Phase Retrieval,
New Results on an Old Problem.

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Support from ERC (project SIPA).
Introduction: diffraction imaging

Diffraction imaging

- Sensors only record the **magnitude** of diffracted rays, and lose the **phase**.
- The phase is required to invert the 2D Fourier transform and reconstruct the sample density.

[Candes et al., 2011]
Focus on the **phase retrieval** problem, i.e. solve

\[
\text{find } \quad x \\
\text{such that } \quad |\langle a_i, x \rangle|^2 = b_i^2, \quad i = 1, \ldots, n
\]

in the variable \( x \in \mathbb{C}^p \).

- Reconstruct a signal \( x \) from the **amplitude of** \( n \) linear measurements \( A \).
- Easy to write, very **hard to solve** in general.
- We seek a **tractable** procedure, i.e. a polynomial time algorithm with explicit approximation and complexity guarantees.
We want **more than uniqueness** of the solution.

- A **tractable** algorithm to solve the phasing problem in polynomial-time.
- A solution that is **stable** and **robust** to noise.

For certain measurement matrices $A$, this is indeed possible. . .
**Introduction**

**Greedy algorithm** [Gerchberg and Saxton, 1972], find $y = Ax$ given $b = |Ax|$

**Input:** An initial $y^1 \in \mathbb{C}^n$, i.e. such that $|y^1| = b$.

1. for $k = 1, \ldots, N - 1$ do
2.   Set $w = AA^\dagger y^k$, \hspace{1em} (project $y$ on $\text{R}(A)$.)
3.   Set $y_{i}^{k+1} = b_i \frac{w}{|w|}$, \hspace{1em} (match $|y|$ with $b$.)
4. end for

**Output:** $y_N \in \mathbb{C}^n$.

Similar to **alternating projections**. Sometimes it works, sometimes it doesn’t.

**Can we do better?**
Given user ratings

Make **personalized** recommendations for other movies. . .
Introduction: collaborative prediction

- A **linear prediction** model

  \[ \text{rating}_{ij} = u_i^T v_j \]

  where \( u_i \) represents user characteristics and \( v_j \) movie features.

- Collaborative prediction is a **matrix factorization** problem

  \[ M = U^T V \]

  \( U \in \mathbb{R}^{n \times k} \) user types, \( V \in \mathbb{R}^{k \times m} \) movie features, \( M \in \mathbb{R}^{n \times m} \) ratings.

- Assume \( M \) is **low rank**.
Introduction: matrix completion

Matrix completion. [Recht et al., 2007, Candes and Recht, 2008, Candes and Tao, 2010].

- The **NETFLIX** problem can be written as

\[
\begin{align*}
\text{Minimize} & \quad \text{Rank}(X) \\
\text{subject to} & \quad \text{Tr}(A_iX) = b_i, \quad i = 1, \ldots, n \\
& \quad X \succeq 0
\end{align*}
\]

- For certain matrices $A_i$, it suffices to solve

\[
\begin{align*}
\text{Minimize} & \quad \text{Tr}(X) \\
\text{subject to} & \quad \text{Tr}(A_iX) = b_i, \quad i = 1, \ldots, n \\
& \quad X \succeq 0
\end{align*}
\]

which is a **convex problem** in $X \in \mathbb{S}_n$. 
Introduction: phase retrieval as a SDP

- [Chai et al., 2011, Candes et al., 2013a], lifting technique from [Shor, 1987]

\[ |\langle a_i, x \rangle|^2 = b_i^2 \iff \text{Tr}(a_i a_i^* x x^*) = b_i^2 \]

to formulate **phase recovery as a matrix completion problem**

\[
\begin{align*}
\text{Minimize} & \quad \text{Rank}(X) \\
\text{such that} & \quad \text{Tr}(a_i a_i^* X) = b_i^2, \quad i = 1, \ldots, n \\
& \quad X \succeq 0
\end{align*}
\]

- [Candes, Strohmer, and Voroninski, 2013a] show that under certain conditions on \( A \) and \( x_0 \), it suffices to solve

\[
\begin{align*}
\text{Minimize} & \quad \text{Tr}(X) \\
\text{such that} & \quad \text{Tr}(a_i a_i^* X) = b_i^2, \quad i = 1, \ldots, n \\
& \quad X \succeq 0
\end{align*}
\]

which is a (convex) **semidefinite program** in \( X \in \mathcal{H}_p \).
Introduction

A very sparse (and incomplete) list of references. . .

Algorithms

- Greedy algorithm [Gerchberg and Saxton, 1972]
- Classical survey of early algorithms by [Fienup, 1982].
- NP-complete [Sahinoglou and Cabrera, 1991].
- Matrix completion formulation [Chai, Moscoso, and Papanicolaou, 2011] and [Candes, Strohmer, and Voroninski, 2013a]

Applications

- X-ray and crystallography imaging [Harrison, 1993], diffraction imaging [Bunk et al., 2007] or microscopy [Miao et al., 2008].
- Audio signal processing [Griffin and Lim, 1984].
Outline

- Introduction
- **Algorithms**
  - Exploiting structure
  - Numerical results
  - Experimental setup?
Introduction: semidefinite programming

A linear program (LP) is written

\[
\begin{align*}
\text{minimize} & \quad c^T x \\
\text{subject to} & \quad Ax = b \\
& \quad x \geq 0
\end{align*}
\]

where \( x \geq 0 \) means that the coefficients of the vector \( x \) are nonnegative.

A semidefinite program (SDP) is written

\[
\begin{align*}
\text{minimize} & \quad \text{Tr}(CX) \\
\text{subject to} & \quad \text{Tr}(A_i X) = b_i, \quad i = 1, \ldots, m \\
& \quad X \succeq 0
\end{align*}
\]

where \( X \succeq 0 \) means that the matrix variable \( X \in S_n \) is positive semidefinite.

- Nesterov and Nemirovskii [1994] showed that the interior point algorithms used for linear programs could be extended to semidefinite programs.
- Efficient solvers, many (unexpected) applications.
Phase problem in phase

We can **decouple** the phase and magnitude reconstruction problems.

- $Ax = \text{diag}(b)u$ where $u \in \mathbb{C}^n$ is a **phase vector** with $|u_i| = 1$.

- The phase recovery problem can be written

$$
\min_{u \in \mathbb{C}^n, \ |u_i| = 1, \ x \in \mathbb{C}^p} \|kAx - \text{diag}(b)uk^2_2, \quad \text{subject to} \quad \|u\|_2 = 1, \quad i = 1, \ldots, n,
$$

- The inner minimization problem in $x$ is a standard least squares, with solution $x = A^\dagger \text{diag}(b)u$, so phase recovery becomes

$$
\begin{align*}
\text{minimize} & \quad u^* Mu \\
\text{subject to} & \quad |u_i| = 1, \quad i = 1, \ldots, n,
\end{align*}
$$

in $u \in \mathbb{C}^n$, where $M = \text{diag}(b)(I - AA^\dagger) \text{diag}(b) - 0$. 

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Exact phase reconstruction in polynomial-time.

- [Candès et al., 2013a,b] show exact recovery w.h.p. for the PhaseLift relaxation
  
  \[
  \begin{align*}
  \text{Minimize} & \quad \text{Tr}(X) \\
  \text{such that} & \quad \text{Tr}(a_i a_i^* X) = b_i^2, \quad i = 1, \ldots, n \\
  X & \succeq 0
  \end{align*}
  \]

  when \( n = O(p) \) observations \( a_i \) picked randomly (sphere or coded Fourier).


  \[
  \begin{align*}
  \text{Minimize} & \quad \text{Tr}(MU) \\
  \text{such that} & \quad \text{diag}(U) = 1, \quad U \succeq 0
  \end{align*}
  \]

  similar to MAXCUT relaxation.

- [Waldspurger et al., 2012] show PhaseCut is tight when PhaseLift is.
Which observations $A$?

[Candes et al., 2013b]: The observations $A$ are constructed from \textbf{multiple} coded diffraction patterns.

More on this later. . .
Block Coordinate Method. PhaseCut & MAXCUT

Input: An initial $U^0 = I_n$ and $\nu > 0$ (typically small). An integer $N > 1$.

1: for $k = 1, \ldots, N$ do
2: Pick $i \in [1, n]$.
3: Compute
   \[
   u = U^k_{i, i^c} M_{i, i^c} \quad \text{and} \quad \gamma = u^* M_{i, i^c}
   \]
4: If $\gamma > 0$, set
   \[
   U^{k+1}_{i, i^c} = U^{k+1*}_{i, i^c} = -\sqrt{1 - \nu} x
   \]
   else
   \[
   U^{k+1}_{i, i^c} = U^{k+1*}_{i, i^c} = 0.
   \]
5: end for

Output: A matrix $U \succeq 0$ with $\text{diag}(U) = 1$.

Writing $i^c$ the index set $\{1, \ldots, i - 1, i + 1, \ldots, n\}$. 

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**Complexity.**

- Each iteration only requires matrix vector products $O(n^2)$.
- Cost per iteration similar to greedy algorithm [Gerchberg and Saxton, 1972].
- Signal applications: matrix vector product computed efficiently using the FFT, cost per iteration reduced to $O(n \log n)$. 
Outline

- Introduction
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- Numerical results
- Experimental setup?
Electronic density: caffeine (left), 2D FFT transform (diffraction pattern, center), reconstructed using 3% of the coefficients at the core of the FFT (right).

- **Molecular imaging**: data is *sparse with known support*.

- Most coefficients in $b$ close to zero, so **most coefficients in $u$ can be set to zero** in

  \[
  \text{minimize} \quad u^*Mu \\
  \text{subject to} \quad |u_i| = 1, \quad i = 1, \ldots n,
  \]

  which means significant computational savings.
We observe the magnitude of the Fourier transform of a discrete signal $x \in \mathbb{R}^p$

$$|F x| = b$$

We seek to reconstruct **positive signals** $x \geq 0$.

A function $f : \mathbb{R}^s \to \mathbb{C}$ is **positive semidefinite** if and only if the matrix $B$ with $B_{i,j} = f(x_i - x_j)$ is Hermitian positive semidefinite for any sequence $x_i \in \mathbb{R}^s$.

**Theorem (Bochner)**

**Fourier on positive signals.** A function $f : \mathbb{R}^s \to \mathbb{C}$ is positive semidefinite if and only if it is the Fourier transform of a (finite) nonnegative Borel measure.
Reconstruct a phase vector $u \in \mathbb{C}^n$ such that $|u| = 1$ and

$$F x = \text{diag}(b) u.$$ 

We define the Toeplitz matrix $B_{ij}(y) = y|i-j|+1$, $i, j = 1, \ldots, p$, so that

$$B(y) = \begin{pmatrix}
y_1 & y_2^* & \cdots & y_n^* \\
y_2 & y_1 & y_2^* & \cdots \\
y_2 & y_1 & y_2^* & \cdots \\
\vdots & \ddots & \ddots & \ddots \\
y_n & \cdots & y_2 & y_1
\end{pmatrix}.$$ 

Bochner’s theorem.

$$x \succeq 0 \iff B(\text{diag}(b) u) \succeq 0,$$

which is a (convex) linear matrix inequality in $u$. 

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Real signals

Real valued signal. Phase problem on real valued signal is

\[
\text{minimize } \| T(A) \begin{pmatrix} x \\ 0 \end{pmatrix} - \text{diag} \begin{pmatrix} b \\ b \end{pmatrix} \begin{pmatrix} \leq(u) \\ u \end{pmatrix} \|_2^2 \\
\text{subject to } u \in \mathbb{C}^n, |u_i| = 1 \\
x \in \mathbb{R}^p.
\]

Here \( x = A_2^\dagger B_2 v \), where

\[
A_2 = \begin{pmatrix} \leq(A) \\ = (A) \end{pmatrix}, \quad B_2 = \text{diag} \begin{pmatrix} b \\ b \end{pmatrix}, \quad \text{and } v = \begin{pmatrix} \leq(u) \\ u \end{pmatrix}
\]

the phase problem is equivalent to

\[
\text{minimize } k(A_2 A_2^\dagger B_2 - B_2) v k_2^2 \\
\text{subject to } v_i^2 + v_{n+i}^2 = 1, \quad i = 1, \ldots, n,
\]

in the variable \( v \in \mathbb{R}^{2n} \).
Real valued signal. The last problem can be relaxed as

\[
\begin{align*}
\text{minimize} & \quad \text{Tr}(VM_2) \\
\text{subject to} & \quad V_{ii} + V_{n+i,n+i} = 1, \quad i = 1, \ldots, n, \\
& \quad V \succeq 0,
\end{align*}
\]

which is a semidefinite program in the variable \( V \in \mathbb{S}_{2n} \), where

\[
M_2 = (A_2A_2^\dagger B_2 - B_2)^T (A_2A_2^\dagger B_2 - B_2) = B_2^T (I - A_2A_2^\dagger) B_2.
\]

- Explicitly constrains the solution \( x \) to be real valued.
- Small increase in complexity.
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Numerical Experiments: PDB molecules

Two molecules, two resolutions: 16x16 and 128x128.

Caffeine

Cocaine
Numerical Experiments: PDB molecules

Solution of the **greedy algorithm** on caffeine molecule, for various values of the **number of masks** and **noise level** $\alpha$.
Numerical Experiments: 2D

Solution of the **PhaseCut SDP** followed by greedy refinements, for various values of the **number of masks** and **noise level** $\alpha$. 

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MSE between reconstructed image and true image for 2 random illuminations without noise, using SDP then Fienup (blue), and Fienup only (red).
Numerical Experiments: comparing algorithms

16x16 caffeine image. No oversampling.

Left: MSE (relative to $b$) vs. number of random masks.
Right: Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.
Numerical Experiments: comparing algorithms

16x16 cocaine image. **No oversampling.**

**Left:** MSE (relative to $b$) vs. number of random masks.  
**Right:** Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.
Numerical Experiments: comparing algorithms

16x16 caffeine image. 2x oversampling.

**Left:** MSE vs. number of random masks.
**Right:** Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.
Numerical Experiments: comparing algorithms

16x16 caffeine image. Mask resolution (1x1 to 8x8 pixels).

Left: MSE vs. mask resolution. (2x oversampling, no noise, 3 masks).
Right: Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.
Numerical Experiments: comparing algorithms

16x16 cocaine image. Mask resolution (1x1 to 8x8 pixels).

Left: MSE vs. mask resolution. (2x oversampling, no noise, 3 masks).
Right: Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.

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Numerical Experiments: comparing algorithms

16x16 cocaine image. **Mask resolution (1x1 to 8x8 pixels).**

*Left:* MSE vs. mask resolution. **(2x oversampling, no noise, 2 masks).**

*Right:* Probability of recovering molecular density (**\(MSE < 10^{-4}\)**) vs. number of random masks.

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Numerical Experiments: comparing algorithms

16x16 caffeine image. **Noise.**

![MSE vs. noise level graph](image1)

**Left:** MSE vs. noise level (2x oversampling, 2 masks).

**Right:** Probability of recovering molecular density ($MSE < 10^{-4}$) vs. number of random masks.

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Numerical Experiments: comparing algorithms

16x16 cocaine image. Noise.

*Left:* MSE vs. noise level *(2x oversampling, 2 masks).*

*Right:* Probability of recovering molecular density *(\(MSE < 10^{-4}\)) vs. number of random masks.
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Observations $A$: implementation

Construct observations $A$ from **multiple** coded diffraction patterns

- Split the beam?
- Mask before/after the sample?
Conclusion

- Tractable algorithms for phase recovery
- Exact recovery results
- Exploit structure

Open questions...

- Is the SDP relaxation optimal?
- Experimental setup?
References


