DIMENSIONALITY AUGMENTATION FOR PHASE RETRIEVAL WITH APPLICATIONS

Projection-based algorithms for high NA case and ...?

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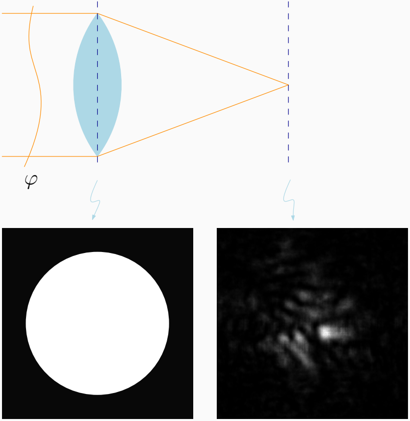
INTRODUCTION

PHASE RETRIEVAL PROBLEM FORMULATION

Only absolute values $|x|$ any $y = |\mathcal{F}x|$ of some signal x and its Fourier transform are known. Find the signal.

$$\text{find } x \in \mathbb{C}^M : \; y = |\mathcal{F}x| \tag{1}$$

Recovering wavefront aberration through the PSF
a.k.a. "Indirect wavefront sensing"



$a(\mathbf{x})$ $I(\xi)$

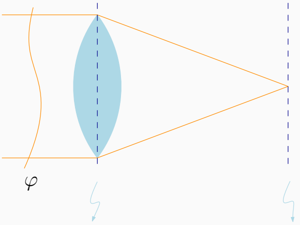
$$I(\boldsymbol{\xi}) = \left| \mathcal{F}_2 \left(a(\boldsymbol{x}) e^{i\varphi(\boldsymbol{x})} \right) \right|^2$$

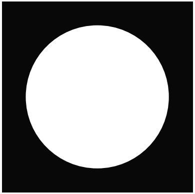
Known information: amplitude (via the intensity) in the pupil and focal planes

Unknown: phase of the field in these plains

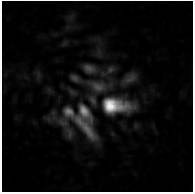
PHASE RETRIEVAL IN OPTICS

Recovering wavefront aberration through the PSF
a.k.a. “Indirect wavefront sensing”





$a(\mathbf{x})$



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Known information: amplitude (via the intensity) in the pupil and focal planes

Unknown: phase of the field in these plains

“The most used algorithm”[a]
Gerchberg and Saxton (1972),
rediscovered by Gonsalves (1976).

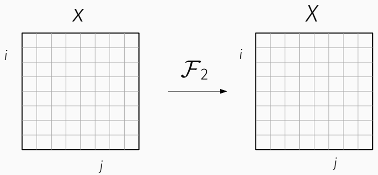
[a] M. A. Fiddy and U. Shahid, “Legacies of the Gerchberg-Saxton algorithm”, *Ultramicroscopy*, **134**, pp. 48–54, 2013.

GERCHBERG, SAXTON, FIENUP

Fig. 1. Owen Saxton (centre) with Ralph Gerchberg (left) and James Fienup (right). Courtesy of James Fienup.

[1] P. W. Hawkes, “A distinguished trio, introduction to the Saxton-Smith-Van Dyck 65th-birthday issue,” *Ultramicroscopy*, **134**, pp. 2–5, 2013.

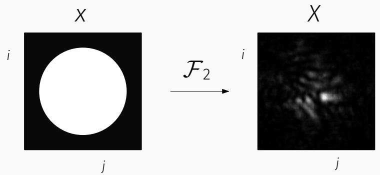
In another form



$$\begin{cases} X = \mathcal{F}_2\, x \\ p = |X| \\ a = |x| \end{cases}, \qquad (2)$$

where $x, X \in \mathbb{C}^{I \times J}$

In another form



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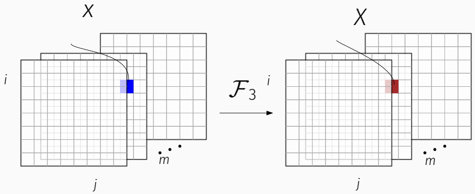
where $x, X \in \mathbb{C}^{I \times J}$

Two amplitudes are known
Both phases are unknown

GENERALISATION TO PR OF HIGHER DIMENSIONS

Easy generalisation to higher dimensions:

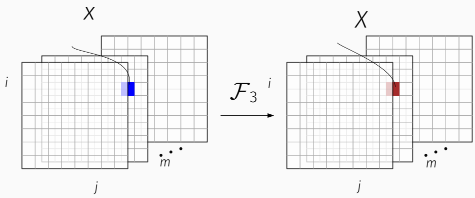


$$\begin{cases} X = \mathcal{F}_3\, x \\ p = |X| \\ a = |x| \end{cases}, \qquad (3)$$

where $x, X \in \mathbb{C}^{I \times J \times M}$

3D phase retrieval problem (aka *phase-diverse phase retrieval*)

Easy generalisation to higher dimensions:



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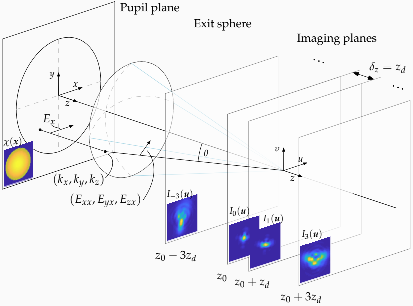
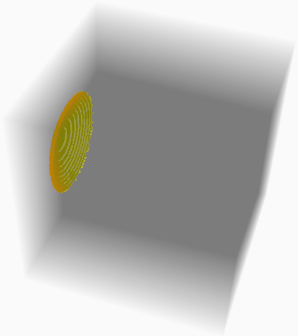
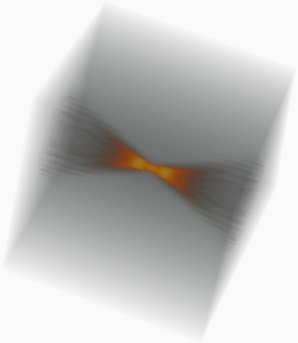
In optics, PR *is* 3D problem
$U(\boldsymbol{r}) = \int A(\boldsymbol{k}) e^{i(k_x x + k_y y + k_z z)} \mathrm{d}\boldsymbol{k}$, where
$|\boldsymbol{k}| = \frac{2\pi}{\lambda}$
Near $z = z_0$, finite size of the aperture introduces limitation $k_x^2 + k_y^2 \leq \mathrm{NA}^2$



EXAMPLE OF 3D PR PAIR





Superposition of plane waves of unit amplitude with the wave vector belonging to a "spherical cap" approximates 3D PSF near focus

$I = J = M = 128$

[1] C. W. McCutchen. *Generalized Aperture and the Three-Dimensional Diffraction Image.* J. Opt. Soc. Am., 54(2):240, 1964

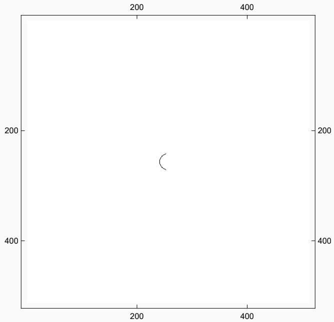
[2] C. W. McCutchen. *Generalized Aperture and the Three-Dimensional Diffraction Image:erratum.* J. Opt. Soc. Am., 19(8):1721, 2002

3D transform is reduced to 2D

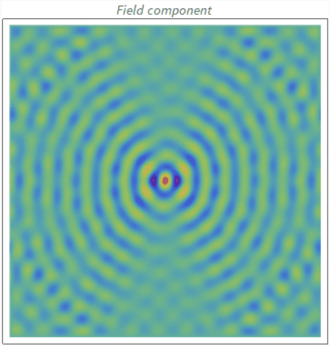
2D PR is originally 3D PR

Support is sparse in $z \Rightarrow \mathcal{F}_3$ can be reduced to $\mathcal{F}_2$ (substitute $k_z = k_z(k_x, k_y) = \sqrt{\left(\frac{2\pi}{\lambda}\right)^2 - k_x^2 - k_y^2}$, with $k_x^2 + k_y^2 \leq \mathrm{NA}^2$)

This can also provide insight on the *phase diverse phase retrieval* or used for PSF simulation along the z-axis



$\xrightarrow{\mathcal{F}_2}$



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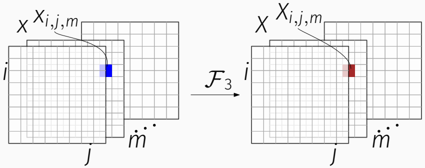

"Coherent" 3D phase retrieval — for $z = z_0$ (or $m = 0$), 2D PSF is the square of the absolute value of sum of (complex-valued) F_2 of each layer

Two superimposed fields U_a, U_b, only intensity is measurable:
$I_a \propto |U_a|^2$, $I_b \propto |U_b|^2$, total intensity is:

Coherent	Incoherent
$I = I_a + I_b + 2\sqrt{I_a I_b}\cos(\Delta\phi)$	$I = I_a + I_b$

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For PSFs as $p = |h|^2$:

$$p_c = |h_1 + h_2|^2 \qquad p_i = |h_1|^2 + |h_2|^2$$

Examples of incoherent sum of PSFs: different sources, different wavelengths, different polarisations

IMAGE FORMATION: SCALAR VS VECTOR DIFFRACTION

PSF FROM PHASE, SCALAR DIFFRACTION THEORY

Scalar light theory:

$$p_\varphi = \left| \mathcal{F}\, a e^{i\varphi} \right|^2, \qquad (4)$$

so input for the phase retrieval problem is

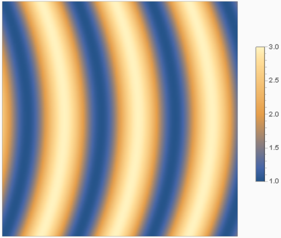
$$y = \sqrt{p_\varphi}, \qquad (5)$$

and it looks for $x : y = |\mathcal{F} x|$,

$$x = a e^{i\varphi}. \qquad (6)$$

$\varphi = \arg x$, hence the name.

Scalar wave example



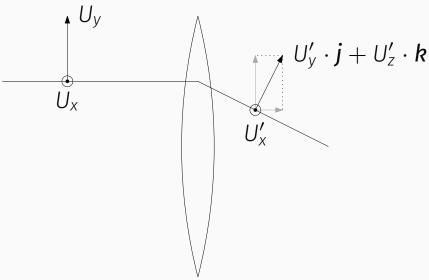
$U(\mathbf{r}, t)$
E.g. sound wave

It can be used as approximation for electromagnetic waves for *small NA values* (that is small angles)

PSF FROM PHASE — HIGH NA CASE, LINEAR POLARISATION

Vector nature of light cannot be neglected for high NA values
$\boldsymbol{U}(\boldsymbol{r},t) = (U_x(\boldsymbol{r},t), U_y(\boldsymbol{r},t), U_z(\boldsymbol{r},t))$

Transverse wave[a] in z direction $\boldsymbol{U}$ before the lens, $\boldsymbol{U'}$ after the lens



[a] $U_z = 0$

$x-$ and $y-$ linear polarizations $E_x = (1,0,0)$ and $E_y = (0,1,0)$ in the entrance pupil after lens change to[1]:

$$
\begin{aligned}
E_{xx} &= 1 - \frac{\sigma_x^2}{1+\sigma_z}, & E_{xy} &= 1 - \frac{\sigma_x \sigma_y}{1+\sigma_z}, \\
E_{yx} &= -\frac{\sigma_x \sigma_y}{1+\sigma_z}, & E_{yy} &= -\frac{\sigma_y^2}{1+\sigma_z}, \\
E_{zx} &= -\sigma_x, & E_{zy} &= -\sigma_y,
\end{aligned}
\tag{7}
$$

where (σ_x, σ_y) are normalised to NA coordinates in the pupil, and $\sigma_z(\sigma_x, \sigma_y) = \sqrt{1 - \sigma_x^2 - \sigma_y^2}$.

Note via duality ray/plane wave $(k_x, k_y, k_z) = \frac{2\pi}{\lambda}(\sigma_x, \sigma_y, \sigma_z)$

[1] M. Mansuripur, *Classical Optics and Its Applications* (Cambridge University Press, 2009).

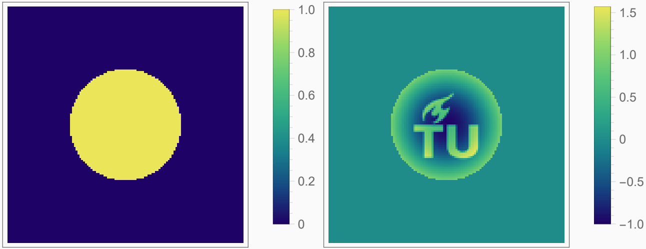
Each of the right-hand-side terms in Eq. (7) can be treated as corresponding amplitude modulation in the entrance pupil for calculation of a PSF with the scalar Fourier method:

$$p_i = \left|\mathcal{F}\left(E_i e^{i\phi + i z_d k_z}\right)\right|^2, \tag{8}$$

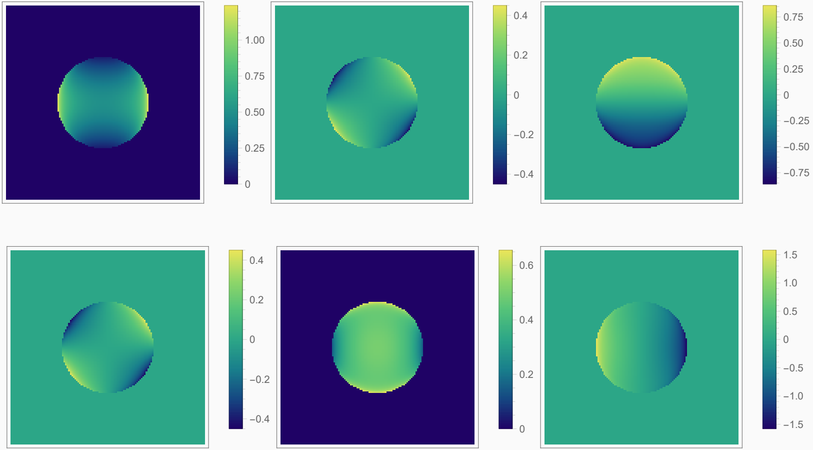
where index i is one of the 6 pairs xx, yx, zx, xy, yy, zy.

One obtains thus 6 PSFs $p_{xx}, p_{yx}, p_{zx}, p_{xy}, p_{yy}, p_{zy}$ which can be used to calculate the *vector* PSF corresponding for any linear polarisation in the entrance pupil. For unspecified polarisation state, all 6 PSFs are summed incoherently:

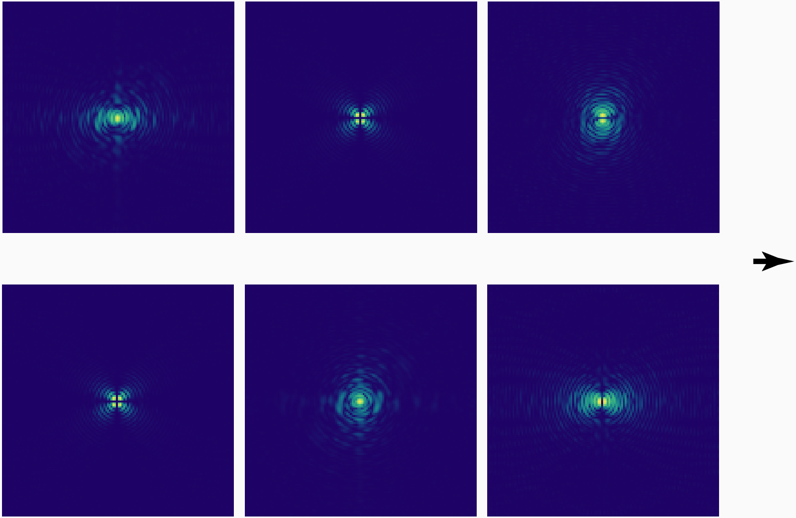
$$p = \sum_i p_i. \tag{9}$$


1.0
0.8
0.6
0.4
0.2
0
1.5
1.0
0.5
0
−0.5
−1.0

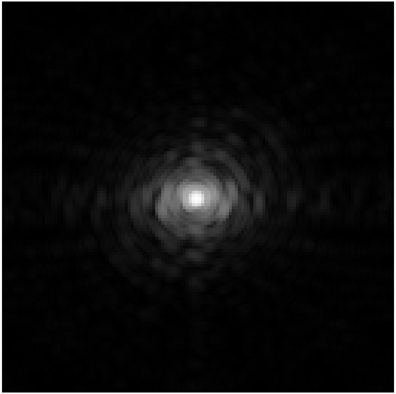
EXAMPLE NA=0.95: APERTURE APODISATIONS



EXAMPLE NA=0.95: PSFS $p_{xx}, p_{yx}, p_{zx}, p_{xy}, p_{yy}, p_{zy}$



EXAMPLE NA=0.95: "VECTOR" PSF



FROM AMPLITUDE CONSTRAINT TO VECTOR NORM CONSTRAINT

Two different polarisation states in the pupil; they do not interfere $\Rightarrow$ measured PSF is incoherent sum of 2D PSFs

Now the 2D phase retrieval problem becomes:

Find $\varphi \in \mathbb{R}^{I \times J}$, if $y, a_1, \ldots, a_M \in \mathbb{R}^{I \times J}$ are known:

$$y^2 = \left| \mathcal{F}_2\, a_1 \mathrm{e}^{\mathrm{i}\varphi} \right|^2 + \ldots + \left| \mathcal{F}_2\, a_M \mathrm{e}^{\mathrm{i}\varphi} \right|^2 \tag{10}$$

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Consider $v = [\mathcal{F}_2\, a_1 \mathrm{e}^{\mathrm{i}\varphi}, \ldots, \mathcal{F}_2\, a_M \mathrm{e}^{\mathrm{i}\varphi}]$. Then Eq. (10) is equivalent to:

$$y^2 = \|v\|_2^2 = \|\mathcal{F}_1\, v\|_2^2 , \tag{11}$$

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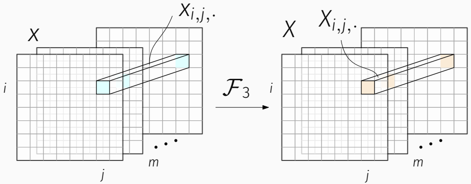
and $\mathcal{F}_1\, v = \mathcal{F}_1([\mathcal{F}_2\, a_1 e^{i\varphi}, \ldots, \mathcal{F}_2\, a_M e^{i\varphi}]) = \mathcal{F}_3([a_1 e^{i\varphi}, \ldots, a_M e^{i\varphi}])$.



Incoherent 3D PR problem

$$\begin{cases} X = \mathcal{F}_3\, x \\ p_{i,j} = \left\|X_{i,j,\cdot}\right\|_2^2 \\ a = |x| \\ \arg x_{i,j,1} = \ldots = \arg x_{i,j,M} \end{cases}, \tag{12}$$

where $x, X \in \mathbb{C}^I \times \mathbb{C}^J \times \mathbb{C}^M$

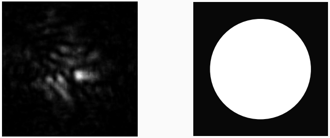
Relaxed constraints on X and additional constraint on x

Also generalisation of scalar PR (with $M = 1$) $\longrightarrow$ we can try to generalise the approach used for 2D PR (demonstrated on “the most used algorithm”)

Iterations $x^k \to X^k \to x^{k+1}, \quad k = 1, 2, \ldots$

PHASE RETRIEVAL AND GS

THE MOST USED ALGORITHM



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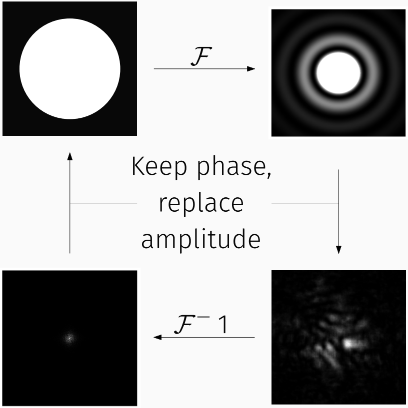
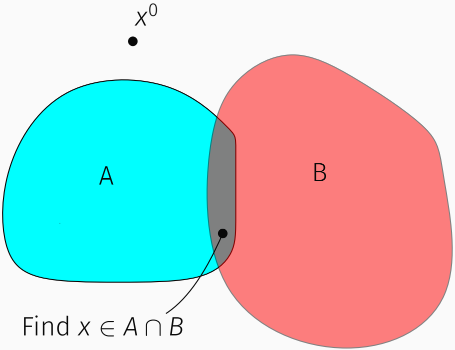
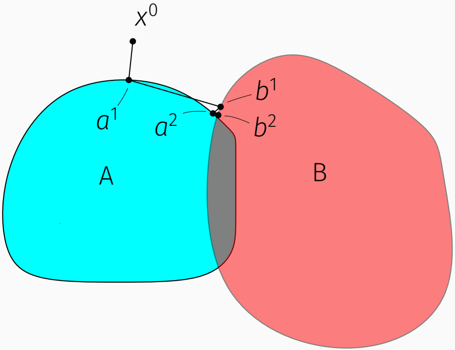


Repeat until convergence



$$A = \{x \in \mathbb{C}^{M\times M} : |x| = p\}$$
$$B = \{x \in \mathbb{C}^{M\times M} : |\mathcal{F}x| = P\}$$
Find $x \in A \cap B$

1) just any would do
2) closest to x^0



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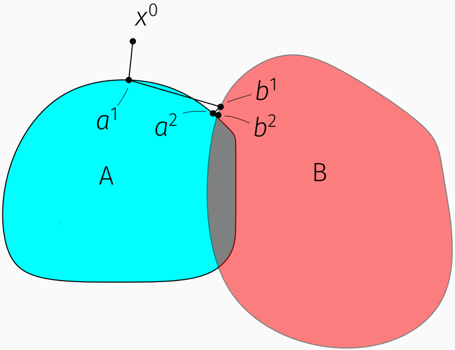
$\dots$
$b^k = \mathrm{Pr}_B\, a^k, a^{k+1} = \mathrm{Pr}_A\, b^k$

- Von Neumann: A, B — convex $\Longrightarrow$ use alternating projections



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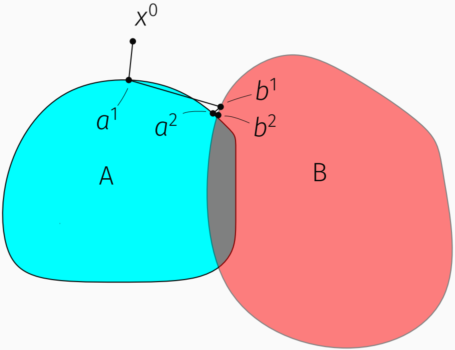
- Kruger, Luke, Thao [1]: A, B should be (sub)transversal

[1] Kruger, A.Y., Luke, D.R., and Thao, N.H. *Set regularities and feasibility problems.* Math. Program. 168, 279–311 (2018)



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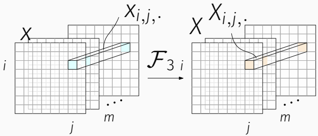
- Von Neumann: A, B — convex $\Longrightarrow$ use alternating projections
- Kruger, Luke, Thao [1]: A, B should be (sub)transversal
- The sets in PR problem are transversal

[1] Kruger, A.Y., Luke, D.R., and Thao, N.H. *Set regularities and feasibility problems.* Math. Program. 168, 279–311 (2018)

vector GS (we need only to update the projections)

$x^k \to X^k$:

$$\hat{X}^k = \mathcal{F}_3 \, x^k \tag{13}$$



$$p_{i,j} = \left\| X_{i,j,.} \right\|_2^2$$

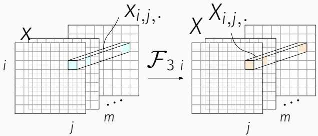
The feasible set defined as Cartesian product of 2M-dimensional spheres

$x^k \to X^k$:

$$\hat{X}^k = \mathcal{F}_3\, x^k \tag{13}$$

This projection is easy to realise — just normalise vector $\hat{X}_{i,j,\cdot}$:

$$X^k_{i,j,\cdot} = \hat{X}^k_{i,j,\cdot} \cdot \frac{\sqrt{p_{i,j}}}{\left\|\hat{X}^k_{i,j,\cdot}\right\|_2}. \tag{14}$$



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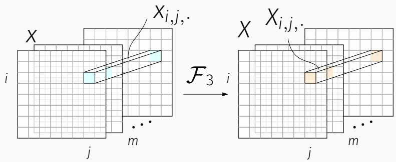
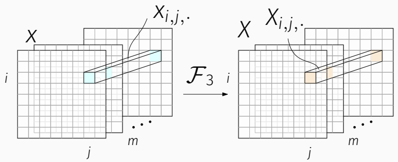


The feasible set defined as Cartesian product of real vector multiplied by a unit complex number

$X^k \to x^{k+1}$:

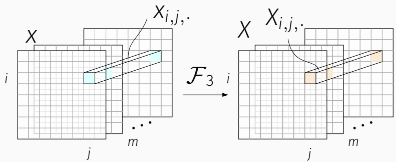
$$\hat{x}^{k+1} = \mathcal{F}_3^{-1} X^k \tag{15}$$



The feasible set defined as Cartesian product of real vector multiplied by a unit complex number

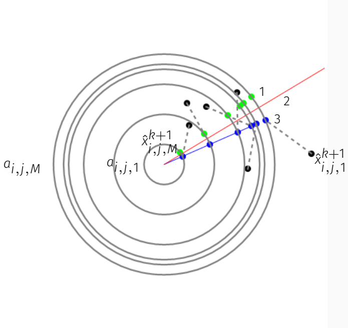
$X^k \to x^{k+1}$:

$$\hat{x}^{k+1} = \mathcal{F}_3^{-1} X^k \qquad (15)$$



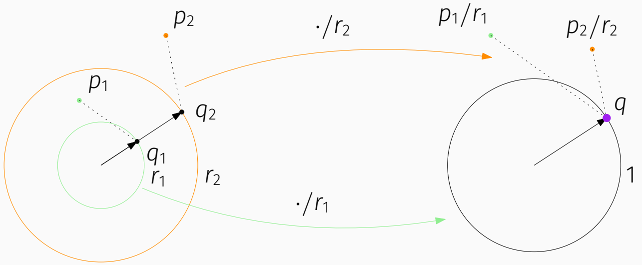
The feasible set defined as Cartesian product of real vector multiplied by a unit complex number

Now some projection point-wise on circles with radii a.

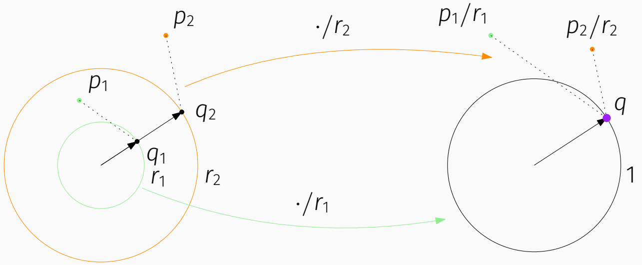


Possible projections

SOLUTION IN THE PUPIL PLANE: LEAST-SQUARES



$$\|p_1 - q_1\|^2 + \|p_2 - q_2\|^2 = (r_1)^2 \|p_1/r_1 - q\|^2 + (r_2)^2 \|p_2/r_2 - q\|^2 \to \min_{q, |q|=1} \quad (16)$$



$$\|p_1 - q_1\|^2 + \|p_2 - q_2\|^2 = (r_1)^2 \|p_1/r_1 - q\|^2 + (r_2)^2 \|p_2/r_2 - q\|^2 \to \min_{q, |q|=1} \quad (16)$$

$$q_0 = \hat{q}/|\hat{q}|, \ \hat{q} = \frac{r_1 p_1 + r_2 p_2}{(r_1)^2 + (r_2)^2} \quad (17)$$

Eq. (16) is the minimiasation of the moment of two-point system with masses r_1^2, r_2^2 in $p_1/r_1, p_2/r_2$, hence q_0 is the closest point on the unit circle to its COG point $\hat{q}$

For a general case:

$$\varphi_{i,j,\cdot}^{k+1} = \arg \frac{\sum_m a_{i,j,m} \cdot \hat{x}_{i,j,m}^{k+1}}{\sum_m a_{i,j,m}^2} \tag{18}$$

and

$$x_{i,j,m}^{k+1} = a_{i,j,m} \mathrm{e}^{\mathrm{i}\varphi_{i,j,\cdot}^{k+1}} \tag{19}$$

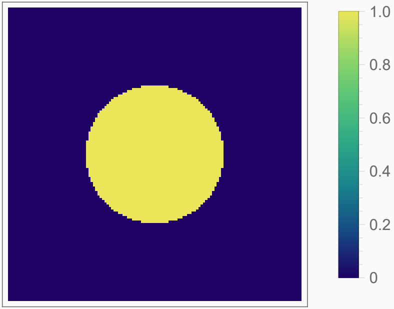
Note: this is the Gonsalves formula / Wiener filter often used in multiframe deconvolution, for instance:

$$I_n = O \cdot H_n \ \Rightarrow O = \frac{\sum_n I_n \cdot H_n^\dagger}{\sum_n H_n \cdot H_n^\dagger} \tag{20}$$

It's easy to show it's a projection (on Cartesian product of 1D complex linear spaces)

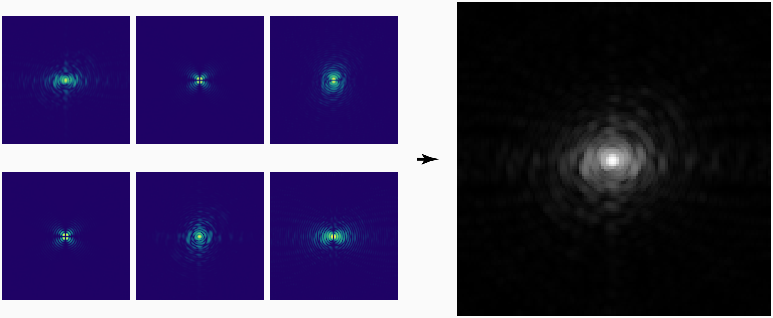
EXAMPLES AND CONCLUSIONS

Input obtained as vectorial PSF (NA = 0.95), 2000 iterations, noiseless case:

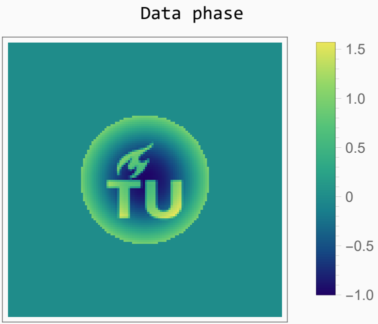


Example 1: High-NA PSF

Input obtained as vectorial PSF (NA = 0.95), 2000 iterations, noiseless case:

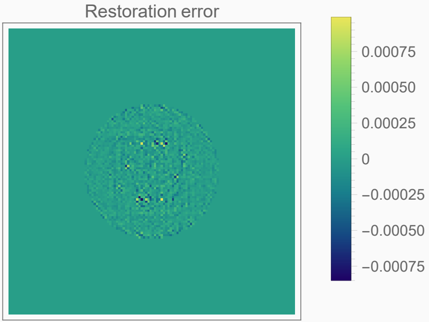


Input obtained as vectorial PSF (NA = 0.95), 2000 iterations, noiseless case:



EXAMPLE 1: HIGH-NA PSF

Input obtained as vectorial PSF (NA = 0.95), 2000 iterations, noiseless case:



More details and more advanced algorithms are provided in [1] and [2]

[1] N. Hieu Thao, O. Soloviev, and M. Verhaegen, *Phase retrieval based on the vectorial model of point spread function,* J. Opt. Soc. Am. A 37, 16 (2020).

[2] N. Hieu Thao, O. Soloviev, R.Luke, and M. Verhaegen, *Projection methods for high numerical aperture phase retrieval,* Inverse Problems 37 (12), 125005 (2021).

OTHER APPLICATIONS OF INCOHERENT PHASE RETRIEVAL

The method can be extended to other incoherent sums (all work in progress), like

- multiple wavelengths
- multiple apertures
- multiple sources

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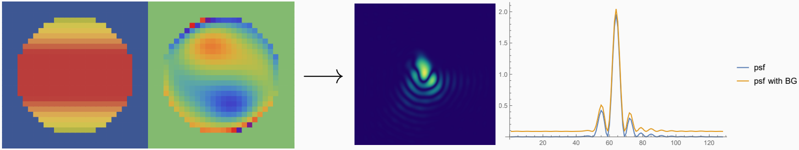
- multiple wavelengths
- multiple apertures
- multiple sources

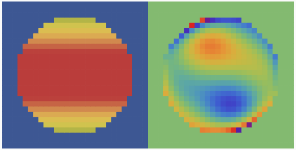
even without apparent “physical meaning”, like in the following example

EXAMPLE 2: LOW-NA PSF + UNKNOWN BACKGROUND

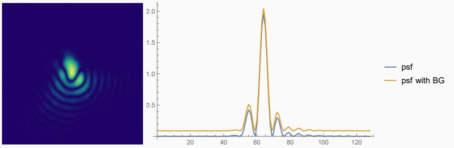


$$I(\boldsymbol{u}) = \left|\mathcal{F}_2\left(a(\boldsymbol{x})e^{i\varphi(\boldsymbol{x})}\right)\right|^2 + b$$

EXAMPLE 2: LOW-NA PSF + UNKNOWN BACKGROUND

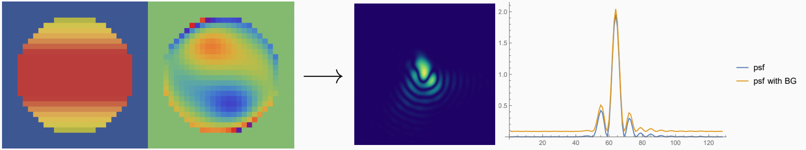


$\longrightarrow$



$$I(\boldsymbol{u}) = \left|\mathcal{F}_2\left(a(\boldsymbol{x})e^{i\varphi(\boldsymbol{x})}\right)\right|^2 + b = \left|\mathcal{F}_2\left(a(\boldsymbol{x})e^{i\varphi(\boldsymbol{x})}\right)\right|^2 + \left|\mathcal{F}_2\left(\sqrt{b}\,\delta(\boldsymbol{x})e^{i\varphi(0)}\right)\right|^2$$

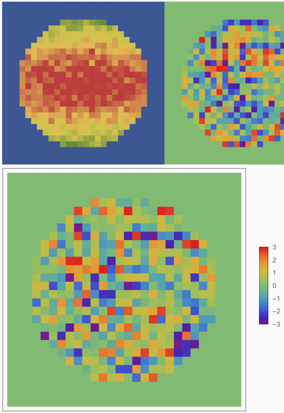
EXAMPLE 2: LOW-NA PSF + UNKNOWN BACKGROUND



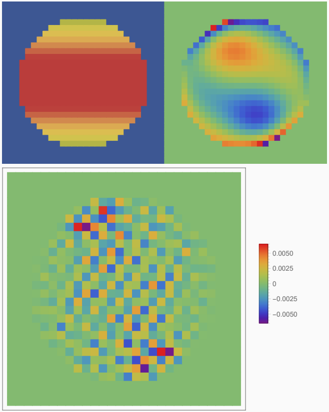
$$I(\boldsymbol{u}) = \left|\mathcal{F}_2\left(a(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\varphi(\boldsymbol{x})}\right)\right|^2 + b = \left|\mathcal{F}_2\left(a(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\varphi(\boldsymbol{x})}\right)\right|^2 + \left|\mathcal{F}_2\left(\sqrt{b}\delta(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\varphi(0)}\right)\right|^2$$

Original pupil function + δ-function modulated aperture, the same algorithm

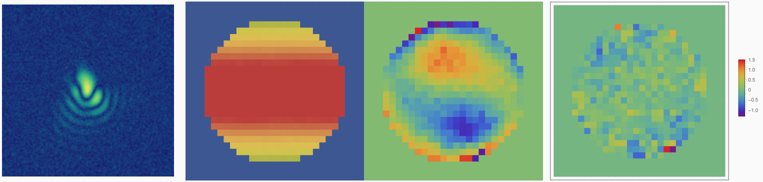
"Traditional PR"
(GS, 20000 iterations), noiseless



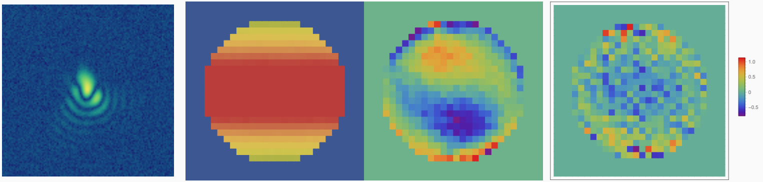
"3D PR", 1000 iterations
noiseless



Poisson noise,



Gaussian noise,



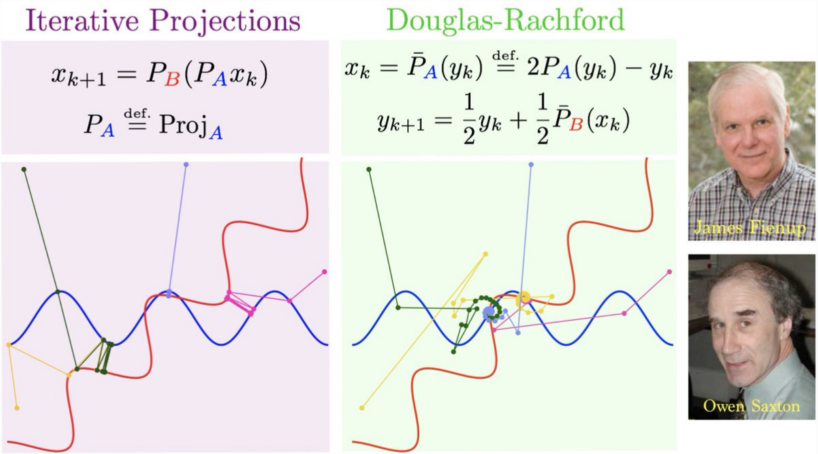
CONCLUSIONS

- 2D PR problem can be generalised to higher dimension setting in two ways, “coherently” and “incoherently”
- Projection-based algorithm can be easily adjusted for both cases
- Incoherent 3D PR can be used for solving PR related problems taking into account the light polarisation or for removing unknown background illumination

For questions: `o.a.soloviev@tudelft.nl`

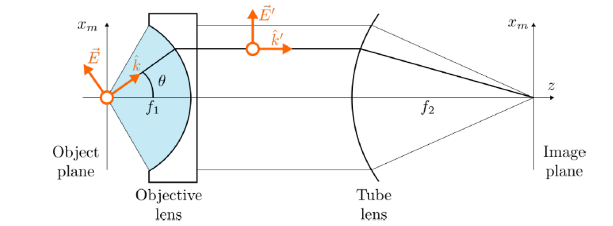
Questions?

GS VS FIENUP OR AP VS DR



[1] Gabriel Peyré, `http://www.gpeyre.com/`

WHY THERE ARE 6 TERMS IN HIGH NA PSF AND NOT 4?



3 components of random orientation of dipole give 6 incoherent components in the collimated beam.

For the tube lens with low NA, the polarisation can be again ignored.