# Reconstruction Algorithms for Blind Ptychographic Imaging

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CARMA

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

NSW/ACT ANZIAM Meeting, November 2015

- 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.

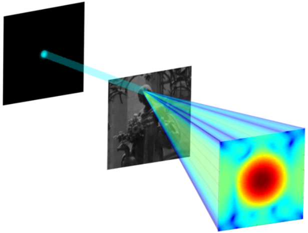

Figure : An illumination function (left), specimen (center), and exit-wave (right).

# Scanning Ptychography: A Crash Course

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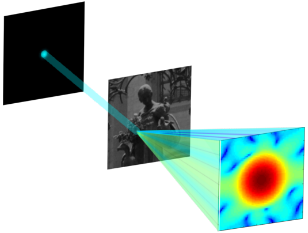

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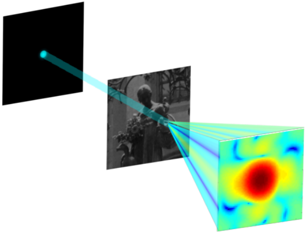
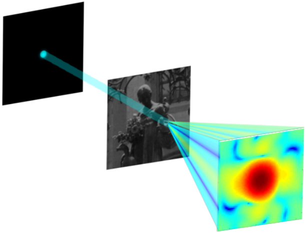


Figure : An illumination function (left), specimen (center), and exit-wave (right).

The forward 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 $j^{\text{th}}$ diffraction pattern measurement.
- The elements of the triple $(x, y, \mathbf{z})$ are related by:

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



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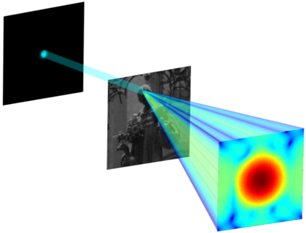

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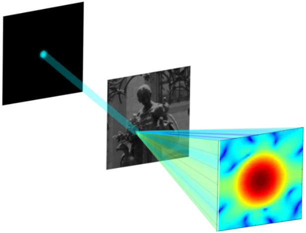

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# Scanning Ptychography: A Crash Course

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

$$b_j \equiv |\mathcal{F}(z_j)| \in \mathbb{R}_+^{n\times n} \quad \forall j \in \{1, 2, \dots, m\},$$

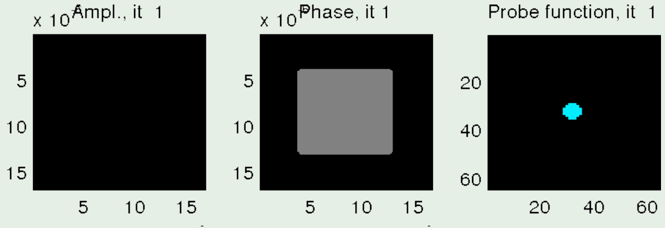
where $\mathcal{F}$ is the *2D Fourier transform*, and $|\cdot|$ is taken element-wise.

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

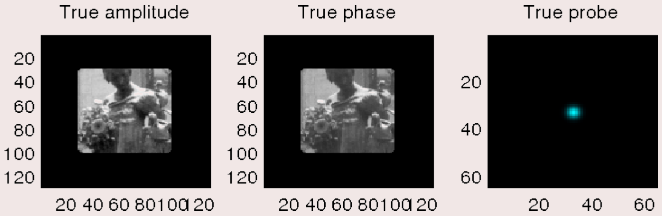
| |
|---|
| Given $b_1, b_2, \dots, b_m \in \mathbb{R}_+^{n\times n}$ reconstruct the triple $(x, y, \mathbf{z})$. |

# Scanning Ptychography: A Crash Course

## Before reconstruction: the specimen and illumination function

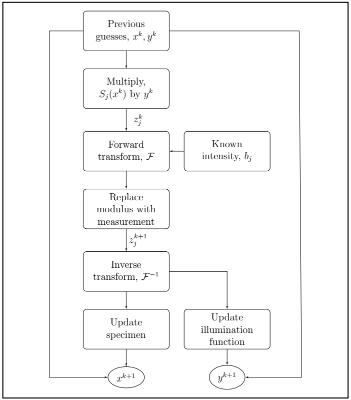



## The actual specimen and illumination function



# Two Algorithms in the Literature

Maiden & Rodenburg proposed:




Update functions are of the form:

$$x^{k+1} = x^k + \underbrace{\alpha \frac{S_j^{-1}(\overline{y}^k)}{\|y^k\|_\infty^2} \odot S_j^{-1}\left(z_j^k - S_j(x^k) \odot y^k\right)}_{\textbf{Think: } \text{Residual}}.$$

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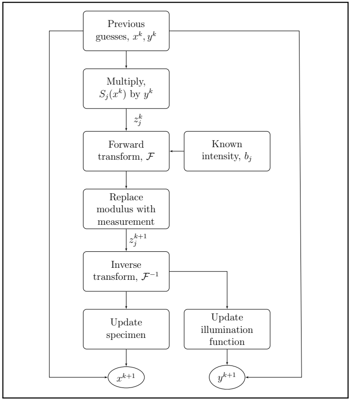


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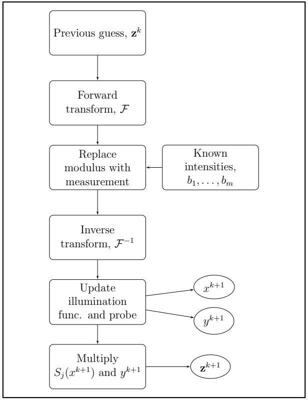


Update step involves solving:

$$y^k = \frac{\sum_{j=1}^m S_j(\bar{x}^k) \odot z_j^k}{\left\|\sum_{j=1}^m x^k \odot \bar{x}^k\right\|_\infty}, \quad x^k = \frac{\sum_{j=1}^m S_j^{-1}(\bar{y}^k \odot z_j^k)}{\left\|\sum_{j=1}^m y^k \odot \bar{y}^k\right\|_\infty}.$$

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 $\hat{P}$

# Our Framework

- Considered the following optimisation problem:

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

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

- Equivalent to the formally unconstrained semi-algebraic problem:

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

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

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

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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.** $(k = 0, 1, \ldots)$

1. Select $$x^{k+1} \in \operatorname*{arg\,min}_{x \in X} F(x, y^k, \mathbf{z}^k),$$
2. Select $$y^{k+1} \in \operatorname*{arg\,min}_{y \in Y} F(x^{k+1}, y, \mathbf{z}^k),$$
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What's involved? Roughly speaking, to compute Step 1 we 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:

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

Replace the objective function $F$ with a better behaved regularisation:

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

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

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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:

**Initialization.** Choose $\alpha, \beta, \gamma > 0$ and $(x^0, y^0, \mathbf{z}^0) \in X \times Y \times Z$.

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

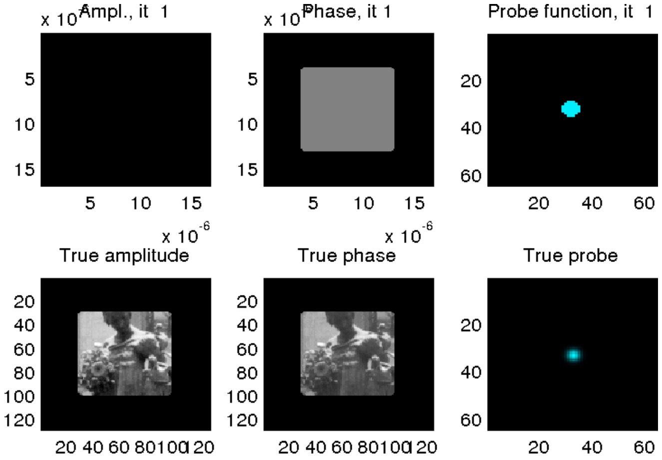
1. Choose $\alpha^k > \alpha$ and select
$$x^{k+1} \in P_X \left( x^k - \frac{2}{\alpha^k} \sum_{j=1}^{m} S_j^{-1}(\overline{y^k}) \odot S_j^{-1} \left( y^k - z_j^k \right) \right).$$

2. Choose $\beta^k > \beta$ and select
$$y^{k+1} \in P_Y \left( y^k - \frac{2}{\beta^k} \sum_{j=1}^{m} S_j(\overline{x^{k+1}}) \odot \left( S_j(x^{k+1}) - z_j^k \right) \right).$$

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 need: $\alpha^k \geq L_x(y^k, z^k)$ 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 constants of $\nabla_x F(\cdot, y^k, z^k)$ and $\nabla_y F(x^{k+1}, \cdot, z^k)$.

# PHeBIE: Example



# 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 $\Psi$. 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.

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For $u \in \text{domain}(f)$, 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: Convergence Theorem (cont.)

*Proof Sketch.*

The proof has three steps:

1. *(Sufficient decrease)* Use structure of the algorithm to establish that there exists of a constant $\rho > 0$ such that
$$\rho\|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|^2 \leq F(x^k, y^k, \mathbf{z}^k) - F(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}).$$
2. *(Subdifferential bound)* Use structure 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, we uses the fact that $\Psi$ satisfied the so-called Kurdyka–Łojasiewicz (KL) Property to deduce Cauchy-ness of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$. □

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The proof strategy is based on an "informal recipe" of *Bolte, Sabach Teboulle (2014)*.

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$$\|w^{k+1}\| \leq \kappa \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|,$$

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, we uses the fact that $\Psi$ satisfied the so-called Kurdyka–Łojasiewicz (KL) Property to deduce Cauchy-ness of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$. □

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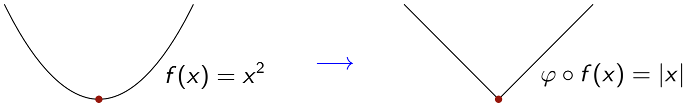
The proof strategy is based on an "informal recipe" of *Bolte, Sabach Teboulle (2014)*.

# The Kurdyka-Łojasiewicz (KL) Property

A functions satisfies the KL-property at a point if it can made "sharp" by reparametrising its range with an increasing function. A simple example: the function $f(x) = x^2$ can be reparametrised by $\varphi(x) = \sqrt{x}$:




**Theorem (Bolte–Danillidis–Lewis 2006)**

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

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

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

The function $f$ has the KL property at $\overline{u} \in \operatorname{dom} \partial f$ if there exists $\eta \in (0, +\infty]$, a neighbourhood $U$ of $\overline{u}$, and a function $\varphi \in \mathcal{C}_\eta$, such that, for all $u \in \{u \in U : f(\overline{u}) < f(u) < f(\overline{u}) + \eta\}$, we have

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

# Interpreting Current State-of-the-Art Algorithms

We summarise the main differences between the three algorithms.

- 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 $\alpha^k$ is given by partial Lipschitz constant of $\nabla_x F(\cdot, y^k, \mathbf{z}^k)$:

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

- Madien & Rodenburg method:
  - Minimisation w.r.t. to three blocks $X$, $Y$ and $Z$.
  - Each $x$-update/$y$-update uses only a single diffraction pattern. In Step 1, the weight when updating using the $j$th diffraction pattern is:

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- Thibault *et al.* method:
  - Minimise w.r.t. three blocks $X, Y, Z$, but many $X, Y$ updates are performed between $Z$ updates.

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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

Summary:

- We have proposed the PHeBIE algorithm for scanning ptychography within a solid mathematical optimisation framework.
- Under practically verifiable assumptions, the algorithm is provably convergent to critical points of the function $\Psi \equiv F + \iota_X + \iota_Y + \iota_Z$.
- Current state-of-the-art ptychography algorithms can be interpreted.

Outlook:

- Can the critical points of of $\Psi$ 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.

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**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).