Reconstruction Algorithms for Blind Ptychographic Imaging

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Joint work with R. Hesse, D.R. Luke and S. Sabach

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Scanning Ptychography: A Crash Course

- An unknown specimen is illuminated by a localized illumination function resulting in an exit-wave whose intensity is observed.
- A ptychography dataset is a series of these observations, each is obtained by shifting the illumination function to a different position relative to the specimen. Neighbouring illumination regions overlap.
- Given a ptychographic dataset, the blind ptychography problem is to simultaneously reconstruct the specimen and illumination function.

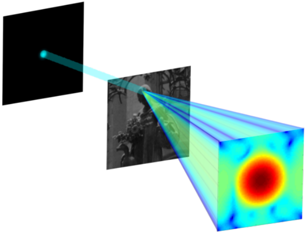

Figure : An illumination function (left), specimen (center), and exit-wave (right).

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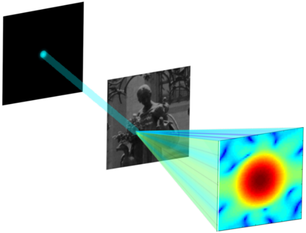

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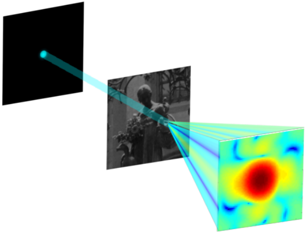

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The mathematical model is:

- The unknown illumination function: $x \in \mathbb{C}^{n\times n}$,
- The unknown specimen: $y \in \mathbb{C}^{n\times n}$,
- An m-tuple of diffraction patterns: $\mathbf{z} = (z_1, \ldots, z_m) \in (\mathbb{C}^{n\times n})^m$,
- The *shift map* $S_j : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ moves x to the position corresponding to the j^{th} diffraction pattern measurement.
- The elements of the triple $(x, y, \mathbf{z})$ are related by:

$$S_j(x) \odot y = z_j \quad \text{for} \quad j = 1, 2, \ldots, m.$$

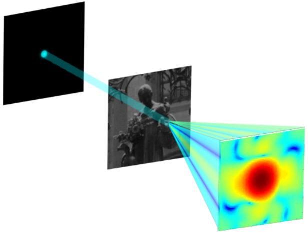

Figure : An example of $S_j(x) \odot y = z_j$ with S_j localising "x" to the jth position.

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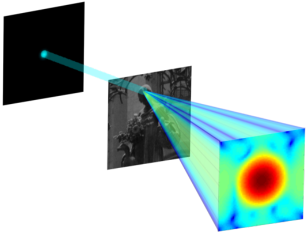

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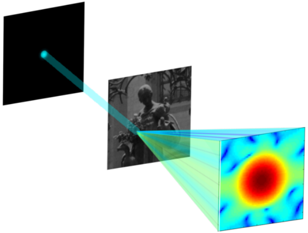

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Scanning Ptychography: A Crash Course

In a ptychography experiment we observe m non-negative matrices:

$$b_1, \ldots, b_m \in \mathbb{R}_+^{n\times n}.$$

Each corresponds to a different illumination region on the specimen:

$$b_j \equiv |\mathcal{F}(z_j)| \quad \text{where} \quad z_j = S_j(x) \odot y,$$

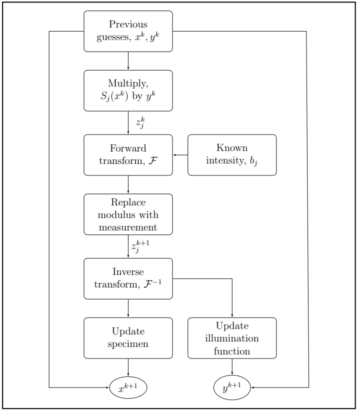
where $\mathcal{F}$ is the *2D Fourier transform*, and $|\cdot|$ is taken element-wise.

The **blind ptychography problem** can now be stated:

> Given $b_1, b_2, \ldots, b_m \in \mathbb{R}_+^{n\times n}$ reconstruct the triple $(x, y, \mathbf{z})$.

Two Algorithms in the Literature

Maiden & Rodenburg proposed:



Update functions are of the form:

$$x^{k+1} = x^k + \alpha \frac{S_j^{-1}(y^k \odot \bar{y}^k)}{\|S_j^{-1}(y^k \odot \bar{y}^k)\|_\infty} \left(z_j^{k+1} - z_j^k\right).$$

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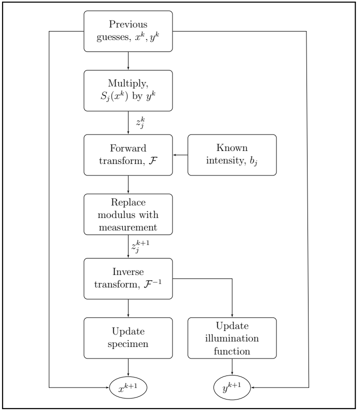

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Thibault *et al.* proposed:

$$P_F(\mathbf{z}) : z_j \to P_F(z_j) \text{ for all } j = 1, 2, \ldots, m. \quad (4)$$

$$P_O(\mathbf{z}) : z_j \to P_O(z_j) \equiv S_j(x) \odot y. \quad (6)$$

$$\mathbf{z}^{k+1} = \mathbf{z}^k + P_F(2P_O(z^k) - z^k) - P_O(z^k). \quad (9)$$

On computing (6):

$$\hat{y}^k = \frac{\sum_{j=1}^m S_j(x^k) \odot z_j^k}{\| \sum_{j=1} x^k \odot \bar{x}^k \|}. \quad (7)$$

$$\hat{x}^k = \frac{\sum_{j=1}^m S_j^{-1}(y^k \odot z_j^k)}{\| \sum_{j=1} y^k \odot \bar{y}^k \|}. \quad (8)$$

In the event the probe P is already known, the overlap projection is given by (6), where $\hat{O}$ is computed with Eq. (7). If $\hat{P}$ also needs to be retrieved, both Eqs. (7) and (8) need to be simultaneously solved. While the system cannot be decoupled analytically, applying the two equations in turns for a few iterations was observed to be an efficient procedure to find the minimum. Within the reconstruction scheme, initial guesses for $\hat{P}$ and $\hat{O}$ are readily available from the previous iteration—apart

Our Framework

- We considered the following optimisation problem:

$$\begin{aligned} \min \quad & F(x, y, \mathbf{z}) := \sum_{j=1}^{m} \|S_j(x) \odot y - z_j\|^2 \\ \text{s.t.} \quad & x \in X := \{x : \|x\|_\infty \le M_x,\ x_{ij} = 0, \forall (i,j) \notin \mathbb{I}_x\}, \\ & y \in Y := \{y : \|y\|_\infty \le M_y\}, \\ & \mathbf{z} \in Z := \{\mathbf{z} : |\mathcal{F}(z_j)| = b_j \text{ for } j = 1, 2, \ldots, m\}, \end{aligned} \tag{P}$$

where $M_x, M_y \in \mathbb{R}$ are bounds, and $\mathbb{I}_x$ is an index set (support of x).

- Separable constraint sets coupled through an objective function.
    - However, all constraints are X, Y, Z are closed semi-algebraic sets.
    - F is a continuous semi-algebraic function (graph F is semi-algebraic).
- (P) is equivalent to the formally unconstrained problem:

$$\min \ \Psi(x, y, z) := F(x, y, z) + \iota_X(x) + \iota_Y(y) + \iota_Z(\mathbf{z}).$$

A set $S \subseteq \mathbb{R}^d$ is semi-algebraic if there exits finitely many polynomials $p_{ij}, q_{ij} : \mathbb{R}^d \to \mathbb{R}$ such that

$$S = \bigcup_{j=1}^{N} \bigcap_{i=1}^{K} \left\{ u \in \mathbb{R}^d : p_{ij}(u) = 0, q_{ij}(u) < 0 \right\}.$$

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A Naïve Algorithm: Alternating Minimisation

Alternating Minimisation Algorithm (over three blocks):

Initialization. Choose $(x^0, y^0, \mathbf{z}^0) \in X \times Y \times Z$.
General Step. $(k = 0, 1, \dots)$

1. Select $$x^{k+1} \in \operatorname*{arg\,min}_{x \in X} F(x, y^k, \mathbf{z}^k),$$
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What's involved? Roughly speaking, to compute Step 1 we need to minimise terms of the form $\|S_j(x) \odot y^k - z_j^k\|^2$. To do so:

$$S_j(x) \odot y^k \approx z_j^k \implies \underbrace{S_j(x) \approx z_j^k \oslash y_k}_{\text{pointwise division } ✗} \implies \underbrace{x \approx S_j^{-1}(z_j^k \oslash y_k)}_{\text{un-shift operator } ✓}.$$

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PHeBIE: Proximal Block Implicit-Explicit Algorithm

From the previous slide, recall our naïve Step 1:

$$x^{k+1} \in \operatorname*{arg\,min}_{x \in X} F(x, y^k, \mathbf{z}^k).$$

Replace the objective function F with a better behaved regularisation:

$$x^{k+1} \in \operatorname*{arg\,min}_{x \in X} \left(F(x, y^k, \mathbf{z}^k) \qquad\qquad\qquad\qquad \right)$$

⋆ No longer requires any ill-conditioned or unstable operations!

Given a set C, its (nearest point) projection, P_C, is given by

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$$= P_X \left(x^k - \frac{2}{\alpha^k} \sum_{j=1}^{m} S_j^{-1}(\overline{y^k}) \odot S_j^{-1} \left(y^k - z_j^k \right) \right).$$

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Proximal Heterogeneous Block Implicit-Explicit Algorithm:

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General Step. $(k = 0, 1, \dots)$

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$$x^{k+1} \in P_X\left(x^k - \frac{2}{\alpha^k}\sum_{j=1}^m S_j^{-1}(\overline{y^k}) \odot S_j^{-1}\left(y^k - z_j^k\right)\right),$$
2. Choose $\beta^k > \beta$ and select
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3. Choose $\gamma^k > \gamma$ and select
$$\mathbf{z}^{k+1} \in P_Z\left(\left[\frac{2}{2+\gamma_k} S_j(x^{k+1}) \odot y^{k+1} + \frac{\gamma_k}{2+\gamma_k} z_j^k\right]_{j=1}^m\right).$$

For convergence we choose: $\alpha^k \geq L_x(y^k, z^k)$ and $\beta^k \geq L_y(x^{k+1}, z^k)$ where $L_x(y^k, z^k)$ and $L_y(x^{k+1}, z^k)$ denote the partial Lipschitz constant of $\nabla_x F(\cdot, y^k, z^k)$ and $\nabla_y F(x^{k+1}, \cdot, z^k)$.

PHeBIE: Convergence Theorem

Theorem (Hesse–Luke–Sabach–T, 2015)

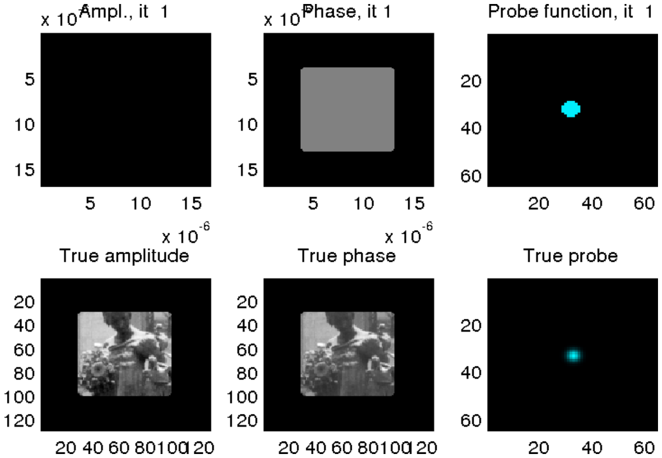
Let $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ be a sequence generated by the PHeBIE algorithm for the blind ptychography problem. Then the following hold.

1. The sequence $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ has finite length. That is,
$$\sum_{k=1}^{\infty} \left\|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\right\| < \infty.$$
2. The sequence $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ converges to point $(x^*, y^*, \mathbf{z}^*)$ which is a critical point of the function Ψ. That is,
$$0 \in \partial\Psi(x, y, z) = \nabla F(x^*, y^*, \mathbf{z}^*) + \partial\iota_X(x^*) + \partial\iota_Y(y^*) + \partial\iota_Z(\mathbf{z}^*),$$
where $\partial(\cdot)$ denotes the limiting Fréchet subdifferential.

For u in the domain of f, the limiting Fréchet subdifferential is given by

$$\partial f(u) := \left\{v : \exists u^k \to u,\ f(u^k) \to f(u),\ v^k \to v,\ v^k \in \widehat{\partial} f(u^k)\right\},\ \text{where } \widehat{\partial} f(u) = \left\{v : \liminf_{\substack{w \neq u \\ w \to u}} \frac{f(w) - f(u) - \langle v, w - u\rangle}{\|w - u\|} \geq 0\right\}.$$

PHeBIE: Example



PHeBIE: Convergence Theorem (cont.)

Proof Sketch.

The proof has three steps:

1. (Sufficient decrease) Use properties of the algorithm to establish that the sequence $\{F(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ is decreasing, converges to some $F^* > -\infty$, and that
$$\sum_{k=1}^{\infty} \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|^2 < \infty.$$
2. (Subdifferential bound) Use properties of the algorithm to show that
$$\|w^{k+1}\| \leq \kappa \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|,$$
for some $w^{k+1} \in \partial\Psi(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1})$ and $\kappa > 0$.
3. To establish convergence of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ to a critical point, uses the fact that Ψ satisfied the so-called Kurdyka–Łojasiewicz (KL) Property which gives Cauchyness of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$. □

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3. To establish convergence of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ to a critical point, uses the fact that Ψ satisfied the so-called Kurdyka–Łojasiewicz (KL) Property which gives Cauchyness of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$.

The proof strategy is based on a paper of *Bolte, Sabach Teboulle (2014)*.

PHeBIE: Convergence Theorem (cont.)

Proof Sketch.

The proof has three steps:

1. (Sufficient decrease) Use properties of the algorithm to establish that the sequence $\{F(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ is decreasing, converges to some $F^* > -\infty$, and that
$$\sum_{k=1}^{\infty} \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|^2 < \infty.$$
2. (Subdifferential bound) Use properties of the algorithm to show that
$$\|w^{k+1}\| \leq \kappa \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|,$$
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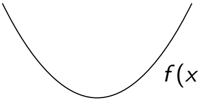
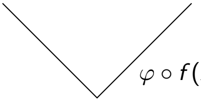
The Kurdyka-Łojasiewicz (KL) Property

Roughly speaking, functions which satisfy the KL-property can made "sharp" by a reparametrisation of their range by an increasing function. A simple example: the function $f(x) = x^2$ can be reparametrised by $\varphi(x) = \sqrt{x}$:



$f(x) = x^2$ $\longrightarrow$



$\varphi \circ f(x) = |x|$

- The utility of the KL-property is that it holds for many real world optimisation problems which lack convexity (*e.g.*, ptychography!).

Theorem (Bolte–Danillidis–Lewis 2006)

Every proper, lower semi-continuous, semi-algebraic function satisfies the KL-property throughout its domain.

Let $f : \mathbb{R}^d \to (-\infty, +\infty]$ be proper. For $\eta \in (0, +\infty]$ define

$$\mathcal{C}_\eta \equiv \left\{\varphi : [0, \eta) \to \mathbb{R}_+ : \varphi(0) = 0, \varphi'(s) > 0 \text{ for all } s \in (0, \eta)\right\}.$$

The function f has KL property at $\overline{u} \in \operatorname{dom} \partial f$ if there exists a neighbourhood U of $\overline{u}$ and a function $\varphi \in \mathcal{C}_\eta$, such that, for all $u \in \{u \in U : f(\overline{u}) < f(u) < f(\overline{u}) + \eta\}$, it holds that

$$\underbrace{\varphi'\left(f(u) - f(\overline{u})\right) \operatorname{dist}(0, \partial f(u)) \geq 1.}_{\textbf{Think: } \text{minimum norm element of } \partial(\varphi \circ g) \text{ where } g = f - f(\overline{u}).}$$

Interpreting Current State-of-the-Art Algorithms

The update steps all of the algorithms: PHeBIE algorithm, Madien & Rodenburg, and Thibault *et al.* are more-or-less the same.

- The PHeBIE algorithm:
  - Minimises w.r.t. three blocks X, Y, Z in cyclic order.
  - Each x-update/y-update uses all m diffraction patterns. In Step 1, the weight α^k given by partial Lipschitz constant of $\nabla_x F(\cdot, y^k, \mathbf{z}^k)$ is

$$L_x(y^k, \mathbf{z}^k) = 2 \left\| \left(\sum_{j=1}^{m} S_j^* (\overline{y^k} \odot y^k) \right) \right\|_\infty .$$

- Madien & Rodenburg method:
  - Can be viewed as minimisation w.r.t. the blocks X, Y and Z.
  - Each x-update/y-update uses only a single diffraction pattern. In Step 1, the weight when updating with the jth diffraction pattern is

$$2 \left\| S_j^* (\overline{y^k} \odot y^k) \right\|_\infty .$$

- Thibault *et al.* method:
  - Minimise w.r.t. three blocks X, Y, Z, but many X, Y updates are performed between Z updates.
  - Updates embedded within a "difference map" algorithmic structure.

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> simultaneously solved. While the system cannot be decoupled analytically, applying the two equations in turns for a few iterations was observed to be an efficient procedure to find the minimum. Within the reconstruction scheme, initial guesses for $\hat{P}$

Concluding Remarks and Ongoing Work

In summary:

- We have presented an algorithm for scanning ptychography within a clear mathematical optimisation framework.
- Under practically verifiable assumptions, the algorithm is provably convergent to critical points of the function $\Psi \equiv F + \iota_X + \iota_Y + \iota_Z$.
- The framework is flexible and allows for an interpretations of current state-of-the-art ptychography algorithms.

Ongoing and future work:

- Can the critical points of of Ψ be characterised in a meaningful way?
- What happens when the data is noisy? Our convergence theorem holds independently of the presence of noise in the data.

Further details can be found in:

Proximal Heterogeneous Block Implicit-Explicit Method and Application to Blind Ptychographic Diffraction Imaging with R. Hesse, D.R. Luke and S. Sabach. *SIAM J. on Imaging Sciences*, 8(1):426–457 (2015).