Partially coherent ptychography

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1 Models

1.1 Coherent model

$$f_j = \left|\mathcal{F}\left(\mathcal{S}_j u \circ \omega\right)\right|^2 \tag{1.1}$$

In a discrete setting, $u \in \mathbb{C}^n$ is a 2D image with $\sqrt{n} \times \sqrt{n}$ pixels, $\omega \in \mathbb{C}^{\bar{m}}$ is a localized 2D probe with $\sqrt{\bar{m}} \times \sqrt{\bar{m}}$ pixels.

$f_j \in \mathbb{R}_+^{\bar{m}} (\forall 0 \leq j \leq J-1)$ is a stack of phaseless measurements. Here $|\cdot|$ represents the element-wise absolute value of a vector, o denotes the elementwise multiplication, and $\mathcal{F}$ denotes the normalized 2 dimensional discrete Fourier transform. Each $\mathcal{S}_j \in \mathbb{R}^{\bar{m} \times n}$ is a binary matrix that crops a region j of size $\bar{m}$ from the image u.

In practice, as the probe is almost never completely known, one has to solve a blind ptychographic phase retrieval (BP-PR) problem:

To find $\omega \in \mathbb{C}^{\bar{m}}$ and $u \in \mathbb{C}^n$ s.t. $|\mathcal{A}(\omega, u)| = \boldsymbol{a}$,

where bilinear operators $\mathcal{A} : \mathbb{C}^{\bar{m}} \times \mathbb{C}^n \to \mathbb{C}^m$ and $\mathcal{A}_j : \mathbb{C}^{\bar{m}} \times \mathbb{C}^n \to \mathbb{C}^{\bar{m}} \forall 0 \leq j \leq J-1$ are denoted as follows:

$\mathcal{A}(\omega, u) := \left(\mathcal{A}_0^T(\omega, u), \mathcal{A}_1^T(\omega, u), \ldots, \mathcal{A}_{J-1}^T(\omega, u)\right)^T$, $\mathcal{A}_j(\omega, u) := \mathcal{F}\left(\omega \circ \mathcal{S}_j u\right)$

and $\boldsymbol{a} := \left(\boldsymbol{a}_0^T, \boldsymbol{a}_1^T, \ldots, \boldsymbol{a}_{J-1}^T\right)^T \in \mathbb{R}_+^m$.

1.2 Specific partially coherent model

1.2.1 Model1[?]

Coherence and vibrations kernels can be combined into one, such that partially coherent ptychography imaging with coherence kernel function κ in a continuous setting:

$$f_{pc,j}(q) = \int \left|\mathcal{F}_{x \to q}\left(\mathcal{S}_j u(x) \omega(x-y)\right)\right|^2 \kappa(y) \mathrm{d}y \tag{1.2}$$

where f_{pc} is the measured partial coherent intensity and $\mathcal{F}_{x\to q}$ is the normalized Fourier transform. κ is a function spikes at 0 like guassians. Setting κ to the Dirac delta function reduces it to the coherent model (**??**).

The partially coherent intensity in a discrete setting is generated as

$$f_{pc,j} = \sum_i \kappa_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\mathcal{T}_i \omega)\right)\right|^2 \tag{1.3}$$

with translation operator $\mathcal{T}_i$, discrete Gaussian weights $\{\kappa_i\}$, and periodical boundary condition for the probe.

Generally speaking, solving (**??**) is a non-linear ill-posed problem with an unknown kernel κ, unknown phobe ω, and unknown target image u.

1.2.2 Model2[?]

Another simpler model mentioned here is:

$$f_{pc} = f * \kappa \tag{1.4}$$

where f_{pc} is the measured partial coherent intensity, f is the coherent intensity in (**??**), $*$ denotes the convolution operator, and κ is the unknown kernel function (Fourier transform of the complex coherence function).

We remark that (**??**) is quite different from (**??**) , since (**??**) illustrates the effects of blurring of images with respect to the probe, while (**??**) can be interpreted as blurring or binning multiple pixels at the detector.

1.3 General partially coherent model

This part explains the partially coherent model proposed by physicists.[**?**]. It is a blind ptychography model based on quantum state tomography[1]. Phobe w is assumed to be in mixed state to represent partially coherent effect.

1.3.1 Decompositon model

$$\begin{gathered}\text{Find } u, r \text{ othogonal } w_k \ s.t. \\ f_{pc,j} = \sum_{k=1}^{r} \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\omega_k)\right)\right|^2\end{gathered} \tag{1.5}$$

Denote $O_j \in C^{\bar{m}\times\bar{m}}$ as a (diagonal) matrix to represent linear transform to w, s.t. $\mathcal{S}_j u \circ \omega = O_j w$. Denote $f_q^* \in C^{1\times\bar{m}}$ as a row vector constructed from Fourier transform $\mathcal{F}$, to represent projection on frepuency element. Construct measurement matrix $\mathcal{I}_{j\mathbf{q}} = O_j^* f_q f_q^* O_j$ and density matrix ρ, we get another form(actually a natural one in quantum state tomography) of the model:

[1] `https://homepage.univie.ac.at/reinhold.bertlmann/pdfs/T2_Skript_Ch_9corr.pdf`Theorem 9.1. Many symbols in quantum mechanics are included here.

$$
\begin{aligned}
&\text{Find } O_j, \rho, s.t. \\
&f_{pc,j}(q) = Tr(\mathcal{I}_{j\mathbf{q}}\rho) \\
&\rho \text{ is positive semi-definite, with rank} \leq r
\end{aligned}
\tag{1.6}
$$

Next we will explain the derivation of this form.

Simple calculation process:

$$
\begin{aligned}
f_{pc,j}(q) = |f_q^* O_j w|^2 = (f_q^* O_j w)^* (f_q^* O_j w) = w^* (O_j^* f_q f_q^* O_j) w \\
= Tr[w^* (O_j^* f_q f_q^* O_j) w] = Tr[(O_j^* f_q f_q^* O_j)(w w^*)] \\
= Tr(\mathcal{I}_{j\mathbf{q}}\rho)
\end{aligned}
$$

It is a bit like the process of phaze-lift.

When w is in pure state(a vector in Hilbert space), $\rho = w^* w$ is a rank-one matirx. In partially coherent case, **we use mixed state to model** w. Fow example, with probability 0.5 in state ψ_1 and 0.5 in ψ_2 (ψ_1 and ψ_2 are not neccesarily orthogonal here). Now w can no longer be represented by a vector(ps. $w \neq p_1\psi_1 + p_2\psi_2$, the latter is still a determined pure state vector). Instead, mixed state is represented by **generalizing the density matrix to one with higher rank**:

$$
\rho = \sum_k p_k \psi_k \psi_k^*
$$

Easy to find ρ is a positive semi-definite matrix, we can decompose ρ using spectral theorem, with r(rank of ρ) othogonal state w_k:

$$
\rho = \sum_{k=1}^{r} w_k w_k^* \tag{1.7}
$$

$$
\begin{aligned}
f_{pc,j}(q) = \operatorname{Tr} \mathcal{I}_{j\mathbf{q}}\rho = \operatorname{Tr}[\mathcal{I}_{j\mathbf{q}} \sum_{k=1}^{r} w_k w_k^*] \\
= \sum_{k=1}^{r} w_k^* \mathcal{I}_{j\mathbf{q}} w_k = \sum_{k=1}^{r} |f_q^* O_j w_k|^2
\end{aligned}
$$

And that is exactly (**??**)$f_{pc,j} = \sum_{k=1}^{r} |\mathcal{F}(\mathcal{S}_j u \circ (\omega_k))|^2$. ($f_{pc,j}(q)$ is a single value at frequency q when $f_{pc,j}$ is the whole diffraction image)

We can write it in another quadratic form:

$$
\begin{aligned}
f_{pc,j}(q) = \operatorname{Tr} \mathcal{I}_{j\mathbf{q}}\rho = Tr[(O_j^* f_q f_q^* O_j)\rho] = Tr[(O_j^* f_q)^* \rho (O_j^* f_q)] = (O_j^* f_q)^* \rho (O_j^* f_q) \\
= g_q^* \rho g_q = \sum_{x_1} \sum_{x_2} \overline{g_q(x_1)} \rho(x_1, x_2) g_q(x_2)
\end{aligned}
\tag{1.8}
$$

where $g_q = O_j^* f_q = \overline{S_j u} \circ f_q$, $\overline{g_q} = S_j u \circ \overline{f_q}$

Then it is a discrete version of the model in [**?**].

1.3.2 The relation between models

In this section we explain how the general model connects with specific models (**??**) and (**??**).

First we consider (**??**). We put the κ_i inside:

$$f_{pc,j} = \sum_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\sqrt{\kappa_i}\mathcal{T}_i \omega)\right)\right|^2 = \sum_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\hat{\omega}_i)\right)\right|^2 \tag{1.9}$$

Multiple modes $\hat{w}_i$ are produced by shifted w. Then we can construct density matrix and use truncated SVD to get a low-rank approximation.

$$\rho = \sum_i \hat{w}_i \hat{w}_i^* \approx \sum_{k=1}^{r} w_k w_k^*$$

As for (**??**), we introduce the definition for coherence function:

$$\gamma(x_1, x_2) = \frac{\rho(x_1, x_2)}{w(x_1)\overline{w(x_2)}}$$

In other word:

$$\gamma = \rho./(ww^*), \rho = \gamma \circ (ww^*) \tag{1.10}$$

where ./ means pairwise division.

In case we assume that coherence function$\gamma(\mathbf{x}_1, \mathbf{x}_2)$ only depends on the difference between the two points $\mathbf{x}_1, \mathbf{x}_2$, i.e. $\gamma(\mathbf{x}_1, \mathbf{x}_2) = \gamma(0, \mathbf{x}_2 - \mathbf{x}_1)$, we can write the far-field intensity as a convolution[**?**] (QU proof unfinished):

$f_{pc} = \kappa * f$. If we know the point spread function $\kappa(q)$, then we get its inverse Fourier transform $\gamma(0, x) = (\mathcal{F}^{-1}\kappa)(x)$. And we get $\gamma(x_1, x_2)$ based on the assumption above. If we also know the phobe w, then we can get ρ, again SVD helps us find the main modes w_k in model (**??**)

With the connection above, we can get the "standard mode decomposition" for simulation experiment which is a good reference.

1.3.3 Alternative Projection

Notation: $P_x - w, O_{x-x_j} - S_j u$. This part introduces the reconstruction algorithm from [**?**] and can be skipped.

The philosophy of the algorithm: Alternative refinement for two constraints – Fourier constraint expresses compliance to the measured intensities $I_{j\mathbf{q}} = \left|\mathcal{F}\left[\phi_{j\mathbf{x}}\right]\right|^2$ and the overlap constraint: $\phi_{j\mathbf{x}} = P_{\mathbf{x}} O_{\mathbf{x}-\mathbf{x}_j}$

Step1: Fourier magnitude projection

Coherent case:

$$\psi_{\mathbf{x}} = \Pi_F\left(\phi_{\mathbf{x}}\right) = \mathcal{F}^{-1}\left[\sqrt{I_{\mathbf{q}}}\frac{\tilde{\phi}_{\mathbf{q}}}{\left|\tilde{\phi}_{\mathbf{q}}\right|}\right]$$

Our partially coherent case:

where we have used the shorthand notation $\tilde{\phi} = \mathcal{F}[\phi]$. Taking the form

$$\begin{aligned}\psi_{j\mathbf{x}}^{(k)} &= \bar{\Pi}_F\left(\phi_{j\mathbf{x}}^{(0)}, \phi_{j\mathbf{x}}^{(1)}, \ldots, \phi_{j\mathbf{x}}^{(r=M_{\mathrm{P}})}\right) \\ &= \mathcal{F}^{-1}\left[\sqrt{I_{j\mathbf{q}}}\frac{\tilde{\phi}_{j\mathbf{q}}^{(k)}}{\sqrt{\sum_k\left|\tilde{\phi}_{j\mathbf{q}}^{(k)}\right|^2}}\right]\end{aligned}$$

again with

$$\tilde{\phi}_{j\mathbf{q}}^{(k)} = \mathcal{F}\left[P_{\mathbf{x}}^{(k)}O_{\mathbf{x}-\mathbf{x}_j}\right]$$

Step2: Overlap projection

Coherent case:

The overlap projection can be computed from the minimization of the distance $E = \left\|\Psi - \Psi^0\right\|^2$, subject to the overlap constraint. The calculation entails to finding $\hat{O}$ and $\hat{P}$ that minimize $\left\|\Psi - \Psi^{\mathrm{O}}\right\|^2 = \sum_j ||\psi_j(\mathbf{r}) - \hat{P}\left(\mathbf{r}\right)\hat{O}(\mathbf{r}-\mathbf{r}_j)||_2^2$ The associated projection is $\Pi_0(\Psi) : \psi_j \to \psi_j^0(\mathbf{r}) = \hat{P}\left(\mathbf{r}\right)\hat{O}(\mathbf{r}-\mathbf{r}_j)$

Minimization of E must be carried numerically as closed form expressions for $\hat{O}$ and $\hat{P}$ cannot be obtained. For this task, setting to zero the derivative of $\left\|\Psi - \Psi^0\right\|^2$ with respect to $\hat{P}$ and $\hat{O}$. Specifically, use variational method, just take $P(\lambda) = P + \lambda\delta$,them $E(\lambda) \geq E(0)$ for all distanbance funtion δ, take the derivative $\dfrac{dE}{d\lambda}E(\lambda)$ and set it to zero at $\lambda = 0$, then use the arbitrariness of δ to give the solution as a system of equations:

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

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

Our partially coherence case:

$$O_{\mathbf{x}} = \frac{\sum_k\sum_j P_{\mathbf{x}+\mathbf{x}_j}^{(k)*}\psi_{j,\mathbf{x}+\mathbf{x}_j}^{(k)}}{\sum_k\sum_j\left|P_{\mathbf{x}+\mathbf{x}_j}^{(k)}\right|^2}$$

$$P_{\mathbf{x}}^{(k)} = \frac{\sum_j O_{\mathbf{x}-\mathbf{x}_j}^*\psi_{j\mathbf{x}}^{(k)}}{\sum_j\left|O_{\mathbf{x}-\mathbf{x}_j}\right|^2}$$

solved numerically by applying them sequentially for a few iterations.

2 ADMM-based numerical algorithm

The AP algorithm above can be rewritten into ADMM form, which is more stable and faster. We generalize the ADMM form in [?] to mixed states.

Now $w \in \mathbb{C}^{(px\times py)\times r}$ is a phobe with r mixed states. $u \in \mathbb{C}^{Nx\times Ny}$ is an image. An auxiliary variable $z = \mathcal{A}(\omega, u) \in \mathbb{C}^{(px\times py)\times N\times r}$ is introduced. $\mathcal{A}$ is a bilinear operator generating diffraction image stacks(N frames for each phobe state) from image u and r different states w_k.

$f \in \mathbb{C}^{(px\times py)\times N}$ is the true(observed) diffraction image stacks. Let $Y = \sqrt{f}$ be the amplitute of stacks. Then $\mathcal{G}(z) = ||\sqrt{\sum_{k=1}^{r}|z(:,:,:,k)|^2} - Y||^2$ measures the difference between values computed by my our model and the groundtruth. Let $\mathcal{X}_1$ and $\mathcal{X}_2$ be the prior range for w and u. Let $l = px \times py$, $\mathcal{X}_3$ be the index function for orthogonal $D\alpha$. (Orthonormal $D \in \mathbb{C}^{l\times r}$, amplitude factors $\alpha \in \mathbb{R}^{r\times r}$). Then we get the following:

$$\begin{aligned}
&\min_{\omega,u,z} \mathcal{G}(z) + \mathbb{I}_{\mathcal{X}_1}(\omega) + \mathbb{I}_{\mathcal{X}_2}(u) + \mathbb{I}_{\mathcal{X}_3}(D\alpha) \\
&s.t. \quad z - \mathcal{A}(\omega, u) = 0, \quad \Omega - w = 0. \\
&where\ D^*D = I, \Omega = reshape(D\alpha, [px, py, r])
\end{aligned} \tag{2.1}$$

The corresponding augmented Lagrangian reads

$$\begin{aligned}
\Upsilon_\beta(\omega, u, z, \Lambda) :=& \mathcal{G}(z) + \mathbb{I}_{\mathcal{X}_1}(\omega) + \mathbb{I}_{\mathcal{X}_2}(u) + \Re(\langle z - \mathcal{A}(\omega, u), \Lambda\rangle) + \frac{\beta}{2}\|z - \mathcal{A}(\omega, u)\|^2 \\
&+ \Re(\langle \Omega - w, \Lambda_2\rangle) + \frac{\beta_2}{2}\|\Omega - \omega\|^2
\end{aligned}$$

where $\Lambda, \Lambda_2 \in \mathbb{C}^{(px\times py)\times N\times r}$ is the multiplier. Let $\Lambda = \Lambda/\beta, \Lambda_2 = \Lambda_2/\beta_2$, we can combine the $\Re$ part and the augmented part to get:

$$\begin{aligned}
\Upsilon_\beta(\omega, u, z, \Lambda) :=& \mathcal{G}(z) + \mathbb{I}_{\mathcal{X}_1}(\omega) + \mathbb{I}_{\mathcal{X}_2}(u) + \mathbb{I}_{\mathcal{X}_3}(D\alpha) \\
&\frac{\beta}{2}\|z - \mathcal{A}(\omega, u) + \Lambda\|^2 - \frac{\beta}{2}||\Lambda||^2 + \frac{\beta_2}{2}\|\Omega - w + \Lambda_2\|^2 - \frac{\beta_2}{2}||\Lambda_2||^2
\end{aligned} \tag{2.2}$$

In ADMM, one seeks a saddle point of the following problem:

$$\max_{\Lambda,\Lambda_2} \min_{\omega,u,z,D,\alpha} \Upsilon_\beta(\omega, u, z, \Lambda, \Lambda_2, D, \alpha)$$

A natural scheme to solve the above saddle point problem is to split them, which consists of four-step iterations for the generalized ADMM (only the subproblems w.r.t. ω or u have proximal terms), as follows:

$$
\begin{aligned}
&\text{Step 1: } \omega^{k+1} = \arg\min_{\omega} \Upsilon_\beta\left(\omega, u^k, z^k, \Lambda^k\right) + \frac{\beta_2}{2}||\omega - (\Omega^k + \Lambda_2)||^2 + \frac{\alpha_1}{2}\left\|\omega - \omega^k\right\|^2_{M_1^k},\\
&\text{Step 2: } u^{k+1} = \arg\min_{u} \Upsilon_\beta\left(\omega^{k+1}, u, z^k, \Lambda^k\right) + \frac{\alpha_2}{2}\left\|u - u^k\right\|^2_{M_2^k},\\
&\text{Step 3: } z^{k+1} = \arg\min_{z} \Upsilon_\beta\left(\omega^{k+1}, u^{k+1}, z, \Lambda^k\right),\\
&\text{Step 4: } D^{k+1} = \arg\min_{D} \mathbb{I}_{\mathcal{X}_3}(D\alpha) + \frac{\beta_2}{2}\|\Omega^k - \omega^{k+1}\|^2\\
&\text{Step 5: } \alpha^{k+1} = \arg\min_{\alpha} \frac{\beta_2}{2}\|\Omega^{k+0.5} - \omega^{k+1}\|^2\\
&\text{Step 6: } \Lambda^{k+1} = \Lambda^k + \left(z^{k+1} - \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right)\right) \qquad (2.3)\\
&\text{Step 7: } \Lambda_2^{k+1} = \Lambda_2^k + (\Omega^{k+1} - \omega^{k+1}) \qquad (2.4)
\end{aligned}
$$

For simplicity, we ignore the stable quadratic terms in Step1 and Step2 in the following analysis.

2.1 Subproblems w and u

w.r.t. the probe ω :

$$
\begin{aligned}
\omega^{k+1} &= \arg\min_{\omega\in\mathcal{X}_1} \frac{1}{2}\left\|z^k + \Lambda^k - \mathcal{A}\left(\omega, u^k\right)\right\|^2 + \frac{\beta_2}{2}||\omega - (\Omega^k + \Lambda_2^k)||^2\\
&= \arg\min_{\omega\in\mathcal{X}_1} \frac{1}{2}\left\|\hat{z}^k - \mathcal{A}\left(\omega, u^k\right)\right\|^2 + \frac{\beta_2}{2}||\omega - \hat{\Omega}^k||^2\\
&= \arg\min_{\omega\in\mathcal{X}_1} \frac{1}{2}\sum_{j,i}\left\|\mathcal{F}^{-1}\hat{z}(:,:,j,i)^k - \omega(:,:,i)\circ\mathcal{S}_j u^k\right\|^2 + \frac{\beta_2}{2}\sum_i ||\omega(:,:,i) - \hat{\Omega}^k(:,:,i)||^2\\
&\text{with } \hat{z}^k := z^k + \Lambda^k, \hat{\Omega}^k := \Omega^k + \Lambda_2^k
\end{aligned}
$$

The close form solution of Step 1 is given as

$$
\omega^{k+1} = \mathrm{Proj}\left(\frac{\beta\sum_j\left(\mathcal{S}_j u^k\right)^*\circ\left[\left(\mathcal{F}^{-1}\hat{z}^k\right)(:,:,j,:)\right] + \beta_2\hat{\Omega}^k}{\beta\sum_j\left|\mathcal{S}_j u^k\right|^2 + \beta_2}; C_\omega\right) \tag{2.5}
$$

with the projection operator onto $\mathcal{X}_1$ defined as $\mathrm{Proj}(\omega; C_\omega) := \min\{C_\omega, |\omega|\}\circ \mathrm{sign}(\omega)$, where $\mathcal{X}_1 = \{\omega : |\omega| \le C_w\}$. $\mathcal{F}^{-1}$ acts on the first two dimensions of $\hat{z}$ (i.e $\hat{z}(:,:,j,i)$).

Similarly we have:

$$
u^{k+1} = \mathrm{Proj}\left(\frac{\sum_{j,i}\mathcal{S}_j^T\left(\left(\omega_i^{k+1}\right)^*\circ\mathcal{F}^{-1}\hat{z}_{j,i}^k\right)}{\sum_{j,i}\left(\mathcal{S}_j^T\left|\omega_i^{k+1}\right|^2\right)}; C_u\right). \tag{2.6}
$$

Here S_j^T is an operator mapping its augument to target postion j in image u.

2.2 Subproblem z

$$z^{k+1} = \arg\min_z \mathcal{G}(z) + \frac{\beta}{2}\left\| z - \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right) + \Lambda^k \right\|^2$$

$$= \arg\min_z \frac{1}{2}||\sqrt{\sum_{i=1}^{r} |z(:,:,:,i)|^2} - Y||^2 + \frac{\beta}{2}\left\| z - z^+ \right\|^2$$

$$= \arg\min_z \sum_{x,y,j} [\frac{1}{2}(\sqrt{\sum_{i=1}^{r} |z(x,y,j,i)|^2} - Y(x,y,j))^2 + \frac{\beta}{2}||z(x,y,j,:) - z^+(x,y,j,:)||^2]$$

where $z^+ = \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right) - \Lambda^k$

For any fixed x, y, j and free i, the problem can be seen as:

$$z^*(x,y,j,:) = \arg \min_{z_{x,y,j} \in \mathbb{C}^r} \frac{1}{2}(||z_{x,y,j}|| - Y_{x,y,j})^2 + \frac{\beta}{2}||z_{x,y,j} - z^+_{x,y,j}||^2$$

Notice that for fixed $||z_{x,y,j}||$, the first term in expression is fixed. To optimize the second term, we should always choose $z_{x,y,j}$ with the same direction as $z^+_{x,y,j}$. So we have $||z_{x,y,j} - z^+_{x,y,j}||^2 = (||z_{x,y,j}|| - ||z^+_{x,y,j}||)^2$

$$\frac{z(x,y,j,i)}{||z_{x,y,j}||} = \frac{z^+(x,y,j,i)}{||z^+_{x,y,j}||}, z(x,y,j,i) = ||z_{x,y,j}|| \frac{z^+(x,y,j,i)}{||z^+_{x,y,j}||}$$

To determine $z_{x,y,j}$, we only need to determine $||z_{x,y,j}||$. Denote it as a.

$$||z_{x,y,j}||^* = \arg\min_{a \in \mathbb{R}} \frac{1}{2}(a - Y_{x,y,j})^2 + \frac{\beta}{2}(a - ||z^+_{x,y,j}||)^2$$

The first optimality condition easily gives:

$$a = \frac{Y_{x,y,j} + \beta||z^+_{x,y,j}||}{1+\beta}$$

The close form solution of Step 3 is given as:

$$z_i^{k+1} = \frac{z_i^k \dfrac{Y}{M^k} + \beta z_i^+}{1+\beta}, 1 \le i \le r \tag{2.7}$$

where $M^k = \sqrt{\sum_i |z^k(:,:,:,i)|^2} \in \mathbb{C}^{px \times py \times N}$

2.3 Subproblem D and α

$$D^{k+1} = \arg\min_D \|\Omega - w^{k+1} + \Lambda_2^k\|^2$$

$$= \arg\min_D \|D\alpha^k - \hat{w}^{k+1}\|^2$$

where $\hat{w}^{k+1} = reshape(\omega^{k+1} - \Lambda_2^k, [px \times py, r])$,$D^*D = I$

This is a special case in Orthogonal Procrustes problem [2]

$$\begin{aligned}
\|D\alpha^k - \hat{w}^{k+1}\|^2 =& Tr[(D\alpha^k - \hat{w}^{k+1})^*(D\alpha^k - \hat{w}^{k+1})] \\
=& ||\alpha^k||_F^2 - Tr[(\alpha^k)^*D^*\hat{\omega}^{k+1}] - Tr[(\hat{\omega}^{k+1})^*D\alpha^k] + ||\hat{\omega}^{k+1}||_F^2
\end{aligned}$$

$$\begin{aligned}
D^{k+1} &= \arg\max_D Tr[(\alpha^k)^*D^*\hat{\omega}^{k+1}] + Tr[(\hat{\omega}^{k+1})^*D\alpha^k] \\
&= \arg\max_D \Re(Tr[(\alpha^k)^*D^*\hat{\omega}^{k+1}]) \\
&\overset{\alpha\in\mathbb{R}^{r\times r}}{=\!=\!=} \arg\max_D \Re(Tr[D^*(\hat{\omega}^{k+1}\alpha^k)])
\end{aligned}$$

Consider the SVD decomposition: $\hat{\omega}^{k+1}\alpha^k = USV^*$

$$\begin{aligned}
D^{k+1} &= \arg\max_D \Re(Tr[D^*USV^*]) = \arg\max_D \Re(Tr[(V^*D^*U)S]) \\
&\overset{\hat{D}=V^*D^*U \text{ is orthonormal}}{=\!=\!=\!=\!=\!=} \arg\max_{\hat{D}} \Re(Tr[\hat{D}S])
\end{aligned}$$

We can easily see $\hat{D} = I$ is optimal, and:

$$D^{k+1} = UV^* \tag{2.8}$$

The updation for α is easier:

$$\alpha^{k+1} = \arg\min_\alpha \|D^{k+1}\alpha - \hat{w}^{k+1}\|^2 = \arg\min_\alpha \sum_i ||\alpha_i D^{k+1}(:,i) - \hat{w}^{k+1}(:,i)||^2$$

Notice that each $\alpha_i \in \mathbb{R}$ can be solved independently, the first optimality condition gives:

$$\alpha_i^{k+1} = \sum_{i_0} \Re[\overline{D^{k+1}(i_0,i)}\hat{w}^{k+1}(i_0,i)] \tag{2.9}$$

3 Numerical experiments

The codes are implemented in MATLAB. First we introduce the setting in experiments, then we conduct experiments on simulation data generated from two specific models in **??** respetively. In each experiment, we compare the reconstructed images and performance metrics in different setting. And we generate ideal modes as in **??** and compare our modes with them.

[2]`https://en.wikipedia.org/wiki/Orthogonal_Procrustes_problem`

Algorithm 1: ADMM for general mixed-state model(**??**)

Initialization: Set the number of states r,
$\omega^0, u^0, z^0 = \mathcal{A}\left(\omega^0, u^0\right), \Lambda^0, \Lambda_2^0 = 0$;
D^0 and α^0 from SVD on ω^0
maximum iteration number Iter $_{\text{Max}}$, and parameter β,β_2

Output: $u^\star := u^{Iter_{Max}}$ and $\omega^\star := \omega^{\text{Iter}_{Max}}$

for $ii = 0$ *to* $Iter_{Max} - 1$ **do**
  Compute ω^{k+1} by (**??**) with $\hat{z}^k := z^k + \Lambda^k$;
  Compute u^{k+1} (**??**). with $\hat{z}^k$ the same as above;
  Compute z_i^{k+1},$1 \leq i \leq r$ by (**??**). with $z^+ = \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right) - \Lambda^k$;
  Compute D^{k+1} (**??**). ;
  Compute $\alpha_i, 1 \leq i \leq r$ (**??**). ;
  Update the multiplier as Step 6 and Step 7 of (**??**) and (**??**);
end

3.1 Experiment setting

3.1.1 Parameters

Parameters	Illustration	Values
N_x, N_y	size of image u	128,128
p_x, p_y	size of phobe w	64,64
$Dist$	scan distance between neighborhood frames	4,8,16
N	number of frames in diffusion image stacks	
r	number of states(modes)	1(coherent) to 15
gridFlag	types of scan methods	1(rectangular lattice), 2(hexagonal),3(randomly disturb on 2)
blurFlag	types of partially coherent effect	1(**??**),2(**??**)

In order to deal with nontrivial ambiguities, nonperiodical lattice based s-canning can be considered experimentally to remove the periodicity of the s-canning geometry, e.g., adding a small amount of random offsets to a set of lattice.($gridFlag = 3$).

$Dist$ is an important parameter for successfull reconstruction. Generally speaking, the smaller the $Dist$, the more the overlapping area and redundancy in data, we can get reconstruction images with higher qualities. Here we find $Dist = 8$ is enough while $Dist = 16$ always fails.

3.1.2 Performance metrics

In order to evaluate performances of algorithms, we introduce 3 metrics.

1. Relative error err and signal-to-noise ratio snr

$$err^k = \frac{||cu^k - u_{true}||_F}{||cu^k||_F}, c = \frac{sum(u_{true} \circ \overline{u^k})}{||u^k||_F^2}$$

$$snr^k = -20 \log_{10}(err^k)$$

$||\cdot||_F$ is the Frobenis norm. err measures the difference between reconstruction image and groundtruth image. c is an estimated scale factor, and sum means the sum of all elements in the target matirx.

2. R-factor R

Let $zz = \mathcal{A}_j\left(\omega^k, u^k\right)$

$$R^k := \frac{\left\|\sqrt{\sum_{i=1}^{r} |zz(:,:,:,i)|^2} - Y\right\|_1}{\|Y\|_1}$$

R measures the difference between the reconstruction diffraction stacks and groundtruth stacks Y. We don't always know u_{true}, Y is the only input data for our algorithm, and R-factor can be used to verify the convergence.

3. Masks approximation error err_M

$$err_M^k = \frac{||c\rho^k - \rho_{true}||_F}{||\rho_{true}||_F}, c = \frac{sum(\rho_{true} \circ \overline{\rho^k})}{||\rho^k||_F^2}$$

err_M measures the difference between the reconstructed density matrix ρ^k from masks and the standard density matirx ρ_{true} from theoretical model.

3.1.3 Operations on modes

1. Initialization

In the following tests, we set $u^0 = \mathbf{1}_{N_x \times N_y}$ and initial phobe $m = \frac{1}{N}\mathcal{F}^{-1}\left(\sum_j Y(:,:,j)\right)$. We generate other modes by randomly disturb intial mask m. r initial probes were created by multiplying the initial mask by different arrays of random complex values (modulus part varies within the range of $[0, 1]$ and phase part $[0, 2\pi]$). Then we get w^0.

2. Orthogonalization

Modes w_k computed in our algorithm are not always orthogonal. However, we can easily orthogonalize them by generating density matrix ρ and perform spectral decompostion on ρ like in (**??**) . The orthogonal representation of modes is always unique(Specifically, when the eigenvalues of ρ are all different, and this always happens in real world data).

Notice that the number of modes is always small i.e. $r \ll l := p_x \times p_y$, we perform SVD on the $l \times r$ phobe matrix directly instead of $l \times l$ density matrix ρ. And we can also select the first $r' \leq r$ modes for an approximation.

Algorithm 2: SVD-based orthogonalization for phobes(Matlab)

Input: $w \in \mathbb{C}^{px \times py \times r}$, the number of modes needed r'

Output: $w_{ort} \in \mathbb{C}^{px \times py \times r'}$

phobe matrix $ss = reshape(w, [l\ r])$;

$[U, S, V] = svd(ss, 'econ')$;

$q = U(:, 1 : r') * S(1 : r', 1 : r')$;

$w_{ort} = reshape(q, [px\ py\ r'])$;

Orthogonalization operation is always performed before we display final modes to get a clearer representation. We also want to figure out whether orthogonalization can be added to improve our Algorithm**??**.

3.2 Experiment for model(**??**)

We set κ in (**??**) as standard guassian kernel with variance $\sigma = 1$, and $gridFlag =$ 3 figures/ex1_u.png

Figure 1: Images reconstructed

figures/ex1_R.png

Figure 2: R-factor, 200 iterations for ADMM and 1000 for AP

3.3 Experiment for model(??)

We set κ as guassian kernel with variance $(\sigma_1, \sigma_2) = (7, 0), (5, 5)$. Here we use $gridFlag = 1$, and we can see the periodical artifects. It seems that 3 modes are enough in this case.

figures/ex2_u_2.png

Figure 3: Images reconstructed

figures/ex2_R.png

Figure 4: R-factor, 300 iterations

And we generate standard modes from (??):

figures/ex_2_standard.png

Figure 5: standard modes

The modes reconstructed by our algorithm:

figures/ex_2_re.png

Figure 6: reconstructed modes

figures/modes_intensity_re.png

Figure 7: Mode intensities

4 Discussion and task

1. Add orthogonal constraint in ADMM
2. Finish the proof in **??** QU.

5 Appendix

5.1 Subproblems in ADMM

5.1.1 ω

Essentially in this subproblem, each state $\omega_i = w(:,:,i)$ is independent. Then we can optimize each w_i seperately.

$$\omega_i^{k+1} = \arg\min_{\omega \in \mathcal{X}_1} \frac{1}{2} \sum_j \left\| \mathcal{F}^{-1} \hat{z}(:,:,j,i)^k - \omega(:,:,i) \circ \mathcal{S}_j u^k \right\|^2$$

Essentially in this subsubproblem, each element in w_i is independent. such that one just needs to solve the following 1D constraint quadratic problem:

$$\omega_i^{k+1}(t) = \arg\min_{|x| \leq C_\omega} \rho_t^k(x).$$

where $\rho_t^k(x) := \frac{1}{2} \sum_j \left| \left(\mathcal{F}^{-1} \hat{z}(:,:,j,i)^k \right)(t) - x \times \left(\mathcal{S}_j u^k \right)(t) \right|^2 \forall x \in \mathbb{C}$

The derivative of $\rho_t^k(x)$ is calculated [3] as

$$\begin{aligned}
\nabla \rho_t^k(x) &= \frac{d\rho_t^k(x)}{dx^*} \\
&= \sum_j \left(x \times \left| \left(\mathcal{S}_j u^k\right)(t) \right|^2 - \left(\mathcal{S}_j u^k\right)^* (t) \left(\mathcal{F}^{-1} \hat{z}_{j,i}^k\right)(t) \right) \\
&= x \times \left(\sum_j \left| \left(\mathcal{S}_j u^k\right)(t) \right|^2 \right) - \sum_j \left(\left(\mathcal{S}_j u^k\right)^* (t) \left(\mathcal{F}^{-1} \hat{z}_{j,i}^k\right)(t) \right)
\end{aligned}$$

The first order optimality condition is $\nabla \rho_t^k(x) = 0$. Then the close form solution of w_i is given as

$$\omega_i^{k+1} = \mathrm{Proj}\left(\frac{\sum_j \left(\mathcal{S}_j u^k\right)^* \circ \left(\mathcal{F}^{-1} \hat{z}_{j,i}^k\right)}{\sum_j \left|\mathcal{S}_j u^k\right|^2}; C_\omega \right)$$

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[3] Notice that here ρ is a real value funtion with complex variable, and we use wirtinger derivatives here. More properties and calculation rules are listed in this link: `https://blog.csdn.net/weixin_37872766/article/details/107673096`