# Phase Retrieval in Coherent Diffractive Imaging

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# **Coherent diffractive imaging**



- Linear propagation + intensity measurement :  $b(j)^2 = |a_i^* x_0|^2$
- ▶ Phase retrieval: Given  $b = (b(j)) \in \mathbb{R}^N_+$  and  $A^* = [a_i^*] \in \mathbb{C}^{N \times M}$ , determine  $x_0$ .
- ► Geometry: Intersection of N-dim real torus of radii {b(j)} and complex linear subspace A<sup>\*</sup>C<sup>M</sup> (N > M).

# Uniqueness for generic frames (Balan-Casazza-Edidin 06)

- ▶ Full-rank  $A \in \mathbb{C}^{M \times N}$ , N > M:  $\{ col(A) \} =$ frame
- Frames form a metric space.
- ► Necessary condition for injectivity (left inverse exists): N ≥ 2M.
- Sufficient condition: If N ≥ 4M − 2 then generic (i.e. an open dense set) frames are injective.

#### Fourier frame is exceptional!

#### **Diffraction = Fourier transform**

Let  $x_0(\mathbf{n})$  be a discrete object function with  $\mathbf{n} = (n_1, n_2, \cdots, n_d) \in \mathbb{Z}^d$ . We assume  $d \ge 2$ .  $\mathcal{M} = \{0 \le m_1 \le M_1, 0 \le m_2 \le M_2, \cdots, 0 \le m_d \le M_d\}$ 

#### Diffraction pattern

$$\left|\sum_{\mathbf{m}\in\mathcal{M}}x_{0}(\mathbf{m})e^{-i2\pi\mathbf{m}\cdot\boldsymbol{\omega}}\right|^{2} = \sum_{\mathbf{n}=-\mathbf{M}}^{\mathbf{M}}\sum_{\mathbf{m}\in\mathcal{M}}x_{0}(\mathbf{m}+\mathbf{n})\overline{x_{0}(\mathbf{m})}e^{-i2\pi\mathbf{n}\cdot\mathbf{w}}$$

$$\mathbf{w} = (w_1, \cdots, w_d) \in [0, 1]^d, \quad \mathbf{M} = (M_1, \cdots, M_d)$$

#### Autocorrelation

$$R(\mathbf{n}) = \sum_{\mathbf{m} \in \mathcal{M}} x_0(\mathbf{m} + \mathbf{n}) \overline{x_0(\mathbf{m})}.$$

 $\widetilde{\mathcal{M}} = \{(m_1, \cdots, m_d) \in \mathbb{Z}^d : -M_1 \le m_1 \le M_1, \cdots, -M_d \le m_d \le M_d\}$ Oversampling ratio = 2^d

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4 / 38

# Ambiguities (Bruck-Sodin 1979, Hayes 1982)

- Oversampling:  $N \ge 4M 4\sqrt{M} + 1$ .
- Global ambiguities for generic objects  $x_0 \in \mathbb{R}^M$

 $\begin{array}{ll} (\text{harmless}) \text{ global phase} & x_0(\cdot) \longrightarrow e^{i\theta} x_0(\cdot) \\ & \text{translation} & x_0(\cdot) \longrightarrow x_0(\cdot + \mathbf{n}), \forall \mathbf{n} \\ & \text{conjugate inversion} & x_0(\cdot) \longrightarrow \overline{x_0}(-\cdot) \end{array}$ 

- ► Generic objects = random vectors according to continuous prior distribution ⇒ nongeneric objects ∈ a measure zero set.
- Problems:
  - → You can not determine if a given object is generic or not since the "world ensemble" may not be absolutely continuous w.r.t. your prior distribution.
  - $\rightarrow$  Global ambiguities may lead to poor reconstruction: bad algorithm or measurement scheme?

# **Coded diffraction pattern**



#### **Measurement matrix**

- Mask function: µ(n).
- Masked object:  $\tilde{x}_0(\mathbf{n}) = \mu(\mathbf{n})x_0(\mathbf{n})$
- Randomly phased mask: μ(n) = exp(iφ(n)) where φ(n) are random variables.
- Measurement matrix:  $\Phi = \text{discrete Fourier transform}$

(1 mask) 
$$A^* = \Phi \operatorname{diag}(\mu)$$
  
(2 masks)  $A^* = \begin{bmatrix} \Phi \operatorname{diag}(\mu_1) \\ \Phi \operatorname{diag}(\mu_2) \end{bmatrix}$ 

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# Uniqueness with coded diffraction patterns

Theorem (F. 2012)

Suppose  $x_0 \in \mathbb{C}^M$  is rank  $\geq 2$  and  $\arg(x_0)$  belongs in a proper sub-interval  $[a, b] \subset [0, 2\pi)$ . Then the object is determined by one coded diffraction pattern up to a constant phase factor with probability at least

$$1 - M \left| \frac{b-a}{2\pi} \right|^{s/2}$$

where s is the number of nonzero pixels.

#### Corollary

Suppose  $x_0 \in \mathbb{R}^M$  and is rank  $\geq 2$ . Then with probability one the object is determined by one coded diffraction pattern up to  $\pm$  sign.

# **Uniqueness** (continued)

#### Theorem (F. 2012)

Suppose  $x_0 \in \mathbb{C}^M$  and is rank  $\geq 2$ . Then the object is determined by two coded diffraction patterns up to a constant phase factor with probability one.

vs Candes-Li-Soltanolkotabi 2015:

- $\rightarrow\,$  PhaseLift: convex programming.
- $\rightarrow\,$  Large number of regularly sampled patterns.
- $\rightarrow\,$  Candes-Strohmer-Voroninski 2013: Gaussian random measurement.
- $\rightarrow$  Lifting  $\Longrightarrow$  huge increase of dimensionality & unpractical computation

#### Nonconvex constraint

Non-linear system:

$$b = |A^*x|, \quad x \in \mathcal{X}$$
  
(1 mask)  $\mathcal{X} = \mathbb{R}^M, \quad A^* = \Phi \operatorname{diag}(\mu)$   
(2 masks)  $\mathcal{X} = \mathbb{C}^M, \quad A^* = \begin{bmatrix} \Phi \operatorname{diag}(\mu_1) \\ \Phi \operatorname{diag}(\mu_2) \end{bmatrix}$ 

Non-convex feasibility problem:

$$\begin{array}{rcl} \mathrm{Find} & \hat{y} & \in & A^* \mathcal{X} \cap \mathcal{Y} \\ & \mathcal{Y} & := & \{ y \in \mathbb{C}^N : |y| = b \} \\ & \hat{x} & = & (A^*)^{\dagger} \hat{y} \end{array}$$

▶ Geometry: Intersection of *N*-dim torus of radii {*b<sub>j</sub>*} and linear subspace *A*<sup>\*</sup>*X* 

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# Alternating projections: feasibility problem

**Two constraints**: Fourier magnitude data (*N*-dim torus of uneven radii)  $\cap$  oversampled Fourier matrix (2*M*-dim subspace)



Non convex: local convergence?





# **Experiments: plain diffraction pattern**











HIO (Fienup 1982)

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12/38

Original images

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# **Reconstruction with coded diffraction patterns**

- Convex method converges surely but (extremely) slowly.
- Nonconvex methods converge fast (with good measurement) without guarantee.
  - 1. Gradient descent algorithms: e.g. Wirtinger flow (Candes-Li-Soltanolkotabi 2015).
  - 2. Iterative projection/fixed point algorithms.
- Initial guess is crucial for non-convex methods: How to put the initial guess in the basin of attraction of the global minimizer?

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# Null vector method (Chen-F.-Liu 2015)

$$A^* = [a_j^*]$$
  
$$a_j^* x_0 = 0 \qquad \qquad b_j = |a_j^* x_0| = a_j^* x_0.$$

If there are sufficiently many data that are small, then the **unique** null vector of the **row** sub-matrix may be a good bet.

$$x_{\text{null}} := \arg\min\left\{\sum_{i \in I} \|a_i^* x\|^2 : x \in \mathcal{X}, \|x\| = \|x_0\|\right\}$$

$$x_{\text{dual}} := \arg \max \left\{ \|A_{I_c}^* x\|^2 : x \in \mathcal{X}, \|x\| = \|x_0\| \right\}$$
  
**Isometry**  $\|A_I^* x\|^2 + \|A_{I_c}^* x\|^2 = \|x\|^2$   
 $x_{\text{null}} = x_{\text{dual}}$  power method  $\frac{2}{14/36}$ 

#### Null vector algorithm

Let  $\mathbf{1}_c$  be the characteristic function of the complementary index  $I_c$  with  $|I_c| = \gamma N$ .

Algorithm 1: The null vector method  
1 Random initialization: 
$$x_1 = x_{rand}$$
  
2 Loop:  
3 for  $k = 1 : k_{max} - 1$  do  
4  $\left| \begin{array}{c} x'_k \leftarrow A(\mathbf{1}_c \odot A^* x_k); \\ \hline x_{k+1} \leftarrow \left[ x'_k \right]_{\mathcal{X}} / \| \left[ x'_k \right]_{\mathcal{X}} \| \\ 6 \text{ end} \\ 7 \text{ Output: } x_{null} = x_{k_{max}}. \end{array} \right.$ 

Algorithm 2: The spectral vector method 1 Random initialization:  $x_1 = x_{rand}$ 2 Loop: 3 for  $k = 1: k_{max} - 1$  do 4  $\begin{vmatrix} x'_k \leftarrow A(|b|^2 \odot A^*x_k); \\ x_{k+1} \leftarrow \begin{vmatrix} x'_k \end{vmatrix}_{\mathcal{X}} / || \begin{vmatrix} x'_k \end{vmatrix}_{\mathcal{X}} ||;$ 6 end 7 Output:  $x_{spec} = x_{k_{max}}.$  **Truncated spectral vector** 

$$\begin{split} x_{\text{t-spec}} &= \arg \max_{\|x\|=1} \|\underline{A\left(\mathbf{1}_{\tau} \odot |b|^2 \odot A^* x\right)} \| \\ & \{i: |A^* x(i)| \leq \tau \|b\|\} \end{split}$$

Netrapalli-Jain-Sanghavi 2015

Candes-Chen 2015

#### **Experiments: Fourier case with two masks**









#### **Experiments: Fourier case with one mask**



Error metrics often poorly reflect the quality of initialization

# Performance guarantee: Gaussian case

Theorem (Chen-F.-Liu 2016)

Let A be drawn from the  $M \times N$  standard complex Gaussian ensemble. Let

 $\sigma := |I|/N < 1, \quad \nu = M/|I| < 1.$ 

Then for any  $x_0 \in \mathbb{C}^n$  the following error bound

$$||x_0x_0^* - x_{\text{null}}x_{\text{null}}^*||^2 \le c_0\sigma ||x_0||^4$$

holds with probability at least

$$1 - 5 \exp\left(-c_1 |I|^2 / N\right) - 4 \exp(-c_2 M).$$

- Nonasymptotic estimate
- ► Asymptotic regime:  $|I|/N \ll 1$ ,  $|I|^2/N \gg 1$  $\implies |I| = N^{\alpha}$ , error  $\sim N^{(\alpha-1)/2}$ ,  $\alpha \in (1/2, 1)$

# **Experiments: Gaussian case**



Empirical scaling law: Relative error ~ L<sup>−β</sup> where L = N/M and β ≈ 1/2.

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19/38

• Theoretical bound: RE  $\sim \sqrt{|I|/N} = L^{(\alpha-1)/2}$  where  $1/2 < \alpha < 1$ .

# **Alternating projectons**

Non-convex feasibility problem:

Find 
$$\hat{y} \in A^* \mathcal{X} \cap \mathcal{Y}$$
  
 $\mathcal{Y} := \{y \in \mathbb{C}^N : |y| = b\}$   
 $\hat{x} = (A^*)^{\dagger} \hat{y}$ 

• Let  $P_1$  and  $P_2$  be projections onto  $A^*\mathcal{X}$  and  $\mathcal{Y}$ , respectively.

(AP) 
$$P_1P_2y = \left[ (A^*)^{\dagger} \left( b \odot \frac{y}{|y|} \right) \right]_{\mathcal{X}}$$

with initial guess  $y^{(1)} = A^* x^{(1)}, x^{(1)} \in \mathcal{X}$ .

▶ Nonconvex optimization:  $U = \{u \in \mathbb{C}^N : |u(j)| = 1\}$  *N*-torus.

$$f(x, u) = \frac{1}{2} ||A^*x - u \odot b||^2$$
  

$$u^{(k)} = \arg\min_{u \in U} f(x^{(k)}, u) \qquad \text{(non-convex)}$$
  

$$x^{(k+1)} = \arg\min_{x \in \mathcal{X}} f(x, u^{(k)}) \qquad \text{(non-smooth)}$$
  

$$20 / 38$$

# Parallel AP (PAP)

$$\begin{aligned} x^{(k+1)} &= \mathcal{F}(x^{(k)}) \\ \mathcal{F}(x) &= \left[ (A^*)^{\dagger} (b \odot \frac{A^* x}{|A^* x|}) \right]_{\mathcal{X}} \quad {}^{(A^*)^{\dagger} = (AA^*)^{-1}A} \\ \end{aligned}$$

$$(2\text{-mask case}) \quad A^* = c \begin{bmatrix} \Phi \operatorname{diag}\{\mu_1\} \\ \Phi \operatorname{diag}\{\mu_2\} \end{bmatrix}$$

21/38

**Fact** every limit point of  $\{x^{(k)}\}$  is a fixed point of the map  $\mathcal{F}$ 

**Proposition** A fixed point preserves the **total signal strength**, iff it is the true solution up to a global phase.  $||A^*x_*|| = ||b||$  iff  $x_* = \alpha x_0$  with  $|\alpha| = 1$ .

Otherwise  $||A^*x_*|| < ||b||$ .

# Serial AP (SAP)

Find  $\hat{y} \in \bigcap_{l=1}^{2} \left( A_{l}^{*} \mathcal{X} \cap \mathcal{Y}_{l} \right), \quad \mathcal{Y}_{l} := \{ y_{l} \in \mathbb{C}^{N/2} : |y_{l}| = b_{l} \}$ 

SAP  $\mathcal{F}_2 \mathcal{F}_1(x)$   $\mathcal{F}_l(x) = A_l \left( b_l \odot \frac{A_l^* x}{|A_l^* x|} \right), \quad l = 1, 2,$ PAP  $\mathcal{F}(x) = A \left( b \odot \frac{A^* x}{|A^* x|} \right) = \boxed{\frac{1}{2} (\mathcal{F}_1(x) + \mathcal{F}_2(x))}$ 

# **Gradient map**

$$B := A \operatorname{diag} \left\{ \frac{A^* x_0}{|A^* x_0|} \right\} \qquad \mathcal{B} := \begin{bmatrix} \Re[B] \\ \Im[B] \end{bmatrix} \in \mathbb{R}^{2n,N}$$

$$G(-id\mathcal{F}\xi) = \mathcal{B}\mathcal{B}^{\mathsf{T}}G(-i\xi), \quad \forall \xi \in \mathbb{C}^{n}$$
  
Isomorphism 
$$G(-iv) := \begin{bmatrix} \Im(v) \\ -\Re(v) \end{bmatrix}, \quad \forall v \in \mathbb{C}^{n}$$

Let  $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{2n} \geq \lambda_{2n+1} = \cdots = \lambda_N = 0$  be the singular values of  $\mathcal{B}$  with the corresponding right singular vectors  $\{\eta_k \in \mathbb{R}^N\}_{k=1}^N$  and left singular vectors  $\{\xi_k \in \mathbb{R}^{2n}\}_{k=1}^{2n}$ .

#### **Proposition**

We have 
$$\xi_1 = G(x_0)$$
,  $\xi_{2n} = G(-ix_0)$ ,  $\lambda_1 = 1$ ,  $\lambda_{2n} = 0$  and  $\eta_1 = |A^*x_0|$ .

$$u^{(k)} := -i(\alpha^{(k)}x^{(k)} - x_0) \longrightarrow \xi_1 \perp G(u^{(k)}), \quad \forall k$$

# Spectral gap

$$\lambda_2 = \max\{\|\Im[B^*u]\| : u \in \mathbb{C}^n, iu \perp x_0, \|u\| = 1\} \\ = \max\{\|\mathcal{B}^\top u\| : u \in \mathbb{R}^{2n}, u \perp \xi_1, \|u\| = 1\}.$$

#### **Proposition**

Suppose  $x_0 \in \mathbb{C}^n$  is rank-2. Then  $\lambda_2 < 1$  with probability one.

# Uniqueness theorem for magnitude retrieval If

$$\measuredangle A^* \hat{x} = \pm \measuredangle A^* x_0$$

where the  $\pm$  sign may be pixel-dependent, then almost surely  $\hat{x} = cx_0$  for some constant  $c \in \mathbb{R}$ .

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24 / 38

One random mask suffices !

#### Local geometric convergence

#### Theorem (Chen-F.-Liu 2015)

For any given  $0 < \epsilon < 1 - \lambda_2^2$ , if  $x^{(1)}$  is sufficiently close to  $x_0$ , then with probability one PAP converges to  $x_0$  geometrically after global phase adjustment

$$\|\alpha^{(k+1)}x^{(k+1)} - x_0\| \le (\lambda_2^2 + \epsilon) \|\alpha^{(k)}x^{(k)} - x_0\|$$

where  $\alpha^{(k)} = x^{(k)*} x_0 / |x^{(k)*} x_0|$ .

#### Theorem (Chen-F.-Liu 2015)

For any given  $0 < \epsilon < 1 - (\lambda_2^{(2)}\lambda_2^{(1)})^2$ , if  $x^{(1)}$  is sufficiently close to  $x_0$  then with probability one SAP converges to  $x_0$  geometrically after global phase adjustment,

$$\|\alpha^{(k+1)}x^{(k+1)} - x_0\| \le ((\lambda_2^{(2)}\lambda_2^{(1)})^2 + \epsilon)\|\alpha^{(k)}x^{(k)} - x_0\|.$$

#### **Experiments: with null initialization**



#### Experiments: null vector with noisy data



# **Experiments: noise stability**



# **Douglas-Rachford splitting**

- ► Feasibility:  $\mathcal{Y} \cap \mathcal{Z} \Longrightarrow \min_{y \in \mathcal{Y}, z \in \mathcal{Z}} \frac{1}{2} \|y z\|^2$ , y = z.
- ADMM (alternating direction method of multiplier)

$$\max_{\lambda} \min_{y \in \mathcal{Y}, z \in \mathcal{Z}} \mathcal{L} := \frac{1}{2} \|y - z\|^2 + \langle \lambda, (y - z) \rangle$$
$$= \max_{\lambda} \min_{y \in \mathcal{Y}, z \in \mathcal{Z}} \mathcal{L} := \frac{1}{2} \|y - z + \lambda\|^2 - \frac{1}{2} \|\lambda\|^2$$

$$\begin{cases} y^{t+1} = \arg\min_{y \in \mathcal{Y}} \frac{1}{2} \|y - z^t + \lambda^t\|^2 &= P_{\mathcal{Y}}(z^t - \lambda^t) \\ z^{t+1} = \arg\min_{z \in \mathcal{Z}} \frac{1}{2} \|y^{t+1} - z + \lambda^t\|^2 &= P_{\mathcal{Z}}(y^{t+1} + \lambda^t) \\ \lambda^{t+1} = \lambda^t + \nabla_{\lambda} \mathcal{L}(y^{t+1}, z^{t+1}) &= \lambda^t + y^{t+1} - z^{t+1} \end{cases}$$

• **DR:**  $x^t := y^{t+1} + \lambda^t \Longrightarrow$ 

 $x^{t+1} = x^t + P_{\mathcal{Y}}(2P_{\mathcal{Z}} - I)x^t - P_{\mathcal{Z}}x^t$ 

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## Fourier domain Douglas-Rachford

$$\mathcal{Y} = \{ y \in \mathbb{C}^{N} : |y| = b \}, \quad \mathcal{Z} = A^{*} \mathcal{X}$$
$$\implies \qquad P_{\mathcal{Y}}(y) = b \odot \frac{y}{|y|}, \quad P_{\mathcal{Z}}(y) = A^{*} A y$$

$$S_{\mathrm{f}}(y) = y + A^* \left[ A \left( 2b \odot \frac{y}{|y|} - y \right) \right]_{\mathcal{X}} - b \odot \frac{y}{|y|}$$

Gradient  $J_{f}v = (I - B^*B)\Re(v) + iB^*B\Im(v)$  $J_{f}$  is a real, but not complex, linear map

$$S(x) = x + \left[\tilde{A}\left(2b \odot \frac{\tilde{A}^*x}{|\tilde{A}^*x|}\right) - x\right]_{\mathcal{X}} - \tilde{A}\left(b \odot \frac{\tilde{A}^*x}{|\tilde{A}^*x|}\right)$$

# Fixed point with two masks

$$S_{\rm f}(y_\infty) = y_\infty, \quad x_\infty = Ay_\infty.$$

#### Theorem (Chen-F. 2016)

The projected fixed point is unique, i.e.  $x_{\infty} = e^{i\theta}x_0$  almost surely.

# FDR locally converges geometrically

Theorem (Chen-F. 2016)

For  $0 < \epsilon < 1 - \lambda_2$ , if  $\alpha^{(1)}x^{(1)}$  is sufficient close to  $x_0$ , then FDR converges geometrically to the solution

$$\|\alpha^{(k)}x^{(k)} - x_0\| \le (\lambda_2 + \epsilon)^{k-1} \|\alpha^{(1)}x^{(1)} - x_0\|.$$

- Explicit measurement schemes.
- Explicit characterization of  $\lambda_2 < 1$ .
- No hard-to-verify assumptions.
- Convex setting (He-Yuan 2012, 2015): k-th error = O(1/k).

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# **Experiments: Two patterns**









33 / 38

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# Fourier domain vs. object domain DR

(FDR) 
$$S_f(x) = y + A^*A\left(2b \odot \frac{y}{|y|} - y\right) - b \odot \frac{y}{|y|}$$
  
(ODR)  $S(x) = x + \tilde{A}\left(2b \odot \frac{\tilde{A}^*x}{|\tilde{A}^*x|}\right) - x - \tilde{A}\left(b \odot \frac{\tilde{A}^*x}{|\tilde{A}^*x|}\right)$ 



# Conclusion

- Two globally convergent schemes in practice:
  - 1. AP+null initialization
  - 2. FDR
- Open problem: proof of global convergence.

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