Algorithmic image reconstruction using iterative phase retrieval schema

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Abstract. X-ray diffraction is potentially a strong candidate for biological imaging since it can in principle reconstruct thick samples at resolutions close to the diffraction limit of the radiation. Due to the non-crystalline nature of such samples, one seeks a phasing method other than that of traditional crystallography; such a method exists in the use of an iterative algorithm based on oversampling [1]. One of the tasks faced by an iterative method is to know when the iteration has given a faithful reconstruction. Past algorithms of this type [1,2,3] have employed the basic Fienup iterative schema [4]. In this paper we report on the use of a newer iterative schema due to Elser [5]; our computer simulations on real and complex test objects using Elser’s schema show that his reconstruction-error function is a reliable measurement of the reconstruction. We also report that a magnitude-based histogram constraint can dramatically speed up the convergence of the reconstruction process.

1. INTRODUCTION

The diffraction of an object illuminated with coherent X-ray light is the Fourier transform of the object’s structural and chemical map within the Born approximation. Therefore, the object can be discovered, if it is unknown, when the complete diffraction data are available. Also, due to the high penetration power of X-rays, diffraction is potentially a valuable tool for mapping a thick sample, for example, a whole cell using 3D data recording such that the reconstruction element is an optically-thin voxel. The well-known phase problem arises when only the diffraction magnitude is measured experimentally and the phase is lost. To handle this, iterative phase recovery based on oversampling has been introduced [1] and successful phase recoveries on known test objects have been reported [1,2,3] especially using Fienup-type iterative schema [4].

When objects are unknown, one has to determine how close the reconstruction of the object is to the true object. Several reconstruction-error functions are available but have been used in limited cases as qualitative tools. The error function defined in Elser’s iterative schema [5] is a vector norm connecting two constraint projections of a current iterate in the vector space, where a n*n pixel array can be represented as a point in the n*n vector space. Our study suggests that the numerical value of this function is a reasonably good measure of the quality of the reconstructions.

\[ 1. \text{Support and positivity constraint: } \rho \rightarrow S(\rho) \]

\[ 2. \text{Fourier moduli constraint: } \rho \rightarrow F(\rho) \]

![constraint projections](image)

(a) support and positivity constraint projection  
(b) Fourier magnitude constraint projection

Figure 1: constraint projections in Elser’s iterative scheme; \( \rho \) is the current iterate in object space during iteration.

In general, phase retrieval algorithms can be thought of as successive projections of the known constraints in order to converge to a set of values which obeys the required constraints simultaneously, for
example, support and Fourier magnitude constraints. One applies a support constraint in the object space and a Fourier magnitude constraint in the Fourier space with Fienup-type iterative schema, so that a current iterate hops between object space and Fourier space. The earlier studies show that this approach might be susceptible to stagnation. In Elser’s iterative schema, the projections of these constraints are both done in object space. Each iterate is modified to create the next iterate by adding the difference between the two projections in object space multiplied by a constant parameter, \( \beta \). The size of \( \beta \) determines how much the current iterate gets modified at each iteration, so that with an optimal \( \beta \) value, the algorithm can move away from a stagnation point. Figure 1 illustrates each projection in Elser’s schema.

2. ALGORITHMIC PROCEDURE

The iteration process based on the difference map is summarized in the following steps. It employs 3 parameters, \( \beta, \gamma_1, \gamma_2 \) \([6]\):

- optimal \( \beta \) value needs to be found experimentally
- \( \gamma_1 = -[4 + s^2 \beta + s (2 + \beta)] / (4 - s + s^2 \beta) \), where \( s \) is the inverse of the oversampling ratio
- \( \gamma_2 = [6 - 2 \beta - s^2 \beta - s (-2 + 3 \beta)] / (4 - s + s^2 \beta) \)

Given these parameters, and support and positivity constraints \( S(p) \) and Fourier magnitude constraint \( F(p) \) of figure 1, the steps in the algorithm are:

1. Start with a random pixel array, \( \rho \), in object-space.
2. Apply the constraints, \( S(p) \) and \( F(p) \) successively, and in opposite orders.
   \[ \rho_{-S-F} = S(1+\gamma_2) F(p) - \gamma_2 \rho \]
   \[ \rho_{-F-S} = F(1+\gamma_1) S(p) - \gamma_1 \rho \]
3. Obtain the new iterate using the expression: new \( \rho = \rho + \beta (\rho_{-S-F} - \rho_{-F-S}) \)
4. Feed new \( \rho \) into step 2 and repeat steps 2 and 3 until the algorithm finds a fixed \( \rho \); fixed \( \rho \) means \( (\rho_{-S-F} - \rho_{-F-S}) = 0 \), which suggests both support and Fourier-magnitude constraints were met.
5. The error of the reconstruction is defined as the distance between \( \rho_{-S-F} \) and \( \rho_{-F-S} \) in the vector space:
   \[ \text{Error} = \| \rho_{-S-F} - \rho_{-F-S} \| \]

\[ \text{Real} \begin{array}{c}
\text{Imaginary}
\end{array} \]
\[ \text{(a) real test object} \quad \text{(b) complex test object} \]

Figure 2: test objects used in the experiments. (a) is a real object. (b) is a complex object with real and imaginary parts.

3. COMPUTER SIMULATION RESULTS

3.1 Real test objects

The reconstructions shown in this section are obtained using support and positivity constraints \( S(p) \) and Fourier magnitude constraint \( F(p) \). Figure 2(a) shows a test real object, a 220*220 pixel array, which is used in the following three reconstructions. The optimal \( \beta \) value is determined experimentally by varying its value from 0.5 to 1.5 and monitoring the convergence rate from the error graphs. The oversampling ratio, total pixel number/unknown-valued pixel number, is 3.71 with a circular support in this experiment. End-of-iteration images with their corresponding error graphs are shown in figure 3 for three different values of \( \beta \). The reconstruction of figure 3 (a) and (b) shows the algorithmic behavior when \( \beta \) is too small and the error graph suggests a stagnation. When \( \beta \) is too large, each iterate makes too big a jump before any mean-
meaningful convergence occurs, shown as a large fluctuation in figure 3(d). $\beta$ is optimized at 1.25 and the error is down to 0.019 after 5000 iterations in this case. The corresponding faithful reconstruction is shown in (e).

![Figure 3: reconstruction images and the corresponding error graph; (a) and (b) are obtained with $\beta = 0.9$. The corresponding reconstruction suffers from overlapping images; (c) and (d) are obtained with $\beta = 1.45$ and the large fluctuation in (d) suggests that $\beta$ is too big; (e) and (f) are obtained with $\beta = 1.25$ and show a faithful reconstruction.](image)

Simulations on other test samples also show a similar result that faithful reconstructions appear when error is down to 0.02. Though not shown here, the algorithm converges to 0 error at less than 100 iterations when $S(p)$ is combined with histogram constraint projection. The similar fast convergence using histogram constraint on real test object was shown earlier in Elser’s paper [5].

### 3.2 Complex test objects

A successful reconstruction of the complex test object is shown in figure 4 and 5 using $S(p)$ and $F(p)$ projections. The test object, a $220 \times 220$ pixel array, with real and imaginary parts is shown in figure 2(b). Optimal $\beta$ is found to be 1.25 and the two reconstructions using different oversampling ratio are shown in figure 4 and 5. The reconstruction of figure 4 is obtained with the oversampling ratio = 3.71. It starts to converge at about 8000 iterations and the error is down to 0.022 after 10,000 iterations. Figure 5 is obtained by reducing the size of the support on the same test object, that is, the algorithm has a bigger oversampling ratio = 4.28 now. The reconstruction converges dramatically at about 2000 iterations in this case and the error is down to 0.018 after 5000 iterations. This suggests that the algorithm may perform better under the tighter support constraints.

![Figure 4: reconstruction of the complex test object, fig.2 (b) with oversampling ratio = 3.71, $\beta = 1.25$](image)
It was reported earlier that histogram constraint can speed up the convergence on real test objects [5]. We have expanded the utility of histogram constraint to complex objects by employing a magnitude-based histogram constraint. That is, pixels of the current iterate are sorted by their magnitudes. The result is once again 0 error when $S(p)$ is modified to incorporate this projection, as shown in fig. 6. (the reconstruction is not shown here).

4. CONCLUSION

We report successful reconstructions on real and complex objects using Elser’s iterative phase retrieval schema. The studies show that, with an optimal $\beta$ value, algorithm can avoid stagnation and give a faithful reconstruction at a reasonable number of iterations. The reconstruction error graphs closely reflect the quality of the reconstruction, which can be a useful tool determining the fidelity of the reconstruction on unknown objects. It is also suggested that histogram constraint can speed up the convergence on both real and complex objects.

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References