Partially coherent ptychography

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Coherent model

$$f_j = \left|\mathcal{F}\left(\mathcal{S}_j u \circ \omega\right)\right|^2 \tag{1}$$

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.

Partially coherent model: a general one

Thibault, Pierre, and Andreas Menzel. "Reconstructing state mixtures from diffraction measurements." Nature 494.7435 (2013): 68-71.

Blind ptychography model + quantum state tomography[1].
Phobe w is assumed to be in mixed state to represent partially coherent effect.

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

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

Step1: Fourier magnitude projection

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

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

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

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

$$P^{(k)}_{\mathbf{x}} = \frac{\sum_j O^*_{\mathbf{x}-\mathbf{x}_j} \psi^{(k)}_{j\mathbf{x}}}{\sum_j \left| O_{\mathbf{x}-\mathbf{x}_j} \right|^2}$$

solved numerically by applying them sequentially for a few iterations.

Outcome

Another form

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:

$$\begin{aligned} &\text{Find } O_j, \rho, s.t. \\ &f_{pc,j}(q) = Tr(\mathcal{I}_{j\mathbf{q}}\rho) \\ &\rho \text{ is positive semi-definite, with rank} \leq r \end{aligned} \tag{3}$$

Derivation

Simple calculation process:

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

When w is in pure state(a vector in Hilbert space), $\rho = ww^*$ is a rank-one matirx. In partially coherent case, **we use mixed state to model** w. Mixed state is represented by **generalizing the density matrix to one with higher rank**:

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

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

And that is exactly (2)$f_{pc,j} = \sum_{k=1}^{r} |\mathcal{F}(\mathcal{S}_j u \circ (\omega_k))|^2$.

Further explaination about mixed state

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).

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

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:

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

Related work

Fannjiang, Albert, and Thomas Strohmer. "The numerics of phase retrieval." Acta Numerica 29 (2020): 125-228. 6.3. Low-rank phase retrieval problems.

The phase retrieval problem has a natural generalization to recovering low-rank positive semidefinite matrices. More precisely, we are concerned with the task of reconstructing a finite-dimensional quantum mechanical system which is fully characterized by its density operator ρ (an n x n positive semidefinite matrix with trace one.)