phase retrieval in x-ray physics: uniqueness, stability, and reconstruction methods

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collaborators

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supported by CRC 755 ”Nanoscale photonic imaging”

SFB 755

Outline

experimental setup

experimental setup:

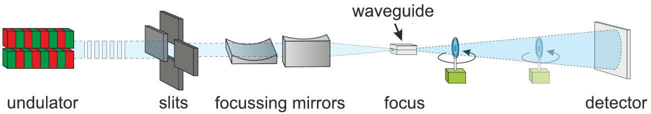
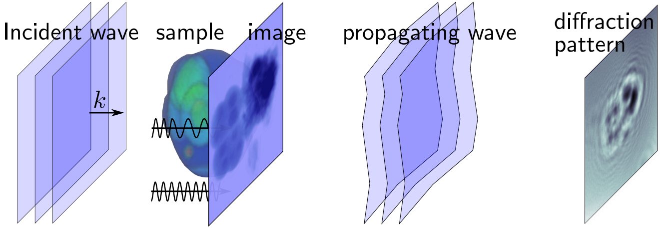


illustration of wave fronts for plane incident wave:



model hierarchy

- time harmonic Maxwell equations for electric field $\mathbf{E}$:

$$\operatorname{curl}\operatorname{curl}\mathbf{E} - \kappa^2 n^2 \mathbf{E} = 0$$

- Helmholtz equation: If $|\kappa^{-1}\nabla n| \ll 1$, the cartesian components of $\mathbf{E}$ satisfy

$$\Delta u + \kappa^2 n^2 u = 0$$

Exact solution in half-space $\{(\mathbf{x}, z) \in \mathbb{R}^2 \times \mathbb{R} : z > 0\}$ for $n \equiv 1$:

$$u(\mathbf{x}, z) = \left(\mathcal{F}_2^{-1} e^{iz\sqrt{\kappa^2 - |\xi'|^2}} \mathcal{F}_2 u_0\right)(\mathbf{x}), \qquad u_0 := u(\cdot, 0)$$

$\mathcal{F}_2 :=$ Fourier transform in $\mathbb{R}^2$

Fresnel approximation

- Fresnel approximation: $\sqrt{\kappa^2 - |\xi|^2} \approx \kappa - \frac{|\xi|^2}{2\kappa}$ if $|\xi| \ll \kappa$

$$u(\mathbf{x}, z) \approx e^{i\kappa z} \left(\mathcal{F}_2^{-1} e^{\frac{-iz|\xi|^2}{2\kappa}} \mathcal{F}_2 u_0 \right) (\mathbf{x}) =: e^{i\kappa z} (\mathcal{D}_{z/\kappa} u_0)(\mathbf{x})$$

The unitary operator $\mathcal{D}_\zeta$ is called *Fresnel transform*.
By the Fourier convolution theorem

$$(\mathcal{D}_{z/\kappa} u_0)(\mathbf{x}) = \int_{\mathbb{R}^2} e^{\frac{i\kappa}{2z}|\mathbf{x}-\mathbf{y}|^2} u_0(\mathbf{y}) d\mathbf{y}$$

- equivalent: Schrödinger approximation of Helmholtz eq.:
$\partial_z^2 + \kappa^2 = (-i\partial_z + \kappa)(i\partial_z + \kappa) \approx i\partial_z + \kappa$ leads to
Schrödinger equation

$$i\partial_z \tilde{u} + \Delta_{\mathbf{x}} \tilde{u} \approx 0 \quad \text{for} \quad \tilde{u}(\mathbf{x}, z) := e^{-i\kappa z} u(\mathbf{x}, z).$$

Fraunhofer approximation

Recall: $u(\mathbf{x}, z) \approx e^{i\kappa z}(\mathcal{D}_{z/\kappa} u_0)(\mathbf{x})$ with

$$(\mathcal{D}_{z/\kappa} u_0)(\mathbf{x}) = \int_{\mathbb{R}^2} e^{\frac{i\kappa}{2z}|\mathbf{x}-\mathbf{y}|^2} u_0(\mathbf{y}) d\mathbf{y}$$

Fresnel number:

$$N_{\mathrm{F}} := \frac{\kappa b^2}{2\pi z}, \qquad b := \mathrm{diam}(\mathrm{supp}\, u_0)$$

If $N_{\mathrm{F}} \ll 1$, the Fraunhofer approximation is valid:

$$\begin{aligned} u(\mathbf{x}, z) &\approx \frac{i\kappa}{2\pi z} e^{i\kappa z + \frac{i\kappa}{2z}|\mathbf{x}|^2} \left[\mathcal{F}_2 u_0 \left(\frac{\bullet}{z}\right)\right](\mathbf{x}) \\ |u(\mathbf{x}, z)| &\approx \frac{\kappa}{2\pi z} \left|\left[\mathcal{F}_2 u_0 \left(\frac{\bullet}{z}\right)\right](\mathbf{x})\right| \end{aligned}$$

Fraunhofer approximation

Recall: $u(\mathbf{x},z) \approx e^{i\kappa z}(\mathcal{D}_{z/\kappa}u_0)(\mathbf{x})$ with

$$(\mathcal{D}_{z/\kappa}u_0)(\mathbf{x}) = e^{\frac{i\kappa}{2z}|\mathbf{x}|^2}\int_{\mathbb{R}^2} e^{-\frac{i\kappa}{z}(\mathbf{x}\cdot\mathbf{y})+\frac{i\kappa|\mathbf{y}|^2}{2z}}u_0(\mathbf{y})d\mathbf{y}$$

Fresnel number:

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basic phase retrieval problems

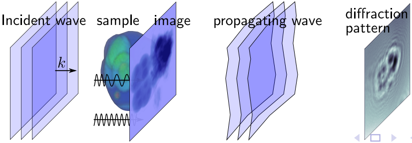
Reconstruct the field u_0 in the object plane from the measured (squared) modulus $|u(\cdot, z)|^2$ of the field in the detector plane and a-priori information on u_0!

- Typical a-priori information: $\operatorname{supp} u_0$, $u_0 \geq 0$, $|u_0| \equiv 1$
- $|u(\cdot, z)|^2$ is the photon density.

mathematical formulation:

- near field data: Given $|\mathcal{D}_\zeta u_0|^2$, find u_0!
- far field data ($z \to \infty$ or $\zeta \to 0$): Given $|\mathcal{F} u_0|^2$ find u_0!

As $\mathcal{F}$ and $\mathcal{D}_\zeta$ are unitary, this is equivalent to finding the missing phase, e.g. $\frac{\mathcal{F} u_0}{|\mathcal{F} u_0|}$.



from n to u_0

- Consider plane incident wave $e^{i\kappa z}$
- Write $u(\mathbf{x}) = \tilde{u}(\mathbf{x}, z)e^{i\kappa z}$ with a *slowly varying envelope* $\tilde{u}$
- Plug this into the Helmholtz equation $\Delta u + \kappa^2 n^2(\mathbf{x})u = 0$:

$$\left[\cancel{\frac{\partial^2}{\partial z^2}} + \cancel{\Delta_{\mathbf{x}}} + 2i\kappa\frac{\partial}{\partial z} + \kappa^2(n^2(x) - 1)\right]\tilde{u}(\mathbf{x}, z) = 0\,.$$

- Fresnel approximation: Neglect $\frac{\partial^2}{\partial z^2}$
  projection approximation: Neglect $\frac{\partial^2}{\partial z^2}$ and $\Delta_{\mathbf{x}}$
- If $\mathrm{supp}(n-1) \subset \{-L < z < 0\}$ and $\tilde{u}(\mathbf{x}, z) = 1$ for $z \leq -L$, then under the projection approximation

$$u_0(\mathbf{x}) \approx \exp\left(\frac{i\kappa}{2}\int_{-L}^{0} \underbrace{(n^2(\mathbf{x}, z) - 1}_{\approx 2(n-1))\text{ as }|n-1| \ll 1}\, dz\right), \qquad \mathbf{x} \in \mathbb{R}^2$$

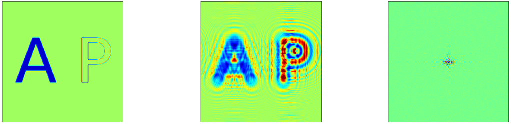
phase and absorption objects

Write contrast as $n - 1 = -\delta + i\beta$ with $0 \leq \delta, \beta \ll 1$.

$$u_0(\mathbf{x}) \approx e^{-i\kappa \int_{-L}^{0} (\delta(\mathbf{x},z) - i\beta(\mathbf{x},z))\, dz}$$

- phase objects: $\delta \gg \beta$ (usual situation)
  If $\beta = 0$, then $|u_0| \equiv 1$ (below in the letter P).
- absorption objects: $\beta \gg \delta$
  If $\delta = 0$, then u_0 is real-valued with $u_0 > 0$ (in letter A).

$N_\mathrm{F} = 100.000$ $\quad$ $N_\mathrm{F} = 1000$ $\quad$ $N_\mathrm{F} = 1$



$|\mathcal{D}_\zeta u_0|$ for different values of $\zeta = \frac{\kappa}{d}$

propagation based phase contrast tomography

- By rotating the sample in the beam we can obtain other line integrals over $n \rightsquigarrow$ tomographic imaging
- Forward operator of phase contrast tomography in terms of the Radon transform R:

$$F : L^2(B) \to L^2(S^1 \times \mathbb{R}^2)$$

$$(F(n))(\theta, \mathbf{x}) = \left| \left(\mathcal{D}_\zeta e^{i\kappa[R(n-1)](\theta,\cdot)} \right)(\mathbf{x}) \right|^2$$

- usual CT: $\zeta = 0$, i.e. $\mathcal{D}_\zeta = I$.
  Usually $\frac{1}{2i\kappa} \ln F$ is considered instead of F.
  No information about $\Re n$, only $\Im n$!

Outline

uniqueness for 2D near field phase retrieval

- Jonas & Louis 2004: Uniqueness of complex-valued *u* if two diffraction patterns at different distances are given
- Nugent 2007: Counterexample for non-uniqueness with one diffraction pattern
- Maretzke 2015: Uniqueness of complex-valued and *compactly supported u* from one diffraction pattern

P. Jonas, A. Louis. *Phase contrast tomography using holographic measurements.* **Inverse Problems** 20:75–102, 2004.

K. Nugent. *X-ray noninterferometric phase imaging. A unified picture.* **JOSA A.** 24:536–547, 2007.

S. Maretzke. *A uniqueness result for propagation-based phase contrast imaging from a single measurement.* **Inverse Problems** 31:065003, 2015.

uniqueness for 2D near field phase retrieval

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- Maretzke 2015: Uniqueness of complex-valued and *compactly supported* u from one diffraction pattern
  - both for full nonlinear and for linearized problem
  - arbitrarily small measurement region
  - implies uniqueness also for phase contrast tomography
  - proof based on complex analysis (theory of entire functions)

P. Jonas, A. Louis. *Phase contrast tomography using holographic measurements.* **Inverse Problems** 20:75–102, 2004.

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well-posedness

Weak object assumption: $u_0 = 1 + u$ with $|u| \ll 1$ such that

$$|\mathcal{D}u_0|^2 = 1 + \underbrace{2\Re\mathcal{D}u}_{=:T_{N_F}u} + \cancel{\mathcal{O}(|u|^2)}$$

Theorem

If the (complex-valued) contrast u vanishes outside of a fixed bounded set Ω, the linearized phase retrieval problem is well posed.
In particular, noise amplification $A_{N_F} := \| T_{N_F}^{-1} \|$ is finite.

- It follows that the nonlinear inverse problem is *locally well-posed.*
- Global well-posedness is an open question.

bounds on noise amplification

Noise amplification determined by two factors:

1. Fresnel number:
   $N_{\mathrm{F}} := \frac{b^2\kappa}{2\pi z}$

   - b sample size
   - z distance sample to detector
   - κ wave number

2. a-priori information.

bounds on noise amplification

Noise amplification determined by two factors:

1. Fresnel number:
   $N_{\mathrm{F}} := \frac{b^2 \kappa}{2\pi z}$

   b sample size
   z distance sample to detector
   κ wave number

2. a-priori information. We considered three cases:
   - none: both phase and absorption constrast

$$A_{N_{\mathrm{F}}} \leq C_1 \exp(c N_{\mathrm{F}})$$

   - pure phase object: $\Re(u) = 0$

$$A_{N_{\mathrm{F}}} \leq C_2 N_{\mathrm{F}}$$

   - single material: $\Re(u) = \mu \Im(u)$ for some $\mu \in \mathbb{R} \setminus \{0\}$

$$A_{N_{\mathrm{F}}} \leq C_3 \sqrt{N_{\mathrm{F}}}$$

Outline

projection methods

- Formulate problem as feasibility problem: Find $u \in A \cap B$ with
  - $A = \{u : u \text{ satisfying a-priori information}\}$ (often convex), e.g. $A = \{u : u \geq 0\}$
  - $B = \{u : u \text{ explains data}\}$, e.g. $B = \{u : |\mathcal{F}u|^2 = y\}$ (non-convex)
- L^2-metric projection onto B:

$$\mathcal{P}_B u := \mathcal{F}^* \left(y \frac{\mathcal{F}u}{|\mathcal{F}u|} \right)$$

- apply splitting methods to $\chi_A(u) + \chi_B(u) = \min!$, e.g.
  - backward-backward = alternating projections = error reduction
  - Douglas Rachford = hybrid input output (HIO)

J.R. Fienup. *Phase retrieval algorithms: a comparison.* **Appl. Opt., OSA** 21:2758–2769, 1982.

H. Bauschke, P. Combettes, R. Luke. *Phase retrieval, error reduction algorithm, and Fienup variants: a view from convex optimization.* **J. Opt. Soc. Amer. A**, 19:1334–1345, 2002.

projection methods: pros and cons

pros:

- easy to implement
- often efficient

cons:

- no provable convergence (only partial results)
- sometimes erratic convergence behaviour
- difficult to respect Poissonian data distribution

phase lift methods

- Consider discrete problem to find $u \in \mathbb{C}^n$ such that $|a_j^* u|^2 = y_j$ for $j = 1, \ldots, m$
- Note: $|a_j^* u|^2 = \mathrm{tr}(u^* a_j a_j^* u) = \mathrm{tr}(a_j a_j^* u u^*)$
- Reformulation with new unknown $U = uu^* \in \mathbb{C}^{n \times n}$:

$$\begin{array}{rll} \text{minimize} & \mathrm{rank}(U) & \text{over } U \in \mathbb{C}^{n\times n}, U \geq 0 \\ \text{s.t.} & \mathrm{tr}((a_j a_j^*)U) = y_j, & j = 1, \ldots, m \end{array}$$

- convex relaxation:

$$\begin{array}{rll} \text{minimize} & \mathrm{tr}(U) & \text{over } U \in \mathbb{C}^{n\times n}, U \geq 0 \\ \text{s.t.} & \mathrm{tr}((a_j a_j^*)U) = y_j, & j = 1, \ldots, m \end{array}$$

E. Candès, T. Strohmer, V. Voroninski. *PhaseLift: exact and stable signal recovery from magnitude measurements via convex programming.* **Comm. Pure Appl. Math.** 66:1241–1274, 2013.

phase lift methods: pros and cons

pros:

- reformulation as a *convex* minimization problem
- mathematically elegant

cons:

- The number of unknowns of an already large problem is squared.
- only applicable to inverse problems, which are linear up to missing phase information
- little flexibility in incorporating a-priori information on unknown and experimental setup

iterative regularization methods

- Formulate inverse problem as an operator equation $F(u) = y$ with an operator F mapping the unknown u to the data y.
- Apply a Newton-type method

$$u_{k+1} \in \operatorname{argmin}_u \left[\mathcal{S}(F(u_k) + F'[u_k](u - u_k), y^{\mathrm{obs}}) + \alpha_k \mathcal{R}(u)\right]$$

  where
  - y^{obs} is observed noisy data (often Poisson distributed)
  - $\mathcal{S}$ is a data fidelity term, e.g. negative log-likelihood
  - $\mathcal{R}$ is a penalty term incorporating a-priori information on u
  - α_k are regularization parameters, $\alpha_k \to 0$

  Minimization problems in each Newton step typically convex, so e.g. the Chambolle-Pock algorithm is applicable.

iterative regularization: pros and cons

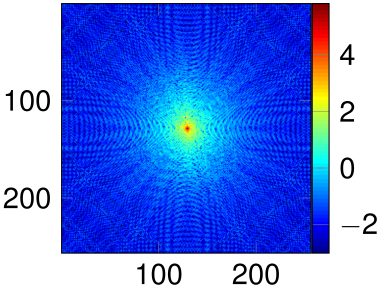
pros:

- great flexibility to incorporate a-priori knowledge
  - on solution (hard constraints as well as smoothness or sparsity)
  - on data distribution (e.g. via Poisson log-likelihood)
  - precise physical model or experimental setup
- more accurate reconstructions

cons:

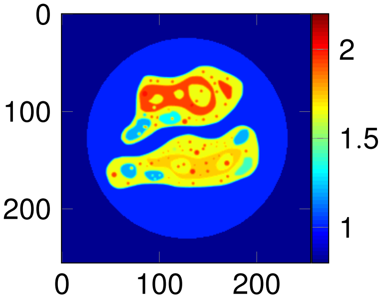
- only local convergence
- often numerically more expensive than projection methods

exact far field data and photon counts



Expected total number of photon counts $= 10^6$

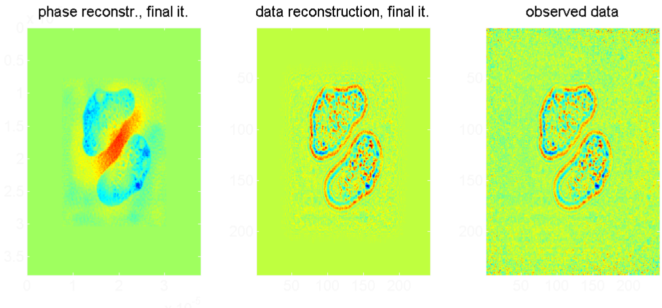
simulated phase object and reconstruction



expected error in terms of #(photons)

t	quadratic	KL
10^3	58.8	53.2
10^4	50.7	39.2
10^5	31.5	29.3
10^6	16.6	13.8
10^7	9.46	8.77
10^8	9.21	7.38

reconstruction of a cell from holographic experimental data in the Fresnel regime



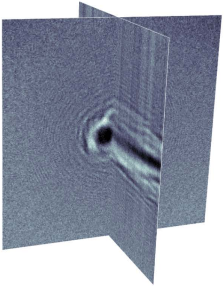
experimental data published in:

K. Giewekemeyer, S.P. Krüger, S. Kalbfleisch, M. Bartels, C. Beta, T. Salditt. *X-ray propagation microscopy of biological cells using waveguides as a quasipoint source.* **Phys. Rev. A** 83:023804. 2011

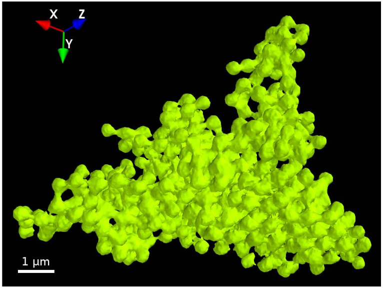
phase contrast tomography

- Straightforward approach: Solve a standard phase retrieval problem for each angle θ and then invert the Radon transform.
- disadvanage: Range of Radon transform has a nontrivial orthogonal complement (Helgason-Ludwig conditions) $\rightsquigarrow$ standard phase retrieval problems unnecessarily unstable.
- All-at-once approach more accurate.
- Inversion by Newton-Kaczmarz method.

3D reconstructions from tomographic experimental data

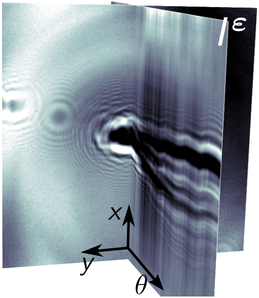


$$\xrightarrow[\text{(by IRNM)}]{F_{\text{tomo}}^{-1}}$$



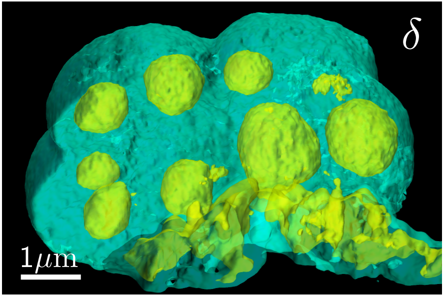
S. Maretzke, M. Krenkel, M. Bartels, T. Salditt, T. Hohage. *Regularized Newton methods for x-ray phase contrast and general imaging problems.* Optics Express 24:6490–6506, 2016.

3d reconstruction of a living cell



Misaligned holograms

$\xrightarrow[\text{(Newton-Kaczmarz)}]{F_{\mathrm{PCT}}^{-1}}$



Sharp 3D-image (*D. radiodurans*) + alignment

Outline

conclusions

- uniqueness for nonlinear near field phase retrieval problems with compactly supported objects
- well-posedness of linearized problems
- explicit stabilty bounds in terms of the Fresnel number
- all-at-once approach for numerical reconstructions

Thank you for your attention!