Introduction To Phase Retrieval

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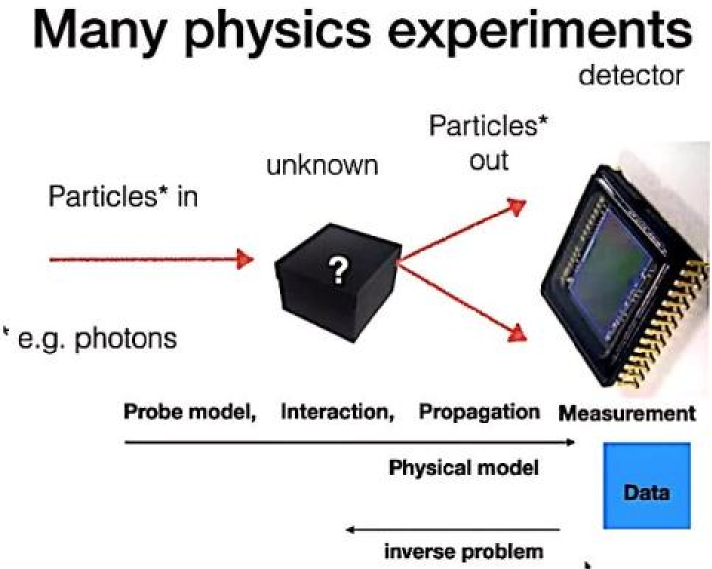
介绍


Many physics experiments
detector
Particles* out
unknown
Particles* in
?
* e.g. photons
Probe model,
Interaction,
Propagation
Measurement
Physical model
Data
inverse problem

Missing phase problem

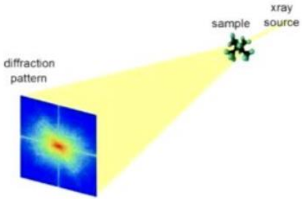
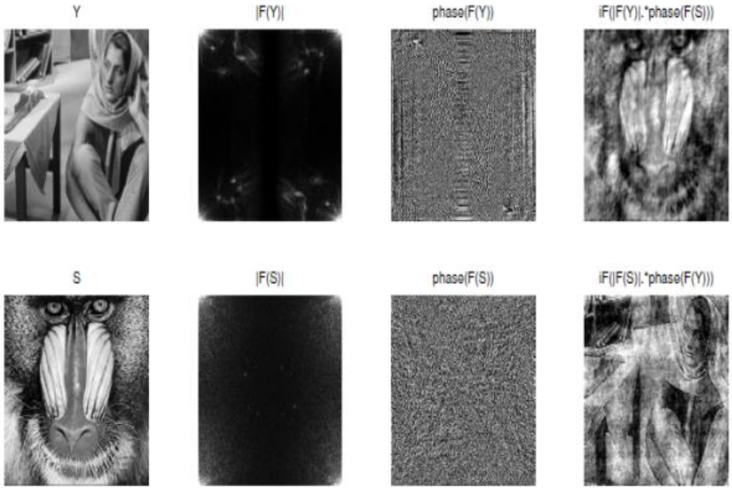


Figure 1: X-Ray Diffraction (Fraunhofer diffraction (far field) $\Rightarrow$ Fourier transform $\mathcal{F}$)

Classical Phase Retrieval

To find complex-valued u, s.t. $|\mathcal{F}u|^2 = b$.

Phase and magnitude



Phase carries more information than magnitude

Classical Phase Retrieval

Feasibility problem

$$\text{find } x \in S \cap \mathcal{M} \text{ or } \text{ find } x \in S_+ \cap \mathcal{M}$$

- given Fourier magnitudes:

$$\mathcal{M} := \{x(r) \mid |\hat{x}(\omega)| = b(\omega)\}$$

  where $\hat{x}(\omega) = \mathcal{F}(x(r))$, $\mathcal{F}$: Fourier transform
- given support estimate:

$$S := \{x(r) \mid x(r) = 0 \text{ for } r \notin D\}$$

  or

$$S_+ := \{x(r) \mid x(r) \geq 0 \text{ and } x(r) = 0 \text{ if } r \notin D\}$$

Error Reduction

Alternating projection:

$$x^{k+1} = \mathcal{P}_{\mathcal{S}}\mathcal{P}_{\mathcal{M}}\left(x^k\right)$$

1. (fit model) projection to S :

$$\mathcal{P}_S(x) = \begin{cases} x(r), & \text{if } r \in D \\ 0, & \text{otherwise} \end{cases}$$

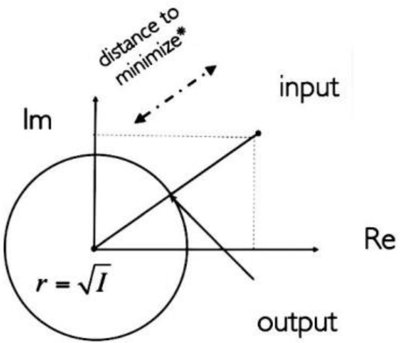
2. (fit data) projection to $\mathcal{M}$:

$E = (|\mathcal{F}(x)|^2 - b)^2$

$\mathcal{P}_{\mathcal{M}}(x) = \mathcal{F}^{-1}(\hat{y})$, where

$\hat{y} =$

$$\begin{cases} b(\omega)\frac{\hat{x}(\omega)}{|\hat{x}(\omega)|}, & \text{if } \hat{x}(\omega) \neq 0 \end{cases}$$



General sample method

1. Phaseless measurements about $x_0 \in \mathbf{C}^n$

$$b_k = |a_k^* x_0|^2, \quad k \in \{1, \dots, m\}$$

2. Phase retrieval is feasibility problem find x_0 s.t. $|a_k^* x_0|^2 = b_k, k = 1, \dots, m$
3. In the case above, $|\mathcal{F} x_0|^2 = b$, we have:

$$b_k = |f_k^* x_0|^2, \quad k \in \{1, \dots, n\}$$

where $f_k^* \in C^{1\times n}$ as a row vector constructed from Fourier transform $\mathcal{F}$, to represent projection on frepuency element. (Detail: 2D and 1D)

PhaseLift (C., Eldar, Strohmer, Voroninski, 2011)

Lifting: $X = xx^*$

$$b_k = |a_k^* x|^2 = a_k^* x x^* a_k = Tr(a_k^* x x^* a_k) = Tr(a_k a_k^* x x^*) = \langle a_k a_k^*, X \rangle$$

Turns quadratic measurements into linear measurements $b = \mathcal{A}(X)$ about xx^*

Phase retrieval problem

find X s.t.

$$\mathcal{A}(X) = b$$

$$X \succeq 0, \mathrm{rank}(X) = 1$$

PhaseLift & Relaxazion

Min $Tr(X)$ s.t.

$$\mathcal{A}(X) = b$$

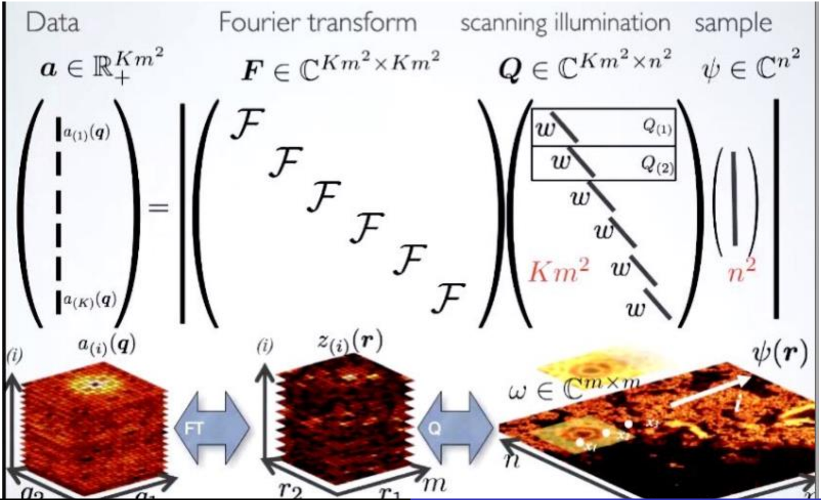
$$X \succeq 0$$

Theorem (C. and Li (' 12); C., Strohmer and Voroninski (' 11))

- a_k independently and uniformly sampled on unit sphere
- $m \gtrsim n$

Ptychographic Phase Retrieval

For practical purposes, we may prefer sets of measurement vectors that obey certain diffraction structure.



Ptychographic Phase Retrieval

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

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

$f_j \in \mathbb{R}_+^{m^2} (\forall 1 \leq j \leq K)$ 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 $\mathcal{S}_j \in \mathbb{R}^{m^2 \times n^2}$ is a binary matrix that crops a region j of size m^2 from the image u.

Ptychographic Phase Retrieval

1. optimization problem

$$\min \rho(u, w) := \sum_{j=1}^{K} \frac{1}{2} \| |\mathcal{F}(\mathcal{S}_j u \circ \omega)| - f_j \|_2^2$$

2. Reformulation:

$$\min \sum_{j=1}^{K} \frac{1}{2} \| |z_j| - f_j \|_2^2 \text{, s.t. } z_j = \mathcal{A}_j(\omega, u) := \mathcal{F}\left(\omega \circ \mathcal{S}_j u\right), j = 1...K$$

3. Combine j:

$z = \mathcal{A}(\omega, u) := \left(\mathcal{A}_1^T(\omega, u), \mathcal{A}_2^T(\omega, u), ..., \mathcal{A}_K^T(\omega, u)\right)^T \in \mathbb{C}^{Km^2}$,
$f := (f_1^T, f_2^T, \ldots, f_K^T)^T$.

$$\min \frac{1}{2} \| |z| - f \|_2^2 \text{, s.t. } z = \mathcal{A}(\omega, u)$$

ADMM

Introduce $\Lambda \in C^{Km^2}$, the corresponding augmented Lagrangian could be formulated as:

$$\begin{aligned} \Upsilon_\beta(\omega, u, z, \Lambda) := \frac{1}{2} \| |z| - f \|_2^2 + \mathbb{I}_{\mathcal{X}_1}(\omega) + \mathbb{I}_{\mathcal{X}_2}(u) \\ + \frac{\beta}{2} \| z - \mathcal{A}(\omega, u) + \Lambda \|^2 - \frac{\beta}{2} ||\Lambda||^2 \end{aligned} \tag{2}$$

$$\begin{aligned} &\text{Step 1:} \omega^{k+1} = \arg\min_{\omega} \Upsilon_\beta \left(\omega, u^k, z^k, \Lambda^k \right) \\ &\text{Step 2:} \;\; u^{k+1} = \arg\min_{u} \Upsilon_\beta \left(\omega^{k+1}, u, z^k, \Lambda^k \right) \\ &\text{Step 3:} \;\; z^{k+1} = \arg\min_{z} \Upsilon_\beta \left(\omega^{k+1}, u^{k+1}, z, \Lambda^k \right), \\ &\text{Step 4:} \;\; \Lambda^{k+1} = \Lambda^k + \left(z^{k+1} - \mathcal{A}\left(\omega^{k+1}, u^{k+1} \right) \right) \end{aligned}$$

Subproblems ω and u

$$\omega^{k+1} = \arg\min_{\omega \in \mathcal{X}_1} \frac{1}{2} \left\| z^k + \Lambda^k - \mathcal{A}\left(\omega, u^k\right) \right\|^2$$
$$= \arg\min_{\omega \in \mathcal{X}_1} \frac{1}{2} \left\| \hat{z}^k - \mathcal{A}\left(\omega, u^k\right) \right\|^2$$

The close form solution of Step 1 is given as:

$$\omega^{k+1} = \mathrm{Proj}\left(\frac{\sum_j \left(\mathcal{S}_j u^k\right)^* \circ [\left(\mathcal{F}^{-1} \hat{z}_j^k\right)]}{\sum_j \mathcal{S}_j \left|u^k\right|^2} ; \mathcal{X}_1 \right) \tag{3}$$

Similarly we have:

$$u^{k+1} = \mathrm{Proj}\left(\frac{\sum_j \mathcal{S}_j^T \left(\left(\omega^{k+1}\right)^* \circ \mathcal{F}^{-1} \hat{z}_j^k \right)}{\sum_j \left(\mathcal{S}_j^T \left|\omega^{k+1}\right|^2 \right)} ; \mathcal{X}_2 \right) . \tag{4}$$

Here S_j^T is an operator mapping its augment to the target position j in image u.

Subproblem z

$$z^{k+1} = \arg\min_{z} \frac{1}{2} \| |z| - f \|_2^2 + \frac{\beta}{2} \left\| z^{+} - \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right) \right\|^2$$

$$= \arg\min_{z} \sum_{x,y,j} [\frac{1}{2}(|z(x,y,j)|^2 - f(x,y,j))^2 + \frac{\beta}{2} ||z(x,y,j) - z^{+}(x,y,j)||^2]$$

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

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

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

Subproblem z

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: $\dfrac{z}{|z|} = \dfrac{z^+}{|z^+|}$, $|z_{x,y,j} - z^+_{x,y,j}|^2 = (|z_{x,y,j}| - |z^+_{x,y,j}|)^2$, $z(x,y,j) = |z_{x,y,j}|\dfrac{z^+(x,y,j)}{|z^+_{x,y,j}|}$

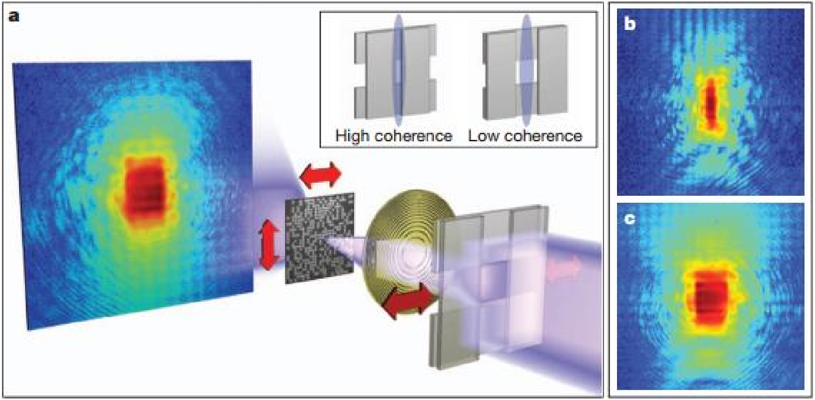
To determine $z_{x,y,j}$, we only need to determine $|z_{x,y,j}|$. Denote it as a.

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

The close form solution of Step 3 is given as:

$$z^{k+1} = \frac{z^+ \dfrac{f}{|z^+|} + \beta z^+}{1+\beta}, \tag{5}$$

New problem: partially coherent



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.

$$\begin{aligned} &\text{Find } u, r\ w_k\ s.t. \\ &f_{pc,j} = \sum_{k=1}^{r} \left| \mathcal{F}\left(\mathcal{S}_j u \circ (\omega_k)\right)\right|^2 \end{aligned} \tag{6}$$

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

Partially coherent model: a general one

Denote $O_j \in C^{m^2 \times m^2}$ as a (diagonal) matrix to represent linear transform to w, s.t. $\mathcal{S}_j u \circ \omega = O_j w$. Denote $f_q^* \in C^{1 \times m^2}$ 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:

$$\begin{aligned} &\text{Find } u, \rho, s.t. \\ &f_{pc,j}(q) = Tr(\mathcal{I}_{j\mathbf{q}}\rho)(1 \le j \le K) \\ &\rho \text{ is positive semi-definite, with rank} \le r \end{aligned} \tag{7}$$

Partially coherent model: a general one

Next, we will explain the derivation of this form.

Simple calculation process:

$$f_{pc,j}(q) = |f_q^* O_j w|^2 = (f_q^* O_j w)^* (f_q^* O_j w) = w^* (O_j^* f_q f_q^* O_j) w$$

$$= Tr[w^* (O_j^* f_q f_q^* O_j) w] = Tr[(O_j^* f_q f_q^* O_j)(ww^*)]$$

$$= Tr(\mathcal{I}_{j\mathbf{q}} \rho), \rho = ww^*$$

Connection to a particular model

Continuous setting:

$$f_{pc,j}(q) = \int \left|\mathcal{F}_{x\to q}\left(\mathcal{S}_j u(x)\omega(x-y)\right)\right|^2 \kappa(y)\mathrm{d}y \tag{8}$$

Discrete setting:

$$f_{pc,j} = \sum_i \kappa_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\mathcal{T}_i\omega)\right)\right|^2 \tag{9}$$

We put the κ_i inside:

$$f_{pc,j} = \sum_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\sqrt{\kappa_i}\mathcal{T}_i\omega)\right)\right|^2 = \sum_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\hat{\omega}_i)\right)\right|^2 \tag{10}$$

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. Then it is exactly (6)

Performance 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 Frobenius norm. *err* measures the difference between a reconstructed image and the groundtruth image. c is an estimated scale factor, and *sum* means the sum of all elements in the target matrix.

2. R-factor R

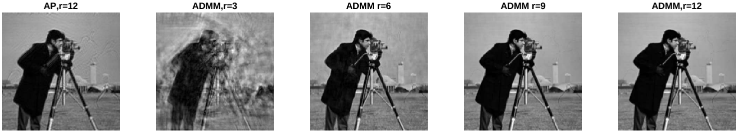
Let $zz = \mathcal{A}_j\left(\omega^k, u^k\right)$

$$R^k := \frac{\||zz| - f\|_1}{\|f\|_1}$$

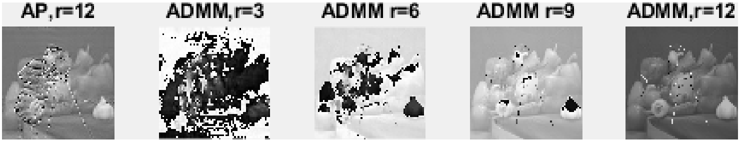
R measures the difference between the reconstruction

Simulation Experiment

$Dist = 8$, regular grid, viberation model, and κ is a guassian kernel with $\sigma = (15, 15)$. $\beta = 0.05$ is chosen as algorithm parameter for ADMM.



(a) Amplitude



(b) Phase

Simulation Experiment

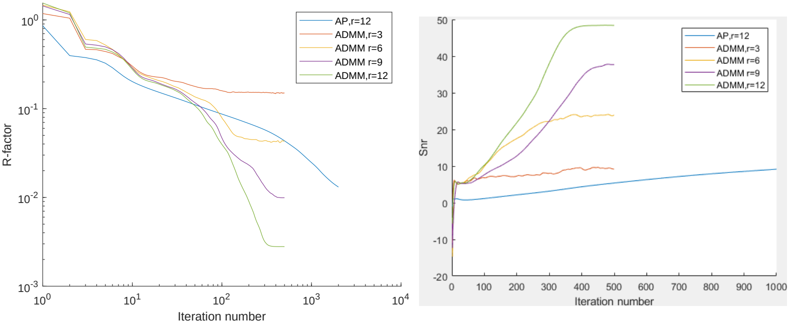


Figure: R and snr.

Simulation Experiment

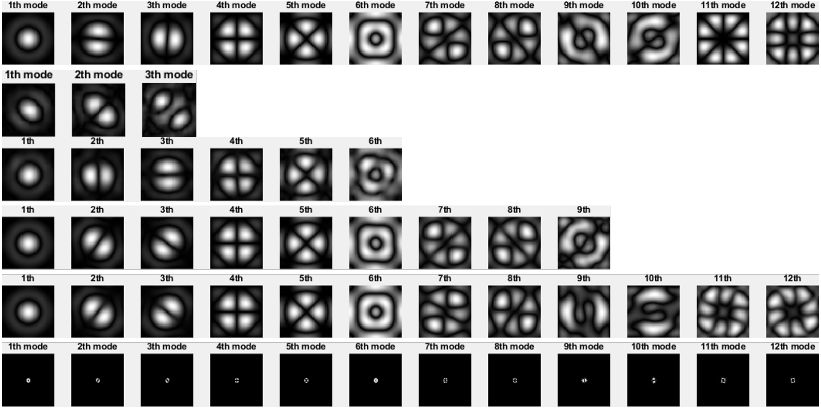


Figure: Mode pattern. The first row represents the standard mode pattern. And the last two rows represent the mode pattern for 12 modes. Mode patterns are in the time domain except that the last row is in the frequency domain.

Discussion

Generally find a low-rank matrix ρ based on (6), which has special structures based on particular models like (9)

Two possible ways:

1. Transfer existing algorithms:

   related to Low-rank Matrix Recovery

2. Exploit new structure:

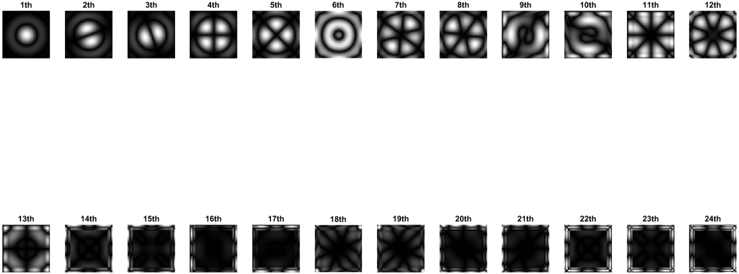
   Rank-1 Matrix + vibration kernel $\kappa \to$ matrix ρ

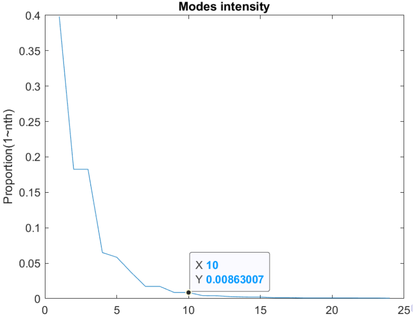
   The rank-1 matrix comes from the main mode (Bessel).

   Why approximated low-rank?

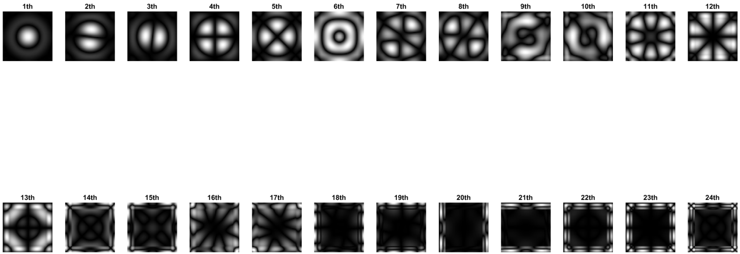
   Why special patterns for modes decomposed from ρ?

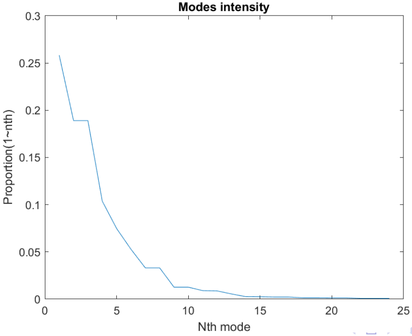
Example: Guassian κ (15 15)



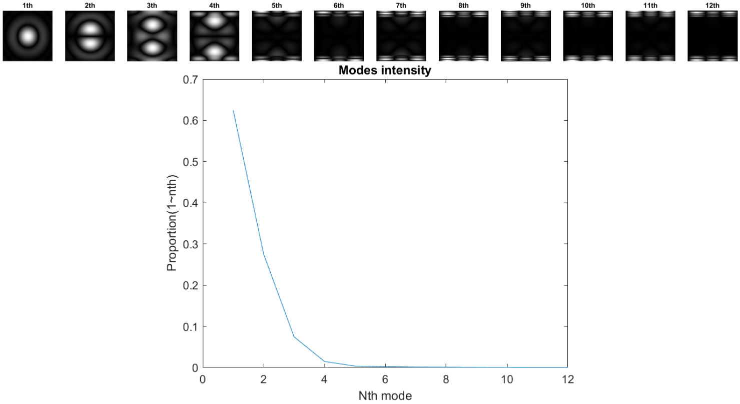


Example: Retangular κ (20 20)

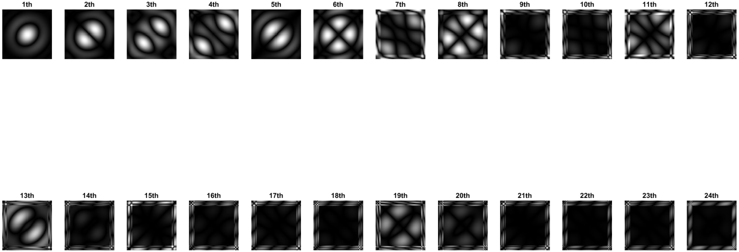


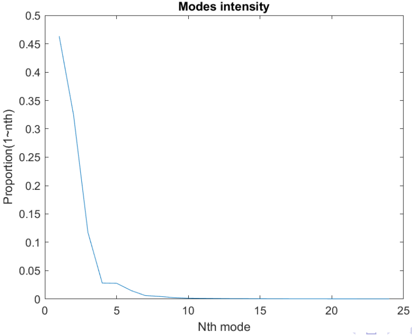


Example: Guassian κ (4 0)



Example: Motion κ (len=20,theta=45)

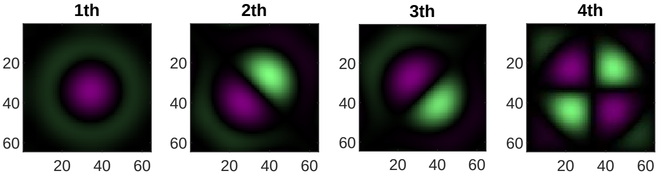


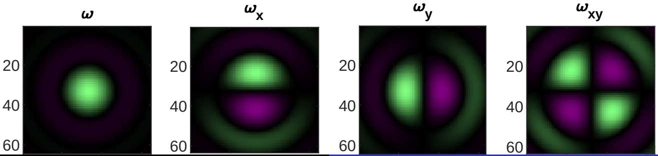


Gradient decomposition

$$f_{pc,j}(q) = \int \left| \mathcal{F}_{x\to q}\left(\mathcal{S}_j u(x)\omega(x-y)\right)\right|^2 \kappa(y)\mathrm{d}y \qquad (11)$$

Expand ω





Thanks!