. 2(a) and 2(b). An infinite number of other examples that are ambiguous even if one knows *a priori* the boundary values (and that satisfy the condition quoted above) can be obtained by replacing the values 1, 1, 1, and 2 of the function shown in Fig. 2(b) by other values w, x, y, and z, respectively, as long as $wz \neq xy$.

The H-Q recursive algorithm involves the solution of $2M-1$ linear equations in $2M-4$ unknowns.[12] One problem with this is that for $m = -M+1$ and for $m = M-1$, Eqs. (5) involve only the known boundary values and not the unknowns. Therefore one really has only $2M-3$ linear equations in $2M-4$ unknowns to begin with. A second problem is that on inspection of those equations one finds that, for the ambiguous cases such as that show in Fig. 1, two or more

1	1	1	1
1	2	0	1
1	1	1	1

(a)

1	1
1	2

(b)

2	3	3	3	1
3	a	b	c	2
3	d	e	f	2
1	2	2	2	1

(c)

Fig. 2. Functions (a) and (b), which generate the object shown in Fig. 1(a) by cross correlation and in Fig. 1(b) by convolution. In (c) is the general form of the objects that have the autocorrelation shown in Fig. 1(c).

of them are dependent equations. Since the number of remaining linear independent equations is fewer than the number of unknowns, the problem is underdetermined, and multiple solutions exist.

Consider the particular example of Fig. 1(c), for which one searches for solutions of the form shown in Fig. 2(c), having the *a priori* known boundary values. The $2M - 3 = 7$ linear equations of Eq. (5), utilizing the second row of Fig. 1(c), are as follows (after rearranging the right-hand sides):

$$27 = 12 + a + 2f, \tag{6a}$$

$$52 = 12 + 2a + b + 2e + 3f, \tag{6b}$$

$$77 = 12 + 2a + 2b + c + 2d + 3e + 3f, \tag{6c}$$

$$88 = 13 + 2a + 2b + 2c + 3d + 3e + 3f, \tag{6d}$$

$$73 = 13 + a + 2b + 2c + 3d + 3e + f, \tag{6e}$$

$$48 = 13 + b + 2c + 3d + e, \tag{6f}$$

$$23 = 13 + c + d. \tag{6g}$$

Note that Eq. (6d) is equal to Eq. (6c) plus Eq. (6g), Eq. (6e) is equal to Eq. (6f) plus Eq. (6b) minus Eq. (6a), and Eq. (6c) is equal to Eq. (6f) plus Eq. (6b) minus Eq. (6g). That is, of these seven equations, three are dependent, leaving only four independent equations in six unknowns. Therefore one can, for example, choose values a and b in Fig. 2(c) arbitrarily, and then the values of c, d, e, and f are determined from Eqs. (6) as follows:

$$c = (15 - a + 2b)/4, \tag{7a}$$

$$d = (25 + a - 2b)/4, \tag{7b}$$

$$e = (35 - a - 2b)/4, \tag{7c}$$

$$f = (15 - a)/2. \tag{7d}$$

At this point the H-Q algorithm would have been stopped, leaving this ambiguity. An alternative is to continue by adding, to the existing set of underdetermined equations, the equations corresponding to the next row of the autocorrelation. Since the previous set of equations was underdetermined, some of this set of equations include terms that are the products of two unknowns, i.e., some of the equations are nonlinear. The first two such equations are (after rearranging the right-hand sides)

$$52 = 12 + 2a + 2c + d + 3f \tag{8a}$$

and

$$100 = 12 + 4b + 3c + 2d + 4e + af. \tag{8b}$$

Combining Eq. (8a) with Eqs. (7) yields

$$a = 15 - 2b, \tag{9}$$

and combining Eq. (8b) with Eqs. (7) and (9) yields

$$b^2 - 10b + 24 = 0 \tag{10a}$$

or

$$b = 4 \text{ or } 6. \tag{10b}$$

Evaluation of the other unknowns by Eqs. (9) and (7) gives the two solutions shown in Figs. 1(a) and 1(b). The equations for the unused points in the autocorrelation are found to be consistent with both solutions. Note that the steps described above for solving for the unknowns is a comprehensive procedure that finds all possible solutions. This modified approach can be generalized as follows. One performs the H-Q algorithm solving the sets of linear equations such as Eqs. (5), using the suggested pseudoinverse matrix[12] or another method such as Gauss elimination. If the number of independent equations is found to be exceeded by the number of unknowns, then one adds to the system of equations additional (possibly nonlinear) equations for the autocorrelation, using points in the next row of the autocorrelation. More equations are added (possibly using points unused by the H-Q algorithm) until the solution is unique or until all the points in the autocorrelation are used (in which case one might be left with multiple solutions). This modification to the H-Q algorithm may be difficult in some cases since it involves the solution of a system of nonlinear equations. Nevertheless, this approach is capable of finding all the solutions when multiple solutions exist. It works even when $\alpha(m)$ is proportional to $\beta(M - 1 - m)$.

Example 2

Figure 3(a) shows an object identical to that shown in Fig. 1(a) except that a value of 4 was replaced by a value of 5 in the fourth column from the left and second row from the top. Figure 3(b) shows its autocorrelation. As we show below, this object is uniquely related to its autocorrelation. On attempting to reconstruct the object from its autocorrelation by the H-Q recursive method using *a priori* knowledge of the boundary values, one finds, similar to the case of Example 1, using Gauss elimination, that three of the seven linear equations of Eqs. (5) are dependent, leaving only four independent equations in six unknowns. Again one can, for example, choose values a and b in Fig. 2(c) arbitrarily, and then the values of c, d, e, and f are determined. At this point the H-Q algorithm would have been stopped, leaving this ambiguity. Similar to the case of Example 1, an alternative is to

2	3	3	3	1
3	7	4	5	2
3	6	5	4	2
1	2	2	2	1

(a)

2	7	13	19	21	17	11	5	1
7	27	52	78	90	75	50	24	5
13	54	103	158	186	153	103	51	11
15	66	130	194	239	194	130	66	15
11	51	103	153	186	158	103	54	13
5	24	50	75	90	78	52	27	7
1	5	11	17	21	19	13	7	2

(b)

Fig. 3. Example 2. An object (a), which is uniquely related to its autocorrelation function (b). For this example Eqs. (5) do not have a unique solution.

carry on and continue to solve for the six unknowns using the equations for the next row of autocorrelation. Then one arrives at only one consistent solution, equal to the original object shown in Fig. 3(a).

Since the modified procedure described above finds all possible solutions having the given boundary values, and since only a single solution was found, the object shown in Fig. 3(a) is the unique solution.

An infinite number of such examples can be generated. If, instead of 5, any other value (except 4) had been used for the fourth column, second row of the object shown in Fig. 3(a), then the same behavior as in Example 2 would be observed: although the underlying phase-retrieval problem is unique, the solution to Eqs. (5) is not.

From the examples discussed above it is seen that the H-Q recursive algorithm, when modified to carry on with unknown variables as suggested above, is reminiscent of the recursive algorithm of Dallas,[5] except that Dallas had a tree of discrete solutions that grew with each recursive step, and ambiguities were resolved when the tree was pruned in later recursive steps. In the present case one must go deeper into the autocorrelation function than suggested in Ref. 12 to obtain enough independent equations to arrive at a solution (or solutions).

Example 3

In the preceding examples and in Refs. 11 and 12 it was assumed that the object was real valued. However, the reconstruction method can be just as well applied to complex-valued objects. Equations (5) simply becomes a system of $2M - 3$ linear equations having complex coefficients in $2M - 4$ complex-valued unknowns. (Alternatively, expressing the real and imaginary parts of each complex-valued equation as two separate equations and solving for the real and imaginary parts of the unknowns, one has a system of $4M - 6$ real linear equations in $4M - 8$ real unknowns. Dealing with the fewer number of equations with complex values is the simpler method.) In either case, if too many of the equations are linearly dependent, then one must resort to using additional (possibly nonlinear) equations as in the modified H-Q algorithm as described in the previous section.

In Figs. 4(a) and 4(b), a complex-valued object and its autocorrelation, respectively, are shown (only the left half of the latter is shown since it is Hermitian). For this example, Eqs. (5) were solved by Gaussian elimination using complex coefficients and the solution (the object) was found to be unique.

SOME UNIQUE CASES

Despite the phase-retrieval problem's not being unique, as demonstrated in Example 1 in the previous section, there are some specific classes of objects for which the solution is known to be unique. These unique objects have supports (or shapes) of special types.

Certain classes of objects having latent reference points can be reconstructed using a simpler recursive algorithm than the one described in the previous section. The simpler recursive algorithm[11] selects the order in which the equations are solved such that at each step one must solve only a single linear equation for a single unknown, which is a trivial computation that always gives a unique result. It is required that no division by zero be allowed, and this is ensured by the requirement that the values of the latent reference points not be zero. The latent reference points act in a similar manner to reference points for holography, but they do not initially satisfy the holographic separation condition.

1+0i	1+i	2-i	-3+2i	0-i
2-2i	2+2i	1-2i	2+i	-1+0i
1+3i	4+i	-2+3i	-1-i	1+2i
1-2i	2+2i	0+i	1-i	-1+i

(a)

-1-i	1-i	-3+0i	11-i	-2+0i
-3-2i	6-4i	-9-5i	9-9i	12-5i
-1-10i	2-i	-4+i	24-22i	9+11i
2+5i	1-23i	18+7i	-17-24i	114+0i
-2-5i	-4+9i	2-9i	6+7i	9-11i
-4+3i	0-14i	-3-5i	20+5i	12+5i
2+i	-9+6i	1-13i	4+i	-2+0i

(b)

Fig. 4. Example 3. A complex-valued object (a), which is uniquely related to its autocorrelation function (b). The right half of (b) (not shown) is the Hermitian conjugate of the left half (shown). For this example Eqs. (5) have a unique solution.

Examples of objects that can be uniquely reconstructed in this manner include (Fiddy *et al.*[16]) objects within a rectangle plus a point off one corner of the rectangle and objects having other supports as well.[11] In most cases the support of the object must be known *a priori* in order to ensure that one obtains a unique reconstruction, since it is usually not possible to deduce the support of the object from the support of its autocorrelation.[10] However, for the objects of Fiddy *et al.*[16] the support can be deduced from the autocorrelation support, and so the reconstruction in that case is unconditionally unique.[11] The objects may be complex valued. Furthermore, for these cases the boundary values need not be known *a priori* since they are computed in the first step of the recursive algorithm.[11,12]

CONCLUSIONS

Although boundary conditions are a powerful constraint for the phase-retrieval problem, it has been proved by counterexample (Example 1) that knowledge of the boundary conditions (the values of the edges of the object) is not sufficient to ensure a unique solution. In practice it may be that a unique solution is usually obtained simply because 2-D phase retrieval is usually unique even when the boundary conditions are not known.[14] It is not yet known what extra constraints are necessary to ensure uniqueness in general.

What seems to be more important to ensure uniqueness is that the object's support be a member of a special class of supports. It is not yet known in general exactly what properties the support must have (except for the special cases mentioned in the previous section) to ensure uniqueness; but it is known that objects with separated supports[17,18] are more likely to be unique (even in the one-dimensional case) and objects having complicated supports tend to be easier to reconstruct than objects with convex symmetric support in the 2-D case.[19]

Even when the underlying phase-retrieval problem is unique, it has been proved by counterexample (Example 2) that the equations of the H-Q recursive algorithm[12] [Eqs. (5)] does not necessarily have a unique solution. This is true even when the condition that $\alpha(m)$ not be proportional to $\beta(M - 1 - m)$ holds. This condition may be necessary to avoid ambiguities, but it is not sufficient. Clearly, for Eqs. (5) to be uniquely solvable it is necessary that the underlying phase-retrieval problem be unique, which is ensured if the object's Fourier transform is an irreducible polynomial, which is usually the case.[14] It is not now known what extra conditions are sufficient to ensure uniqueness for the solution of Eqs. (5), nor is it known whether it will usually be unique. Even if the solution to Eqs. (5) is not unique, one can find the solution or solutions if one uses the modified algorithm suggested here, which employs more of the points of the autocorrelation.

The value of the recursive algorithms may be more in their predictions of uniqueness than in their ability to reconstruct images, since they tend to be very sensitive to noise.[11,12] A more stable reconstruction method would be the iterative Fourier transform algorithm,[6] which repeatedly reinforces both the measured data and the *a priori* constraints on the reconstructed image.

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