层叠成像中的相位恢复问题

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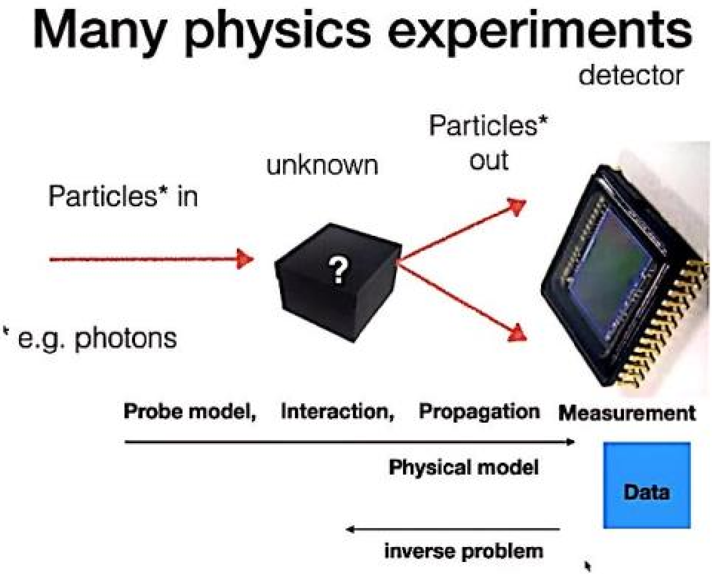
Contents

研究背景


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

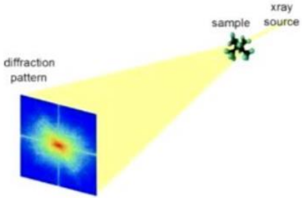


Figure 1: X-Ray Diffraction (Fraunhofer diffraction (far field) $\Rightarrow$ Fourier transform $\mathcal{F}$)

Classical Phase Retrieval

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

层叠成像

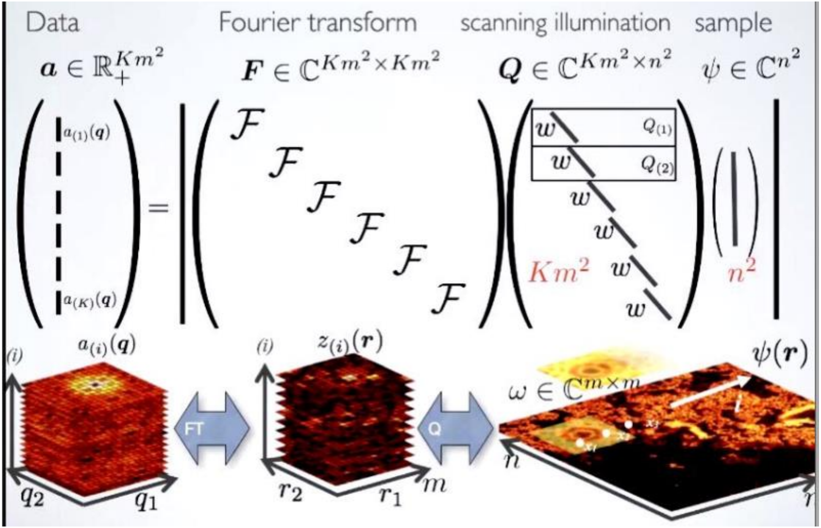
Ptychographic Phase Retrieval

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

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.

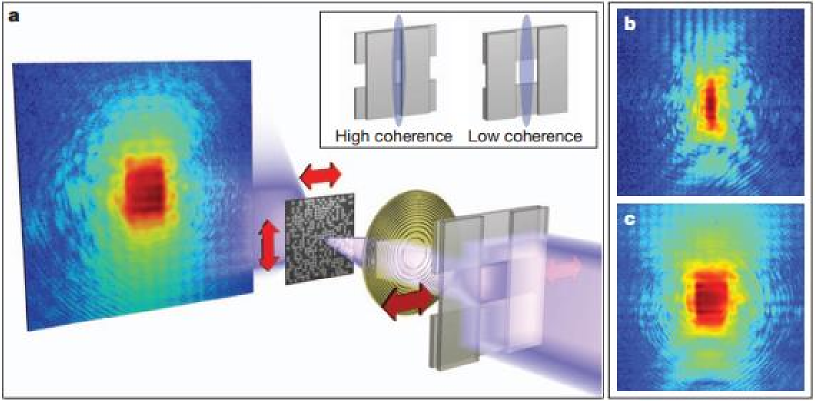
$f_j \in \mathbb{R}_+^{m^2} (\forall 1 \leq j \leq K)$ is a stack of phaseless measurements. Here $|\cdot|$ represents the element-wise absolute value of a vector, o denotes the elementwise multiplication, and $\mathcal{F}$ denotes the normalized 2 dimensional discrete Fourier transform. Each $\mathcal{S}_j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

Ptychographic Phase Retrieval



偏向干层叠成像

New problem: partially coherent



模型

Target model: phobe vibration

Continuous setting:

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

Discrete setting:

$$f_{pc,j} = \sum_i \kappa_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\mathcal{T}_i \omega)\right)\right|^2 \tag{3}$$

Density matrix

$$
\begin{aligned}
f_{pc,j}(q) &= \int \left|\mathcal{F}_{x\to q}\left(\mathcal{S}_j u(x)\omega(x-y)\right)\right|^2 \kappa(y)\mathrm{d}y \\
&= \int\int \mathcal{S}_j u(x_1)e^{-iqx_1}\omega(x_1-y)\overline{\mathcal{S}_j u(x_2)e^{-iqx_2}\omega(x_2-y)}\int \kappa(y)dydx_1dx_2 \\
&= \int\int \mathcal{S}_j u(x_1)e^{-iqx_1}\overline{\mathcal{S}_j u(x_2)e^{-iqx_2}}\left(\int \omega(x_1-y)\overline{\omega(x_2-y)}\kappa(y)dy\right)dx_1dx_2
\end{aligned}
$$

Density matrix in time space:

$$\rho(x_1,x_2) = \int \omega(x_1-y)\overline{\omega(x_2-y)}\kappa(y)dy \tag{4}$$

In discrete setting:

$$\rho = \sum_i \hat{w}_i\hat{w}_i^*, \hat{w}_i = \sqrt{\kappa_i}\mathcal{T}_i\omega \tag{5}$$

$$
\begin{aligned}
f_{pc,j}(q) &= \int \left|\mathcal{F}_{x\to q}\left(\mathcal{S}_j u(x)\omega(x-y)\right)\right|^2 \kappa(y)\mathrm{d}y \\
&= \int\int \mathcal{S}_j u(x_1)\omega(x_1-y)e^{-iqx_1}dx_1 \overline{\int \mathcal{S}_j u(x_2)\omega(x_2-y)e^{-iqx_2}dx_2} \kappa(y)dy \\
&= \int\int \mathcal{S}_j u\widehat{(x_1)e^{-iqx_1}}\omega\widehat{(x_1-y)}dx_1' \overline{\int (\mathcal{S}_j u)\widehat{(x_2)e^{-iqx_2}}\omega\widehat{(x_2-y)}dx_2'} \kappa(y)dy \\
&= \int\int \mathcal{S}_j u\widehat{(x_1)e^{-iqx_1}}\widehat{\omega}(x_1')e^{-iyx_1'}\overline{\mathcal{S}_j u\widehat{(x_2)e^{-iqx_2}}\widehat{\omega}(x_2')e^{-iyx_2'}} \int \kappa(y)dydx_1'dx_2' \\
&= \int\int \widehat{(\mathcal{S}_j u)}(x_1'+q)\widehat{\omega}(x_1')\overline{\widehat{(\mathcal{S}_j u)}(x_2'+q)\widehat{\omega}(x_2')}(\int \kappa(y)e^{-iy(x_1'-x_2')}dy) \\
&= \int\int \widehat{(\mathcal{S}_j u)}(x_1'+q)\overline{\widehat{(\mathcal{S}_j u)}(x_2'+q)}(\hat{\kappa}(x_1'-x_2')\widehat{\omega}(x_1')\overline{\widehat{\omega}(x_2')})dx_1'dx_2'
\end{aligned}
$$

Density matrix in Fourier space:

$$\widehat{\rho}(x_1', x_2') = \int\int \rho(x_1, x_2) e^{-ix_1x_1'} e^{-ix_2x_2'} dx_1' dx_2' = \hat{\kappa}(x_1' - x_2') \widehat{\omega}(x_1') \overline{\widehat{\omega}(x_2')} \tag{6}$$

In discrete setting:

$$\hat{\rho} = F \rho F^* = \hat{\kappa}. * (\hat{\omega}\hat{\omega}^*) \tag{7}$$

ρ is psd, and so is $\hat{\rho}$. Use truncated SVD to get a low-rank approximation:

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

General model

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

Blind ptychography model + quantum state tomography.

Phobe w is assumed to be in mixed state to represent partially coherent effect.

$$\text{Find } u, r\ w_k\ s.t.$$
$$f_{pc,j} = \sum_{k=1}^{r} \left| \mathcal{F}\left(\mathcal{S}_j u \circ (\omega_k)\right)\right|^2 \tag{8}$$

算法

1. optimization problem

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

2. Reformulation: $\min \sum_{j=1}^{K} \frac{1}{2} \left\| \sqrt{\sum_{i=1}^{r} |z_{j,i}|} - f_j \right\|_2^2$
, s.t. $z_{j,i} = \mathcal{A}_j(\omega_i, u) := \mathcal{F}\left(\omega_i \circ \mathcal{S}_j u\right), j = 1...K$

3. Combine
$z_i = \mathcal{A}(\omega_i, u) := \left(\mathcal{A}_1^T(\omega_i, u), \mathcal{A}_2^T(\omega_i, u), ..., \mathcal{A}_K^T(\omega_i, u)\right)^T \in \mathbb{C}^{Km^2}$,
$f := (f_1^T, f_2^T, \ldots, f_K^T)^T$; $z = (z_1^T, z_2^T, ..., z_r^T)^T \in \mathbb{C}^{Krm^2}$

$$\min \mathcal{G}(z) := \frac{1}{2} \left\| \sqrt{\sum_{i=1}^{r} |z_i|} - f \right\|_2^2, \text{ s.t. } z_i = \mathcal{A}(\omega_i, u), i = 1, ..., r$$

ADMM(Alternating Direction Method Of Multipliers)

$$
\begin{aligned}
&\min_{\omega,u,z} \mathcal{G}(z) + \mathbb{I}_{\mathcal{X}_1}(\omega) + \mathbb{I}_{\mathcal{X}_2}(u) + \mathbb{I}_{\mathcal{X}_3}(D\alpha) \\
&s.t. \quad z - \mathcal{A}(\omega, u) = 0, \quad \Omega(D\alpha) - \omega = 0.
\end{aligned}
\tag{9}
$$

The corresponding augmented Lagrangian reads

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

$$\text{Step 1: } \omega^{k+1} = \arg\min_{\omega} \frac{\beta}{2}\|z - \mathcal{A}(\omega, u) + \Lambda\|^2 + \tag{10}$$

$$\frac{\beta_2}{2}||\omega - (\Omega(D^k\alpha^k) + \Lambda_2)||^2 + \frac{\alpha_1}{2}\left\|\omega - \omega^k\right\|_{M_1^k}^2,$$

$$\text{Step 2: } u^{k+1} = \arg\min_{u} \frac{\beta}{2}\|z - \mathcal{A}(\omega, u) + \Lambda\|^2 + \frac{\alpha_2}{2}\left\|u - u^k\right\|_{M_2^k}^2,$$

$$\text{Step 3: } z^{k+1} = \arg\min_{z} \frac{\beta}{2}\|z - \mathcal{A}(\omega, u) + \Lambda\|^2,$$

$$\text{Step 4: } D^{k+1} = \arg\min_{D} \mathbb{I}_{\mathcal{X}_3}(D\alpha) + \frac{\beta_2}{2}\|\Omega(D^k\alpha^k) - \omega^{k+1}\|^2$$

$$\text{Step 5: } \alpha^{k+1} = \arg\min_{\alpha} \frac{\beta_2}{2}\|\Omega(D^{k+1}\alpha^k) - \omega^{k+1}\|^2$$

$$\text{Step 6: } \Lambda^{k+1} = \Lambda^k + \left(z^{k+1} - \mathcal{A}\left(\omega^{k+1}, u^{k+1}\right)\right) \tag{11}$$

$$\text{Step 7: } \Lambda_2^{k+1} = \Lambda_2^k + (\Omega(D^{k+1}\alpha^{k+1}) - \omega^{k+1}) \tag{12}$$

Subproblems ω and u

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

The close form solution of Step 1 is given as:

$$
\omega^{k+1} = \mathrm{Proj}\left(\frac{\beta\sum_j\left(\mathcal{S}_j u^k\right)^* \circ \left[\left(\mathcal{F}^{-1}\hat{z}^k\right)(:,:,j,:)\right]+\beta_2\hat{\Omega}^k}{\beta\sum_j\left|\mathcal{S}_j u^k\right|^2+\beta_2};\mathcal{X}_1\right) \tag{13}
$$

$$
u^{k+1} = \mathrm{Proj}\left(\frac{\sum_{j,i}\mathcal{S}_j^T\left(\left(\omega_i^{k+1}\right)^*\circ\mathcal{F}^{-1}\hat{z}_{j,i}^k\right)}{\sum_{j,i}\left(\mathcal{S}_j^T\left|\omega_i^{k+1}\right|^2\right)};\mathcal{X}_2\right). \tag{14}
$$

Subproblem z

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

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

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

The close form solution of Step 3 is given as:

$$z_i^{k+1} = \frac{z_i^+ \dfrac{Y}{M^k} + \beta z_i^+}{1+\beta}, 1 \le i \le r \tag{15}$$

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

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

The close form solution for D^{k+1} is:

$$D^{k+1} = UV^* \tag{16}$$

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

The close form solution for α^{k+1} is:

$$\alpha_i^{k+1} = \sum_{i_0} \Re[\overline{D^{k+1}(i_0, i)}\hat{w}^{k+1}(i_0, i)](1 \leq i \leq r) \tag{17}$$

数值实验

Experiment setting

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(3)

Performance Metrics

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

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

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

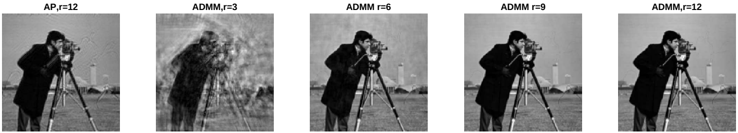
c is an estimated scale factor

2. R-factor R

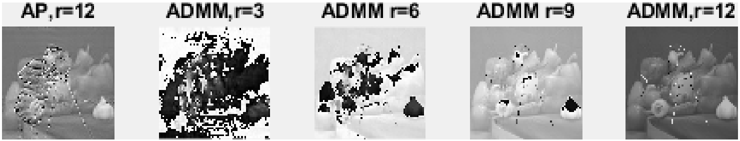
Let $zz = \mathcal{A}_j\left(\omega^k, u^k\right)$

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

Simulation Experiment



(a) Amplitude



(b) Phase

Simulation Experiment

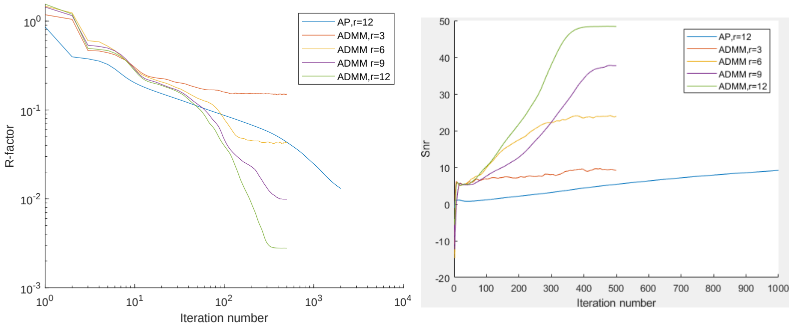


Figure: R and snr.

Simulation Experiment

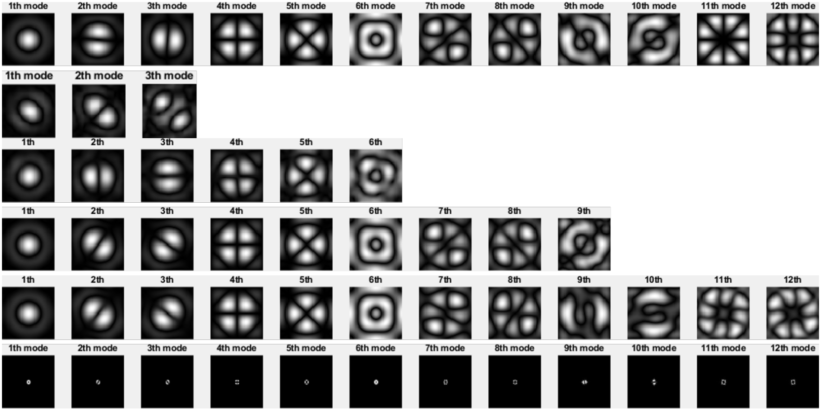


Figure: Mode pattern

Add the orthogonal constraint

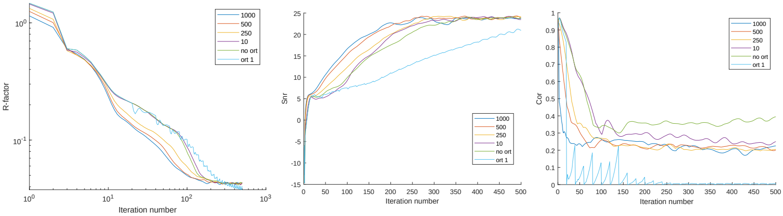


Figure: The vertical axis and horizontal axis are set in log-scale in the first subfigure for R-factor. The blue line represents $\beta_2/\beta = 1000$ and works the best in this case. The green line represents the result without orthogonalization. 'ort 1' means performing orthogonalization every 20 iterations.

总结和讨论

Conclusion

主要贡献：

验证了将目标模型放入通用模型框架下求解合理而且有效

1. 模型：具体刻画了目标模型密度矩阵的结构，将它放入通用模型的框架中
2. 算法：改进了求解通用模型的相位恢复算法。将多模态AP改进为多模态的ADMM; 尝试在里面加入对不同模态的正交约束
3. 实验：用模型生成仿真数据进行数值实验，并与传统AP 的计算结果和基于模型得到的“标准答案”进行对比，验证的算法的有效性

Discussion

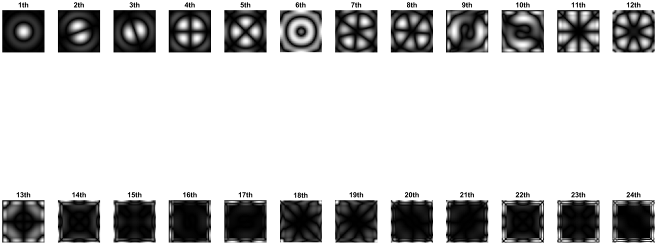
不足：

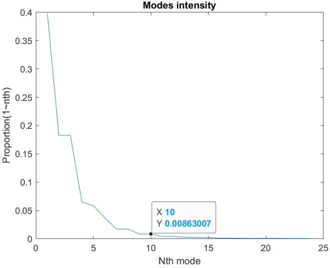
通用模型可以求解任何近似$rank-r$ 的密度矩阵，而我们目标模型中的密度矩阵结构更特殊：一个toeplitz 矩阵与一个秩一矩阵逐个元素相乘。没有利用到里面的特殊结构十分可惜。

$$\widehat{\rho}(x_1', x_2') = \hat{\kappa}(x_1' - x_2')\widehat{\omega}(x_1')\overline{\widehat{\omega}(x_2')}$$

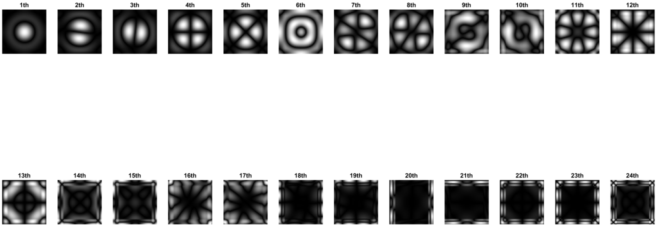
$$\hat{\rho} = F\rho F^* = \hat{\kappa}.*(\hat{\omega}\hat{\omega}^*)$$

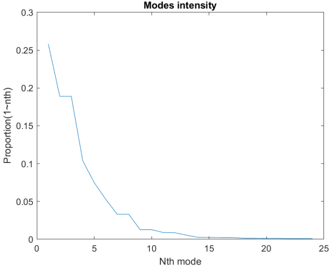
Example: Guassian κ (15 15)



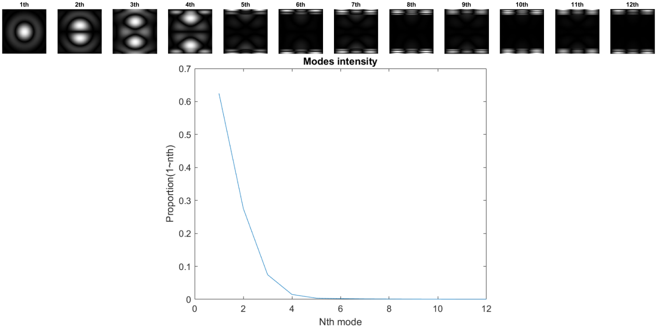


Example: Retangular κ (20 20)

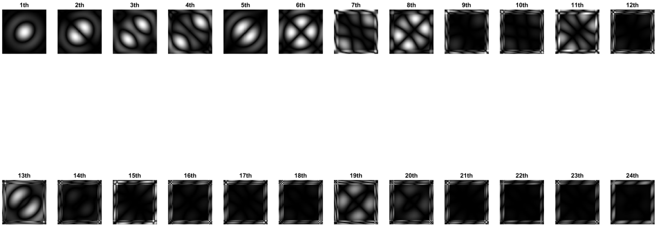


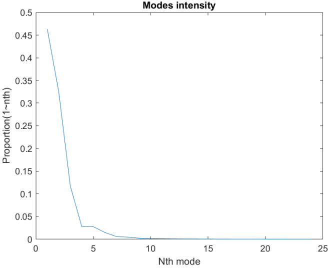


Example: Guassian κ (4 0)



Example: Motion κ (len=20,theta=45)





Thanks!