Reconstruction Algorithms for Blind Ptychographic Imaging

Matthew K. Tam
School of Mathematical and Physical Sciences
University of Newcastle Australia

THE UNIVERSITY OF NEWCASTLE AUSTRALIA

CARMA

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

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What is Ptychography?

- 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 of which 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 relative phase of the specimen and illumination function.

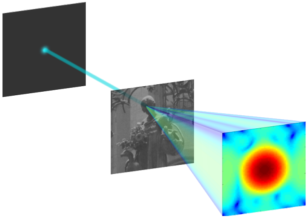


Figure : An illumination function (left), specimen (center), and exit-wave (right).

What is Ptychography?

The mathematical model is:

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

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

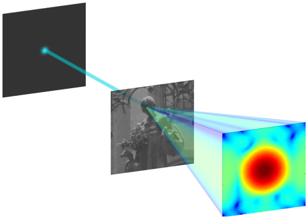


Figure : An example of $S_j(x) \odot y = z_j$ with S_j localising "x" to the girl's head.

What is Ptychography?

In a ptychography experiment we observe the m-matrices

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

where b_j, for $j = 1, 2, \ldots, m$, are given by

$$b_j = |\mathcal{F}(z_j)| = |\mathcal{F}(S_j(x) \odot y)|.$$

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

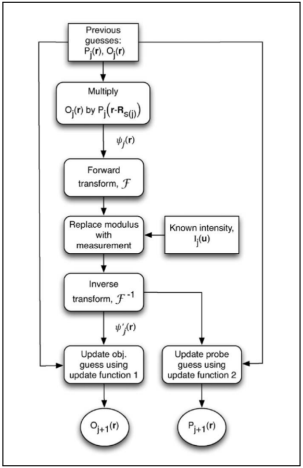
The blind ptychography problem is:

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

- Ill-posed, inverse problem with many solutions $\Rightarrow$ hopeless without *a priori* knowledge.

Two Algorithms in the Literature

Maiden & Rodenburg proposed:



With update functions:

$$O_{j+1}(\mathbf{r})=O_j(\mathbf{r})+\alpha\frac{P_j^*(\mathbf{r}-\mathbf{R}_{s(j)})}{|P_j(\mathbf{r}-\mathbf{R}_{s(j)})|^2_{\max}}(\psi'_j(\mathbf{r})-\psi_j(\mathbf{r})). \quad P_{j+1}(\mathbf{r})=P_j(\mathbf{r})+\beta\frac{O_j^*(\mathbf{r}+\mathbf{R}_{s(j)})}{|O_j(\mathbf{r}+\mathbf{R}_{s(j)})|^2_{\max}}(\psi'_j(\mathbf{r})-\psi_j(\mathbf{r})).$$

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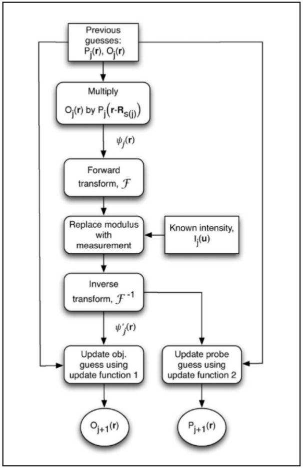

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Thibault *et al.* proposed:

$$\Pi_{\mathrm{F}}(\Psi):\psi_j\to\psi_j^{\mathrm{F}}=p_{\mathrm{F}}(\psi_j). \tag{4}$$

$$\Pi_{\mathrm{O}}(\Psi):\psi_j\to\psi_j^{\mathrm{O}}(\mathbf{r})=\hat{P}(\mathbf{r}-\mathbf{r}_j)\hat{O}(\mathbf{r}). \tag{6}$$

$$\Psi_{n+1}=\Psi_n+\Pi_{\mathrm{F}}[2\Pi_{\mathrm{O}}(\Psi_n)-\Psi_n]-\Pi_{\mathrm{O}}(\Psi_n). \tag{9}$$

On computing (6):

$$\hat{O}(\mathbf{r})=\frac{\sum_j\hat{P}^*(\mathbf{r}-\mathbf{r}_j)\psi_j(\mathbf{r})}{\sum_j|\hat{P}(\mathbf{r}-\mathbf{r}_j)|^2}, \tag{7}$$

$$\hat{P}(\mathbf{r})=\frac{\sum_j\hat{O}^*(\mathbf{r}+\mathbf{r}_j)\psi_j(\mathbf{r}+\mathbf{r}_j)}{\sum_j|\hat{O}(\mathbf{r}+\mathbf{r}_j)|^2}. \tag{8}$$

In the event the probe $\hat{P}$ 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

- Perfectly good algorithmic schemes, which have been shown to work.
- Not clear what (optimisation?) problem the algorithms solve.
  - Cannot be cast as projection-type algorithms solving feasibility problems, although they seem closely related.
- We considered the following optimisation problem:

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

  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 a "nice" objective function.
- (P) is equivalent to the formally unconstrained problem:

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

  where $\iota_C(w)$ is the indicator function of the set C which takes the value 0 if $w \in C$, and $+\infty$ if $w \notin C$.

A Naive Approach: 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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3. Select $$\mathbf{z}^{k+1} \in \operatorname*{arg\,min}_{\mathbf{z} \in Z} F(x^{k+1}, y^{k+1}, \mathbf{z}).$$

What's involved? Roughly speaking, to compute Step 1 we must minimise the terms of the form $\|S_j(x) \odot y^k - z_j^k\|^2$. If this is zero, then

$$S_j(x) \odot y^k = z_j^k \implies S_j(x) = z_j^k \oslash y_k \implies x = S_j^{-1}(z_j^k \oslash y_k).$$

- Inverting S_j is stable (just "un-shift").
- Division by y_k is unstable (divide by zero)
- Similar observations apply to Step 2.
- Step 3 is unstable but there are regularisation schemes in the literature.

PHeBIE: Proximal Block Implicit-Explicit Algorithm

We regularise doing the following to F:

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- Linearising Steps 1 & 2. For Step 1, we have

$$F(x, y^k, \mathbf{z}^k) \quad \longrightarrow \quad F(x^k, y^k, \mathbf{z}^k) + \langle x - x^k, \nabla_x F(x^k, y^k, \mathbf{z}^k)\rangle.$$

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- Adding a proximal term to Steps 1, 2 & 3. For Step 1, such a term looks like

$$+\frac{\alpha^k}{2}\|x - x^k\|^2,$$

where $\alpha^k > 0$ is dependent on y^k and $\mathbf{z}^k$.

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The regularised version of Step 1 becomes:

$$x^{k+1} \in \underset{x \in X}{\arg\min} \left\{ \langle x - x^k, \nabla_x F(x^k, y^k, z^k)\rangle + \frac{\alpha^k}{2}\|x - x^k\|^2 \right\}.$$

The other steps are similar.

PHeBIE: Proximal Block Implicit-Explicit Algorithm

Proximal Block Implicit-Explicit Algorithm:

Initialization. Choose $\alpha, \beta > 1$, $\gamma, \eta_x, \eta_y > 0$, $\left(x^0, y^0, \mathbf{z}^0\right) \in X \times Y \times Z$.

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

1. Set $\alpha^k = \alpha \max\{L_x\left(y^k, \mathbf{z}^k\right), \eta_x\}$ 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. Set $\beta^k = \beta \max\{L_y\left(x^{k+1}, \mathbf{z}^k\right), \eta_y\}$ 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. Select, for $j = 1, 2 \dots, m$,
$$\mathbf{z}_j^{k+1} \in P_Z\left(\left[\frac{2}{2+\gamma_k}S_j(x^{k+1}) \odot y^{k+1} + \frac{\gamma_k}{2+\gamma_k}z_j^k\right]_{j=1}^{m}\right).$$

Here $L_x(y^k, z^k)$ (resp $L_y(x^{k+1}, z^k)$) denotes the partial Lipschitz constant of $\nabla_x F(x, y^k, z^k)$ (resp. $\nabla_y F(x^{k+1}, y, z^k)$), and the projection onto a set C is given by

$$P_C(w) := \underset{u \in C}{\arg\min} \|u - w\|^2.$$

PHeBIE: Convergence Theorem

Theorem (Hesse–Luke-Sabach–T, 2015)

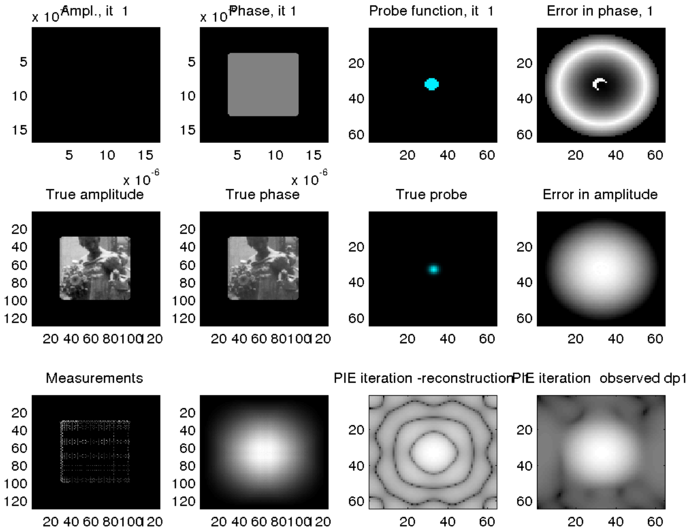
Let $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ be a sequence generated by PHeBIE for blind ptychography problem. Then the following hold.

1. The sequence $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$ has finite length. That is,
$$\sum_{k=1}^{\infty} \left\|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\right\|^2 < \infty.$$
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.)

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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
$$\sum_{k=1}^{\infty} \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|^2 < \infty.$$

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2. (Subdifferential bound) Use properties of the algorithm to show that
$$\|w^{k+1}\| \le \kappa \|(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1}) - (x^k, y^k, \mathbf{z}^k)\|,$$
for some $w^{k+1} \in \partial\Psi(x^{k+1}, y^{k+1}, \mathbf{z}^{k+1})$ and $\kappa > 0$.

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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 appeal to a result of *Bolte, Sabach & Teboulle, 2014*. Here the important ingredient is that Ψ satisfied the Kurdyka–Łojasiewicz (KL) Property which gives Cauchyness of $\{(x^k, y^k, \mathbf{z}^k)\}_{k\in\mathbb{N}}$.

□

The Kurdyka-Łojasiewicz (KL) Property

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

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

The function f is said to have the 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

$$\varphi'\left(f(u) - f(\overline{u})\right) \operatorname{dist}(0, \partial f(u)) \geq 1.$$

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it holds that

$$\varphi'(f(u) - f(\overline{u}))\operatorname{dist}(0, \partial f(u)) \geq 1.$$

Why is the KL property useful? It holds for many important nonconvex optimisation problems.

In particular, any proper, lsc, semi-algebraic function is satisfies the KL property everywhere in its domain.

Exploiting Block Structure

The present algorithm:

- Alternatively minimizes w.r.t. three blocks: X, Y and Z.
- At each iteration the "step-size" is inversely proportional to a parital Lipschitz constant. For instance,

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

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When X or Y has separable structure, they can be decomposed as

$$X \equiv X_1 \times X_2 \times \cdots \times X_N, \quad Y \equiv Y_1 \times Y_2 \times \cdots \times Y_M.$$

- Algorithm variant: alternatively minimizes w.r.t. $(N + M + 1)$-blocks.
- The jth "sub-block", X_j, has partial Lipschitz constant

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

⋆ More sub-blocks → small sub-blocks → small constant → larger step-size.

- Sub-blocks can be updated sequentially or in parallel. In both cases, an analogous convergence theorem holds (see the paper for details).

Explaining Maiden & Rodenburg

In our framework, we can interpret Maiden & Rodeburg's algorithm as alternating minimisation w.r.t. the blocks (in order)

$$X_1, Y_1, Z, X_2, Y_2, Z, X_3, Y_3, Z, \ldots, X_1, Y_1, Z, \ldots$$

where sub-blocks X_j and Y_j correspond to restrictions related to the support of the jth exit wave.

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where sub-blocks X_j and Y_j correspond to restrictions related to the support of the jth exit wave.

Moreover, Maiden & Rodenburg's update rules:

$$O_{j+1}(\mathbf{r}) = O_j(\mathbf{r}) + \alpha \frac{P_j^*(\mathbf{r} - \mathbf{R}_{s(j)})}{|P_j(\mathbf{r} - \mathbf{R}_{s(j)})|^2_{\max}} (\psi_j'(\mathbf{r}) - \psi_j(\mathbf{r})). \quad P_{j+1}(\mathbf{r}) = P_j(\mathbf{r}) + \beta \frac{O_j^*(\mathbf{r} + \mathbf{R}_{s(j)})}{|O_j(\mathbf{r} + \mathbf{R}_{s(j)})|^2_{\max}} (\psi_j'(\mathbf{r}) - \psi_j(\mathbf{r})).$$

are what is obtain by by taking $X = Y = \mathbb{C}^{m \times m}$. Note that the "normalisations" are precisely the partial Lipschitz constants!

Explaining Thibault *et al.*

If it were not a difference-map algorithm, Thibault *et al.* could be interpreted as the two block alternating proximal linearisation minimisation of:

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

1. Select $$(x^{k+1}, y^{k+1}) \in \underset{(x,y)\in X\times Y}{\arg\min}\; F(x, y, \mathbf{z}^k),$$
2. Select $$\mathbf{z}^{k+1} \in \underset{\mathbf{z}\in Z}{\arg\min}\, F(x^{k+1}, y^{k+1}, \mathbf{z}).$$

However Step. 1 is not so easy to solve:

$$\hat{O}(\mathbf{r}) = \frac{\sum_j \hat{P}^*(\mathbf{r} - \mathbf{r}_j)\psi_j(\mathbf{r})}{\sum_j |\hat{P}(\mathbf{r} - \mathbf{r}_j)|^2}, \tag{7}$$

$$\hat{P}(\mathbf{r}) = \frac{\sum_j \hat{O}^*(\mathbf{r} + \mathbf{r}_j)\psi_j(\mathbf{r} + \mathbf{r}_j)}{\sum_j |\hat{O}(\mathbf{r} + \mathbf{r}_j)|^2}. \tag{8}$$

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So the actual computation is the following heuristic approximation to 1.:

Input. $(\hat{x}^0, \hat{y}^0) := (x^k, y^k) \in X \times Y, \mathbf{z}^k$, and $L \in \mathbb{N}$.
General Step. $(l = 0, 1, \ldots, (L-1))$

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

In our framework, this is alternating minimisation w.r.t. the blocks (in order)

$$X, Y, X, Y, \ldots, X, Y, Z, X, Y, X, Y, \ldots, X, Y, Z, \ldots.$$

Concluding Remarks and Ongoing Work

In summary:

- We presented a ptychography algorithm with a clear mathematical framework.
- Under practically verifiable assumption, it is provably convergent to critical points of a function Ψ.
- The flexibility of the framework allows interpretation of current state-of-the-art ptychography algorithms.

Ongoing and future work:

- Is there a useful characterisation of the critical points of of Ψ?
- Can the algorithm structure be exploited on specific architectures?

For further details see:

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).