The Geometry of the Phase Retrieval Problem

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I want to thank Christian and Patrick for inviting me to speak.

What I will discuss today is somewhat unconventional, ongoing work, at the intersection of pure mathematics, numerical analysis and mathematical physics.

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Outline

1. Introduction
2. The Discrete Phase Retrieval Problem
3. Geometry of the Torus
4. Reconstruction Algorithms
5. Numerical Examples in Phase Retrieval
6. Other Auxiliary Conditions
7. Short History of CDI
8. Bibliography
Today I will speak about inverse problems that arise in *Coherent Diffraction Imaging*. This is a technique that uses very high energy, monochromatic light, either electrons or x-rays, to form high resolution images of animate and inanimate materials. The goal is to achieve resolutions in the 1–10nm range.
The photons used to illuminate the samples are in the 0.1-10KeV range; the light is typically assumed to be monochromatic, produced either by a laser or as synchrotron radiation. The object being imaged is typically many wavelengths across and the measurement is made very far from the object and light source, hence in the far field (the Fraunhofer regime). As is well known, if $\rho(x)$ describes the density of the object, then the leading order term in the far field expansion of the scattered radiation is proportional to the square of the Fourier transform, $\hat{\rho}(k)$, of $\rho$. At such small wavelengths, one can only measure the intensity of the scattered field, $|\hat{\rho}(k)|^2$, and not its phase.
Here are computed far field diffraction patterns produced by (a) a semi-circle, (b) an equilateral triangle.
Here is an actual diffraction pattern produced by frozen-hydrated yeast spore at 520 eV. Courtesy E. Lima PhD thesis, Stony Brook U, from [8].
Of course we would like to reconstruct $\rho(x)$ from this measurement, but we need to, at least, estimate the unmeasured phase of $\hat{\rho}(k)$. This is called the *phase retrieval problem*. It also arises in x-ray crystallography, but is really quite a different problem for a periodic structure. In the context of a compact object, the possibility of solving this problem was first suggested by D. Sayre in 1952. He saw it as a consequence of Nyquist’s sampling theorem! See [1].

For this problem to be solvable, even in principle, some auxiliary information is required, such as an estimate for the support of the object, or knowledge that the function $\rho(x)$ is non-negative and an estimate on the support of its autocorrelation function. Many attempts have been made to solve this problem, but with rather limited success. Today we’ll discuss the underlying reasons for the difficulty of this problem...which may suggest better approaches.
Outline of this Lecture

We will try to cover the following material:

- The Discrete Phase Retrieval Problem (a simpler model)
- Geometry of the Amplitude Torus
- Reconstruction Algorithms
- What We Learn from Numerical Examples
The phase retrieval problem encountered in coherent diffraction imaging is fraught with many practical difficulties. For the remainder of the talk we focus on a simpler model problem, which already proves very difficult to solve. We call this the \textit{discrete, classical phase retrieval} problem. We imagine that the unknowns are samples of an object on a finite uniform grid:

$$\mathbf{x}_j = \rho(j_1 \Delta x, j_2 \Delta x), \text{ where } j \in J. \quad (1)$$

Here $J = [n_1 : N_1] \times [n_2 : N_2]$, is a rectangular grid. We call such collections of data indexed by \textit{J images}.
The Measurements

In our model problem, the measured data are the magnitudes of the DFT of these samples:

\[ \{a_j = |\hat{x}_j| : j \in \hat{J}\}, \quad (2) \]
where \( \hat{J} \) is a set of sample frequencies, with \(|J| = |\hat{J}|\). If \( J = [0 : N - 1]^d \), then

\[ \hat{x}_j = \sum_{k \in J} x_k e^{-\frac{2\pi i j \cdot k}{N}}. \quad (3) \]

We let \( \mathcal{M} : \mathbb{R}^J \rightarrow \mathbb{R}_+^J \) denote the measurement map:

\[ \mathcal{M}(x) = (|\hat{x}_j|)_{j \in J}. \quad (4) \]

There are important differences between these model measurements and the samples of a continuum Fourier transform that would actually be collected.
As noted above we need to have auxiliary information to be able to solve the phase retrieval problem. We imagine that the support of the unknown image $x$, $S_x$, is contained in a rectangular subset $R \subset J$ with the side lengths of $R$ at most half those of $J$. In the literature it is often said that we “oversample,” but really we just need to sample in $k$-space on a fine enough grid for the data set to contain information about the support of $x$.

Our auxiliary information will be an estimate for $S_x$. This is a subset $S$ with $S_x \subset S \subset R \subset J$. We are therefore looking for an image $x$ so that $x_j = 0$ for $j \notin S$, and

$$|\hat{x}_j| = a_j \text{ for all } j \in \hat{J}. \quad (5)$$

This problem usually does not have a unique solution, but generically, the non-uniqueness is of a simple sort.
If \( x \) is an image indexed by \( J \), then we think of it as being periodic in \( \mathbb{Z}^2 \), with \( \{ j \in J \} \) representing a single period cell. We can then translate an image by any lattice vector \( k \in \mathbb{Z}^2 \), defining

\[
x_j^{(k)} \overset{d}{=} x_{j-k}.
\]

We can also define the inverted image by setting

\[
\tilde{x}_j = x_{-j}.
\]

Translation and inversion lead to images with the same magnitude Fourier data; these are called the trivial associates of \( x \).
Hence there are always many images with the same magnitude Fourier data, and support in a translate of $R$, but there is a theorem, due to Monson Hayes (see [5]) which states that generically this is the only form of non-uniqueness one encounters: with sufficiently fine sampling in the Fourier domain, the only images with the given magnitude Fourier data are the trivial associates of a given image with this data.

Let $S_x \subset S \subset R$, as above; the support condition $S$ defines a linear subspace of $\mathbb{R}^J$,

$$B_S = \{x \in \mathbb{R}^J : x_j = 0 \text{ if } j \notin S\}. \ (8)$$

In all cases $\mathcal{M}^{-1}(\mathcal{M}(x)) \cap B_S$ is a finite set, and generically it consists of trivial associates of $x$. 

Uniqueness
The better our estimate, $S$, for the support is, the fewer trivial associates there are, with the given magnitude Fourier data, that will also satisfy the condition that $S_x \subseteq S$. One might expect that if $S = S_x$, then the phase retrieval problem should be “easy,” but that, in fact, is not usually the case.

For numerical experiments we often quantify our knowledge of the support of $x$ in terms of \textit{$p$-pixel neighborhoods}. The $p$-pixel neighborhood of a set $U \subset \mathbb{Z}^2$ is obtained as the union of all translates of $U$ by integer vectors $(j_1, j_2)$ lying in the square with vertices at $(\pm p, \pm p)$.

Before turning our attention to methods for solving the phase retrieval problem, we consider its underlying geometry.
As we’ve assumed that the image is real, the phase retrieval problem takes place in the ambient space $\mathbb{R}^J$. The magnitude Fourier data of $x : \{a_j : j \in \hat{J}\}$, defines a torus, which we call the *magnitude torus* defined by $x$:

$$\mathbb{A}_a = \{y \in \mathbb{R}^J : |\hat{y}_j| = a_j \text{ for all } j \in \hat{J}\}. \quad (9)$$

The cardinality of $J$ is typically in the hundreds of thousands, or millions. For a small, low resolution image $|J| = 4096 = 64 \times 64$. The dimension of $\mathbb{A}_a$ is about $\frac{|J|}{2}$, and (in $2d$) $\text{dim} \mathbb{B}_S$ is about $\frac{|J|}{4}$. 
Geometric Statement of the Phase Retrieval Problem

Geometrically the phase retrieval problem is the problem of finding points in the intersection $\mathbb{A}_a \cap B_S$.

Alternately we can imagine trying to find a local inverse for the measurement map $\mathcal{M} \upharpoonright B_S$ defined above.

A very important difference between our model problem and the actual problem in CDI (with finitely many samples of the continuum Fourier transform) is that the model problem has exact solutions, but the actual problem does not: A function with only finitely many non-zero Fourier coefficients cannot be either compactly supported or non-negative.
Generalized phase retrieval has enjoyed a recent resurgence of interest, with work of Candes, Daubechies, et al. The problems that these authors have considered are usually quite different from the classical phase retrieval problem.

Briefly, one begins with a Hilbert space \((\mathcal{H}, \langle \cdot, \cdot \rangle)\) and a frame \(\Phi = \{\varphi_n : n \in \mathcal{I}\}\) for \(\mathcal{H}\). The measurements at one’s disposal are the magnitudes of the frame coefficients:

\[ M_{\Phi}(x) = (\|\langle x, \varphi_n \rangle\|)_{n \in \mathcal{I}}. \]  

The phase retrieval problem is then to recover \(x\), up to a global phase (or sign) from the measurements \(M_{\Phi}(x)\). From the definition of a frame it follows that

\[ \|M_{\Phi}(x) - M_{\Phi}(y)\|_2 \leq C_1 \|x - y\|_\mathcal{H}. \]
Other Phase Retrieval Problems, II

If dim $\mathcal{H} < \infty$ and $\mathcal{H}$ complex, (real) then generically, for a frame, $\Phi$, with $|\mathcal{I}| > 4 \dim \mathcal{H} + 4$, ($|\mathcal{I}| > 2 \dim \mathcal{H} + 2$) the map $x \mapsto M_\Phi(x)$ is injective and the generalized phase retrieval problem it defines is, in principle, solvable.

In this case one can show that the inverse satisfies a Lipschitz estimate: there exists a $0 < C < \infty$ so that

$$\inf_{\alpha} \| x - e^{i\alpha} y \|_{\mathcal{H}} \leq C \| M_\Phi(x) - M_\Phi(y) \|_2.$$ (11)

The problem we consider is quite different in that the measurements $M(x)$ never determine a unique solution. The question about the Lipschitz estimate is quite interesting, and rather subtle.

Many real physical measurements can only be modeled by the classical Fourier measurements, and the generalized theory simply does not apply.
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The underlying problem in phase retrieval is that of finding the intersection between two subsets, $A, B$ of a vector space, where we know that $A \cap B$ consists of a finite set of points. In most analyses of this class of problems, it is assumed that the sets $A$ and $B$ are convex and meet \textit{transversally}; that is, $A$ and $B$ are convex submanifolds and if $x \in A \cap B$, then the tangent spaces meet only at $x$ itself:

$$T_x A \cap T_x B = \{x\}. \quad (12)$$

Transversality is more or less necessary for the linearized problem, that of locating $T_x A \cap T_x B$, to provide a good model for problem of locating points in $A \cap B$.

The magnitude torus is never convex and, as we see below, the transversality assumption almost always \textit{fails} in the classical phase retrieval problem.
A surprising feature of the classical problem is the extent to which we can explicitly describe the tangent space to a magnitude torus. Let \( y \in \mathbb{A}_a \) and let \( \hat{y} \) be the DFT of \( y \). The following vectors contain a spanning set for the fiber of \( T_y \mathbb{A}_a \):

\[
    t_j = \mathcal{F}^{-1} \left[ i \hat{y}_j e_j - i \hat{y}_{j'} e_{j'} \right] \quad \text{for } j \in J. \tag{13}
\]

Here \( j' \) is the “conjugate index” to \( j \), for which reality of \( y \) implies that

\[
    \hat{y}_{j'} = \overline{\hat{y}_j}. \tag{14}
\]

Each non-zero vector appears twice, and we let \( J_1 \subset J \) be chosen so that

\[
    \left\{ \frac{t_j}{\sqrt{2|\hat{x}_j|}} : j \in J_1 \right\}. \tag{15}
\]

is a basis for the fiber of \( T_y \mathbb{A}_a \).
In all cases, a basis for the fiber of the tangent space can be described (in the Fourier domain) by the list of the indices in $J_1$ paired with $|J_1|$ complex numbers of modulus 1. Notice that an orthonormal basis for a subspace of this dimension generically requires a matrix with dimensions $|J_1| \times |J|$. Hence these subspaces admit a *highly* compressed representation, which requires only the FFT to access and use.

In fact, there is a different description of the tangent space that is even more useful for analyzing the relationship of $T_y \mathbb{A}_a$ to $B_S$, when $y \in \mathbb{A}_a \cap B_S$. 
A Second Basis for $T_{y}^{0} \mathbb{A}_a$ and $N_{y}^{0} \mathbb{A}_a$

We state this as a lemma:

**Lemma**

Let $y \in \mathbb{A}_a$ and $v \in \mathbb{N}^2$, then the vectors

\[
\tau(v) = y(v) - y(-v) \in T_{y}^{0} \mathbb{A}_a \quad \text{and} \quad v(v) = y(v) + y(-v) \in N_{y}^{0} \mathbb{A}_a.
\]

If $x_j \neq 0$, for any $j \in J$, then these sets contain spanning sets for these vector spaces.

Recall that $x_j^{(v)} = x_j - v$, is just a translate of $x$. This allows us to examine the intersection $T_{y} \mathbb{A}_a \cap B_S$ in detail. If $S_y \subset S$, and $v$ is a vector so that both $S_y(v) \subset S$ and $S_y(-v) \subset S$. Then the tangent vector $\tau(v) \in T_{y}^{0} \mathbb{A}_a \cap B_S$. 
Suppose that $S_p$ is the $p$-pixel neighborhood of $S_x$, for some image $x$, with small support.

It turns out that the dimension of the “numerical” intersection $T_y \bigcap_a \cap B_{S_p}$ depends on both the smoothness of the image and the size of the neighborhood. A simple combinatorial argument shows that

$$\dim T_y \bigcap_a \cap B_{S_p} \geq 2p(p + 1).$$  \hspace{1cm} (17)

This does not depend on the ambient dimension, i.e. $|J|$. For a piece-wise constant image this gives the exact dimension of the intersection (again independently of $|J|$). As the image becomes smoother this becomes a lower bound.
We examine these intersections for “small” examples. Test images are obtained as samples of random collections of disks, which have been smoothed by a Gaussian whose width is determined by a parameter $0 \leq k$. 

![Test Images](image-url)
As noted above, we quantify our knowledge of the support of $x$ in terms of $p$-pixel neighborhoods. Let $S_p$ be the $p$-pixel neighborhood of $S_x$. This figure shows $S_1, S_2, S_3, S_4$ for the $k = 1$ case in the previous slide.
In the table below we show the dimensions of the “numerical” intersections $T_x \mathbb{A}_a \cap B_{S_p}$ for various values of $k$ and $p$. These are subspaces where the angle is less than $10^{-7}$ radians. The ambient dimension is 4096, and $\dim T_y \mathbb{A}_a = 2046$.

<table>
<thead>
<tr>
<th>diff\supp</th>
<th>$p = 1$</th>
<th>$p = 2$</th>
<th>$p = 3$</th>
<th>$p = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k = 0$</td>
<td>4</td>
<td>12</td>
<td>24</td>
<td>40</td>
</tr>
<tr>
<td>$k = 1$</td>
<td>12</td>
<td>24</td>
<td>40</td>
<td>60</td>
</tr>
<tr>
<td>$k = 2$</td>
<td>48</td>
<td>72</td>
<td>100</td>
<td>132</td>
</tr>
<tr>
<td>$k = 3$</td>
<td>96</td>
<td>128</td>
<td>164</td>
<td>204</td>
</tr>
</tbody>
</table>

In the table the dimensions are always positive, indeed it is very rare for this dimension to be zero! That is: the intersection $\mathbb{A}_a \cap B_S$ is not usually transversal.
For the smoother examples ($k > 0$) it is not clear if the dimensions of the exact intersections are increasing, or if there are subspaces, whose dimension increases with $k$, where $B_S$ and $T_y \hat{A}_a$ make a very shallow angle. Indeed, it seems likely that the latter possibility is the correct interpretation.
Non-transversality renders the problem of finding points in $\mathbb{A}_a \cap B_S$ ill-conditioned in a neighborhood of $y$ : Suppose that $y \in \mathbb{A}_a \cap B_S$ and $v$ is a unit vector belonging to $T_y \mathbb{A}_a \cap B_S$. Because this direction is tangent to both submanifolds it is clear that, $y + tv \in B_S$ and for small $t$,

$$\text{dist}(y + tv, \mathbb{A}_a) \propto t^2$$

$$\text{dist}(y + tv, \mathbb{A}_a \cap B) \approx t.$$
This shows that if our numerical computations are accurate to $\varepsilon_{\text{Mach}}$, then the set of vectors

$$\{ y + tv : |t| \leq \sqrt{\varepsilon_{\text{Mach}}} \text{ and } v \in T_y A_a \cap T_y B_S \text{ with } \|v\| = 1 \}$$

all lie in $A_a \cap B_S$ to accuracy $\varepsilon_{\text{Mach}}$.

Because these intersections are non-transversal, at machine precision, there will be many equally valid “solutions,” which actually lie quite far from a true intersection point.

This is entirely independent of the algorithm.
As noted above, the map $\mathcal{M} \upharpoonright_{B_S}$ is always locally invertible on its range. But note:

**Theorem**

Suppose that $x$ satisfies $\hat{x}_j \neq 0$, for all $j \in J$, and $S_x \subset S \subset R$, with $R$ at most half the size of $J$. There exists $\eta > 0$ and a finite $C$ so that

$$\|x - y\|_2 \leq C \|\mathcal{M}(x) - \mathcal{M}(y)\|_2$$

for $y \in B_S$, with $\|x - y\|_2 < \eta$, if and only if

$$T_x \Delta_a \cap B_S = \{x\}.$$  

That is the local inverse is Lipschitz if and only if the intersection $\Delta_a \cap B_S$ is transversal at $x$. The “if” part follows from the observations on the previous two slides. The “only if” is a little harder to prove.
The failure to have a Lipschitz lower bound shows that the local inverse of $\mathcal{M}$ cannot be Lipschitz continuous. This means that the solution to this problem can be expected to have great sensitivity to noise and measurement errors. These geometric considerations also have a significant impact on the performance of standard algorithms.
The most classical approach to finding points in $\mathbb{A} \cap B_S$ is called \textit{alternating projection}. In Functional Analysis it was introduced by von Neumann, and, in image reconstruction, by Gerchberg and Saxton, see [2]. We let $P_{B_S} : \mathbb{R}^J \to B_S$ be the orthogonal projection, and $P_A : \mathbb{R}^J \to A$ be the closest point map. This map is defined on the complement of a union of codimension 2 linear subspaces.

The idea for alternating projection is very simple. We choose a random collection of phases $\{e^{i\theta_j} : j \in \hat{J}\}$ and use the inverse DFT to find the initial image $x^{(0)} = \mathcal{F}^{-1}([a_j e^{i\theta_j}])$, which is a random point on the magnitude torus.
We define the alternating projection sequence

$$x^{(n+1)} = P_{\mathbb{A}} \circ P_{B_S}(x^{(n)}).$$

(22)

It is clear that any point $x \in \mathbb{A} \cap B_S$ is a fixed point of this iteration, and it was hoped for many years that these iterates would converge to such a fixed point. In fact AP has many attracting fixed points that do not come from intersection points.
These additional fixed points are local minima of the map from 
\( A \times B_S \rightarrow [0, \infty) \) defined by

\[
d_{AB}(x, y) = \|x - y\|_2 \text{ (The Euclidean distance).} \tag{23}
\]

A priori, it is not obvious that any such points exist, but this is quickly clarified by numerical experiments.

The next slide shows the results of running AP for 10,000 iterates with 25 different randomly chosen starting points. The 256 \( \times \) 256-image is piecewise constant, with a support neighborhood of 3-pixels.
Experiments with AP

(a) The target for the flow.

Figure: In (b), blue is the log$_{10}$ of the distance to $A \cap B_{S_3}$, the cyan curves are plots of the “residual:” log$_{10}$ $\|x^{(n)} - P_{BS_3}(x^{(n)})\|$, and red is the distance between successive iterates of the algorithm, log$_{10}$ $\|x^{(n)} - x^{(n+1)}\|$.
On the previous slide we saw the results of starting the AP-algorithm at 25 random initial point on the magnitude torus. It is quite apparent, from the behavior of the red curves, which show \( \log_{10} \| x^{(n)} - x^{(n+1)} \| \), that the iterates of the AP-algorithms converge. Indeed the sum \( \sum_n \| x^{(n)} - x^{(n+1)} \| < \infty \).

The limit points, however, do not lie on \( \mathbb{A} \cap B_S \). A careful examination of these limits shows that they are all different, which gives strong evidence that \( d_{AB} \) has many local minima, where \( d_{AB}(x_A, y_B) \neq 0 \).

Contrary to what is stated in the many places, Alternating Projection does not stagnate, it just converges to limit points that are far from \( \mathbb{A} \cap B_S \).
Stagnation versus Convergence

We use these terms a little differently from most people working in this field.

**Definition**

A sequence of points \( \{x^{(n)}\} \) converges to \( x^* \) if

\[ \lim_{n \to \infty} \| x^{(n)} - x^* \| = 0. \]

**Definition**

A sequence of points \( \{x^{(n)}\} \) stagnates if the sequence remains in a bounded set \( D \), but the successive differences \( \| x^{(n)} - x^{(n+1)} \| \) do not converge to zero.

These aren’t all the possibilities, but these are the outcomes we have observed, experimentally, in the phase retrieval problem.
It has been known for a long time that algorithms based on the AP-map do not work very well. A different class of maps, which we call difference maps, were introduced to correct this problem. The first such algorithms were proposed by Fienup, using a map given by

\[ D_{BA}^\beta = x \mapsto x + P_B[(1 + \beta)P_A(x) - x] - \beta P_A(x). \]  

(24)

Here \( \beta \in (0, 1] \). This is call the “hybrid input-output method;” there were later additions by Elser, Miao, etc. See [3], [4], [6], [7]. There are many variants, which all behave similarly.
A representative case is given by the map:

\[ D_{AB}(x) = x + P_A \circ R_B(x) - P_B(x), \]  

which, in the notation of the previous slide, is \( D_{AB}^1 \). Here \( R_B \) is the “reflection around \( B \)” defined by

\[ R_B(x) = 2P_B(x) - x. \]

If \( B \) is a linear subspace, then \( R_B \) is just the usual orthogonal reflection with fixed point set equal to \( B \).
A easy calculation shows that $x^*$ is a fixed point for $D_{AB}$ if and only if
\[ P_A \circ R_B(x^*) = P_B(x^*). \] (27)

The fixed points do not necessarily belong to $A \cap B_S$, but once a fixed point is found, then the point
\[ x^{**} = P_A \circ R_B(x^*) = P_B(x^*) \]
automatically does lie on the intersection.

Thus we would like to understand the fixed point sets of difference maps.
The Center Manifold, I

Suppose that \( x^{**} \in \mathbb{A} \cap B_S \), then we let

\[
L_A = P_A^{-1}(x^{**}) \quad \text{and} \quad L_B = P_B^{-1}(x^{**}).
\]

The set of fixed points that “find” \( x^{**} \) consists of

\[
C_{AB}^{x^{**}} = R_B^{-1}(L_A) \cap L_B.
\]

We call this the center manifold defined by \( x^{**} \). The set \( L_B = B_S^\perp \), and, at least near enough to \( x^{**} \),

\[
L_B = N_{x^{**}} \mathbb{A}.
\]

This is the fiber of the normal bundle to the torus at \( x^{**} \).

At least near to \( \mathbb{A} \cap B \) the maps \( D_{AB}^\beta, D_{BA}^\beta \) all have the same center manifolds.
The Center Manifold, II

$B_S$ is a linear subspace, and $R_B^{-1} = R_B$, acts as the identity map on $B_S$ and as $-\text{Id}$ on $B_S^\perp$. Hence we easily compute that

$$C_{AB}^{x**} = R_B(N_{x**} \cap B_S^\perp).$$

(30)

The set $N_{x**} \cap B_S^\perp$ is an affine space consisting of vectors, $x** + v$, where $v$ is orthogonal to the tangent space to the torus at $x**$, and supported in $S^c$.

This means that, in its initial steps, an algorithm based on iterating a difference map is searching for a neighborhood of a subset of dimension

$$\dim C_{AB}^{x**} = \dim N_{x**} \cap B_S^\perp$$
$$= |J| - \dim T_{x**} \cap B_S^\perp$$

which is usually about $|J|/4$. The dimension of the center manifold increases along with $\dim T_{x**} \cap B_S^\perp$!
Other Invariant Sets for Difference Maps

While it is true that the *fixed points* of difference maps are always related to points in $\mathbb{A} \cap B_s$, there are other invariant sets that are not. For example, if there exists points $x_1 \in \mathbb{A}$ and $x_2 \in B_s$, with $x_1 \neq x_2$, which are critical for $d_{\mathbb{A}B_s}$, the distance between $\mathbb{A}$ and $B_s$, then $C_{x_1x_2} = N_{x_1} \mathbb{A} \cap B_s^\perp$ (as affine subspaces of $\mathbb{R}^J$) is non-empty. Many such critical points exist.

If $C_{x_1x_2} \cap \mathbb{A} \cap B_s = \emptyset$, then $C_{x_1x_2}$ is an invariant set without a fixed point. In examples, we have seen that this sort of set may be dynamically attracting. The map $D_{AB}$ translates by a fixed vector along such an invariant set.
The Linear Case, I

To have somewhat better intuition for the behavior of these algorithms near to their fixed point sets it pays to consider how they behave if we replace $A, B$ with arbitrary linear subspaces of $\mathbb{R}^N$, which we denote by $A, B$, with similar dimensions.

Suppose that $A \cap B = F$, and let $A_0 = A \cap F^\perp$, $B_0 = B \cap F^\perp$ and $C = (A + B)^\perp$. It is easy to see that $C$ is the center manifold. If we let $U, V, W, Z$ denote orthonormal bases for $A_0, B_0, F, C$ respectively, then we can represent the action of $D_{AB}$ on $x = Ux_1 + Vx_2 + Wx_3 + Zx_4$. 
The Linear Case, II

\( \mathbb{R}^J = A_0 \oplus B_0 \oplus F \oplus C \)

We have the formula

\[
D_{AB}(x_1, x_2, x_3, x_4) = \begin{pmatrix} A_H & 0 & 0 \\ 0 & \text{Id} & 0 \\ 0 & 0 & \text{Id} \end{pmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}, \tag{31}
\]

where \( H = V^t U \), and

\[
A_H \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} 2H^t H & H^t \\ -H & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{32}
\]

One can show that the map \( A_H \) is a contraction, and therefore

\[
\lim_{n \to \infty} D_{AB}^n(x_1, x_2, x_3, x_4) = (0, 0, x_3, x_4). \tag{33}
\]

That is: transverse to the \( F \oplus C \)-directions the map is contracting, but in the \( F \oplus C \)-directions the map acts as the identity, and is therefore only neutrally stable.
For completeness we observe that, in the linear case, the AP-map in the $A_0 \oplus B_0 \oplus F \oplus C$-decomposition is given by

$$P_B \circ P_A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ H & HH^t & 0 & 0 \\ 0 & 0 & \text{Id} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (34)$$

Near enough to intersection points these algorithms should behave similarly, but practically speaking iterates of neither the AP-algorithm, nor difference maps converge to intersection points.
Even if $F = \{0\}$, the analysis above shows that, in the linear case, the iterates converge to a point on the center manifold, $C$. Near $A \cap B$ the map is only neutrally stable in these directions; convergence is therefore a non-linear phenomenon. The rate of convergence in the remaining directions is determined by the singular values of $H$. These are all less than 1, and equal the cosines of angles between vectors in $A_0$ and $B_0$. The smaller these angles, the slower this iteration converges.
In the case of interest $A = \mathbb{A}$, which is non-linear. Under the best of circumstances, the iterates of a difference map converge to a point on the center manifold which is quite distant from $\mathbb{A} \cap B_S$. So it’s not clear if this linear analysis is applicable to the non-linear case. It is surprisingly informative. To get some intuition we consider a very low dimensional example.
We consider two low dimensional examples. The first is a circle and a line. The circle, $A$, is the unit circle in the $xy$-plane, and the line $B_\theta = \{(1, 0, 0) + \lambda(0, \cos \theta, \sin \theta)\}$. We show two possibilities below

(a) Center manifold is $x$-axis.

(b) Center manifold is $xz$-plane.

**Figure:** A circle and a line.
In these examples we run $D_{AB}$ until the error reaches $10^{-10}$. Observe the how the lengths of the trajectories depends on the angle.
Low Dimensional Examples, II

The iteration is the following map:

\[
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \mapsto \begin{pmatrix} x_1 + 1 - x_1/r \\ x_2 \left( \sin^2 \theta + \frac{\cos 2\theta}{r} \right) - \frac{x_3 \sin 2\theta}{2} \\ x_2 \left( \frac{2}{r} - 1 \right) \frac{\sin 2\theta}{2} + x_3 \cos^2 \theta \end{pmatrix}, \tag{35}
\]

where \( r = \sqrt{x_1^2 + x_2^2} \). The \( x_1 \)-coordinate is monotonically increasing and converges to a value larger than 1. The \( x_2 \) coordinate rapidly approaches zero, independently of \( \theta \); whereas, for small \( \theta \), after the initial iterates, the \( x_3 \)-coordinate is dominated by the \( x_3 \cos^2 \theta \) term. This is the linearization at the point of intersection.
We see that the number of iterates required to get 10-digits of accuracy grows quickly as the angle decreases, until the angle reaches 0, when the number drops from 200,000 to 30. The iterates always converge to a point on the center manifold quite distant from $A \cap B$. Nonetheless the linearized analysis at $A \cap B$ does a very good job predicting the behavior of the algorithm except when $\theta = 0$. This is essentially because when $\theta \neq 0$, both $y$ and $z$ need to converge to zero, and this process is governed by the linearized analysis at $A \cap B$.

When $\theta = 0$, then only $y$ needs to converge to zero, and this is governed by non-linear effects that essentially “choose” a point on the center manifold where this coordinate decreases geometrically.
We now consider the effects of almost intersections, and nearby intersections. Trajectories are ordered blue to red.
The first images shows a near miss. There is a center manifold defined by the closest approach of \( A \) to \( B \), which is attracting, and sends the trajectories spiraling out to infinity.

The second example is a tangent intersection. Once again, the single coordinate that needs to converge to zero is governed by a non-linear process that finds a point on the 2-dimensional center manifold near which this coordinate goes quickly to zero.

The third example is the result of two very nearby intersection points. The center manifold defined by the local maximum of the \( d_{AB} \) between these points is attracting and, again, translates the iterates out to infinity.

Finally a transversal intersection is attracting, but the angle between the two tangent spaces is very small, leading to slow spiraling convergence.
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Low Dimensional Examples, VI

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- Finally a transversal intersection is attracting, but the angle between the two tangent spaces is very small, leading to slow spiraling convergence.
Despite the fact that the iterates converge to points on center manifolds far from $A \cap B$, the linearized analysis of the iteration in the non-common tangent directions remains qualitatively correct.

Critical points of the function $d_{AB}$ define generalized center manifolds that can be attracting sets for the difference map. These do not have to be local minima.

Convergence in the common tangent directions is non-linear, and governed by the location on the center manifold. It can occur very rapidly.

Difference maps have attracting basins that are not defined by intersection points.
Lessons from Low Dimensional Examples

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- Difference maps have attracting basins that are not defined by intersection points.
The linearization of the torus is the tangent space at \( x^{**} \), denoted \( T_{x^{**}}A \). As we have seen, it is often the case that \( \dim T_{x^{**}}A \cap B_S > 0 \); this subspace is the analogue of the \( F \)-directions above. Hence there are directions transverse to the center manifold at \( A \cap B_S \) where the difference map is only neutrally stable. Convergence in these directions is a non-linear phenomenon.

There can also be large dimensional subspaces where these vector spaces make very small, but non-zero angles. The behavior of the iterations in these directions is accurately predicted by the linear analysis at exact intersection points, even though these points are quite far from \( A \cap B_S \).
What Low-d Examples Tell Us, I

The low dimensional examples suggest the sorts of phenomena we should expect to see in the phase retrieval problem. These examples certainly suggest that small, non-zero angles between subspaces of $T_x^* \mathbb{A}$ and $B_S$ can lead to very slow convergence, or even stagnation, far from the center manifolds defined by points in $\mathbb{A} \cap B_S$. 

When there are subspaces $T_x^* \Lambda$ and $B_S$ that make very small, non-zero angles, the iteration of a difference map displays two phases:

1. In the first phase the maps behave as if the small angles were in fact zero. The interates converge toward a higher-dimensional pseudo-center manifold, but not quite what would result from these angles being zero. The reconstruction error remains “large.”

2. In the second phase the coefficients from the directions that make very small non-zero angles might tend very slowly to zero, as predicted by the linearization at the exact intersection point.

Because of the existence of multiple nearby attracting basins other more complicated things also happen.
Outline

1. Introduction
2. The Discrete Phase Retrieval Problem
3. Geometry of the Torus
4. Reconstruction Algorithms
5. Numerical Examples in Phase Retrieval
6. Other Auxiliary Conditions
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8. Bibliography
In the real phase retrieval there is only one reasonable measure of success; it is the data error:

$$\| P_A(x^{(n)}) - P_{B_S}(x^{(n)}) \|.$$ (36)

Once this falls below a certain threshold then one has, to all intents and purposes, solved the problem. But do solutions in this sense correspond to accurate reconstructions?
Guide to the Plots

In the plots below, the red curves are the $\log_{10}$ of the residuals

$$\| P_{BSp} (x^{(n)}) - P_A \circ R_{BSp} (x^{(n)}) \| = \| x^{(n+1)} - x^{(n)} \|;$$

The point $r^{(n)} = P_{BSp} (x^{(n)})$ is our best guess for the reconstruction, given $x^{(n)}$; this residual gives an upper bound for the data error

$$\| P_{BSp} (x^{(n)}) - P_A \circ R_{BSp} (x^{(n)}) \| \geq \| \mathcal{M}(r^{(n)}) - a \|. \quad (37)$$

If $x^{(v)}$ is the trivial associate of the target image closest to $r^{(n)}$, then the blue curves show the $\log_{10}$ of the distance

$$\| r^{(n)} - x^{(v)} \|. \quad (38)$$
The Effect of the Support Condition

In this slide we show the effect on the behavior of a difference algorithm of loosening the support condition with a piecewise constant image.

- (a) $D_{A|B_{S_0}}$ with $p = 0$.
- (b) $D_{A|B_{S_1}}$ with $p = 1$.
- (c) $D_{A|B_{S_2}}$ with $p = 2$.
- (d) $D_{A|B_{S_3}}$ with $p = 3$.
- (e) $D_{A|B_{S_4}}$ with $p = 4$.
- (f) $D_{A|B_{S_5}}$ with $p = 5$. 
Once the support condition reaches \( p = 2 \), the iterates, \( \{x^{(n)}\} \) of \( D_{A \cap B_{Sp}} \) stagnate and approach the center manifold so that the reconstructions \( \{r^{(n)}\} \) are approaching \( x^{**} \) along a trajectory lying largely in \( T_{x^{**} \cap B_{Sp}} \). Examining exactly which trivial associate the \( \{r^{(n)}\} \) are approaching, we can see in each of these cases the dimension of this intersection is positive. In the \( p = 3 \) case we see that

\[
\| P_{B_{Sp}}(x^{(n)}) - P_{A \cap R_{B_{Sp}}}(x^{(n)}) \| \propto \| r^{(n)} - x^{(v)} \|^m, \tag{39}
\]

for an \( 2 < m \). This is not because the iterates have found a direction in \( B_{Sp} \) that makes higher order contact with \( A \) at \( x^{(v)} \), but rather because

\[
\dim T_{x^{(v)} \cap B_{S}} \approx \dim N_{x^{(v)} \cap B_{S}}. \tag{40}
\]
In this slide we show 5000 iterates from two runs of $D_{\mathbb{A}B_{S_2}}$ on a piecewise constant image.

(a) Errors and residuals for $D_{\mathbb{A}B_{S_2}}$ with $k = 0$, $p = 2$, where the iterates lie in an attracting basin with dim $T_{x_0^{(2,2)}} \mathbb{A} \cap B_{S_2} = 0$.

(b) Errors and residuals for $D_{\mathbb{A}B_{S_2}}$ with $k = 0$, $p = 2$, where the iterates lie in an attracting basin with dim $T_{x_0^{(1,-1)}} \mathbb{A} \cap B_{S_2} = 4$.

The plot on the left shows geometric convergence, that on the right shows either very slow convergence, or stagnation. In the phase retrieval problem, non-transversality alone can lead to very slow convergence.
The Effect of Smoothness

In this slide we show the effects of varying the level of smoothness of the image on the behavior of a difference algorithm. In all cases we use a 1-pixel support neighborhood.

(a) $D_{ABC_1}$ with $k = 0, p = 1$
(b) $D_{ABC_1}$ with $k = 1, p = 1$
(c) $D_{ABC_1}$ with $k = 2, p = 1$
(d) $D_{ABC_1}$ with $k = 3, p = 1$
(e) $D_{ABC_1}$ with $k = 4, p = 1$
(f) $D_{ABC_1}$ with $k = 5, p = 1$
Once the image is no longer piecewise constant, i.e. $k \geq 1$, the iterates, $\{x^{(n)}\}$ of $D_{\mathbb{A} \mathbb{B}}S_1$ stagnate and approach the center manifold so that the reconstructions $\{r^{(n)}\}$ are approaching $x^{**}$ along a trajectory lying largely in $T_{x^{**}}\mathbb{A} \cap B_{S_1}$, and the large dimensional subspace of the tangent space that makes a very small angle with $B_{S_1}$. 
In this slide we show 250,000 iterates of $D_{A B S_1}$ on a 256 × 256-image with $p = 1, k = 2$. It seems very plausible that this iteration has stagnated!
It is a remarkable fact that the iterates of these algorithms fall into attracting basins in which they remain, without converging for a very large number of iterates, e.g. $5 \times 10^6$. In fact the sizes of the successive differences, $\|x^{(n+1)} - x^{(n)}\|$, are essentially constant, and large enough that these iterates could easily have wandered far out of the attracting basin. But they don’t!

The bulk of the differences $x^{(n+1)} - x^{(n)}$ lie in the $F \oplus C$-directions defined by $x_0$, and in directions where $T_{x_0}\mathbb{A}$ and $B_S$ make a very small angle. It may be that the iterates are trapped in some sort of “strange attractor” lying in a small neighborhood of $C_{\mathbb{A}B_S}^{x_0}$.

We examine this possibility by looking at low-dimensional projections of these trajectories.
(a) 3-principal components of iterates 1,500,000 to 6,500,000.

(b) 3-principal components of reconstructions 1,500,000 to 6,500,000.

Figure: An example with $k = 0$, $p = 3$, with closest exact intersection $F_0^{[0,0]}$. 
(a) 3-principal components of iterates 1,500,000 to 6,500,000.

(b) 3-principal components of reconstructions 1,500,000 to 6,500,000.

Figure: Example with $k = 2$, $p = 1$, with closest exact intersection $\mathcal{F}_0^{[0,0]}$. 
Outline

1. Introduction
2. The Discrete Phase Retrieval Problem
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There are circumstances where it is reasonable to assume that the unknown image is non-negative. Clearly non-negativity alone is not a strong enough constraint to imply uniqueness up to trivial associates. The measured data \{|\hat{x}_j|\} suffices to determine the autocorrelation image

\[ x \star x_j = \sum_k x_k x_{k-j}. \]  

This is because \(|\hat{x} \star x_j| = |\hat{x}_j|^2\). We have shown that if \(S_{x \star x}\) is small enough and \(x\) is known to be non-negative, then we can prove that \(S_x\) is also small. Without the sign constraint this is false. We can then conclude that the set of images with the given data \(\mathcal{M}(x)\) is finite and generically consists of trivial associates of \(x\).
Using the Positivity Constraint

If we set $B_+ = \{x : 0 \leq x_j \text{ for } j \in J\}$, then we can looks for points in the intersection $A_a \cap B_+$. Assuming that $S_{x \star x}$ is small enough, there will be finitely many of these points on the $\partial B_+$. The boundary of the orthant is not a smooth manifold, but is instead a stratified space, stratified by the number of vanishing coordinates. In general, the intersections we seek lie in a stratum of high codimension. These strata are much more convex than a linear subspace, so it is reasonable to expect that the intersections have a better chance of being transversal. But what do we mean by that?
Transversality of the Positivity Constraint

While $\partial B_+$ is not smooth, it is a union of orthants in Euclidean spaces, so it is piecewise linear. With that in mind, it makes sense to measure transversality of intersections by examining

$$T_x A_a \cap \partial B_+.$$  \hspace{1cm} (42)

To analyze this intersection it turns out to be useful to study the $\ell_1$-norm as a function on $T_x A_a$.

If $x$ is a non-negative image, then $\|x\|_1 = \hat{x}_0$, moreover the $\ell_1$-norm on $A_a$ assumes its minimum value at images that are either non-negative or non-positive. If $B_r^1$ is the $\ell_1$-ball with radius $r = \|x\|_1$, then

$$A_a \cap B_+ = A_a \cap B_r^1.$$  \hspace{1cm} (43)

There is a fast algorithm for projection onto $\partial B_r^1$ and so this leads to different algorithms for finding these intersections.
The \( \ell_1 \)-norm on \( T_x \mathbb{A}_a \)

The understand the transversality of the intersections in (43) we need to study the \( \ell_1 \)-norm on \( T_x \mathbb{A}_a \), where \( \mathbf{x} \) is a non-negative image.

The \( \ell_1 \)-norm always assumes its minimum value at \( \mathbf{x} \in T_x \mathbb{A}_a \), however, this minimum may not be strict. If it is not, then there is a convex set \( \mathcal{W} \) where the \( \ell_1 \)-norm assumes the value \( \| \mathbf{x} \|_1 \); in fact:

\[
\mathcal{W} = T_x \mathbb{A}_a \cap \partial B_+ = T_x \mathbb{A}_a \cap B_r^1. \tag{44}
\]

In light of this, algorithms based on \( P_{B_+} \) can be expected to work about as well as those based on \( P_{B_r^1} \). Experimentally this is true, but, being non-linear, individual runs can be quite different. As expected, the \( \dim \mathcal{W} \) grows much more slowly with the smoothness of \( \mathbf{x} \) than \( \dim T_x \mathbb{A}_a \cap B_S \).
This analysis suggests that finding methods to more effectively recover the unmeasured phase information will require a different experimental protocol. Simply changing the algorithm is unlikely to produce substantial improvements. We have considered two possible modifications that lead to better reconstructions. The first involves cutting a soft object off along a known hard edge. The second involves adding a known hard object exterior to the object we are trying to image; we call this external holography. It is important to have accurate information about the shape of the edge along which the object is cut, or of the hard external object. This is needed to break the infinitesimal symmetry that leads to non-transversal intersections. In the next two slides we show examples of these approaches indicating how well they work.
Using a Sharp Cut-off

(a) The image in [a] cut-off along a circular edge.

(b) Histograms comparing log_{10}-errors with and without a hard-edge.

Figure: $k = 4$-image cut-off along a circular edge, known to 1-pixel.

The errors are computing by randomly choosing 400 runs out of a pool of 20,000 trials, and then using the minimum residual image as the reconstruction.
Figure: Improvement of convergence properties of $D_{AaB_{S_1}}$ by addition of a hard external object. The original object is $k = 6$, and the shape of the external object is known to 1-pixel.
Thanks for your attention!

And thanks to Flatiron Institute of the Simons Foundation for supporting this research.
The Geometry of the Phase Retrieval Problem

Charles L. Epstein

Introduction

Discrete Problem

Torus Geometry

Reconstruction Algorithms

Numerical Examples

Other Auxiliary Conditions

Short History of CDI

Bibliography
Short History of Coherent Diffraction Imaging

This slide courtesy Malcolm Howells, ESRF


COHERENT X-RAY DIFFRACTION IMAGING: HISTORY

Sayre (1952) - Fundamentals of sampling the wave amplitude and wave intensity

Gerchberg and Saxton (1972) - First phase-retrieval algorithm successful on test data

Sayre (1980) - Idea to do "crystallography" with non-periodic objects (i.e. attempt phase retrieval) and exploit the cross-section advantage of soft x-rays

Sayre, Yun, Chapman, Miao, Kirz (1980’s and 1990’s) - development of the experimental technique

Fienup (1978-) - Development of practical phase-retrieval algorithms including use of the combination of support constraint and oversampling of the amplitude pattern

Miao, Charalambous, Kirz and Sayre (1999) - first demonstration of 2-D CXDM using a Fienup-style algorithm at 0.73 keV x-ray energy, 75 nm resolution

Miao et al (2000) - imaging of a fixed biological sample in 2-D at 30 nm resolution

Miao et al (2001) - improved resolution in 2-D: 7 nm achievement of 3-D with moderate resolution: 55 nm

Robinson et al (2001-3) - Application to microcrystals and defects - 3D reconstruction - hardest x-rays

ALS group 2002-5 - reconstruction without use of other microscopes - 3D reconstructions with many (up to 280) views and 10 nm resolution
Outline

1. Introduction
2. The Discrete Phase Retrieval Problem
3. Geometry of the Torus
4. Reconstruction Algorithms
5. Numerical Examples in Phase Retrieval
6. Other Auxiliary Conditions
7. Short History of CDI
8. Bibliography
Some References