Well-conditioned ptychographic imaging via lost subspace completion

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Abstract

Ptychography, a special case of the phase retrieval problem, is a popular method in modern imaging. Its measurements are based on the shifts of a locally supported window function. In general, direct recovery of an object from such measurements is known to be an ill-posed problem. Although for some windows the conditioning can be controlled, for a number of important cases it is not possible, for instance for Gaussian windows. In this paper we develop a subspace completion algorithm, which enables stable reconstruction for a much wider choice of windows, including Gaussian windows. The combination with a regularization technique leads to improved conditioning and better noise robustness.

Keywords: phase retrieval, ptychography, regularization

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

1. Introduction

The aim in the phase retrieval problem is to recover a vector \(x_0 \in \mathbb{C}^d\) from measurements given by

\[
y_j = |\langle x_0, a_j \rangle|^2 + n_j \quad \text{or} \quad y = |Ax_0|^2 + n,
\]

where the measurement vectors \(a_j\) (or the measurement matrix \(A\), respectively) is known and the noise \(n\) is unknown, but small. Note that no recovery method can distinguish the solution candidates \(\{e^{i\theta} \cdot x_0 : \theta \in [0, 2\pi]\}\), since they all generate the same set of measurements, so at

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best, reconstruction is possible up to a global phase factor. To account for this ambiguity, one typically measures the quality of reconstruction via
\[
d(x, x_0) = \min_{\theta \in [0, 2\pi]} \| x - e^{i\theta} x_0 \|_2.
\]

Phase retrieval is a central problem in various applied fields such as optical imaging [1], crystallography [2], or imaging of noncrystalline materials [3]. In these fields, the aim is to draw conclusions about an object of interest based on diffraction measurements made from illuminating the object with some sort of radiation such as light waves or x-ray beams. These measurements, however, only measure the intensity of the optical wave that is reaching a detector and are not capable to measure any information about the phase [1], although it encodes important structural information [4]. Thus, some restrictive model assumption or measurement redundancy is crucially required for recovery.

1.1. Ptychography and locally supported measurements

Ptychography is a specific form of a redundant phase retrieval problem that received considerable attention in recent years. Instead of a full illumination of the specimen \(x_0\), multiple measurements are obtained where in each of them the x-ray beam is focused on a small region of the object. For each focus region the intensities of the resulting far field diffraction patterns are captured by a detector. In the experimental setup, this is realized by moving the object after each measurement. To obtain redundancies, the regions are chosen to be overlapping. The whole process is summarized in figure 1.

The history of ptychography dates back to works by Hoppe [5] from the late 1960s. In the following decades it was studied mainly in a number of works by Rodenburg and coauthors [6–8]. Only in 2007 with the development of new imaging methods and devices, ptychography was rediscovered and became more popular, especially in the synchrotron community [9].

Ptychography has applications in many different research areas across life science and materials science and has been successfully used to get image resolutions at a nanometer scale. For example it was used to image the internal structure of silk fibers [10], the 3D pore structure of a catalyst [11], and to visualize stereocilia, hair cells in the inner ear, necessary for hearing and balancing that have a diameter in the nanometer range [12].

At the core of the measurement process is a detector that samples the intensities of the far field diffraction pattern of the illuminated region. The measurements can be modeled by squared magnitudes of the Fourier coefficients of the windowed image, that is,
\[
(y_{j, \ell})_j = \left| \sum_{n=1}^{d} w_n(x_0)_{n+j, \ell} e^{-\frac{2\pi i}{d} (j-1)(n-1)} \right|^2 + n_{j, \ell}, \quad (j, \ell) \in [d] \times P,
\]
where \(P \subset \{0, 1, \ldots, d - 1\}\) is the set of shifts of the object, \(w \in \mathbb{C}^d\) is a localized illumination or window function and \(n_{j, \ell}\) is noise.

1.2. Overview of related work

The general phase retrieval problem has been widely discussed along the time period of the last 50 years in the scientific community and a lot of research has focused on developing algorithms to tackle it efficiently. Earliest attempts are alternating projection algorithms developed in the 1970s by Gerchberg and Saxton [13] and Fienup [14]. An overview and a numerical evaluation of such methods can be found in [15, 16]. In general, algorithms based on alternating projection are popular among practitioners because they are easy to implement, often have
low computational complexity, and produce reasonable solutions in many cases. Nevertheless, these iterative methods are difficult to analyze mathematically and their performance heavily relies on a good initial guess [17]. In particular, there are no global convergence guarantees for alternating projection approaches.

Following the emergence of compressed sensing in 2004 a number of works aimed to analyze the phase retrieval problem from a similar viewpoint. These include works deriving conditions for injectivity under generic measurements [18] and recovery guarantees for various algorithms under random measurement scenarios—first for Gaussian random measurements with full randomness [19–22] and later for derandomized measurements such as subsampled spherical designs [23] and coded diffraction patterns [21, 24–26]. The algorithms analyzed in these results include convex optimization approaches such as PhaseLift [19]—these mainly show that recovery in polynomial time is possible and are not feasible for larger problem sizes—and non-convex alternatives such as the Wirtinger Flow algorithm [21], which pursues a gradient descent strategy and, thus, is computationally more efficient. None of the rigorous error bounds derived in these works, however, apply in ptychographic measurement scenarios.

With rising interest in ptychography, several methods were developed specifically for measurements of the form (2). An approach based on the combination of gradient descent steps and alternating projections known as ptychographic iterative engine (PIE) [27, 28] and its extensions such as ePIE [29] are commonly used by practitioners, but not yet understood mathematically. Alternatives that come with some mathematical guarantees include frame based approaches [30], numerical integration strategies [31], methods based on the properties of the Wigner distribution [7, 32, 33], and the so called BlockPR algorithm [34].

The last mentioned method, which is also the starting point for our paper, uses deterministic measurement masks and a lifting scheme similar to PhaseLift [19]. However, it is much more efficient as it exploits the locality of the measurement masks to reduce the dimension of the problem from $d^2$ in PhaseLift to $d(2\delta - 1)$ in BlockPR, with $\delta$ denoting the size of the illuminated region. The idea is to solve a linear system in a first step to recover a number of central diagonals of the outer product $x_0 x_0^*$, from which, in a second step, the missing phases are estimated. In the initial version of BlockPR [35], the second step was based on a greedy algorithm. Later, the second step was significantly improved by estimating the phases via angular synchronization [34, 36] and the BlockPR algorithm was extended to subsampled scenarios.

![Figure 1](image.png)

**Figure 1.** A typical one-dimensional ptychographic setup.
[37, 38]. All of these works focus on rather restrictive classes of measurement windows; as we will see this is due to inherent invertibility and conditioning problems. In this paper, we address this issue proposing a strategy that allows for recovery even in the case of singularities. Note that parts of our results have already been announced in a conference paper [39].

1.3. Summary of main contribution and outline of the paper

In this paper we enhance the BlockPR algorithm by extending it to a broader and more realistic class of measurement windows, including symmetric windows such as windows that are well described by Gaussian functions. For such windows in even dimension, the BlockPR algorithm in its original form cannot be applied, as stated in our following first result, which we summarize as follows (see theorem 2 below for the precise formulation).

**Theorem A.** Consider discretized ptychographic measurements in even dimensions generated using a symmetric window. Then the linear system to be solved in the first step of the BlockPR algorithm is singular.

The idea of our extension is that the information contained in the diagonals to be recovered in the first step of BlockPR is still redundant. The enhanced method we propose, stated in algorithm 2, completes the information missing due to singularities or conditioning problems by exploiting these redundancies.

Our main contribution is to demonstrate, in theory and numerical experiments, that algorithm 2 is indeed able to solve the ptychographic phase retrieval problem even in the case of singularities as discussed above. More precisely, we formulate two conditions, (A1) and (A2), that we empirically show to hold in many situations, and under which we establish a recovery guarantee that is summarized as follows (see theorem 6 below for the precise formulation).

**Theorem B.** If the linear system to be solved in the first step of the BlockPR algorithm satisfies assumptions (A1) and (A2), then the information lost due to singularities can be completed, and the underlying signal can be recovered up to a global phase using algorithm 2.

Numerical experiments in section 4 confirm the performance guarantees predicted by our results and explore the use of the new method as a regularized BlockPR algorithm to provide improved reconstruction quality for noisy measurements.

The paper is structured as follows. We start with introducing notation and important preliminaries in section 2. In section 3 we first show why the BlockPR algorithm is not suitable for symmetric windows. After this we describe our generalization, elaborate on its functionality, and state our main result. Next, we perform numerical experiments in section 4 and, finally, present our proofs in section 5. The paper is finalized with a short conclusion and outlook in section 6.

2. Preliminaries

2.1. Notation and Fourier transform basics

Index sets will be expressed by the notation

\[ [n]_k := \{k, \ldots, k + n - 1\} \subset \mathbb{N}^0, \quad k \in \mathbb{N}^0, \]

where we set \([n] := [n]_1\). For a complex number \(a = |a|e^{i\phi}\) the argument of \(a\) is defined as \(\arg(a) = \phi \in [-\pi, \pi)\). The Hadamard product \(u \circ v \in \mathbb{C}^d\) of two vectors \(u, v \in \mathbb{C}^d\) is given
entrywise by \((u \circ v)_j = u_j v_j\). Recall that for a complex vector \(u \in \mathbb{C}^d\) its discrete Fourier transform (DFT) \(\hat{u} \in \mathbb{C}^d\) is given by
\[
\hat{u}_k = \sum_{n=1}^{d} u_n e^{-2\pi i (n-1)(k-1)/d}.
\] (3)

We define the discrete circular convolution of two vectors \(u\) and \(v\) according to [40] as a vector \(u * v\) with
\[
(u * v)_\ell = \sum_{k=1}^{d} u_{\ell - k + 1} v_k, \quad \ell \in [d].
\] The (discrete version of the) convolution theorem states that the Fourier transform of the Hadamard product of two signals \(u\) and \(v\) in \(\mathbb{C}^d\) is the (circular) convolution of the Fourier transforms of the two signals, i.e.,
\[
\hat{u} \circ \hat{v} = \hat{u} * \hat{v}.
\] (4)

A proof of this result can be found for example in [40].

The (discrete) circular shift operator \(S_\ell : \mathbb{C}^d \rightarrow \mathbb{C}^d\), \(\ell \in \mathbb{Z}\) and the modulation operator \(W_k : \mathbb{C}^d \rightarrow \mathbb{C}^d\), \(k \in \mathbb{Z}\) are given by
\[
(S_\ell u)_j := u_{\ell + j}, \quad u \in \mathbb{C}^d, \ j \in [d]
\] (5) and
\[
(W_k u)_j := e^{2\pi i (j-1)(k-1)/d} u_j, \quad u \in \mathbb{C}^d, \ j \in [d].
\] (6)

The next lemma summarizes some well-known basic properties of the DFT, which are relevant for this paper.

**Lemma 1 (Elementary Fourier transform properties).** Let the modulation operator \(W_k\) be defined as in (6), the DFT be defined as in (3) and the shift operator \(S_\ell\) be defined as in (5). Then, the following properties hold for every complex vector \(x \in \mathbb{C}^d\):

\((a)\) \(S_\ell \hat{x} = \hat{x}_{\ell + 1}\),
\((b)\) \(\hat{(x)}_k = \hat{(x)}_{d-k+2} \ \forall \ k \in [d]\).

**2.2. Model**

One diffraction measurement \((y_\ell)_j\) in (2) corresponds to the \(j\)th Fourier mode of the illuminated specimen shifted by \(\ell\). The window \(w\) that describes the illumination is assumed to have compact support
\[
\text{supp}(w) = [\delta] \subset [d],
\]
where \(\delta\) denotes the support size. By combining the window with the modulation in (2) we obtain masks \(m_j, \ j \in [d]\), given by
\[
(m_j)_n := \frac{w_{n+1-j} e^{-2\pi i (n(1-j)-1)}}{d}.
\] (7)
With this definition the squared magnitude measurements are of the form
\[ (y_j)_j = |\langle S_0^j, m_j \rangle|^2 + n_{j,\ell} = |\langle x_0, S_0^j m_j \rangle|^2 + n_{j,\ell}, \quad (j, \ell) \in [K] \times P, \tag{8} \]
with \( K = d \) and \( m_j \) given by (7). Further, we consider another set of masks, obtained by subsampling in frequency domain, i.e.,
\[ (m_j)_n = \begin{cases} \frac{1}{\sqrt{2\delta - 1}} m_n \cdot e^{\frac{2\pi i n j}{2\delta-1}} & \text{if } n \leq \delta, \\ 0 & \text{if } n > \delta, \end{cases} \quad j \in [2\delta-1]. \tag{9} \]
In particular we are interested in a Gaussian window given by the formula
\[ u_n = \exp \left\{ -\frac{(n - \frac{\delta + 1}{2})^2}{2\sigma^2\delta^2} \right\}, \quad n \in [\delta], \tag{10} \]
which is a good approximation of windows appearing in ptychography [41].

2.3. Idea of the BlockPR algorithm

The eigenvector-based angular synchronization BlockPR algorithm proposed by [34, 36] uses a linear measurement operator to describe how to retrieve the measurements (8) from the signal \( x_0 \). In order to introduce this linear operator, we first observe that in the noiseless case the quadratic measurements can be lifted up and interpreted as linear measurements of the rank one matrix \( x_0 x_0^* \) as done in [4]. Indeed,
\[ (y_j)_j = |\langle x_0, S_0^j m_j \rangle|^2 = |\langle x_0, S_0^j m_j \rangle| \cdot |\langle S_0^j m_j, x_0 \rangle| = m_j^* S_0 x_0^* S_0^j m_j = \operatorname{tr}(S_0^j m_j m_j^* S_0), \]
where \( \langle \cdot, \cdot \rangle_F \) denotes the Frobenius inner product defined as \( \langle A, B \rangle_F := \operatorname{tr}(A^* B) \). By this reformulation, the phase retrieval problem is lifted to a linear problem on the space of Hermitian \( d \times d \) matrices \( \mathcal{H}^d \). We consider all shifts \( \ell \in P = [d]_0 \) and recall that the masks are compactly supported. Thus, we observe that for every matrix \( A \in \operatorname{span}\{S_0^j m_j m_j^* S_0\}_{j \in [K], \ell \in [d]_0} \) we have \( A_{k,j} = 0 \) when \( |k-j| < \delta \) or \( |k-j| > d - \delta \). Based on this observation we introduce a family of orthogonal projection operators \( T_\delta : \mathcal{H}^d \to \mathbb{C}^{d \times d} \), given by
\[ (T_\delta(A))_{k,j} = \begin{cases} A_{k,j} & \text{if } |k-j| < \delta \text{ or } |k-j| > d - \delta, \\ 0 & \text{else.} \end{cases} \]
We see that \( T_\delta \) is the orthogonal projection operator from the space \( \mathcal{H}^d \) onto range \( T_\delta(\mathcal{H}^d) \supseteq \operatorname{span}\{S_0^j m_j m_j^* S_0\}_{j \in [K], \ell \in [d]_0} \). Consequently, we can write
\[ \langle x_0 x_0^*, S_0^j m_j m_j^* S_0^j \rangle = \langle T_\delta(x_0 x_0^*), S_0^j m_j m_j^* S_0^j \rangle. \]

Finally we define the linear operator \( A : \mathcal{H}^d \to \mathbb{C}^D, D := K \times d \), describing the measurement process as
\[ A(X) = [(X, S_0^j m_j m_j^* S_0^j)]_{(j,\ell)} \tag{11} \]
We will denote the restriction of the operator \( A \) to the domain \( T_\delta(\mathcal{H}^d) \) by \( A|_{T_\delta(\mathcal{H}^d)} \).
Algorithm 1. Fast phase retrieval from local measurements \([34]\)

**Input:** Measurements \(y \in \mathbb{R}^D\) as in (8)

**Output:** \(x \in \mathbb{C}^d\) with \(x \approx e^{j\theta_0}x_0\) for some \(\theta \in [0, 2\pi]\)

1. Compute \(X = [A|_{\mathcal{T}_3(H^d)}]^{-1}y \in \mathcal{T}_3(H^d)\) as an Hermitian estimate of \(T_3(x_0, x_0^*)\).
2. Form the banded matrix of phases \(X \in \mathcal{T}_3(H^d)\) defined in (12).
3. Compute the normalized top eigenvector of \(X\), denoted by \(\tilde{x} \in \mathbb{C}^d\) with \(\|\tilde{x}\|_2 = \sqrt{d}\).
4. Set \(x_j = \sqrt{X}_{\tilde{j}j}\) for all \(j \in \{d\}\) to form \(x \in \mathbb{C}^d\).

The operator \(A|_{\mathcal{T}_3(H^d)}\) allows to reformulate (8) in the absence of noise as

\[
(y_j)_j = \|\langle x_0, S_j^*m_j \rangle\|^2 = \langle T_3(x_0, x_0^*), S_j^*m_j S_j \rangle = \langle A|_{\mathcal{T}_3(H^d)}T_3(x_0, x_0^*) \rangle_{\{d\}}
\]

which we wish to invert in order to obtain the lifted and on \(T_3\) projected rank 1 object

\(X_0 := T_3(x_0, x_0^*)\).

From this matrix we form a banded matrix \(\tilde{X}_0\) by entrywise normalization of non-zero entries of \(X_0\), i.e.,

\[
(\tilde{X}_0)_{k,j} = \begin{cases} 
\frac{(X_0)_{k,j}}{(X_0)_{k,j}}, & (X_0)_{k,j} \neq 0, \\
0, & \text{otherwise,}
\end{cases} \tag{12}
\]

The magnitudes of the entries of the signal \(x_0\) can be recovered as square roots of the diagonal elements of \(X_0\) as in [35]. The phases of \(x_0\) can be obtained from the entrywise normalization of the top eigenvector of matrix \(X_0\) as a result of solving the angular synchronization problem. The whole reconstruction of \(x_0\) as proposed in [34] is summarized in algorithm 1.

When the measurements are noisy, this approach needs to be refined for stable approximate recovery. This gives rise to block magnitude estimation [34, 36, 38], which we also use as a building block of our implementation to obtain the magnitudes. This technique utilizes the banded structure of \(X_0\) by decomposing it into smaller fixed size block matrices from which then separate magnitude estimates are made. The actual estimation is realized via calculating and averaging the top eigenvector of each single block matrix which serves as a guess of the underlying signal magnitude.

Note that invertibility and well-conditioning of the operator \(A|_{\mathcal{T}_3(H^d)}\) are crucial for a proper recovery by algorithm 1. In fact, invertibility of the operator \(A|_{\mathcal{T}_3(H^d)}\) strongly depends on the selection of the measurement masks \(m_j, j \in \{K\}\), which determines if the condition \(T_3(H^d) = \text{span}\{S_j^*m_j S_j\}_{j \in \{K\}/\{d\}}\) holds, which is equivalent to invertibility of \(A|_{\mathcal{T}_3(H^d)}\). In [35] measurement masks

\[
(m_j)_n = \begin{cases} 
\frac{1}{\sqrt{2\delta - 1}} e^{-n/\alpha} e^{2\pi(-1)^{n-1}(-1)^{n-1}} & \text{if } n \leq \delta, \\
0, & \text{if } n > \delta,
\end{cases} \tag{13}
\]

where \(\alpha \in [4, \infty)\) and \(m_j \in \mathbb{C}^d, j = 1, \ldots, 2\delta - 1\), are proven to be a good choice. They resemble the structure of ptychographic masks (7) and at the same time allow for a stable inversion as proven in lemma 2 of [35].
2.4. Gerchberg–Saxton and Wirtinger Flow algorithms

In section 4, we will evaluate the numerical performance of our algorithm by comparing it to state-of-the-art methods in the literature. To put our numerical findings into perspective, we will now briefly summarize the key ideas of these algorithms.

The Gerchberg–Saxton algorithm [13] is an alternating minimization scheme whose iterations consist of the following three steps. First, a current iterate $x_t$ is mapped to the diffraction plane using the measurement matrix $A$ as in (1) to obtain $z_t := Ax_t$. Second, the entrywise magnitudes of $z_t$ are then adjusted to satisfy the intensity constraint $|\hat{z}_t|^2 = y$, resulting in $(\hat{z}_t)_j := \sqrt{y_j} \cdot (z_t)_j / |(z_t)_j|$. Finally, to obtain the next iterate $x_{t+1}$ one inverts the measurement matrix $A$ by solving the least squares problem $\arg \min_{x_{t+1}} \|Ax_{t+1} - \hat{z}_t\|^2$. These three steps are iterated until a predefined stopping criterion is satisfied.

The Wirtinger Flow algorithm [21] is a gradient descent method that minimizes the squared error $\|Ax - y\|^2$ between the intensities of the diffraction patterns generated by the estimate $x$ and the measurements $y$. Since this objective is not a holomorphic function, the algorithm employs the Wirtinger derivatives as an alternative to the standard gradient. This leads to the update step

$$x_{t+1} = x_t - \mu_t A^* \text{diag}(|Ax_t|^2 - y)Ax_t,$$

where the learning rate $\mu_t$ is a tuning parameter, which is chosen via the Armijo–Goldstein condition. The algorithm iterates until the gradient vanishes or a predefined stopping criterion is satisfied.

3. A BlockPR method with subspace completion—algorithm formulation and performance guarantees

Under the model (13), it is shown in lemma 2 of [35] that the operator $A|_{T_\delta(\mathcal{H}_d)}$ is invertible. However, it is also shown that its minimal singular value behaves proportional to $\delta^{-1}$ which leads to severe conditioning problems as the support size increases. In addition, this analysis is specific to masks of the form (13). First steps toward a more general choice of windows were taken in [36, 38], but for many windows including Gaussian windows (10), the reconstruction remained an open problem. The difficulty is that for many windows, the measurement operator $A|_{T_\delta(\mathcal{H}_d)}$ is not even invertible. An example is the following statement.

**Theorem 2.** Consider masks of the form (9). Assume that $d$ is even and the window $w$ satisfies the symmetry condition

$$w_n = w_{\delta - n + 1} \text{ for all } n \in [\delta].$$

Then, $A|_{T_\delta(\mathcal{H}_d)}$ is not invertible.

Theorem 2 is equivalent to saying that $T_\delta(\mathcal{H}_d) \supset \text{span}\{S_\ell m_j m_j^* S_\ell\}_{j \in [K], \ell \in [d], \ell \leq J}$, which is for symmetric windows there exists a nontrivial ‘lost subspace’ $\mathcal{L} \subset T_\delta(\mathcal{H}_d)$ with $T_\delta(\mathcal{H}_d) = \text{span}\{S_\ell m_j m_j^* S_\ell\}_{j \in [K], \ell \in [d], \ell \leq J} \oplus \mathcal{L}$. The main idea of this paper is that the redundancy in $X_0$ can be utilized to complete the information about the ‘lost subspace’ $\mathcal{L}$. Moreover, this technique can be extended to the ‘approximately lost subspace’ corresponding to the ill-conditioned part of the operator $A|_{T_\delta(\mathcal{H}_d)}$ and, by doing so, better robustness to noise is achieved. The resulting method, the main contribution of our work, is summarized in algorithm 2. Its fundamental ideas are presented in the remainder of this section.
Algorithm 2. Fast phase retrieval from locally supported measurements with subspace completion.

**Input:** Measurements \( y \in \mathbb{R}^D \) as in (8), truncation parameter \( \varepsilon \geq 0 \)

**Output:** \( x \in \mathbb{C}^d \) with \( x \approx e^{-i \theta} x_0 \) for some \( \theta \in [0, 2\pi] \)

1. Compute \( X_S = A|_{S} y \in T_{\delta}(H^d) \).
2. Evaluate Fourier coefficients of diagonals \( L' \) corresponding to columns of \( V_1 \) by corollary 4.
3. Recover missing entries of \(  \hat{L}' \) for columns of \( V_2 \) by solving (19).
4. Form \( X \) with diagonals \( L' \).
5. Form the banded matrix of phases \( \tilde{X} \in T_{\delta}(H^d) \) defined in (12).
6. Compute the normalized top eigenvector of \( \tilde{X} \), denoted by \( \tilde{x} \in \mathbb{C}^d \) with \( \| \tilde{x} \|_2 = \sqrt{d} \).
7. Set \( x_j = \sqrt{X_j} \cdot (\tilde{x})_j \) for all \( j \in [d] \) to form \( x \in \mathbb{C}^d \).

3.1. Generalized inversion step

As discussed in section 2, the measurement operator \( A \) is a linear function of \( X_0 \), the restriction of \( x_0 x_0^* \) to the \( 2\delta - 1 \) significant diagonals. Consequently, as observed in [35], by reorganizing the entries of these diagonals as a vector, i.e.,

\[
\text{vec}(X_0) := \left( (x_0)_{\left(\frac{j-1}{2}\right)+1} \right|_{j=1}^{(2\delta-1)+1} (x_0)_{\left(\frac{j-1}{2}\right)+\left(\frac{2\delta-1}{2}\right)+1} \quad \forall \ j \in [D], \quad (14)
\]

one can describe the measurement process as a matrix-vector product

\[
M \text{ vec}(X_0) = y
\]

for an appropriate matrix \( M \in \mathbb{C}^{D \times D} \). Note that \( M \) is obtained by deleting the columns of the matrix form of \( A|_{T_{\delta}(H^d)} \) corresponding to the entries in the kernel of the projection \( T_{\delta} \). Thus, to understand the invertibility and stability of the operator \( A|_{T_{\delta}(H^d)} \) it is sufficient to analyze the conditioning of the matrix \( M \).

We split the singular value decomposition of this matrix \( M \) into two parts corresponding to all singular values above some threshold \( \varepsilon \)—these will form the matrix \( \Sigma_1 \)—and all singular values less or equal to \( \varepsilon \)—these will form the matrix \( \Sigma_2 \). The matrices \( U \) and \( V \) of the left and right singular vectors are split accordingly into \( U_1, U_2 \) and \( V_1, V_2 \), respectively. That is, we obtain

\[
M = U \Sigma V^* = (U_1 \quad U_2) \left( \begin{array}{cc} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{array} \right) (V_1 \quad V_2)^*.
\]

The subspace \( S \) is defined as

\[
S := \text{span}\{V_1^{(q)} : \text{column of } V_1\}
\]

As it was shown in theorem 2, the inverse of operator \( A|_{T_{\delta}(H^d)} \) and hence of \( M \) does not exist. To account for this and possible ill-conditioning we will work with a regularized inverse, which for \( \varepsilon = 0 \) agrees with the Moore–Penrose pseudoinverse and which is defined as

\[
M_S^{-1} := \begin{pmatrix} V_1 & V_2 \end{pmatrix} \begin{pmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} U_1 & U_2 \end{pmatrix}^*.
\]

For \( \varepsilon > 0 \) this thresholding yields a more noise robust version of the pseudoinverse operator. Note that in all cases one has

\[
M_S^{-1} M = V_1 V_1^*.
\]
By construction, this operation yields a matrix in $T_{\delta}(H^d)$ in vectorized form. Combined with an embedding step that maps this vectorization back to matrix form, we obtain a regularized inverse operator, which we denote by $A_{\xi}^{-1}$.

The strategy of our approach will be to first reconstruct the well-conditioned portion of the signal $X_S := A_{\xi}^{-1}y$ and then use the underlying structure to recover $X_0$ from $X_S$.

3.2. Subspace completion algorithm

The matrix $X_0$ can be expressed through its diagonals $L_r$, $r \in [2\delta - 1]$, which are defined componentwise as

$$L_r = \begin{cases} (x_0)_z(x_0)_{z+r-1} & \text{if } 1 \leq r \leq \delta, \\ (x_0)_{z+1}(x_0)_{z+1+r-2\delta} & \text{if } \delta + 1 \leq r \leq 2\delta - 1, \end{cases}$$  \hspace{1cm} (17)

where $z \in [d]$.

As a matter of fact, each of the columns of $V$, that is, each right singular vector of $M$, is exclusively supported on a single diagonal. Even stronger, each Fourier coefficient of a diagonal $L'$ can be computed using just one of the singular vectors, as given by the following theorem.

Theorem 3. Consider measurement masks of the form (9). Then,

$$\hat{L}'_\xi = \sqrt{d} \langle \text{vec}(X_0), V^{(q)} \rangle,$$  \hspace{1cm} (18)

where $q$ is decomposed as

$$q = (2\delta - 1)(\xi - 1) + r$$

with $\xi \in [d]$ and $r \in [2\delta - 1]$ and $\hat{a}$ denotes the DFT of the vector $a \in \mathbb{C}^d$ as in (3).

Note that equality (18) will not change if we replace $X_0$ by an orthogonal projection $X_S$ onto a truncated singular space, as long as $V^{(q)} \in \mathcal{S}$. Consequently, one obtains

Corollary 4. Under assumption of theorem 3 in the noiseless case where $X_S = A_{\xi}^{-1}y$ it holds that

$$\sqrt{d} \langle \text{vec}(X_S), V^{(q)} \rangle = \begin{cases} \hat{L}'_\xi & \text{if } V^{(q)} \text{ is a column of } V_1, \\ 0 & \text{if } V^{(q)} \text{ is a column of } V_2. \end{cases}$$

Thus, completion of the lost subspace information is equivalent to finding the missing Fourier coefficients of the diagonals $L'$. For that, we exploit the redundancy in $X_0$ as a projection of a rank one matrix via the following lemma.

Lemma 5. Let $L'$ and $L'_\ell$, $r, \ell \in [\delta]$ be diagonals as defined in (17). Then, the following relation holds

$$L' \circ S_{r-1}(L')^* = L'_\ell \circ S_{r-1}(L')^*.$$  \hspace{1cm} (19)

This allows us to summarize the lost subspace completion in algorithm 2.

In general equation (19) establishes a quadratic system. Arguably however, it is a common case that at most one Fourier coefficient of each diagonal is missing and then (19) becomes a linear system. Indeed, the singular values corresponding to a single diagonal $L'$ are given by

$$\sum_{\ell=1}^{\delta-r+1} u'_\ell w_{\ell+r-1} e^{\frac{2\pi i k (\ell - 1)}{d^2}}, \quad k \in [d].$$
Since this expression as a function of $k$ and extended to the full interval $[1, d]$ is highly oscillating, hitting zero at an integer point is a rare event, except for a zero that results from the symmetry for $k = d/2 + 1$ on some diagonals. Thus, encountering two zeros on one diagonal is much less common than just one. For the same reason it is commonly the case that on at least one of the diagonals one does not encounter any zeros. This heuristic leads to the assumptions of the following theorem, which are indeed sufficient to guarantee recovery.

**Theorem 6.** Assume that

(a) At least one diagonal $L'$ is fully recovered in step 2 of algorithm 2.

(b) At most one Fourier coefficient of each diagonal is missing.

Then (19) can be expressed as a linear system and step 3 of algorithm 2 recovers the lost Fourier coefficients via standard solution strategies.

The numerical experiments presented in the following section confirm that assumptions (a) and (b) are justified in realistic scenarios such as for Gaussian windows, and hence algorithm 2 yields improved reconstruction quality.

The computational complexity of the algorithm 1 is $O(d^2 \log d)$ [34] when using the fast Fourier transforms in step 1. Since steps 1–2 and 4–7 of algorithm 2 directly correspond to steps of algorithm 1, it only remains to estimate the number of operations required in step 3 to bound the computational complexity of 2. Our solver for equation (19) finds each missing coefficient as a solution to a system of at most $d$ linear equations with 2 unknowns, which requires $O(d^2 \cdot D_2)$ operations. Here $0 < D_2 < (2\delta - 1)d$ denotes the number of singular values below the threshold $\epsilon$. Alternatively, solving the linear regression problem using gradient descent decreases the complexity to $O(d \cdot D_2)$. For $\epsilon$ large, where many singular values are to be replaced, this contribution scales quadratically in the dimension and hence dominates the computational complexity of algorithm 2, for smaller values of $\epsilon$, however, the complexity of the original steps dominates and the algorithm is fast. Indeed, numerical trials below confirm that in these cases its runtime is comparable to state-of-the-art algorithms.

4. **Numerics**

In this section we present numerical trials to assess the performance of algorithm 2. Our main objective is to demonstrate the positive effect of the additional completion step between steps 1 and 2 of algorithm 1. In the following, we will denote by BlockPR the algorithm without that additional step as originally proposed in [34] and summarized in algorithm 1 above. As discussed in section 3, the subspace completion step is not only useful when information gets lost due to zero singular values, but also in case of very small singular values that can give rise to instabilities. In that case, algorithm 2 is applied after deleting all the information which corresponds to singular values of the measurement operator $A|_{T_\infty(h_d)}$ below some threshold $\epsilon \geq 0$. We will refer to this combined procedure by BlockPR + SC$_\epsilon$, where $\epsilon$ indicates the truncation level.

We study two different examples for illumination windows in this section, the Gaussian window (10) with $\sigma = 0.3$ and the exponential window as in (13) with $\alpha = 2$. The windows are normalized, so that $\|w\|_2 = 1$ and the maximal singular value of the matrix $M$ is equal to $\|w\|_2^2 = 1$, which provides an easy interpretation of the truncation parameter $\epsilon$.

We first illustrate the guarantees of theorem 6. Indeed, Gaussian windows in even dimensions fulfill the assumptions of theorem 2 and also of theorem 6, which indicates that BlockPR + SC$_{0}$ should significantly outperform the original BlockPR algorithm. Figure 2 demonstrates
Figure 2. Comparison of the reconstruction accuracy between the BlockPR algorithm and the BlockPR + SC₀ algorithm for Gaussian window with support size $\delta = 8$ and dimension $d = 256$ (a) and $d = 255$ (b).

Table 1. Distribution of the singular values for $d = 256$ for Gaussian windows.

| $\delta$ | $\{0\}$ | $(10^{-5}, 10^{-4})$ | $(10^{-4}, 10^{-3})$ | $(10^{-3}, 10^{-2.5})$ | $(10^{-2.5}, 0.01)$ | $(0.01, 0.1)$ | $(0.1, 10)$ | Total |
|----------|----------|---------------------|---------------------|---------------------|---------------------|----------------|----------------|-------|
| 8        | 8        | 7                   | 4                   | 28                  | 86                  | 220            | 2324          | 1171  |
| 32       | 31       | 20                  | 598                 | 1582                | 5922                | 6748           | 1227          | 16128 |

that this is the case for additive Gaussian noise. We continue by comparing the reconstruction accuracy achieved for different choices of truncation parameters $\varepsilon$ again under additive Gaussian noise.

Figures 3 and 4 show that larger truncation thresholds yield better results for larger noise levels and smaller thresholds are better suited for smaller noise levels. We observe that our approach significantly outperforms the competitor algorithms Wirtinger Flow and Gerchberg–Saxton in scenarios that are less well-conditioned such as Gaussian masks of a small size relative to the dimension and exponential masks. In scenarios with better conditioning, we observe a comparable decay rate, but a worse constant.

In the second line of experiments, we analyze a measurement scenario designed to mimic actual ptychographic measurements. As in this initial contribution, we focus on the one-dimensional setup, our algorithm cannot be applied to real data yet, but we aim to capture two important features. Firstly, we consider piecewise constant signals as one-dimensional analogs of phantoms commonly used as benchmarks. Secondly, we consider Poissonian noise as it more realistically describes ptychographic experiments. For such measurements, we assess the reconstruction quality achieved by BlockPR + SC (figures 5 and 6) and show examples of the reconstructed signals (table 2). Furthermore, in figure 7 we explore a hybrid approach, in which the solution of BlockPR + SC is used as the initialization for iterative methods. Finally, figure 8 explores the runtime complexity of discussed algorithms. We again observe best performance for small window size, both in terms of the mean squared error (MSE) and visually.

We consider two metrics to compare the different approaches: runtime complexity and the relative error between the true underlying signal $x_0 \in \mathbb{C}^d$ and its estimate $x \in \mathbb{C}^d$ up to a global
Figure 3. Comparison of the reconstruction accuracy for different truncation parameters $\varepsilon$ for the BlockPR + SC algorithm, Gerchberg–Saxton and Wirtinger Flow for Gaussian windows with support size $\delta = 8$ (left) and $\delta = 32$ (right), and dimension $d = 256$.

Figure 4. Reconstruction of a $d = 256$ dimensional signal with exponential windows with support size $\delta = 32$ for BlockPR, BlockPR + SC $10^{-3.5}$, Gerchberg–Saxton, and Wirtinger Flow.

For more representative results each data point of the following figures is the average of reconstructing 100 different test signals. All experiments were performed on the laptop computer running Windows 10 Pro with an Intel(R) Core(TM) i7-8550U processor, with 16 GB RAM and Matlab R2018b.
Figure 5. Reconstruction of a $d = 256$ dimensional piecewise constant signal (15 jumps) with Gaussian windows with support size $\delta = 8$ (left) and $\delta = 32$ (right) for different truncation parameters $\epsilon$ for BlockPR + SC, Gerchberg–Saxton, and Wirtinger Flow in the case of the Poisson noise model.

Table 2. Visualized reconstruction and pixelwise phase error for the worst out of 100 realizations of ptychographic measurements affected by Poissonian noise for a fixed piecewise constant $d = 256$ dimensional signal (15 jumps) using a Gaussian windows with support sizes $\delta = 8$ and $\delta = 32$ and $10^7$ photons per pixel. The signal and its reconstructions are visualized using the HSV color scheme with brightness indicating magnitude and color indicating phase. For the phase error, white corresponds to the perfect reconstruction and black to an error of at least $\pi/2$.

| Reconstructed signal | Phase error $|\arg(x_j) - \arg((x_0)_j)|$ |
|----------------------|-----------------------------|
| Gerchberg–Saxton     | $\delta = 8$                |
| Wirtinger Flow       |                             |
| BlockPR + SC$_{10^{-3}}$ |                     |
| BlockPR + SC$_{10^{-4}}$ |                     |
| Original signal      |                             |
| Gerchberg–Saxton     | $\delta = 32$                |
| Wirtinger Flow       |                             |
| BlockPR + SC$_{10^{-3}}$ |                     |
| BlockPR + SC$_{10^{-4}}$ |                     |

The experimental setup for the first line of trials is the following. We generate synthetic signals using i.i.d. zero-mean complex random multivariate Gaussian vectors. To model noisy data we add random Gaussian noise to our measurements. The signal to noise ratios (SNRs) will be measured in decibels (dB), that is, we consider

$$\text{SNR(dB)} = 10 \log_{10} \left( \frac{\sum_{i=0}^{d-1} \sum_{j=1}^{2d-1} (y_{ij})^2}{d(2\delta - 1)\mu^2} \right),$$

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Figure 6. Histogram of the MSE for 100 realizations of ptychographic measurements affected by Poissonian noise with $10^7$ photons per pixel for a fixed $d = 256$ dimensional piecewise constant signal (15 jumps) with a Gaussian window of support size $\delta = 8$ with Gerchberg–Saxton, Wirtinger Flow, BlockPR + SC10−3 and BlockPR + SC $10^{-4}$.

where $(y_j)$ are measurements as in (8) and $\nu^2$ denotes the variance of the Gaussian noise.

We begin with a first experiment demonstrating the improved reconstruction accuracy of the BlockPR + SC0 algorithm over the BlockPR algorithm for the masks of the form (9) with Gaussian window (10). Figure 2(a) shows the result of reconstructing a test signal of dimension $d = 256$ for a window size $\delta = 8$ and different noise levels. As predicted by theorem 2, the BlockPR algorithm yields a large reconstruction error due to zero singular values resulting from the symmetry of the window. The reconstruction error of the BlockPR + SC0 algorithm, in contrast, shows significant decay for decreasing noise levels, similar to odd dimensions, where no singularities arise (see figure 2(b)) for an example, where the results of BlockPR and BlockPR + SC0 agree as there are no zero singular values. This decay is in line with theorem 6. Indeed, table 1 shows that there are only $\delta - 1$ zero singular values for both $\delta = 8$ and $\delta = 32$. So, by corollary 8 below, there is at most one zero singular value per diagonal. That is, assumptions (A1) and (A2) are satisfied, which explains the improved performance of BlockPR + SC0 as compared to BlockPR.

Nevertheless, figure 2 shows that without truncation ($\varepsilon = 0$) algorithm 2 struggles with high noise. The reason behind the suboptimal reconstruction quality is due to the large condition number of the operator $A|^{-1}_S$, whose application is at the core of the BlockPR algorithm. With the subspace completion technique at hand we improve the conditioning by disregardign information corresponding to the small singular values and completing it after the inversion step.
Figure 7. Quality of reconstruction and runtime of a \( d = 256 \) dimensional piecewise constant signal (15 jumps) with Gaussian windows of support size \( \delta = 8 \) (left) and \( \delta = 32 \) (right) with BlockPR + SC being an initialization for Wirtinger Flow and Gerchberg–Saxton in the case of the Poisson noise model. The truncation parameter for BlockPR + SC is chosen as \( 10^{-\frac{k^2}{30} - \frac{k}{10} - \frac{2}{3}} \), where \( k = \log_{10}(\text{photons per pixel}) \).

The effect of different choices of \( \varepsilon \) is illustrated in figure 3 for dimension \( d = 256 \) and support sizes \( \delta = 8 \) and \( \delta = 32 \). For comparison, we also include the Gerchberg–Saxton method [13] and the Wirtinger Flow [21] algorithm (implementations provided by PhasePack library [42]). We observe that for increased truncation parameters \( \varepsilon \) reconstruction at low and medium SNRs improves significantly. However, the error does not converge to zero anymore when noise diminishes as assumptions (a) and (b) are no longer universally satisfied. In this case one can no longer solve a linear system; rather, our implementation proceeds sequentially treating all unknown values as zero. This is of course only a heuristics and not covered by our theory. In fact, large truncation thresholds lead to a significant loss of information—e.g., for \( \varepsilon = 10^{-1} \) table 1 shows that more than 2/3 of singular values are deleted, so complete reconstruction is no longer possible even for very low noise. Thus, the optimal choice of \( \varepsilon \) depends on the noise level and should be based on a trade-off between noise robustness for low SNRs and perfect reconstruction for high SNRs. For a suitable choice of \( \varepsilon \), we observe that our method outperforms the state-of-the-art approaches for a window size of \( \delta = 8 \) and small to medium noise levels.

Increasing the support size from \( \delta = 8 \) to \( \delta = 32 \) leads to the larger overlaps of the measured regions and, consequently, better conditioning of the problem. It results in better performance.
of iterative algorithms, so our method no longer outperforms the state of the art, but scales comparably up to constant factors.

We point out that the good performance of algorithm 2 is not limited to Gaussian windows. In our final example of the first series of trials, we show that the subspace completion technique can be used for recovery from ptychographic measurements with exponential masks (13) beyond the range of stable invertibility. Figure 4 illustrates the performance of algorithms 1 and 2 in comparison with Gerchberg–Saxton and Wirtinger Flow for such masks with parameter $\alpha = 2$ and of sizes $\delta = 8$ and $\delta = 32$ in dimension $d = 256$. In both cases BlockPR alone already outperforms both iterative methods for moderate noise levels. For $\delta = 32$, we improve the accuracy even further by the application of algorithm 2 with regularization parameter $\varepsilon = 10^{-3.5}$, while for $\delta = 8$, including the subspace completion method does not affect the results.

In the second line of experiments, we consider the Poisson noise model, i.e., each pixel of the resulting diffraction pattern is modeled by a random variable following the Poisson distribution with parameter $\lambda_{\ell,j}$ given by

$$
\lambda_{\ell,j} = \left| \langle x_0, S^{\ast}_{\ell,m_j} \rangle \right|^2 \cdot \mu_p, \quad j \in [2\delta - 1], \quad \ell \in [d]_0,
$$

where $\mu_p$ denotes the number of photons per pixel. To generate the piecewise constant test signals we draw $n - 1$ jump locations at random from $[d]$ without replacement, sort them in increasing order, and assign $n$ complex standard Gaussian i.i.d random variables as values to all points in the intervals between the jump locations.

We start by looking at the impact of the truncation parameter $\varepsilon$ on the reconstruction quality (figure 5). Again we observe that our method with suitable truncation parameter outperforms the state of the art for small window size and small to medium noise levels, while exhibiting error decay of comparable order for larger window size. In contrast to the case of additive Gaussian noise (figure 3), however, higher truncation thresholds turn out to be somewhat more useful. For instance, when $\delta = 32$, BlockPR + SC$_{10^{-1}}$ exhibits a reconstruction quality similar to Wirtinger Flow when the number of photons is low, while for Gaussian noise, the reconstruction is meaningless for any noise level. Another striking difference between the two noise
models is that for large numbers of photons, our method outperforms Wirtinger Flow, which is not observed in figure 3.

As the MSE can sometimes be misleading as a measure for reconstruction quality, we illustrate in table 2 the visual reconstruction quality for the example of worst quality in terms of MSE among the 100 trials for $\delta = 8$ and $\delta = 32$. As the signals are complex, we represent them via the HSV color scheme, in which the phase is translated into color and the modulus into brightness. For comparison, we also depict the pixel-wise phase error in a second column. For $\delta = 32$, all the methods yield a reconstruction that visually resembles the true signal, but the BlockPR + SC reconstructions exhibit some artifacts. For $\delta = 8$, only BlockPR + $\text{SC}_{10^{-4}}$ yields a visually similar reconstruction, both BlockPR + $\text{SC}_{10^{-4}}$ and the iterative methods show strong visible differences in various parts. Thus the worse reconstruction quality in terms of the MSE (and the reconstructed phases, cf second column) is also reflected in the visual quality.

Figure 6 provides a better inside, why iterative methods show worse performance in the case $\delta = 8$. While the BlockPR + SC methods yield a consistently small error, the other methods yield some good reconstructions and some with rather large error, which we conjecture to correspond to suboptimal initializations. This motivates a combination of the two classes of approaches, with the solution of BlockPR + SC as an initialization of an iterative method.

In figure 7 we numerically observe that for a medium to large number of photons per pixels, such a hybrid method outperforms any individual approach, not only providing a better reconstruction error, but, in the case of Gerchberg–Saxton, also significantly reducing the runtime. Here the truncation parameter $\varepsilon$ is adaptively reduced with the noise level. This, however, is not necessary: for constant $\varepsilon = 10^{-3}$, its performance is comparable both in runtime and accuracy for small to medium noise levels. For larger noise, constant $\varepsilon = 10^{-3}$ yields only slightly worse accuracy, while the runtime is significantly reduced. We omit the details here.

Finally, we look at the runtime complexity of BlockPR + SC (figure 8). As discussed in section 3, BlockPR + SC shows a near-linear time complexity for $\varepsilon$ small. For greater $\varepsilon$, more singular values are truncated and the number of operations exhibits quadratic scaling as a result of having to recover a larger number of unknowns from the linearized quadratic system (19). As the value of the appropriate truncation level $\varepsilon$ decays with the dimension, a plot with fixed $\varepsilon$ and varying dimension is not meaningful, which is why we fix a proportion of truncated entries rather than a threshold.

5. Proofs

5.1. Singular values of measurement operator and proof of theorem 2

As discussed in section 3, the action of the measurement operator $\mathcal{A}$ can be described as a matrix-vector product

$$M\text{ vec}(X_0) = y.$$  

As shown in sections 2.2 and 4.4 of [35], the matrix $M$ takes the form

$$M = \begin{pmatrix}
M_1 & M_2 & \cdots & M_\delta & 0 & 0 & \cdots & 0 \\
0 & M_1 & \cdots & M_{\delta-1} & M_\delta & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
M_2 & M_3 & \cdots & 0 & 0 & 0 & \cdots & M_1
\end{pmatrix},$$

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where $M_1, \ell \in [\delta]$, are $(2\delta - 1) \times (2\delta - 1)$ matrices given by

\[
(M_1)_{n,j} = \begin{cases} 
\frac{\bar{w}_n w_{n+\ell-1}}{\sqrt{2\delta - 1}} e^{-\frac{2\pi i n (j-1)}{2\delta - 1}} & \text{if } 1 \leq j \leq \delta - \ell + 1, \\
0 & \text{if } \delta - \ell + 2 \leq j \leq 2\delta - \ell - 1, \\
\frac{\bar{w}_{n+1} w_{n+\ell+1}}{\sqrt{2\delta - 1}} e^{-\frac{2\pi i n (j-1)}{2\delta - 1}} & \text{if } 2\delta - \ell \leq j \leq 2\delta - 1, \ell < \delta,
\end{cases}
\]

if $j > 1$ and $\ell = \delta$.

As shown in [35], $M$ can be block diagonalized using the unitary block Fourier matrix $U_{2\delta-1} \in \mathbb{C}^{D \times D}$ defined as

\[
U_{2\delta-1} := \frac{1}{\sqrt{d}} \begin{pmatrix}
I_{2\delta-1} & I_{2\delta-1} & \cdots & I_{2\delta-1} \\
I_{2\delta-1} & I_{2\delta-1} & \cdots & I_{2\delta-1} \\
\vdots & \vdots & \ddots & \vdots \\
I_{2\delta-1} & I_{2\delta-1} e^{\frac{2\pi i (\delta-2d)}{d}} & \cdots & I_{2\delta-1} e^{\frac{2\pi i (\delta-1d-1)}{d}}
\end{pmatrix},
\]

where $I_{2\delta-1}$ denotes an $(2\delta - 1) \times (2\delta - 1)$ identity matrix. More precisely,

\[M = U_{2\delta-1} J U_{2\delta-1}^*,
\]

where $J \in \mathbb{C}^{D \times D}$ is a block diagonal matrix of the form

\[
J := \begin{pmatrix}
J_1 & 0 & \cdots & 0 & 0 \\
0 & J_2 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & J_{\delta-1} & 0 \\
0 & 0 & \cdots & 0 & J_{\delta}
\end{pmatrix},
\]

with blocks

\[J_k := \sum_{\ell=1}^{\delta} M_{k,\ell} e^{\frac{2\pi i k (\ell-1)}{d}}, \quad k \in [d].\]

A single block matrix $J_k \in \mathbb{C}^{(2\delta-1) \times (2\delta-1)}$ can be expressed as

\[
J_k = F_{2\delta-1} \begin{pmatrix}
z_{k,1} & 0 & \cdots & 0 \\
0 & z_{k,2} & 0 & \vdots \\
0 & 0 & \ddots & 0 \\
0 & 0 & \cdots & z_{k,2\delta-1}
\end{pmatrix}
\]

where $F_{2\delta-1}$ denotes a DFT matrix of size $\mathbb{C}^{(2\delta-1) \times (2\delta-1)}$. As $U_{2\delta-1}$ and $F_{2\delta-1}$ are unitary matrices, the absolute values of the $z_{k,j}$’s are the singular values of $M$. For masks of the form (13) upper bounds on the condition number of these matrices have been shown in [35]; they guarantee the stable invertibility of the operator $A|_{T_{s}(2\delta)}$ and matrix $M$ respectively. The next proposition, however, shows that this is specific to exponentially decaying masks and that for
a large class of masks naturally appearing in ptychography the operator $A_{|T_{\delta}(\mathbb{R}^d)}$ is not only ill-conditioned but even singular.

**Proposition 7.** Consider masks of the form (9). Assume that $d$ is even and the window $w$ satisfies the symmetry condition

$$u_n = w_{\delta-n+1} \quad \text{for all } n \in [\delta].$$

Then it holds that

$$z_{4+1,j} = 0 \quad \text{if} \quad \begin{cases} \delta - j \text{ is odd where } j \in [\delta], \\
\delta - j \text{ is even where } j \in [\delta - 1]_{\delta+1}. \end{cases} \quad (21)$$

To fully understand the implications of proposition 7 we note that the singular value decomposition of the matrix $M$ takes the form

$$M = U_{2\delta-1} J U^*_{2\delta-1} = U_{2\delta-1} \begin{pmatrix} F_{2\delta-1} & 0 \\ 0 & F_{2\delta-1} \end{pmatrix} \text{sign}(Z) |Z| U^*_{2\delta-1}, \quad (22)$$

where $Z$ is the diagonal matrix in $\mathbb{C}^{\delta \times \delta}$, which contains all $z_{k,j}$ for $k \in [d], j \in [2\delta - 1]$ on its main diagonal and the operations sign and $| \cdot |$ are taken entrywise.

With this expression for the SVD at hand, proposition 7 directly yields theorem 2, as every vanishing $z_{k,j}$ corresponds to a zero singular value of $M$. Therefore, the matrix $M$ cannot be invertible and, consequently, neither can the operator $A_{|T_{\delta}(\mathbb{R}^d)}$, as stated in theorem 2.

Moreover, proposition 7 provides explicit expressions for the index set $I$ corresponding to these zero singular values of $M$, as we will see below.

**Proof of Proposition 7.** We first consider the case $1 \leq j \leq \delta$. By (20),

$$z_{k,j} = (F_{2\delta-1} \cdot J_k)_{j,j} = \sum_{\ell=1}^{\delta-j+1} w_{\ell} w_{j+\ell-1} e^{2\pi i (\ell-1)j/\delta}.$$

Setting $k = \frac{\delta}{2} + 1$, we get

$$z_{4+1,j} = \sum_{\ell=1}^{\delta-j+1} w_{\ell} w_{j+\ell-1} e^{2\pi i j(\ell-1)/\delta} = \sum_{\ell=0}^{\delta-j} w_{\ell+1} w_{j+\ell} (-1)^{\ell}$$

$$= \sum_{\ell=0}^{\delta-j} w_{j+\ell} w_{\delta-j-\ell+1} (-1)^{\ell} = \sum_{\ell=0}^{\delta-j} w_{j+\ell+1} w_{\ell+1} (-1)^{\delta-j-\ell},$$

where in the third equality we used the symmetry of the window $w$ and in the last one we changed the summation order. We continue by averaging the first and last reformulation of $z_{4+1,j}$ obtaining

$$z_{4+1,j} = \frac{1}{2} z_{4+1,j} + \frac{1}{2} z_{4+1,j} = \sum_{\ell=0}^{\delta-j} w_{j+\ell+1} w_{\ell+1} \frac{1}{2} \left( (-1)^{\ell} + (-1)^{\delta-j-\ell} \right)$$

$$= \sum_{\ell=0}^{\delta-j} w_{j+\ell+1} w_{\ell+1} \frac{(-1)^{\ell}}{2} \left( 1 + (-1)^{\delta-j-2\ell} \right).$$
When $\delta - j$ is odd, the last factor vanishes in all the summands and hence
\[ z_{4+1,j} = 0. \]

For the case $\delta + 1 \leq j \leq 2\delta - 1$, we get analogously
\[ z_{4+1,j} = 0 \quad \text{if } \delta - j \text{ is even.} \]

Proposition 7 can be reformulated in terms of the matrix $V_2$ as follows.

**Corollary 8.** Consider measurement masks of the form (9). Assume that $d$ is even and the window $w$ satisfies the symmetry condition
\[ w_n = w_{\delta-n+1} \quad \text{for all } n \in [\delta]. \]

Then the right singular vector $V^{(q)}$ corresponding to the singular value $|z_{4+1,j}|$ is a column of $V_2$ provided the index $q$ is of the form
\[ q = (2\delta - 1)(d^2 + 1) + r \]
with $r \in I$, where the set $I$ of size $|I| = \delta - 1$ is given by
\[ I = \{ j \in [\delta] : \delta - j \text{ is odd} \} \cup \{ j \in [\delta - 1]_{\delta+1} : \delta - j \text{ is even} \}. \]

Equivalently, $L'_{4+1}, r \in I$, are not recovered in the step 2 of algorithm 2.

5.2. Proof of theorem 3 and corollary 4

**Proof of Theorem 3.** First we use the definition of the DFT (3) and the diagonals $L'_{\xi}$ (17) to obtain
\[ L'_{\xi} = \sum_{n=1}^{d} e^{2\pi i (\xi-1)(n-1) / d} L_n' \]
\[ = \begin{cases} \sum_{n=1}^{d} e^{2\pi i (\xi-1)(n-1) / d} (x_0)_n (x_0)_{n+r-1} & \text{if } 1 \leq r \leq \delta, \\
\sum_{n=1}^{d} e^{2\pi i (\xi-1)(n-1) / d} (x_0)_{n+1} (x_0)_{n+1+r-2\delta} & \text{if } 1 + \delta \leq r \leq 2\delta - 1. \end{cases} \]

To reformulate the right-hand side of (18), we need an alternative representation of the vectorization of $X_0$ as given in the following lemma.

**Lemma 9.** Decomposing $q \in [D]$ as
\[ q = (2\delta - 1)(\xi - 1) + r \quad \text{with } \xi \in [d], r \in [2\delta - 1], \]
one can express the vectorization of $X_0$ from formula (14) as
\[ \text{vec}(X_0)_q = \begin{cases} (x_0)_{\xi+r-1} & \text{if } 1 \leq r \leq \delta, \\
(x_0)_{\xi+1+r-2\delta+1} & \text{if } 1 + \delta \leq r \leq 2\delta - 1. \end{cases} \]
The proof of the lemma can be found in the appendix A.

Recall that by (22), one has that \( V = U_{2\delta - 1} \). Thus, as for every column of \( U_{2\delta - 1} \), the indices of \( V^{(\ell)} \) can be expressed as

\[
(v^{(\ell)})_i = \left( U_{2\delta - 1} \right)_i^\ell = \begin{cases} \frac{1}{\sqrt{d}} \cdot 2^{2\lfloor \ell(\delta - 1) \rfloor} & \text{if } \ell \mod (2\delta - 1) = r, \\ 0 & \text{else,} \end{cases}
\]

where \( s = \lfloor \frac{d+1}{2\delta - 1} \rfloor \). We obtain that

\[
\sqrt{d} \langle \text{vec}(X_0), V^{(\ell)} \rangle = \sum_{i=1}^d e^{-\frac{2\pi i (\ell(\delta - 1) - 1)}{\delta}} \text{vec}(X_0)_{2\delta - 1(n-1)+r}
\]

\[
= \begin{cases} \sum_{i=1}^d e^{-\frac{2\pi i (\ell(\delta - 1) - 1)}{\delta}} (x_0)_h(x_0)_{n+r-1} & \text{if } 1 \leq r \leq \delta, \\ \sum_{i=1}^d e^{-\frac{2\pi i (\ell(\delta - 1) - 1)}{\delta}} (x_0)_{n+1}(x_0)_{n+1+r-2\delta} & \text{if } 1+\delta \leq r \leq 2\delta - 1, \end{cases}
\]

where the last equality follows from lemma 9.

\[\square\]

Corollary 4 now follows directly from the definition of \( X_S \).

**Proof of Corollary 4.** Combining the definition of \( X_S \) with (16), we obtain

\[
\text{vec}(X_S) = M_S^{-1}y = M_S^{-1}M \text{ vec}(X_0) = V_1V_1^* \text{ vec}(X_0)
\]

and

\[
\sqrt{d} \langle \text{vec}(X_S), V^{(\ell)} \rangle = \sqrt{d} \langle V_1V_1^* \text{ vec}(X_0), V^{(\ell)} \rangle = \sqrt{d} \langle \text{vec}(X_0), V_1V_1^* V^{(\ell)} \rangle
\]

\[
= \begin{cases} \sqrt{d} \langle \text{vec}(X_0), V^{(\ell)} \rangle & \text{if } V^{(\ell)} \text{ column of } V_1, \\ 0 & \text{if } V^{(\ell)} \text{ column of } V_2, \end{cases}
\]

which concludes the proof.

\[\square\]

### 5.3. Recovery of lost coefficients and proof of theorem 6

In this section we will show that under the assumptions of theorem 6, algorithm 2 provides a feasible and reliable procedure to complete the restricted low-rank matrix \( X_0 \). We first prove lemma 5, which establishes that, under the assumptions that the algorithm is tractable and the solution of (19) is unique, algorithm 2 yields the right answer.

**Proof of Lemma 5.** Observe that for arbitrary \( j \in [d] \)

\[
\left( L^J \circ S_{\ell-1}(L^J)^* \right)_j = (x_0)_{j+1-\ell-1} \cdot (x_0)_{j+\ell-1}(x_0)_{j+\ell+r-2} = (x_0)_{j+1-\ell-1} \cdot (x_0)_{j+\ell-1}(x_0)_{j+\ell+r-2} = \left( L^J \circ S_{\ell-1}(L^J)^* \right)_j.
\]

\[\square\]

In the remainder of this section, we will show tractability and uniqueness, which will both follow from the fact that under assumptions (a) and (b), (19) is in fact a linear relation.
The main idea is that for the index \( r \) corresponding to the diagonal that is fully known by (a), the left-hand side of (19) is known, and all but one Fourier coefficients of the right-hand side consists of products of different coefficients. Thus, one obtains linear equations in the real and imaginary parts of the single unknown coefficient. This is formalized in the following proof of theorem 6.

**Proof of Theorem 6.** Let us denote by \( L' \) the diagonal with all known entries, provided by assumption (A1). Due to assumption (A2) we are missing at most one Fourier coefficient on each of the other diagonals \( L^d \), say at position \( q \in [d] \). To estimate this missing coefficient, we work with the DFT of the quadratic relationship (19). Using the convolution theorem (4) and lemma 1, we obtain the following expression for the \( j \)th Fourier coefficient.

\[
\begin{align*}
c_j := (L' \circ S_{-1}(L')^*)_j &= (L' \circ S_{-1}(L')^*)_j \\
&= (L_j^*(W_j(L_j^*))_j = \sum_{p=1}^{d} L_{j-p+1}^* W_p(L_j^*)_p \\
&= \sum_{p=1}^{d} e^{\frac{2\pi i r (q-1)p}{d}} L_{j-p+1}^* L_{d-p+2}^*.
\end{align*}
\]

We note that for \( p \in C := \{ j + 1 - q, d + 2 - q \} \) the corresponding summand on the right-hand side contains \( L_q^j \) or \( L_q^j \), all other summands are known by assumption (A2). For \( j = 1 \), \( C \) is a single index, which leads to a quadratic term \( |L_q^j|^2 \). For this reason we skip the case \( j = 1 \) in the following considerations. For \( j \neq 1 \), let

\[
\begin{align*}
z_j := \sum_{p=1}^{d} e^{\frac{2\pi i r (q-1)p}{d}} L_{j-p+1}^* L_{d-p+2}^*.
\end{align*}
\]

We obtain

\[
\begin{align*}
c_j - z_j &= L_q^j e^{\frac{2\pi i r (q-1)j}{d}} L_{d-j+q+1}^* e^{\frac{2\pi i r (q-1)d}{d}} L_{j-d+q+1}^*。
\end{align*}
\]

By decomposing the complex numbers in the previous equation into their real and imaginary part we get

\[
\begin{align*}
\begin{bmatrix} \text{Re}(a_j) + \text{Re}(b_j) & -\text{Im}(a_j) + \text{Im}(b_j) \\ \text{Im}(a_j) + \text{Im}(b_j) & \text{Re}(a_j) - \text{Re}(b_j) \end{bmatrix} \begin{bmatrix} \text{Re}(L_q^j) \\ \text{Im}(L_q^j) \end{bmatrix} = \begin{bmatrix} \text{Re}(c_j - z_j) \\ \text{Im}(c_j - z_j) \end{bmatrix}.
\end{align*}
\]

Combining these linear systems for all \( j = 2, \ldots, d \) we obtain the overdetermined linear system

\[
\begin{align*}
\begin{bmatrix} Q_2 \\ Q_3 \\ \vdots \\ Q_d \end{bmatrix} \begin{bmatrix} \text{Re}(L_q^j) \\ \text{Im}(L_q^j) \end{bmatrix} = \begin{bmatrix} v_2 \\ v_3 \\ \vdots \\ v_d \end{bmatrix} = Q \begin{bmatrix} \text{Re}(L_q^j) \\ \text{Im}(L_q^j) \end{bmatrix} = v.
\end{align*}
\]

(23)
This system can be solved using least squares to approximate the missing component \( \hat{L}_q^\ell \). After this estimation step all entries of the diagonal \( \hat{L}_q^\ell \) are available and one can obtain an estimate for the vector \( L^\ell \) via the inverse DFT. This procedure is repeated for all diagonals \( L^\ell \) with \( 1 \leq \ell \leq \delta \) that have missing Fourier coefficients. This recovers the upper triangular part of \( X_0 \). To obtain the remaining entries, we use that \( X_0 \) is a Hermitian matrix.

6. Conclusion and future work

In this paper, we proposed a subspace completion technique, which extends the range of applicability of the BlockPR algorithm in ptychography to a larger class of windows. Furthermore, our technique can be used as a regularizer for better noise robustness. The next step will be to analyze the case of more than one zero entry per diagonal in more detail. As this scenario gives rise to nonlinear dependencies, this will likely require a very different set of tools. Also, we plan to consider the extension of the technique to models with shifts longer than 1 as proposed in [37, 38], and to two-dimensional images.

Another aspect to explore for further improvement is to use weighted angular synchronization techniques in the second step of the BlockPR, as discussed in [36, 43]. The idea is to incorporate magnitude information of the matrix \( X \) obtained in step 4 of the algorithm 2 as weights for the phase reconstruction in step 6, which can lead to better reconstruction quality.

A long-term objective will be to extend our analysis to scenarios, where the illumination is partly of fully unknown, the so-called blind ptychography problem. The development of the algorithms for this problem has been a very active area of research for some years—see, e.g., recent works regarding the identifiability [44] and local convergence of alternating projections [45]—but, to the best of our knowledge, no global recovery guarantees are available yet.

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Appendix A. Proof of lemma 9

We start by considering the case that \( 1 \leq r \leq \delta \). Then to rewrite the index of the first factor on the right-hand side of (14), we observe that it follows from the decomposition of \( q \) that

\[
\frac{q + \delta - 1}{2\delta - 1} = \frac{(2\delta - 1)(\xi - 1) + r + \delta - 1}{2\delta - 1} = \xi - 1 + \frac{r + \delta - 1}{2\delta - 1}.
\]

Since \( r \in [\delta] \), it follows that

\[
\frac{1}{2} \leq \frac{\delta}{2\delta - 1} \leq \frac{r + \delta - 1}{2\delta - 1} \leq \frac{2\delta - 1}{2\delta - 1} = 1,
\]
and, thus, 
\[ \left\lceil \frac{q + \delta - 1}{2\delta - 1} \right\rceil = \xi. \]
Furthermore, we have
\[ (q + \delta - 2) \mod(2\delta - 1) = ((2\delta - 1)(\xi - 1) + r + \delta - 2) \mod(2\delta - 1) = (r + \delta - 2) \mod(2\delta - 1) = r + \delta - 2. \]
Thus, the index of the second factor on the right-hand side of (14) can be rewritten as
\[ \left\lceil \frac{q + \delta - 1}{2\delta - 1} \right\rceil + [(q + \delta - 2) \mod(2\delta - 1)] - \delta + 1 = \xi + r - 1. \]
Consequently, we obtain that vec\((X_0)_q\) defined in (14) can be written as
\[ \text{vec}(X_0)_q = (x_0)_{\xi}(x_0)_{\xi + r - 1} \text{ if } 1 \leq r \leq \delta \text{ and } \xi \in [d]. \]
In the second case we have \(1 + \delta \leq r \leq 2\delta - 1\), which immediately gives
\[ 1 < \frac{2\delta}{2\delta - 1} \leq \frac{r + \delta - 1}{2\delta - 1} \leq \frac{3\delta - 2}{2\delta - 1} \leq 2, \]
and, thus, the index of the first factor on the right-hand side of (14) is given by
\[ \left\lceil \frac{q + \delta - 1}{2\delta - 1} \right\rceil = \xi + 1. \]
Furthermore, analogous to the previous case we get
\[ (q + \delta - 2) \mod(2\delta - 1) = r - (\delta + 1), \]
so that the index of the second factor in (14) becomes
\[ \left\lceil \frac{q + \delta - 1}{2\delta - 1} \right\rceil + [(q + \delta - 2) \mod(2\delta - 1)] - \delta + 1 = \xi + r - 2\delta + 1. \]
Finally, we get that vec\((X_0)_q\) as defined in (14) can be written equivalently as
\[ \text{vec}(X_0)_q = (x_0)_{\xi + r - 2\delta + 1}(x_0)_{\xi + r - 2\delta + 1} \text{ if } 1 + \delta \leq r \leq 2\delta - 1 \text{ and } \xi \in [d]. \]

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