Augmented projections for ptychographic imaging

Stefano Marchesini 1, Andre Schirotzek 1, Chao Yang 2, Hau-tieng Wu 3 and Filipe Maia 4

1 Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
2 Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
3 Statistics, University of California, Berkeley, CA 94720, USA
4 NERSC, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

E-mail: smarchesini@lbl.gov, aschirotzek@lbl.gov, cyang@lbl.gov, hauwu@berkeley.edu and frmaia@lbl.gov

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Abstract

Ptychography is a popular technique to achieve diffraction limited resolution images of a two- or three-dimensional sample using high frame rate detectors. We introduce a relaxation of common projection algorithms to account for instabilities given by intensity and background fluctuations, position errors, or poor calibration using multiplexing illumination. This relaxation introduces an additional phasing optimization at every step that enhances the convergence rate of common projection algorithms. Numerical tests exhibit the exact recovery of the object and the perturbations when there is high redundancy in the data.

(Some figures may appear in colour only in the online journal)

1. Introduction

Ptychography was proposed in 1969 to improve the resolution in electron or x-ray microscopy [1–4]. In a scanning microscope, a small beam is focused onto the sample via a lens, and the transmission is measured in a single-element detector. The image is built up by plotting the transmission as a function of the sample position as it is rastered across the beam. In such microscope, the resolution of the image is given by the beam size. In ptychography, one replaces the single-element detector with a two-dimensional array detector such as a CCD and measures the intensity distribution at many scattering angles. Each recorded diffraction pattern contains short-spatial Fourier frequency information about features that are smaller than the beam size, enabling higher resolution. At short wavelengths however it is only possible to measure the intensity of the diffracted light. To reconstruct an image of the object, one needs to retrieve the phase information. With measured amplitude and phase information, a high resolution image can be readily computed, phase contrast imaging becomes possible, and the depth of focus for three-dimensional (3D) micro-tomography is no longer a problem. While...
phase retrieval problems are notoriously difficult to solve numerically, the problem is made tractable in ptychography by using redundant measurements. In practice, multiple views of the same region of the object are recorded by using a small step size—relative to the size of the illuminating beam—when scanning the sample. With high speed detectors [5, 6] and ever brighter light sources, ptychographic imaging is becoming increasingly popular.

A practical issue in ptychographic reconstruction are the strict requirements of the experimental geometry to achieve high quality data. For example, the need for stable, well controlled coherent illumination of the sample, limited detector speed and response function all contribute to limit the specifications of a ptychographic microscope. New methods to work with unknown illuminations were proposed [7–10]. They are now used to calibrate high quality x-ray optics [11–13] and space telescopes. More recently, position errors [14–16], background [17, 18], noise statistics [19, 20] and partially coherent illumination [21–25], or vibrations have been added to the nonlinear optimization to fit the data.

Existing methods iterate between an object space—an image representing an estimate of the object—and a measurement space given by the measured diffraction frames. For example in the approach first described by [14], one starts from an estimate of the positions of the illuminating beam and an estimate of the object under study. From this starting point one minimizes the discrepancy with the data using local—gradient based—optimization and obtains a new estimate of the object and positions.

In this paper we introduce an additional optimization step in the measurement space which is—since in ptychographic experiments one records multiple views of the same region of the object—of higher dimensionality than the object space. We form pairwise comparisons between neighboring frames and update the unknown parameters of each diffraction frame so that each frame is consistent with each other.

The approach described in this work achieves accelerated convergence for large scale phase retrieval problems spanning multiple length-scales. We also show that this approach can recover experimental fluctuations over a large range of time-scales.

Notation and background

In a ptychography experiment [3, 7, 8, 10, 26–28] (see figure 1), a two-dimensional small beam with distribution \( w(r) \) of dimension \( m \times m \) illuminates a subregion centered at \( x_{(i)} \)—referred to as frame—of an unknown object of interest \( \psi \) of dimension \( n \times n \). Here \( 0 < m < n \), \( i = 1, \ldots, k \), \( k \) is the number of frames, \( r > 0 \) is a length-scale (the diffraction limited resolution of the microscope), and

\[
\begin{align*}
  r &= (r\mu, r\nu), \quad \mu, \nu \in \{0, \ldots, m - 1\}, \\
  x_{(i)} &= (r\mu', r\nu'), \quad \mu', \nu' \in \{0, \ldots, n - m\}.
\end{align*}
\]

As \( x_{(i)} \) is rastered on a typically coarser grid, \( r + x_{(i)} \) spans a finer grid of dimension \( n \times n \). Here for simplicity we consider square matrices, and generalization to non-square matrices is straightforward but requires more indices and complicates notation. In other words, we assume that a sequence of \( k \) diffraction intensity patterns \( I_{(i)}(q) = a_{(i)}^2(q) \) are collected as the position of the object is rastered on the position \( x_{(i)} \), where

\[
q = \left( \frac{2\pi}{mr} \mu, \frac{2\pi}{mr} \nu \right), \quad \mu, \nu \in \{0, \ldots, m - 1\}.
\]

The relationship among the amplitude \( a_{(i)} \), the probe \( w \) and an unknown object \( \psi \) to be estimated can be expressed as follows:
Figure 1. Left: experimental geometry in ptychography: an unknown sample with transmission \( \psi(\mathbf{r}) \) is rastered through an illuminating beam \( w(\mathbf{r}) \), and a sequence of diffraction measurements \( |a_i|^2 \) are recorded on an area detector as the sample is rastered around. The point-wise product between illuminating function and sample \( z_i(\mathbf{r}) = w(\mathbf{r})\psi(\mathbf{r} + \mathbf{x}_i) \)—which we refer to as ‘frame’ throughout the paper—is related to the measurement by a Fourier magnitude relationship \( a_i = |\mathcal{F}z_i| \).

\[
\begin{align*}
a_i(q) &= |\mathcal{F}w(\mathbf{r})\psi(\mathbf{r} + \mathbf{x}_i)|, \\
(\mathcal{F}f)(q) &= \sum_\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} f(\mathbf{r}),
\end{align*}
\]

where the sum over \( \mathbf{r} \) is given on all the indices \( m \times m \) of \( \mathbf{r} \), and \( \mathcal{F} \) is the two-dimensional discrete Fourier transform.

We introduce the illumination operator \( Q_{(i)} \), \( i = 1, 2, \ldots, k \), associated with \( x_{(i)} \) that extracts a frame \( z_{(i)} \) out of \( \psi \), and scales the frame point-wise by the illumination function \( w(\mathbf{r}) \) (see figure 1):

\[
z_{(i)}(\mathbf{r}) = w(\mathbf{r})\psi(\mathbf{r} + \mathbf{x}_{(i)}) = [Q_{(i)}\psi](\mathbf{r}),
\]

where \( z_{(i)} \) represents the frames extracted from \( \psi \) and multiplied by the probe \( w(\mathbf{r}) \).

To have a compact representation for numerics, we introduce the following notations. We represent \( \psi \) as a vector of length \( n^2 \), that is, \( \psi \in \mathbb{C}^{n^2} \). The moving beam associated with the illumination function \( w(\mathbf{r}) \) can be represented as an \( n^2 \times n^2 \) sparse ‘illumination matrix’ associated with the illumination operator, which is again denoted as \( Q_{(i)} \). To express \( Q_{(i)} \) in the matrix form, we introduce a restriction matrix \( R_{(i)} \), which restricts the \( n \times n \) region onto the \( m \times m \) subregion centered at \( x_{(i)} \), that is,

\[
Q_{(i)} = \text{diag}(w)R_{(i)}.
\]

The relationship between the diffraction measurements collected in a ptychography experiment and the unknown object to be recovered can be represented compactly as:

\[
a = |\mathcal{F}Q\psi|,
\]
if we stack the diffraction measurements \(a_{(i)}\) into a long vector \(a\), and define various matrices as follows:

\[
\begin{align*}
  a &= \begin{pmatrix} a_{(1)} \\ \vdots \\ a_{(k)} \end{pmatrix}, \\
  Q &= \begin{pmatrix} Q_{(1)} \\ \vdots \\ Q_{(k)} \end{pmatrix}, \\
  z &= \begin{pmatrix} z_{(1)} \\ \vdots \\ z_{(k)} \end{pmatrix}, \\
  F &= \begin{pmatrix} F \\ \vdots \\ F \end{pmatrix}.
\end{align*}
\]

We call the domain of \(Q\) the object space, and the range of \(FQ\) the measurement space.

Geometrically, \(Q\) is the matrix that extracts \(k\) frames out of an object \(\psi\) and multiplies them by the probe \(w\); \(Q^*\) is the conjugate transpose that merges \(k\) frames onto the object space; in addition, \(Q^*Q\) can be viewed as the normalization factor given by the sum of the illumination functions. In particular, by a direct calculation, \(Q^*Q\) is a \(n \times n\) diagonal matrix whose \(l\)th diagonal entry is \(\sum_{k,l=r_k-l} |w(r_k)|^2\), where we abuse the notation by using \(l\) to indicate the point on the object space. Physically \(l\) is the index of the grid point on the unknown object of interest which is covered by the point \(r_k\) of the \(l\)th illumination window. See table 1 for the relationship between probe \(w\), translation \(x_{(j)}\), \(Q_{(j)}\) and \(Q\).

The objective of the ptychographic reconstruction problem is to find \(\psi\) given \(a\) from (equation (1)). This is often formulated using a ‘divide and conquer’ approach referred to as projection algorithms, iterative transform methods, or alternating direction methods (ADMs) [29]. One formulates the relationship (equation (1)) as

\[
\begin{align*}
  a &= |Fz|, \\
  z &= Q\psi. 
\end{align*}
\]

These algorithms are often defined in terms of two projection operators \(P_F^x\) and \(P_Q\) that project onto the solution \(z\) to equations ((2) and (3)) that is closest to the current estimate described in section 2.

Alternative approaches include formulating the problem as

\[
\min_{\psi} \|a - |FQ\psi|\|
\]
we formulate equation (4) using the frames \( z \) as slack variables as discussed in section 2 and solve

\[
\min_{z} \|a - |Fz|\|
\]

with the conditions that \( z \) satisfies equation (3) using projected gradient, Newton and quasi-Newton methods [30, 31].

Another approach uses a \( n^2 \times n^2 \) phase-space described in terms of a ‘Wigner Distribution’ function [3, 7]. More recently [32–34] a convex relaxation of the quadratic problem is obtained by lifting to an \( n^2 \times n^2 \) space and minimizing the rank of the matrix.

**Main results**

The main contribution of this paper is the introduction of an additional optimization step in the measurement space, which with a dimensionality of \( km^2 \), is larger than the object space, \( n^2 \). It is aimed to deal with fluctuating intensities, position errors, poor calibration using multiplexing illumination, and an unknown offset (background) for every pixel but constant throughout the acquisition (or vice versa). Specifically, instead of solving equation (4), we wish to minimize the gap between the measurement space and the smaller object space:

\[
\min_{z,|Fz|=a} \|I - P_Q|z|\|
\]

where \( I \) is the identity operator and \( P_Q \) represents a projection onto the object space and will be described in the following section.

Recently it was proposed to use maxcut algorithms to solve a similar problem [35]. Here we approach the problem differently. We start from the redundant measurement space and compute pairwise comparison between frames before merging into the object space.

In section 3 we consider the case that the diffraction measurement \( a(i) \) is contaminated (i.e. multiplied) by an unknown scalar factor \( \omega(i) \). We encounter this problem if the intensity or integration time of the incident beam is unknown. If we fix the relative amplitude and phase within every frame \( z(i) \) and minimize the gap equation (6) with respect to the vector \( \omega \) for a given \( z \), we can express equation (6) as

\[
\min_{\omega} \omega^* H \omega
\]

\[
H_{i,j} = z(i)^* \left( \delta_{i,j} I - \frac{Q(i)Q(i)^*}{e_i^*(Q^*Q)e_j} \right) z(j),
\]

where the \( k \times k \) matrix \( H \) is calculated by computing the pairwise dot product between overlapping frames. While this problem arises from the need to account for intensity fluctuations, it turns out to be a useful technique to improve the convergence rate for large scale problems. The phase vector obtained by normalizing \( \omega \) enables us to adjust for the relative phase between frames and accelerate the rate of convergence in iterative algorithms.

We use a similar approach to optimize perturbations of the illumination matrix \( Q \): the position among frames (section 4). Alternative approaches optimizing the positions from the reduced object space have been proposed by others [14, 15]. By minimizing the gap between measurement space and constraint, we obtain a first-order correction formula that relies on pairwise scalar products between neighboring frames. We expect a method based on pairwise comparisons to work well in large scale problems when long range position drifts may arise.

In section 6 we report the following numerical results:

- Exact reconstruction with intensity fluctuation given by the coefficients \( \omega(i) \) (see figure 4).
- Accelerated convergence (figure 5) even when no intensity fluctuation is present in the data (Table 3).
• Exact reconstruction with multiplexing using four simultaneous illuminations adding incoherently on the detector, with perturbation of the amplitudes (figure 6).
• Position recovery (figure 7) of the illuminating probe.
• Joint reconstruction of the sample and fluctuating background noise independent from the sample (figures 8 and 9).
• Exact reconstruction with missing (corrupted) data entries (see figures 11 and 12).

In the following section 2 we will describe the standard operators commonly used in the literature.

2. Standard Projection algorithms

The projection operator \( P^a_F \) mentioned in the previous section is often known as the Fourier magnitude projection operator. Applying this operator to a vector \( z \) yields

\[
P^a_F z = F^* \left( \frac{Fz}{|Fz|} \cdot a \right)
\]

(8)

where division and multiplication are intended as element-wise operations. It is easy to verify that

\[
|P^a_F z| = |a|
\]

(9)

and therefore \( P^a_F \) satisfies equation (2) for any \( z \). We mention that \( P^a_F \) is a projection in the sense that

\[
P^a_F z = \arg \min_{\tilde{z}} \| z^{(i)} - \tilde{z}^{(i)} \|
\]

subject to \( |F\tilde{z}| = a \),

(9)

where \( \| \| \) denotes the Euclidean norm. The matrix \( Q \) defines an orthogonal projection operator \( P_Q \) that projects any vector in \( \mathbb{C}^k \) onto the range of \( Q \):

\[
P_Q = QQ^* - I_Q
\]

(10)

when \( (Q^*Q)^{-1} \) exists. An alternative formulation uses projection operators that apply on the Fourier frames \( \hat{z} = Fz \):

\[
P^a_F = FF^* , \quad \tilde{P}^a_F = FP^a_F F^*.
\]

Line search straategies to solve equation (9) can be implemented more efficiently using this formulation [30].

In the simple alternating projection algorithm, the approximation to the solutions of (equations (2) and (3)) are updated by

\[
z^{(i)} = [P_Q P^a_F] z^{(i-1)},
\]

(11)

where typically the initial guess \( z^{(0)} \) is a random vector. Clearly \( P^a_F \) from (9) forces \( z^{(i-1)} \) to have the right amplitude in the Fourier domain, and \( P_Q \) forces \( P^a_F z^{(i-1)} \) to be located in the range of \( Q \). We note that the projector \( P_Q \) can be expressed by computing the running estimate of \( \psi \) denoted as \( \psi^{(i)} \)

\[
\psi^{(i)} = \arg \min_{\tilde{z}} \| P^a_F z^{(i-1)} - Q\tilde{z} \|, \quad (i)
\]

(12)

which is solved by taking equation (10) into account:

\[
\psi^{(i)} = [(Q^*Q)^{-1} Q^*] P^a_F z^{(i-1)},
\]

(13)

when \( (Q^*Q)^{-1} \) exists. Notice that \( P_Q P^a_F z^{(i-1)} = Q\psi^{(i)} \).

We mention two practical issues regarding the updating steps (12) and (9). First, since \( (Q^*Q)^{-1} \) may not exist, one may introduce a regularization factor \( \epsilon \) into (12) and update the running estimate as

\[
\psi^{(i)} = (Q^*Q + \epsilon)^{-1} (Q^*P^a_F z^{(i-1)} + \epsilon \psi^{(i-1)})
\]

(14)
Table 2. Popular fix-point algorithms used in phase retrieval. HIO: hybrid input–output algorithm. RAAR: Relaxed averaged alternating reflections algorithm.

| Projection algorithm | Updating formula $z^{(t+1)} = $ |
|----------------------|----------------------------------|
| Alternating Projection [37] | $P_Q P_F |z^{(t)}| \sqrt{a + |Fz| \sigma^2}$ |
| HIO [37]               | $P_Q P_F + (I - P_Q)(I - \beta P_F)|z^{(t)}|$ |
| Difference Map [8]     | $P_F P_Q + (I - P_F)(I - \beta P_Q)|z^{(t)}|$ |
| RAAR [38]              | $2\beta P_F P_Q + (1 - 2\beta)P_F + \beta(P_Q - I)|z^{(t)}|$ |

with typically $\psi^{(0)} = 0$. $\epsilon$ is a regularization factor that leaves unchanged the entries that are never illuminated, and gradually reduces the correction from $\psi^{(t-1)}$ where the sum of the illuminating probe intensities is small. If we replace equation (13) by equation (14) we obtain an operator that is no longer a projection operator but can be viewed as a relaxed projection.

If the entries of $a(i,q)$ are corrupted by Gaussian random noise with known variance $\sigma_i^2(q)$, which is expressed as a $m^2$ long column vector, one may replace equation (9) modifying $P^\ast_F$ with

$$P_F^{(\sigma^2)} z = F^\ast \left( \begin{array}{c} Fz \\ |Fz| \sigma^2 \end{array} \right),$$

(15)

where $\sigma$ is viewed as a regularization factor that leaves unchanged the entries of $z$ when the data entries are completely corrupted ($\sigma^2 \to \infty$). Clearly $\frac{a + |Fz| \sigma^2}{1 + \sigma^2} \to 1$ when $\sigma^2 \to \infty$. When $\sigma^2 \to 0$, (equation (15)) reverts to the regular projection operator (equation (8)).

The simple alternating projection algorithm can be viewed as the projected steepest descent algorithms. Projected conjugate gradient methods have also been proposed in [14, 19, 30] to accelerate convergence rate.

A number of heuristic first-order algorithms have been proposed that outperform the simple algorithms, a few examples are given in table 2, with $\beta \in [0, 1]$ is a relaxation parameter. Very recently, an ADM was proposed to work with a special augmented Lagrangian function [29]. This function is minimized by applying a block coordinate descent scheme [36] (or alternating search directions) akin to these projection operators.

3. Fluctuating intensities, and augmented phase retrieval

Intensity fluctuations can be accounted for by introducing a scalar scaling factor $\omega_i \in \mathbb{C}$ multiplying every $(m^2)$ pixel of a diffraction frame. This can be expressed in various forms (frame by frame or all at once) as

$$|F_{z(i)}| \cdot |\omega(i)| = a(i), \quad \forall i$$

(16)

$$\text{diag} (Fz) \omega = a.$$  

(17)

where $\omega = [\omega_1, \ldots, \omega_k] \in \mathbb{C}^k$ and $B$ is a $k \times k$ diagonal block matrix with the diagonal entry $1_{m^2}$, which is the $m^2 \times 1$ matrix with 1 in all entries. In other words, $B$ copies the scalar factors $\omega_i$ before multiplying by $Fz$. In practice $\omega_i$ is unknown and needs to be estimated. If we know $z$ or its approximation, to estimate $\omega_i$, we find the vector $\omega$ that minimizes the gap with the object space:

$$\arg \min_{\omega} \| (I - P_Q) \text{diag} (z) B \omega \|^2.$$  

(18)
We can write equation (18) as
\[ \arg \min_{\omega} \omega^T H \omega, \]
where the \( k \times k \) matrix \( H \) is computed by performing the scalar product between every pair of overlapping frames. We can eliminate the trivial solution \( \omega = 0 \) by setting an additional constraint such as \( \sum_\omega \), or \( \| \omega \| = \text{constant} \). A simple way to solve this problem (see appendix A) is to start with \( 1 \) as our first guess for \( \omega \) and solve
\[ H \omega = \alpha 1, \]
where \( \alpha \) is chosen to normalize the average flux \( \| \omega \| / \| 1 \| \).

In order to take the intensity fluctuation problem into account while applying the projection algorithm (2) and (3), we introduce the following solution. First, we replace the operator \( P Q \) used in the standard projection algorithms listed in table 2 by an augmented projection operator \( P^\omega Q \) defined as
\[ P^\omega Q = D^{-1} P Q D^\omega, \quad D^\omega = \text{diag} (\omega), \]
where \( \omega \) is the solution to equation (19) or equation (20). An alternative modification is to recompute the normalization factor \( Q^* Q \) with the scaling factors \( |\omega_i|^2 \). This yields an orthogonal projection:
\[ \bar{P}^\omega Q = Q^\omega (Q^* Q)^{-1} Q^\omega, \quad Q^\omega = D^{-1} Q. \]

When no intensity fluctuations are present, we normalize \( \omega \) and replace \( D^\omega \) with:
\[ D^\circ \omega = \text{diag} \left( \frac{\omega}{|\omega|} \right). \]

Although the construction of \( P^\omega Q \) is motivated by the need to account for intensity fluctuations among different diffraction frames in the measured data, it turns out to be a useful technique for accelerating the convergence of projection algorithms even when no intensity fluctuation is present in the data. The minimization problem in (equation (18)) is similar to the phase problem of how to merge frames \( z_{(i)} \) with unknown phase factor \( \omega \), which can be written as
\[ \arg \min_{\omega, |\omega| = 1} \omega^T H \omega. \]
Replacing the condition \( |\omega| = 1 \) with weaker conditions such as \( \sum_\omega \) or \( \| \omega \| = \text{constant} \) enables us to solve this problem more efficiently. A similar approach is discussed in [39].

The problem of the incoherent superposition of different signals can be treated in a similar way.

3.1. Multiplexing and incoherent measurements

The incoherent measurement model is as follows. We consider \( z_i \) the highly redundant set of frames generated for all the positions of the illumination function during an exposure. For example, a single exposure \( a_{(i)} \) may represents the sum of the intensities generated by an illumination beam that translates during the exposure, or may represent a binned sample of a continuous signal. Assume we have \( k \) redundant measurement \( z_{(i)}, \) where \( i = 1, \ldots, k. \) The
incoherent measurement is introduced by summing $s < k$ illumination windows according to a weight factor, where we assume $k/s$ is an integer for convenience. The weight factor, or the integration time, for each frame, is represented by $|\omega|^2$. In particular, the redundant set of frames $z_{i(\ell)}$ is not measured directly; instead it is multiplied by a known averaging operator, which is expressed as $|\omega|^2$ and a $(k/s)m^2 \times km^2$ real matrix $\Omega$ with all non-zero entries 1. Geometrically, $\Omega$ groups the frames, which are weighted by $|\omega|^2$, and then the weighted frames in each group are summed. The incoherent measurement can thus be expressed by modifying (17):

$$a^2 = \Omega(|Fz|^2 \cdot B|\omega|^2),$$

where $\cdot$ and $| \cdot |^2$ are intended as element-wise operations $z$ is a given $km^2$ complex column vector and $a^2$ is a $(k/s)m^2$ real column vector. The projection operator associated with this problem can be expressed as follows:

$$P_{\Lambda \Omega} z = F^* \left( \text{diag} \left( \frac{|a^2|}{\Lambda (|Fz|^2 \cdot B|\omega|^2)} \right) Fz \right),$$

when all non-zero entries of $\Lambda$ are 1 and $\Omega \Omega^* = sI_{(k/s)m^2}$. Here $\Omega^*$ copies the entries over all the frames that contribute to an exposure $a_{ij}$. We can directly check that equation (25) satisfies equation (24). Replacing this operator in the reconstruction process is a subject of recent interest by several groups [21, 40]. Other approaches for incoherent averaging over wavelengths, orientation, coherence, etc have been discussed by others [22–25].

If $|\omega|^2$ is unknown, we can derive it from solving a minimization problem of the type equation (4), from the object space, but with an incoherent measurement model. Another approach is to obtain $\omega$ by solving a minimization problem of the type equation (6), from the measurement space with the incoherent measurement model by solving equation (20) and using equation (21) .

Numerical tests described in section 6 show the exact recovery (within numerical precision) of the object and a multiplexing array of beam positions averaged incoherently with errors in the calibration of the amplitude factors. The ability to recover the relative precision) of the object and a multiplexing array of beam positions averaged incoherently.

The number of frames used in the calculation however increases, and with it, the computational cost increases as well. To reduce the number of parameters to optimize we can describe the change in measurement space using Taylor expansion.

4. Position retrieval

We consider the case in which the probe $w$ is translated from the input coordinate by an unknown distance $\xi$. We call $Q_\xi$ the unknown illumination matrix used to generate the data. To determine the illumination matrix, we determine the parameter $\xi$ so that the error $\varepsilon_{Q_\xi}$ is minimized:

$$\varepsilon_{Q_\xi} := \|I - P_{Q_\xi}\|_2^2.$$

Given the illumination function $w$, we can compute the first- and second-order derivatives with respect to translation.

We denote by $Q_{(\ell)}$, $R_{1,(\ell)}$, $R_{2,(\ell)}$, $S_{11,(\ell)}$, $S_{12,(\ell)}$, $S_{21,(\ell)}$, and $S_{22,(\ell)}$ the illumination matrices that extract a frame out of an image and multiply by $w_{(\ell)}(r)$, $\partial_{\xi} w_{(\ell)}(r)$, $\partial_{\xi} w_{(\ell)}(r)$, $\partial_{\xi, \gamma} w_{(\ell)}(r)$, $\partial_{\xi, \gamma} w_{(\ell)}(r)$, and $\partial_{\xi, \gamma}^2 w_{(\ell)}(r)$ respectively. Build up
the frames\( Q_{\xi} \) satisfies the following second-order perturbation from \( Q \):

\[
Q_{\xi} = Q + \text{diag}(B\xi_1)R_1 + \text{diag}(B\xi_2)R_2 + \text{Diag}(B\xi_3^2)S_{11} + 2\text{diag}(B(\xi_1 \cdot \xi_2))S_x + \text{Diag}(B\xi_3^2)S_{22}
\]

where \( \cdot \) and \( \cdot^2 \) are intended as element-wise operations, \( \xi_1 \) (resp. \( \xi_2 \)) is a \( k \times 1 \) matrix so that the \( i \text{th} \) entry is the translation distance in the \( x \)-axis (resp. \( y \)-axis) of the \( i \text{th} \) illumination window, and \( S_x \equiv \frac{1}{2} (S_{12} + S_{21}) \). Using this Taylor expansion into equation (26) and setting \( \partial_{z_i} \parallel \cdot \parallel \) to 0 gives (see appendix B for the detailed derivation for the 1-dim case)

\[
\begin{pmatrix} H_1 & H_x \\ H_x & H_2 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \begin{pmatrix} z^*zR_{11} + z^*_Rz_R \\ z^*zR_{21} + z^*_Rz_R \end{pmatrix}, \tag{27}
\]

using the definition \( z_{11}, \ldots, z_{22} = [R_1, \ldots, S_{22}] \frac{1}{Q} Q^* z, \ z \equiv [I - R Q] z, \) and where the matrices \( H_1, H_2 \) and \( H_x \) are defined as

\[
\begin{align*}
(H_1)_{ij} &= (z^*_Rz_{R_{11}} - 2z^*_Rz_{S_{12}})\delta_{ij} - z^*_j (O_{11})_{ij} z_j + \text{cc}, \\
(H_2)_{ij} &= (z^*_Rz_{R_{22}} - 2z^*_Rz_{S_{22}})\delta_{ij} - z^*_j (O_{22})_{ij} z_j + \text{cc}, \\
(H_x)_{ij} &= (z^*_Rz_{R_{12}} - 2z^*_Rz_{S_{21}})\delta_{ij} - z^*_j (O_x)_{ij} z_j + \text{cc},
\end{align*}
\]

where \( \text{cc} \) denotes the complex conjugate term,

\[
\begin{align*}
(O_{11})_{ij} &= (R_1)_{ij} \frac{1}{Q} Q^* (R_1)_{ij}^*, \\
(O_{22})_{ij} &= (R_2)_{ij} \frac{1}{Q} Q^* (R_2)_{ij}^*, \\
(O_x)_{ij} &= (R_1)_{ij} \frac{1}{Q} Q^* (R_2)_{ij}^*.
\end{align*}
\]

The system of equations (equation (27)) can be solved efficiently by sparse linear algebra solvers. The entries of the equation are given by the dot product between frames \( (z, z, z_R, \ldots, z_{S_{22}}) \) with partial overlap and scaling factors given by \( R_{1,2} \frac{1}{Q} Q^* R_{1,2}^* \). The terms \( z^*_Rz \) in \( H \) are higher order corrections close to the solution and can be neglected in practice.

In section 6 we will show that this method can recover the position perturbations to numerical accuracy when the perturbations are smaller than the probe width.

5. Background noise

For completeness we consider an unknown offset \( b(q) \geq 0 \) (background) added to each frame. A similar problem is discussed in [17] where Thurman and Fienup consider the case of a constant signal bias \( b(q) = b(0) \). Here we extend this approach to a fluctuating background that is different for every pixel but constant throughout the illumination window. When \( b \) is constant, the method described here reverts to [17, 18]. We express the relationship between the frames \( z(\iota) \), the data \( a(\iota) \) and the background \( b \) as:

\[
|z(\iota)|^2 + b = a^*_G(\jmath), \quad \tilde{z}(\iota) = \mathcal{F}z(\iota). \tag{28}
\]
A less trivial variation of the problem is when \( b_i(q) \geq 0 \) is different for every frame but the same for every pixel \( q \).

At each iteration, we solve the following offset minimization problem with an additional scaling parameter:

\[
\min_{b, \eta} \sum_i |\hat{z}(i) - \hat{z}(i)^{(\ell)}|^2
\]

subject to \( |\hat{z}(i)^{(\ell)}|^2 = \eta(i)\left(a_i^2 - b(i)^{(\ell)}\right)\), (29)

where we set the initial value of \( b(i)^{(\ell=0)} = 0 \), and \( \eta \in \mathbb{R}^{m^2} \) is a shrinkage parameter that accounts for the fact that \( |\hat{z}^{(\ell)}|^2 \) is on average smaller than \( a_i^2 \). This is because \( \hat{z} \) is obtained from a sequence of linear projections that reduce the overall norm. Since \( \hat{z} \) is smaller, the solution to the offset projection problem (29) is biased toward a larger offset. Introducing the shrinkage parameter \( \eta \) equal for every frame provides the flexibility to avoid this problem.

By solving for \( \eta \) first, we obtain the first- and second-order terms:

\[
\eta(i)^{(\ell)} = \frac{\sum_i d(i)|\hat{z}(i)^{(\ell)}|^2}{\sum_i d(i)^2},
\]

where \( d(i) = a_i^2 - b(i) \). Solving for \( b(i) \) for a fixed \( \eta(i) \) gives

\[
b(i)^{(\ell)} - b(i)^{(\ell-1)} = \frac{1}{k} \sum_i \left( d(i) - \frac{|\hat{z}(i)^{(\ell)}|^2}{\eta(i)} \right)
\]

\[
= \langle d(i) \rangle - \frac{1}{\eta(i)} \langle |\hat{z}(i)^{(\ell)}|^2 \rangle
\]

\[
= \langle d(i) \rangle - \frac{\langle d(i)^2 \rangle |\hat{z}(i)^{(\ell)}|^2}{\langle |\hat{z}(i)^{(\ell)}|^2 \rangle}.
\]

To avoid strong perturbations, however, we set \( \eta(q) = 0.8 \) if \( \eta(q) < 0.8 \). When optimizing for a fluctuating offset \( b(i)(q) = b(i)(0) \) constant for every frame), we simply replace the sum over \( i \) with the sum over \( q \). The update of \( z \) is then computed as a regular Fourier magnitude projection operator with an intensity offset:

\[
\tilde{P}\left[a_i^2 - b(i)^{(\ell)}\right] \hat{z}(i)^{(\ell)} = \hat{z}(i)^{(\ell)} \left[ a_i^2 - b(i)^{(\ell)} \right],
\]

where we used the notation \( \tilde{P} = \mathcal{F}P\mathcal{F}^* \).

In the following section we will show that common projection methods can recover the background even if the SNR is much smaller than 1.

6. Numerical tests

The object used to simulate the diffraction pattern is obtained from an SEM image of a cluster of commercial 50 nm colloidal gold spheres. The image is shown in figure 2. The gray scale values were converted to a sample thickness varying between 0 and 50 nm, and we assigned the complex index of refraction of a 750 eV x-ray photon going through an organic compound (PMMA). Here the numerical tests are done assuming periodic boundary conditions. These boundary conditions ensure that every region of the object \( \psi \) is illuminated with an equal number of overlapping frames, in other words the null space of \( Q \) is empty. We use frame width 16 × 16, probe width 8, step size 5, number of frames \( 8 \times 8 \ldots 64 \times 64 \),
RAAR algorithm, $\beta = 0.75$. The initial guess of the phase chosen to be random. There is no padding of the illumination function shown in figure 3 (the intensity measurement is slightly under-sampled).

The metrics $\varepsilon_F$, $\varepsilon_Q$ used to monitor progress are functions depending on $z^{(l)}$:

$$
\varepsilon_F(z^{(l)}) = \frac{\| [P_F - I] z^{(l)} \|}{\| a \|},
$$

$$
\varepsilon_Q(z^{(l)}) = \frac{\| [P_Q - I] z^{(l)} \|}{\| a \|},
$$

where $I$ is the identity operator. This has to be compared to $\varepsilon_0$, the error w.r.t. the known solution:

$$
\varepsilon_0(z^{(l)}) = \frac{1}{\| a \|} \min_{\varphi} \| e^{i\varphi} z^{(l)} - Q \psi \|,
$$

where $\varphi$ is an arbitrary global phase factor.

We report the following observations

- **Fluctuating intensities**: (figure 4). The intensity fluctuation in this test is 20%. By solving the new LSQ problem introduced in (21), we obtain accelerated convergence and exact reconstructions every time we tested the problem, see (figure 4). No degradation (above numerical precision) introduced by intensities perturbed by 20%.
- **Scaling**: (figure 5). We show improved convergence in the larger scale problems. The results are summarized in table 3. As we increase the number of frames, convergence slows down for standard projection operators. The parameters used in this simulation are

Figure 2. The object $\psi$ used to simulate diffraction data obtained from an SEM image of a cluster.
Figure 3. Absolute value of the probe $|w(r)|$ used in simulations (16×16 pixels).

Table 3. Performance of projection algorithms using Matlab R2012a 64-bit (maci64) (Lapack version 3.3.1, MKL 10.3.5) on 2×2.2 GHz Quad-core Intel Xeon using frames of dimension 16×16.

\begin{tabular}{cccc}
  No. of frames & Clock time(s) & Iteration & $\epsilon_0^2$ \\
  \hline
  Standard & & & \\
  4×4 & 0.7 & 121 & $<1 \times 10^{-11}$ \\
  8×8 & 1.4 & 125 & $<1 \times 10^{-11}$ \\
  16×16 & 4.9 & 144 & $<1 \times 10^{-11}$ \\
  24×24 & 26.3 & 400 & $4.3 \times 10^{-10}$ \\
  32×32 & 36.3 & 400 & $4.3 \times 10^{-4}$ \\
  48×48 & 90.7 & 400 & $3.4 \times 10^{-4}$ \\
  64×64 & 137.5 & 400 & $5.3 \times 10^{-3}$ \\
  \hline
  Augmented & & & \\
  4×4 & 1.9 & 138 & $<1 \times 10^{-11}$ \\
  8×8 & 2.7 & 141 & $<1 \times 10^{-11}$ \\
  16×16 & 6.5 & 138 & $<1 \times 10^{-11}$ \\
  24×24 & 14 & 134 & $<1 \times 10^{-11}$ \\
  32×32 & 25.6 & 139 & $<1 \times 10^{-11}$ \\
  48×48 & 60.4 & 142 & $<1 \times 10^{-11}$ \\
  64×64 & 96.2 & 149 & $<1 \times 10^{-11}$ \\
  \hline
\end{tabular}

$m = 16, D_x = 4, k$ varies and $n = kD_x + m$, where $D_x$ is the step size of the illumination windows.

• Incoherent multiplexing: (figure 5). Deconvolution of the incoherent sum of frames translated by three times the illuminating beam width.
Figure 4. Convergence rate with an $I_0$-error of ±20%. Top left: old projection operator, top right: new projection operator. Bottom: reconstruction from data with $I_0$-error, and solution (reconstruction using the new projection operator is within the computer numerical precision, i.e. the figure on the right looks identical to the exact solution.

Figure 5. Convergence rate ($\varepsilon_F, \varepsilon_Q, \varepsilon_0$ versus number of iteration $\ell$) for (top) regular reconstruction. (bottom) using augmented projection ($m = 16$ and step size $x_1 - x_2 = 3$).
Figure 6. Convergence rate with incoherent illumination of four beams, separated by $3 \times$ the probe width (FWHM) using standard projection algorithms (top left), with intermediate phase optimization (top-right), phase and amplitude (bottom-left), and phase and amplitude with initial amplitude error of 20% (bottom right), frame width $16 \times 16$, $16 \times 16$ frames, step size $3.5$ pixels close packing with $\pm 1$ pixel known random perturbations.

Figure 7. Reconstruction with position errors using the method described in section 4, where $\epsilon_{x_0} = \|\xi - \xi_0\|/\|\xi_0\|$, and the perturbations in position are randomly distributed with $(\xi_0) = \frac{1}{k} \sum \|\xi_i\| = 2.5$ resolution elements. (number of frames: $16 \times 16$, frame dimensions $32 \times 32$, step size: $3.5$ pixels, hexagonal packing with known random perturbations of $\pm 1$ pixels and unknown $\xi$ random perturbations).

- **Incoherent beams with fluctuations:** (figure 6). Deconvolution of the incoherent sum of frames translated by three times the illuminating beam width, with unknown amplitude.
- **Positions:** (figure 7). Recovery of the positions perturbed by an unknown factor randomly distributed between $\pm 2.5$ pixels.
- **Background:** (figures 8 and 9). $\langle \|z_i\|\rangle/\|b\| = 0.5$. In figures 8 and 9 we obtain exact reconstruction of the object and background (background ratio $\|a\|/\|b\| = 10^{-6}$).
Figure 8. Two measured intensities with additive background (SNR = 0.5). In a separate test the diffraction data was buried by the background (in other figures not included, the background was $10^6 \times$ the signal).

Figure 9. Top: reconstructed image with background optimization (left) and without (right). The figure on the left looks identical to the exact solution. Bottom: reconstructed background (left), convergence behavior (right).
Exact recovery (within numerical precision) was obtained with step size $\delta x = 3r$. No degradation (above numerical precision) introduced by the background, nearly no influence on convergence rate.

- **Missing data:** (figures 10–12). Exact recovery (within numerical precision) using equation (15). Frame size: $32 \times 32$, number of frames: $16 \times 16$, step size: 3.5 pixels.
Conclusions

While phase retrieval problems are notoriously difficult to solve numerically, the high redundancy in ptychographic data enables not only robust phase recovery [19, 20] but the recovery of other parameters such as the illuminating function itself [9], position [14–16], coherence function [21], etc.

In this paper we introduce a modified projection operator for the ptychographic reconstruction problem that accounts for fluctuating intensities, position errors, partial coherence or poor calibration using multiplexing illumination, and an unknown offset (background) difference for every pixel but constant throughout the acquisition (or vice versa). Our approach starts from the redundant measurement space and computes pairwise comparison between frames before merging into the object space. We describe first-order methods to minimize the gap between measurement space and object space w.r.t. the perturbation parameter. We show that our method enhances the convergence rate of common projection algorithms. We show several cases where missing information (phases, bad pixels, positions, incoherence, etc) was retrieved exactly (to within numerical precision) starting from random phases. This method appears to be robust when the amount of overlap between neighboring frames is around 50% or more.

Further theoretical analysis on the relative merits between object-space minimization and measurement space minimization will be the subject of the future work.

Here some numerical details deserve further developments. By optimizing the phase of each frame from the redundant measurement space, we solve the phase problem at a resolution given by the step size between frames. This intra-frame phase optimization may be applied to merge subregions reconstructed independently by distributed computer systems. For 3D objects, we could apply similar approach to merge two-dimensional views reconstructed independently into one 3D object. Finally, this intra-frame optimization could be applied to multi-scale reconstructions where frames are divided in regions of Fourier space, or it could be applied to correct low-order phase aberrations between frames. More work is needed to establish the optimal frequency of communication and the amount of overlap between sub-reconstruction regions.
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Appendix A. Intensity fluctuations

One of the practical issues one may face in ptychography is the intensity fluctuation among different diffraction frames introduced by instabilities in the light source, optics and shutters. Such fluctuation can be accounted for by introducing a scaling factor \( \omega \in \mathbb{C} \) for each diffraction frame. As a result, the definition \( \hat{z}_i \) is modified so that the equation

\[
\omega_i z_i(i) = Q(i) \psi, \quad (A.1)
\]

holds for \( i = 1, 2, \ldots, k \).

Since both \( \omega_i \) and \( \psi \) are unknown in (A.1), the solution to (A.1) is clearly not unique. To exclude the trivial solution \( \omega_i = 0 \), for \( i = 1, 2, \ldots, k \) and \( \psi = 0 \), we introduce an additional constraint and solve

\[
(\psi_{\text{min}}, \omega_{(i)}) = \arg \min_{\psi, \omega_{(i)}} \sum_i \|Q(i) \psi - \omega_i z_i(i)\|^2
\]

subject to \( \sum_{(i)} \omega_i = \sum_{(i)} 1 = k \),

(A.2)

which is equivalent to solve

\[
\min_{\psi, \omega_i, \lambda} \mathcal{L}(\psi, \omega_i, \lambda), \quad \text{where} \quad \mathcal{L} = \sum_i \|Q(i) \psi - \omega_i z_i(i)\|^2 + 2\lambda \left( \sum_i \omega_i - \|1\|^2 \right), \quad (A.3)
\]

where \( \lambda \) is a Lagrange multiplier. To find the coefficients \( \omega_i \), we use the normal equation associated with the LSQ problem (equation (A.3)):

\[
\begin{pmatrix}
\sum_i Q(i)^* Q(i) & -Q(i)^* z_i & 0 & \cdots & 0 \\
-Q(i)^* z_i & z_i^* z_i & 0 & \cdots & 0 \\
0 & 0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & -Q_k^* Q_k & z_k^* z_k \\
0 & \cdots & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\psi \\
\omega_1 \\
\vdots \\
\omega_k \\
\lambda
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
\|1\|^2
\end{pmatrix}.
\]

We can partition the equation above as

\[
\begin{pmatrix}
A & B^* & 0 \\
B & D & 1 \\
0 & 1^* & 0
\end{pmatrix}
\begin{pmatrix}
\psi \\
\omega
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
\|1\|^2
\end{pmatrix},
\]

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where

\[
A = \sum_{i=1}^{k} Q_i^* Q_i, \quad B = \begin{pmatrix} -z_1^* Q_1 \\
\vdots \\
-\sum_{i=1}^{k} Q_i \\
\end{pmatrix}, \quad D = \begin{pmatrix} z_1^* z_1 & 0 & \cdots & 0 \\
0 & z_2^* z_2 & \cdots & \vdots \\
\vdots & \vdots & \ddots & 0 \\
0 & 0 & \cdots & z_k^* z_k \\
\end{pmatrix}, \quad \omega = \begin{pmatrix} \omega_1 \\
\vdots \\
\omega_k \\
\end{pmatrix}.
\]

By the block factorization

\[
\begin{pmatrix}
I & 0 & 0 \\
-BA^{-1} & I & 0 \\
0 & -1^* H^{-1} & 1
\end{pmatrix} \begin{pmatrix} A & B^* & 0 \\
0 & H & 1 \\
0 & 0 & -1^* H^{-1} \end{pmatrix} \begin{pmatrix} \psi \\
\omega \\
\lambda \end{pmatrix} = \begin{pmatrix} 0 \\
0 \\
\|1\|^2 \end{pmatrix} \tag{A.4}
\]

where the Schur complement \(H = D - BA^{-1}B^*\) is given by

\[
H_{i,j} = z_i^* \left( \delta_{i,j} I - \sum_{\iota} Q_{\iota}^* Q_{\iota} \right)^{-1} Q_j^* z_j.
\]

By block-wise inversion of equation (A.4), we obtain \(\omega\) and the scaling factor \(\lambda\) from a sparse linear equation:

\[
H\omega = -\lambda 1, \quad \lambda = -\frac{\|1\|^2}{1^* H^{-1} 1}.
\]

**Eigenvalue method**

If we make a change of variable, \(v_{\iota} = \|z_{\iota}\| \omega_{\iota}\), we can re-write the problem \(\arg\min_{\omega} \omega^* H\omega\) as

\[
\arg\min_{v} \|v\|^2 - v^* K v,
\]

\[
K_{i,j} = \frac{z_{\iota}^*}{\|z_{\iota}\|} \sum_{\iota} Q_{\iota}^* Q_{\iota} \left( \sum_{\iota} Q_{\iota}^* Q_{\iota} \right)^{-1} Q_j^* \frac{z_j}{\|z_j\|}.
\]

The solution to this problem assuming \(\|v\|=\text{constant}\) is the eigenvector corresponding to the largest eigenvalue of the sparse matrix \(K\). This can be computed efficiently using packages such as [41]

**Appendix B. Taylor expansion**

We consider the case in which the probe \(w\) is translated from the input coordinate by an unknown distance \(\xi\). We restrict ourselves to the 1-dim ptychography problem to simplify the discussion. We call \(Q_{\xi}\) the unknown illumination matrix used to generate the data. To determine the illumination matrix, we determine the parameter \(\xi\) so that the error \(\varepsilon_{Q_{\xi}}\) is minimized:

\[
\arg\min_{\xi \in \mathbb{R}^k} \|I - P_{Q_{\xi}}\|^2, \tag{B.1}
\]

where the \(i\)th entry of \(\xi \in \mathbb{R}^k\) represents the translation distance of the \(i\)th frame. Given the illumination function \(w\), we can compute the first- and second-order derivatives with respect to translation. We denote by \(Q, R, S\) the illumination matrices that extract a frame out of an image and multiplies by \((w(x), \partial_x w(x), \partial_x^2 w(x))\) respectively. Build \(Q, R, S\) from \(Q, R, S\), which are tall and skinny matrices of the same size as \(Q\) discussed earlier, with
identical location of the non-zero entries. Assume that the probe is perturbed to second-order as follows:

$$Q_\xi = Q + \xi R + \xi^2 S.$$  

where, by a slight abuse of notation, $\xi$ denotes a diagonal and real matrix so that the $i$th diagonal entry, denoted as $\xi_i$, represents the translation distance of the $i$th frame. With $Q_\xi$ plugged into (B.1), we now minimize

$$\arg \min_{\xi \in \mathbb{R}} \| (I - (Q + \xi R + \xi^2 S)(Q + \xi R + \xi^2 S)^\ast (Q + \xi R + \xi^2 S)^{-1} (Q + \xi R + \xi^2 S)^\ast \| \xi \|^2.$$  

(B.2)

By Taylor expansion,

$$[\cdot]^{-1} \simeq \frac{1}{Q\ast Q} \left( 1 - (R\ast \xi Q + Q\ast \xi R + O(\xi^2)) - \frac{1}{Q\ast Q} \right),$$

when $Q\ast Q$ is invertible. The second-order term $O(\xi^2)$ includes other second-order terms that we will not need. We write the expansion of the residual in equation (B.2) $f_0 + f_1(\xi) + f_2(\xi^2)$ as

$$f_0 = [I - P_Q]\xi \equiv \xi.$$  

(B.3)

We define $\phi^\ast \equiv \frac{1}{Q\ast Q} Q\ast$, and express the first order as

$$f_1(\xi) = [-\xi R \phi^\ast - \phi R\ast \xi + \phi (R\ast \xi Q + Q\ast \xi R) \phi^\ast] \xi.$$  

By setting $z_R \equiv R \phi^\ast \xi$, using $P_Q = Q \phi^\ast = Q$, and rearranging, we get

$$f_1(\xi) = -\xi z_R - \phi R\ast \xi (z - Q \phi^\ast \xi z) + \phi Q\ast \xi z_R$$

$$= -(1 - P_Q)\xi z_R - \phi R\ast \xi z.$$  

(B.4)

By using the equality $\xi (I - P_Q)\xi \equiv \xi$, setting $O_R \equiv R \phi^\ast \phi R^\ast = R \frac{1}{Q\ast Q} R^\ast$ and rearranging, we obtain

$$f_2(\xi) = -\left[ \xi R \frac{1}{Q\ast Q} R\ast \xi + \xi^2 S \phi + Q O (\xi^2) \right] \xi$$

$$= -\xi O_R \xi \xi z - \xi^2 z_S + QO (\xi^2) \xi z.$$  

(B.5)

where $z_S \equiv S \phi^\ast \xi$. We rewrite equation (B.2) above as

$$\| U - P_Q \| \xi \|^2 = f_0 f_0 + f_1 f_1 + f_2 f_0 + f_0 f_1 + f_0 f_0 + f_0 f_0 + O(\xi^3).$$

Note that $\xi^\ast \phi = \xi \phi = 0$. Set $z_0 \equiv Q \phi \xi z$ and obtain the first- and second-order terms of equation (B.2):

$$f_0 f_1 + f_1 f_0 = -z_0^\ast \xi z_R - z_R^\ast \xi z$$

$$f_1 f_1 + f_0 f_2 + f_2 f_0 = z_R^\ast \xi (I - P_Q) \xi z_R + z_R^\ast \xi O_R \xi \xi z - z_R^\ast \xi O_R \xi z - z_0^\ast \xi Z_S - z_0^\ast \xi O_R \xi \xi z - z_0^\ast \xi O_R \xi z - z_0^\ast \xi O_R \xi z_R.$$  

(B.6)

By using the definition of $z_Q$, $z_R$, $P_Q$ and $O_R$ it is easy to show that $z_R^\ast \xi O_R \xi z_Q = z_R^\ast \xi P_Q \xi z_R$ and simplify as:

$$f_1 f_1 + f_0 f_2 + f_2 f_0 = z_R^\ast \xi Z_R - z_R^\ast \xi Z_S - z_R^\ast \xi O_R \xi \xi z.$$  

(B.7)

By setting $\delta_{\xi} \| \xi \|^2 = 0$ in equation (B.2), we obtain the linear equation for solving $\xi$:

$$\sum_j (2(z_R^\ast z_R + z_R^\ast z_S + z_R^\ast \xi) \delta_{ij} - z_R^\ast O_R z_j - z_R^\ast O_R z_i) \xi_j = \xi^\ast z_R + z_R^\ast \xi.$$
We note that \(-z_i^2 \xi_j z_i - z_i \xi_i z_i^2 - z_i^2 \xi_i z_i z_i^2\) is a second-order correction if we assume that \(z\) is in that range of an unknown \(Q_\xi\) for small \(\xi\). We thus have the following approximation:

\[
f_j f_0 + f_j f_2 + f_j f_0 \approx z_i \xi_i z_i^2 z_i^2 - z_i^2 \xi_i Q_\xi z_i.
\] (B.8)

We can thus consider solving the following approximation equation in practice:

\[
\sum_j (2z_i^2 \xi_i z_i^2 - z_i^2 \xi_i z_i - z_i^2 \xi_i z_i) \xi_j \approx z_i^2 \xi_i z_i^2 + z_i^2 \xi_i z_i^2
\]

Extension to the two-dimensional case is given in section 4.

References

[1] Hoppe W 1969 Beugung im inhomogenen Primärrstrahlwellenfeld: I. Prinzip einer Phasenmessung von Elektronenbeugungsinterferenzen Acta Crystallogr. A 25 495–501
[2] Hegerl R and Hoppe W 1970 Dynamic theory of crystalline structure analysis by electron diffraction in inhomogeneous primary wave field Ber. Bunsenges. Phys. Chem. 74 1148
[3] Rodenburg J M and Bates R H T 1992 The theory of super-resolution electron microscopy via Wigner-distribution deconvolution Phil. Trans. R. Soc. Lond. A 339 521–53
[4] Spence J CH 2003 High-Resolution Electron Microscopy vol 60 (Oxford: Clarendon)
[5] Broennimann Ch et al 2006 The Pilatus 1 m detector J. Synchrotron Radiat. 13 120–30
[6] Doering D et al 2011 Development of a compact fast CCD camera and resonant soft x-ray scattering endstation for time-resolved pump-probe experiments Rev. Sci. Instrum. 82 073303
[7] Chapman H N 1996 Phase-retrieval x-ray microscopy by Wigner-distribution deconvolution Ultramicroscopy 66 153–72
[8] Thibault P, Dierolf M, Menzel A, Bunk O, David C and Pfeiffer F 2008 High-resolution scanning x-ray diffraction microscopy Science 321 379–82
[9] Thibault P, Dierolf M, Bunk O, Menzel A and Pfeiffer F 2009 Probe retrieval in ptychographic coherent diffractive imaging Ultramicroscopy 109 338–43
[10] Rodenburg J M and Faulkner H M L 2004 A phase retrieval algorithm for shifting illumination Appl. Phys. Lett. 85 4705–7
[11] Kushwah C M, Thibault P, Dierolf M, Bunk O, Menzel A, Vila-Comamala J, Jefimovs K and Pfeiffer F 2010 Ptychographic characterization of the wavefield in the focus of reflective hard x-ray optics Ultramicroscopy 110 325–9
[12] Hönig S, Hoppe R, Patommel J, Schropp A, Stephen S, Schöder S, Burghammer M and Schroer C G 2011 Full optical characterization of coherent x-ray nanobeams by ptychographic imaging Opt. Express 19 16324–9
[13] Guizar-Sicairos M, Narayanan S, Stein A, Metzler M, Sandy A R, Fienup J R and Evans-Lutterodt K 2011 Measurement of hard x-ray lens wavefront aberrations using phase retrieval Appl. Phys. Lett. 98 111108
[14] Guizar-Sicairos M and Fienup J R 2008 Phase retrieval with transverse translation diversity: a nonlinear optimization approach Opt. Express 16 7264–78
[15] Maiden A M, Humphry M J, Sarahan M C, Kraus B and Rodenburg J M 2012 An annealing algorithm to correct positioning errors in ptychography Ultramicroscopy 120 64–72
[16] Beckers M, Senkeil T, Giorkn T, Giewekemeyer K, Salditt T and Rosenhahn A 2013 Drift correction in ptychographic diffractive imaging Ultramicroscopy 126 44–47
[17] Thurman S T and Fienup J R 2009 Phase retrieval with signal bias J. Opt. Soc. Am. A 26 1008–14
[18] Guizar-Sicairos M and Fienup J R 2009 Measurement of coherent x-ray focused beams by phase retrieval with transverse translation diversity Opt. Express 17 2670–85
[19] Thibault P and Guizar-Sicairos M 2012 Maximum-likelihood refinement for coherent diffractive imaging New J. Phys. 14 063004
[20] Godard P, Allain M, Chamard V and Rodenburg J 2012 Noise models for low counting rate coherent diffraction imaging Opt. Express 20 25914–34
[21] Jesse N C and Andrew G P 2011 Simultaneous sample and spatial coherence characterisation using diffractive imaging Appl. Phys. Lett. 99 154103
[22] Fienup J R, Marron J C, Schulz J T and Seldin J H 1993 Hubble space telescope characterized by using phase-retrieval algorithms Appl. Opt. 32 1747–67
[23] Abbey B, Nugent K A, Williams G J, Clark J N, Peel A G, Pfeiffer M A, de Jonge M and Mcnulty I 2008 Keyhole coherent diffractive imaging Nature Phys. 4 394–8
[24] Whitehead L W, Williams G J, Quiney H M, Vine D J, Dilanian R A, Flewett S, Nugent K A, Peele A G, Balaur E and McNulty I 2009 Diffractive imaging using partially coherent x rays Phys. Rev. Lett. 103 243902
[25] Jinsong Wu, Leinenweber K, Spence J CH and O’Keeffe M 2006 Ab initio phasing of x-ray powder diffraction patterns by charge flipping Nature Mater. 5 647–52
[26] Rodenburg J M 2008 Ptychography and related diffractive imaging methods Adv. Imaging Electron Phys. 150
[27] Faulkner H M L and Rodenburg J M 2004 Movable aperture lensless transmission microscopy: a novel phase retrieval algorithm Phys. Rev. Lett. 93 023903
[28] Dierolf M, Menzel A, Thibault P, Schneider P, Kewish C M, Wepf R, Bunk O and Pfeiffer F 2011 Ptychographic x-ray computed tomography at the nanoscale Nature 467 436–9
[29] Wen Z, Yang C, Liu X and Marchesini S 2012 Alternating direction methods for classical and ptychographic phase retrieval Inverse Problems 28 115010
[30] Yang C, Qian J, Maia A S F and Marchesini S 2011 Iterative algorithms for ptychographic phase retrieval Technical Report 4598E (Berkley, CA: Lawrence Berkeley National Laboratory) arXiv:1105.5628
[31] Qian J, Yang C, Schirotzek A, Maia F and Marchesini S 2013 Efficient algorithms for ptychographic phase retrieval Contemp. Math. at press (available at www.math.msu.edu/~qian/papers/Paper4Phase.pdf)
[32] Candès E J, Strohmer T and Voroninski V 2013 PhaseLift: exact and stable signal recovery from magnitude measurements via convex programming Commun. Pure Appl. Math. 66 1241–74
[33] Ohlsson H, Yang A Y, Dong R and Shankar Sastry S 2011 Compressive phase retrieval from squared output measurements via semidefinite programming arXiv:1111.6323
[34] Candès E, Eldar Y, Strohmer T and Voroninski V 2013 Phase retrieval via matrix completion SIAM J. Imaging Sci. 6 199–225
[35] Waldspurger I, d’Aspremont A and Mallat S 2012 Phase recovery, MaxCut and complex semidefinite programming arXiv:1206.0102
[36] Wen Z, Goldfarb D and Scheinberg K 2012 Block coordinate descent methods for semidefinite programming Handbook on Semidefinite, Conic and Polynomial Optimization (International Series in Operations Research and Management Science vol 166) ed M F Anjos and J B Lasserre (Berlin: Springer) pp 533–64
[37] Fienuj J R 1982 Phase retrieval algorithms: a comparison Appl. Opt. 21 2758–69
[38] Luke R 2005 Relaxed averaged alternating reflections for diffraction imaging Inverse Problems 21 37–50
[39] Singer A 2011 Angular synchronization by eigenvectors and semidefinite programming Appl. Comput. Harmon. Anal. 30 20–36
[40] Thibault P and Menzel A 2013 Reconstructing state mixtures from diffraction measurements Nature 494 68–71
[41] Lehoucq R B, Sorensen D C and Yang C 1998 Arpack Users Guide (Society for Industrial and Applied Mathematics) DOI:10.1137/1.9780898719628