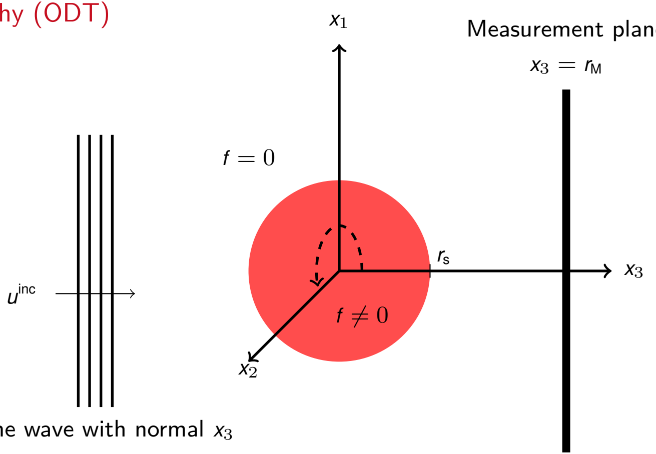
 

Fourier Reconstruction in Diffraction Tomography of an Irregularly Moving Object

Michael Quellmalz | TU Berlin | SIAM Imaging Science, 21 March 2022
joint work with Robert Beinert, Florian Faucher, Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl

Optical Diffraction Tomography (ODT)

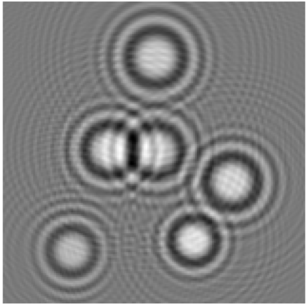


Incident field: Plane wave with normal x_3

C Kirisits, M Quellmalz, M Ritsch-Marte, O Scherzer, E Setterqvist, G Steidl.
Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations.
Inverse Problems 37, 2021.

Optical Diffraction

Optical diffraction occurs when the wavelength of the imaging beam is large $\approx$ the size of the object (μm scale)



Simulation of the scattered field from spherical particles (size $\approx$ wavelength)

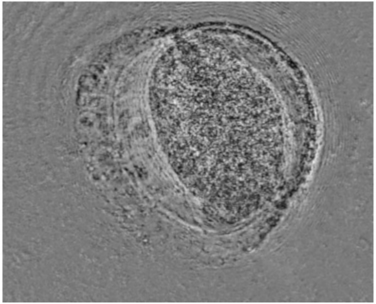


Image with diffraction

Modeling of Optical Diffraction Tomography

- We have field $u^{\mathrm{tot}}(x_1, x_2, r_{\mathrm{M}})$ at measurement plane $x_3 = r_{\mathrm{M}}$
- We want scattering potential $f(\boldsymbol{x})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_{\mathrm{s}}} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$
- Total field $u^{\mathrm{tot}}(\boldsymbol{r}) = u^{\mathrm{sca}}(\boldsymbol{r}) + u^{\mathrm{inc}}(\boldsymbol{r})$ solves the wave equation

$$-\left(\Delta + f(\boldsymbol{r}) + k_0^2\right) u^{\mathrm{tot}}(\boldsymbol{r}) = 0$$

- Rearranging yields

$$-\left(\Delta + k_0^2\right) u^{\mathrm{sca}}(\boldsymbol{r}) - \underbrace{\left(\Delta + k_0^2\right) u^{\mathrm{inc}}(\boldsymbol{r})}_{=0} = f(\boldsymbol{r}) \left(u^{\mathrm{sca}}(\boldsymbol{r}) + u^{\mathrm{inc}}(\boldsymbol{r})\right)$$

Born approximation

Assuming $\left|u^{\mathrm{sca}}\right| \ll \left|u^{\mathrm{inc}}\right|$, we obtain

$$-\left(\Delta + k_0^2\right) u^{\mathrm{sca}}(\boldsymbol{r}) = f(\boldsymbol{r}) u^{\mathrm{inc}}(\boldsymbol{r})$$

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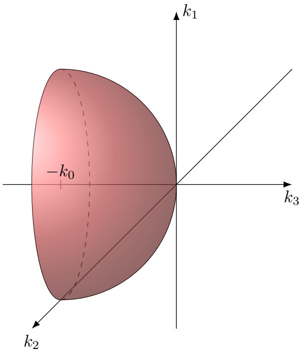
Fourier diffraction theorem [Kirisits Q. Ritsch-Marte Scherzer Setterqvist Steidl 2021]

1. scattering potential $f \in L^p$, $p > 1$, where $\operatorname{supp}(f) \subset \mathcal{B}_{r_s}$, $0 < r_s < r_M$,
2. incident field is a plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$,
3. Born approximation is valid and u^{sca} satisfies the Sommerfeld condition (u^{sca} is an outgoing wave),
4. scattered field u^{sca} is measured at the plane $r_3 = r_M$.

Then

$$\sqrt{\frac{2}{\pi}}\kappa \mathrm{i} \mathrm{e}^{-\mathrm{i}\kappa r_M} \mathcal{F}_{1,2} \underbrace{u^{\mathrm{sca}}(k_1, k_2, r_M)}_{\text{measurements}} = \mathcal{F} f(\boldsymbol{h}(k_1, k_2)), \quad (k_1, k_2) \in \mathbb{R}^2,$$

where $\boldsymbol{h}(k_1, k_2) := \begin{pmatrix} k_1 \\ k_2 \\ \kappa - k_0 \end{pmatrix}$ and $\kappa := \sqrt{k_0^2 - k_1^2 - k_2^2}$.



Semisphere $\boldsymbol{h}(\boldsymbol{k})$ of available data in Fourier space

based on [Wolf 1969] [Natterer Wuebbeling 2001] [Kak Slaney 2001]

Fourier diffraction theorem (with rotation)

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2. incident field is a plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = e^{ik_0 x_3}$,
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Then

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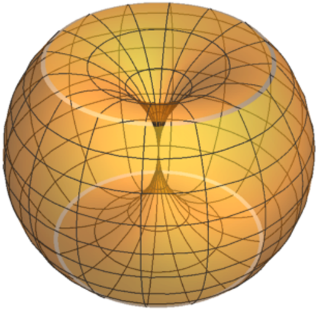


Set of available Fourier space data for full rotation

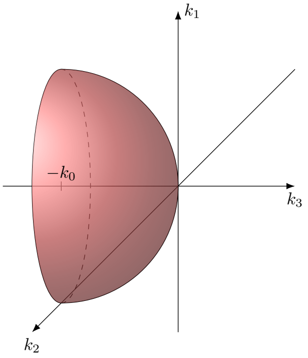
Rotation $R_t \in \mathrm{SO}(3)$ at time $t \in [0, T]$

Comparison with Computerized Tomography

Optical diffraction tomography (ODT)

diffraction of imaging beam

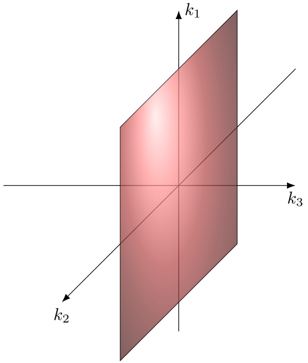
Data: Fourier transform on semispheres containing $\mathbf{0}$



Computerized tomography (CT)

light travels on lines

Data: Fourier transform on planes containing $\mathbf{0}$



Discretization

- Uniform sampling of $f(\boldsymbol{x}_{\boldsymbol{k}} = \boldsymbol{k}\frac{2L_{\mathrm{s}}}{K})$, $\boldsymbol{k} \in \mathcal{I}_K^3 := \{-K/2, \dots, K/2-1\}^3$
- Uniform sampling of measurements $u^{\mathrm{tot}}_{t_m}(\boldsymbol{y}_{\boldsymbol{n}}, r_{\mathrm{M}})$, $\boldsymbol{y}_{\boldsymbol{n}} = \boldsymbol{n}\frac{2L_{\mathrm{M}}}{N}$, $m = 1, \dots, M$, $\boldsymbol{n} \in \mathcal{I}_N^2$
- **discrete Fourier transform** (DFT)

$$\left[\boldsymbol{F}_{\mathrm{DFT}}\, u^{\mathrm{sca}}_{t_m}\right]_{\boldsymbol{\ell}} := \sum_{\boldsymbol{n}\in\mathcal{I}_N^2} u^{\mathrm{sca}}_{t_m}(\boldsymbol{y}_{\boldsymbol{n}}, r_{\mathrm{M}})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{n}\cdot\boldsymbol{\ell}/N}, \qquad \boldsymbol{\ell} \in \mathcal{I}_N^2,$$

- **Non-uniform discrete Fourier transform** (NDFT)

$$\left[\boldsymbol{F}_{\mathrm{NDFT}}\boldsymbol{f}\right]_{m,\boldsymbol{\ell}} := \sum_{\boldsymbol{k}\in\mathcal{I}_K^3} f_{\boldsymbol{k}}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{x}_{\boldsymbol{k}}\cdot\left(R_{t_m}\boldsymbol{h}(\boldsymbol{y}_{\boldsymbol{\ell}})\right)}, \qquad m \in \mathcal{J}_M,\ \boldsymbol{\ell} \in \mathcal{I}_N^2$$

Discretized forward operator

$$\boldsymbol{D}^{\mathrm{tot}}\boldsymbol{f} := \boldsymbol{F}_{\mathrm{DFT}}^{-1}(\boldsymbol{c} \odot \boldsymbol{F}_{\mathrm{NDFT}}\boldsymbol{f}) + \mathrm{e}^{\mathrm{i}k_0 r_{\mathrm{M}}}, \qquad \boldsymbol{f} \in \mathbb{R}^{K^d},$$

where $\boldsymbol{c} = \left[\frac{\mathrm{i}}{\kappa(\boldsymbol{y}_{\boldsymbol{\ell}})}\, \mathrm{e}^{\mathrm{i}\,\kappa(\boldsymbol{y}_{\boldsymbol{\ell}})\, r_{\mathrm{M}}} \left(\frac{N}{L_{\mathrm{M}}}\right)^{d-1} \left(\frac{L_{\mathrm{s}}}{K}\right)^{d}\right]_{\boldsymbol{\ell}\in\mathcal{I}_N^2}$

Reconstruction algorithm

Input: Scattered wave $\boldsymbol{v}^{\mathrm{sca}}_{m,\boldsymbol{n}} := u^{\mathrm{tot}}_{t_m}\left(\boldsymbol{n}\frac{2L_{\mathrm{M}}}{N}, r_{\mathrm{M}}\right) - \mathrm{e}^{\mathrm{i}k_0 r_{\mathrm{M}}}$, $m \in \mathcal{J}_M$, $\boldsymbol{n} \in \mathcal{I}_N^{d-1}$.

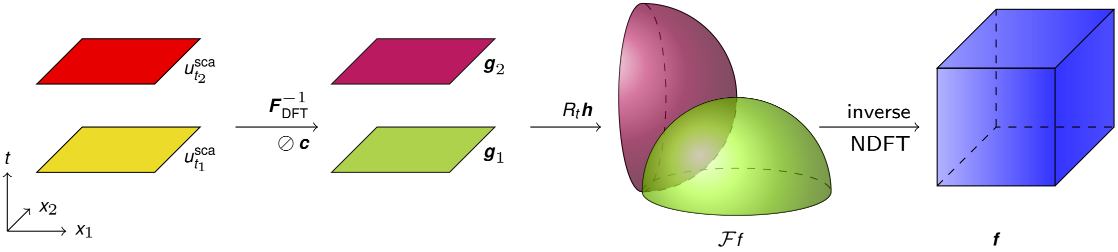
for $m = 1, \dots, M$

$\quad \tilde{\boldsymbol{g}}_m := \boldsymbol{F}_{\mathrm{DFT}} \boldsymbol{v}^{\mathrm{sca}}_m$

$\quad \boldsymbol{g}_m := \tilde{\boldsymbol{g}}_m \oslash \boldsymbol{c}$, where $\oslash$ is the Hadamard (entrywise) division

Compute the inverse NDFT by solving $\boldsymbol{F}_{\mathrm{NDFT}} \boldsymbol{f} = \boldsymbol{g}$ for $\boldsymbol{f}$

Output: Scattering potential $\boldsymbol{f} \approx [f(\boldsymbol{x}_{\boldsymbol{k}})]_{\boldsymbol{k} \in I_K^d}$.



Method 1: Backpropagation

Idea: Compute inverse Fourier transform of $\mathcal{F}f$ restricted to the set of available data $\mathcal{Y}$:

$$f_{\mathrm{bp}}(\boldsymbol{x}) := (2\pi)^{-\frac{3}{2}} \int_{\mathcal{Y}} \mathcal{F}f(\boldsymbol{k})\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\, \mathrm{d}\boldsymbol{k}.$$

Theorem [Kirisits, Q, Ritsch-Marte, Scherzer, Setterqvist, Steidl 2021]

Consider the rotation R_t round axis $\boldsymbol{n} \in C^1([0,T], \mathbb{S}^2)$ with angle $\alpha \in C^1[0,T]$. Then

$$f_{\mathrm{bp}}(\boldsymbol{x}) = (2\pi)^{-\frac{3}{2}} \int_0^T \int_{\mathcal{B}_{k_0}} \mathcal{F}f(R_t\boldsymbol{h}(k_1,k_2))\, \mathrm{e}^{\mathrm{i}R_t\boldsymbol{h}(k_1,k_2)\cdot\boldsymbol{x}} \frac{|\det \nabla T(k_1,k_2,t)|}{\mathrm{Card}\, T^{-1}(T(k_1,k_2,t))}\, \mathrm{d}(k_1,k_2)\, \mathrm{d}t,$$

where

$$|\det \nabla T(k_1,k_2,t)| = \frac{k_0}{\kappa} \Big| \left((1-\cos\alpha)\left(n_3\,\boldsymbol{n}'\cdot\boldsymbol{h} - n_3'\boldsymbol{n}\cdot\boldsymbol{h}\right) - n_3\,\boldsymbol{n}\cdot\left(\boldsymbol{n}'\times\boldsymbol{h}\right)\sin\alpha\right)$$
$$-\alpha'\,(n_1k_2 - n_2k_1) + (\boldsymbol{n}\cdot\boldsymbol{h})\left(n_1n_2' - n_2n_1'\right)\sin\alpha \Big|,$$

and $T(k_1,k_2,t) := R_t\boldsymbol{h}(k_1,k_2)$.

It is complicated to determine the Crofton symbol $\mathrm{Card}(T^{-1}(\boldsymbol{y}))$ algebraically (except for a constant $\boldsymbol{n}$).

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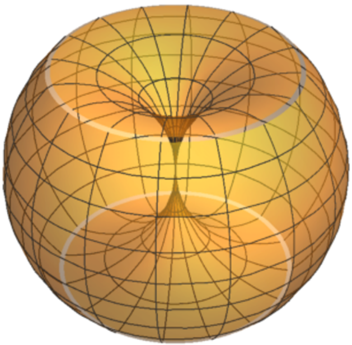
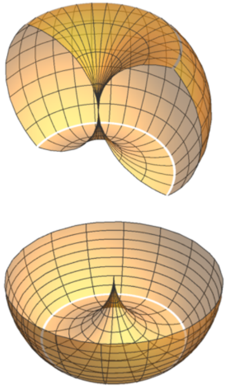
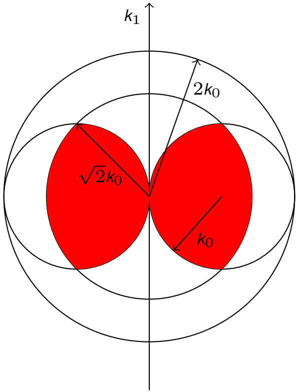
Example: Rotation Around the First Axis

Backpropagation formula $f_{\mathrm{bp}}(\boldsymbol{x}) = (2\pi)^{-\frac{3}{2}} \int_0^T \int_{\mathcal{B}_{k_0}} \mathcal{F}f(R_t\boldsymbol{h}(k_1, k_2))\, \mathrm{e}^{R_t\boldsymbol{h}(k_1,k_2)\cdot\boldsymbol{x}}\, \frac{k_0\,|k_2|}{2\kappa}\, \mathrm{d}(k_1, k_2)\, \mathrm{d}t$

[Kak, Slaney 2001] [Müller, Schürmann, Guck 2016]







Approach 2: Conjugate Gradient (CG) Method

- Inversion of the NDFT

- Find a solution $\boldsymbol{f} \in \mathbb{R}^{K^3}$ of

$$\underset{\boldsymbol{f}\in\mathbb{R}^{K^d}}{\text{minimize}} \qquad \|\boldsymbol{F}_{\text{NDFT}}\boldsymbol{f} - \boldsymbol{g}\|_{2,\boldsymbol{w}}^2 = \sum_{\boldsymbol{x}} \left(\boldsymbol{F}_{\text{NDFT}}\boldsymbol{f}(\boldsymbol{x}) - g(\boldsymbol{x})\right)^2 w(\boldsymbol{x})$$

- Use Conjugate gradients on the normal equations

Approach 3: TV (Total Variation) Regularization

- Inversion of the NDFT

- Find a solution $\boldsymbol{f} \in \mathbb{R}^{K^3}$ of

$$\underset{\boldsymbol{f}\in\mathbb{R}^{K^d}}{\text{minimize}} \qquad \chi_{\mathbb{R}^{K^d}_{\geq 0}}(\boldsymbol{f}) + \frac{1}{2}\|\boldsymbol{F}_{\mathrm{NDFT}}(\boldsymbol{f}) - \boldsymbol{g}\|_{2,\boldsymbol{w}}^2 + \lambda \mathrm{TV}(\boldsymbol{f}),$$

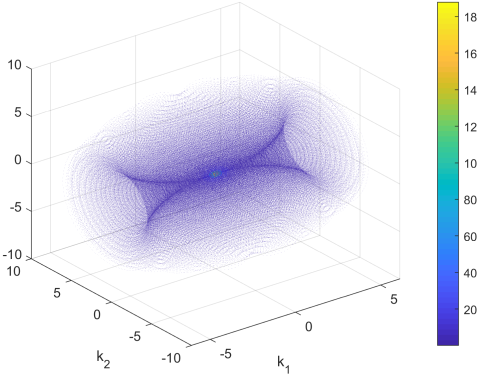
  with the total variation

$$\mathrm{TV}(\boldsymbol{f}) := \sum_{\boldsymbol{k}\in\mathcal{I}_K^3} \|\operatorname{grad} \boldsymbol{f}(\boldsymbol{x}_{\boldsymbol{k}})\|_2$$

- Solve with primal-dual (PD) iteration [Chambolle & Pock 2010]
- Adaptive selection of step sizes [Yokota & Hontani 2017]

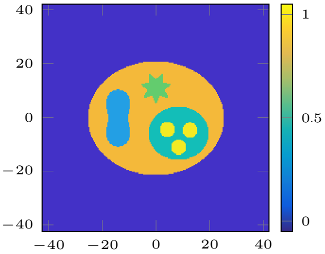
Test Setup

- Normalized wavelength $\lambda = 1 \Rightarrow k_0 = \frac{2\pi}{\lambda} = 2\pi$
- Test function f given analytically
- Generate simulated data via direct convolution with the Green function (also based on Born approximation) to avoid the “inverse crime”
- “missing cones” around the axis of rotation
- NFFT (Non-uniform fast Fourier transform): for computing $\boldsymbol{F}_{\mathrm{NDFT}}\mathbf{f}$ in $\mathcal{O}\left(N^3 \log N\right)$ steps [Dutt Rokhlin 93], [Beylkin 95], [Potts Steidl Tasche 01], [Potts Kunis Keiner 04+]

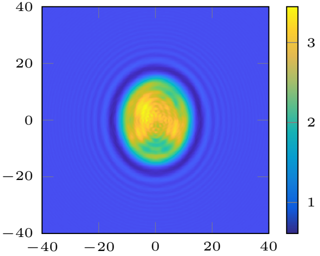


Simulated data: Fourier transform $|\mathcal{F}f|$ at 496944 nodes (constant rotation axis)

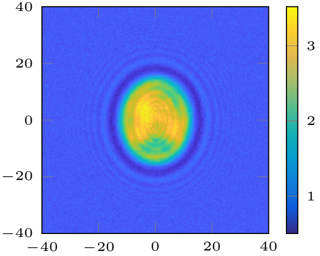
Test data



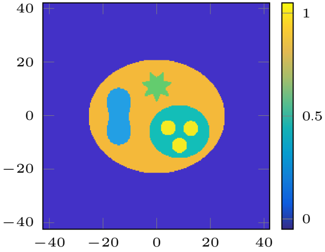
Ground truth f
$(240 \times 240 \times 240$ grid)
Slice at $x_3 = 0.35$



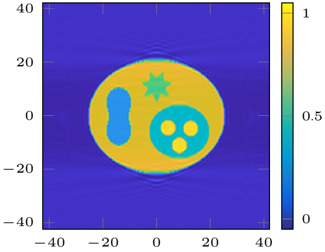
Exact data $|u_t^{\text{tot}}(\cdot, r_{\text{M}})|$
$(240 \times 240$ grid and 240 rotations



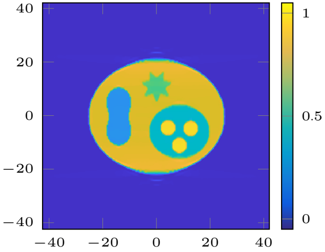
Data with $5\,\%$ Gaussian noise



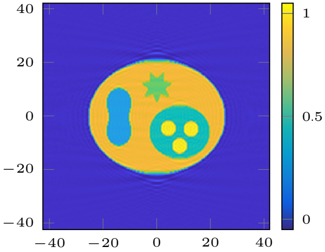
(a) Ground truth $\boldsymbol{f}$



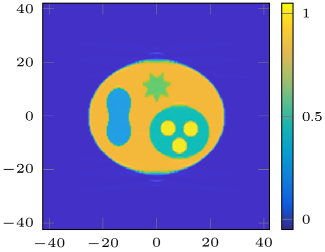
(b) Backpropagation
PSNR 29.07, SSIM 0.614
4 sec



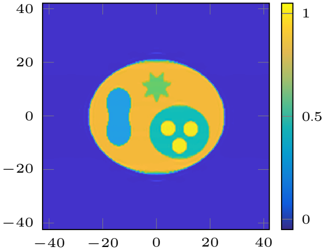
(c) Backprop. and TVdenoise ($\lambda = 0.02$)
PSNR 32.79, SSIM 0.987
37 sec



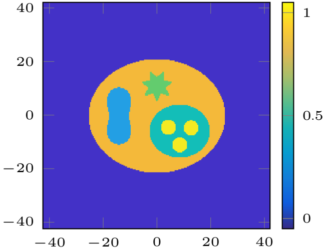
(d) CG Reconstruction
PSNR 33.36, SSIM 0.955
79 sec



(e) CG and TVdenoise ($\lambda = 0.02$)
PSNR 33.82, SSIM 0.988
31 sec



(f) PD with TV ($\lambda = 0.02$)
PSNR 34.36, SSIM 0.957
21 min



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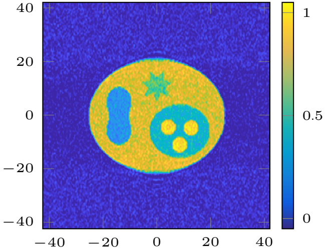
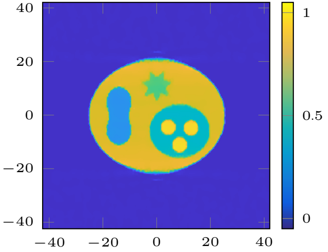
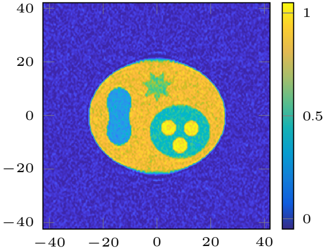


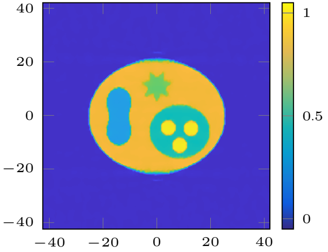
(b) Backpropagation
PSNR 24.53, SSIM 0.178



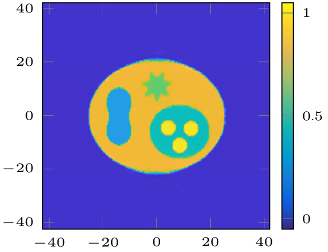
(c) Backpropagation and TVdenoise ($\lambda = 0.05$)
PSNR 32.51, SSIM 0.968



(d) CG Reconstruction
PSNR 26.74, SSIM 0.309

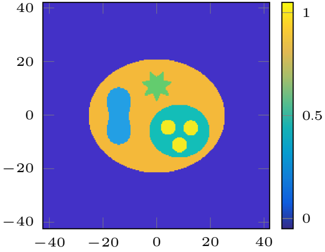


(e) CG and TVdenoise ($\lambda = 0.02$)
PSNR 33.53, SSIM 0.965

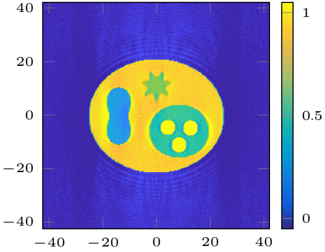


(f) PD with TV ($\lambda = 0.02$)
PSNR 33.58, SSIM 0.736

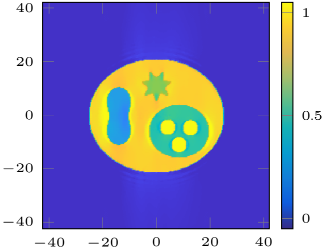
Figure: Slice of 3D reconstruction with 5 % Gaussian noise (grid $240 \times 240 \times 240$)



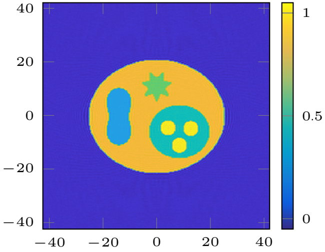
(a) Ground truth $\boldsymbol{f}$



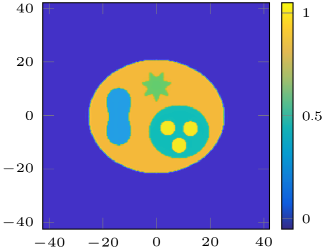
(b) Backpropagation
PSNR 24.17, SSIM 0.171



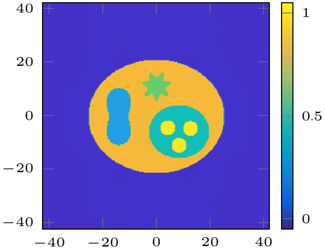
(c) Backpropagation and TVdenoise $(\lambda = 0.02)$
PSNR 29.17, SSIM 0.783



(d) CG Reconstruction
PSNR 35.84, SSIM 0.962



(e) CG and TVdenoise $(\lambda = 0.02)$
PSNR 36.88, SSIM 0.995



(f) PD with TV $(\lambda = 0.02)$
PSNR 40.95, SSIM 0.972

Figure: Slice of 3D reconstruction from exact data with moving rotation axis (grid $240 \times 240 \times 240$)

Phase Retrieval

[Beinert & Q. 2022]

– In practice, one can often measure only the intensity

$$\left|u_t^{\text{tot}}(\boldsymbol{y}, r_{\text{M}})\right| = \left|u_t^{\text{sca}}(\boldsymbol{y}, r_{\text{M}}) + e^{ik_0 r_{\text{M}}}\right|, \qquad \boldsymbol{y} \in \mathbb{R}^2, t \in [0, T]$$

– Existing phase retrieval methods in diffraction tomography

- require more measurements [Gbur & Wolf 2002] [Wedberg & Stamnes 1995]
- use far zone approximations [Cheng & Han 2001] [Gureyev & Davis 2004]
- Consider phase retrieval separate from reconstruction [Maleki & Devaney 1993]
- Use techniques of ptychography [Horstmeyer Chung Ou Zheng & Yang 2016]

– We require additional information:

- $f \geq 0$
- f has bounded support
- total variation of f

All-at-Once Approach for Phase Retrieval

Forward operator $\boldsymbol{D}f(t,\boldsymbol{y}) = u_t^{\text{tot}}(\boldsymbol{y}, r_{\text{M}})$

Hybrid input-output (HIO) algorithm [Fienup 1982]

Input: Data $\boldsymbol{d} = |\boldsymbol{D}(\boldsymbol{f})| = |u^{\text{tot}}|$, parameter $\beta \in [0,1]$, support radius $r_{\text{s}} > 0$.

Initialize $\boldsymbol{g}^{(0)} := \boldsymbol{d}$

for $j = 0, 1, 2, \dots$

$$\boldsymbol{f}^{(j)} := \boldsymbol{D}^{-1}\boldsymbol{g}^{(j)}$$

$$\tilde{f}^{(j)}_{\boldsymbol{k}} := \begin{cases} \max\{f^{(j)}(\boldsymbol{x_k}), 0\}, & \|\boldsymbol{x_k}\|_2 \le r_{\text{s}}, \\ 0, & \|\boldsymbol{x_k}\|_2 > r_{\text{s}}, \end{cases}$$

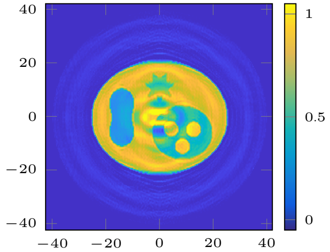
$$f^{(j+1/2)}(\boldsymbol{x_k}) := \begin{cases} f^{(j)}(\boldsymbol{x_k}), & \text{if } f^{(j)}(\boldsymbol{x_k}) = \tilde{f}^{(j)}(\boldsymbol{x_k}) \\ f^{(j-1/2)}(\boldsymbol{x_k}) - \beta\big(f^{(j)}(\boldsymbol{x_k}) - \tilde{f}^{(j)}(\boldsymbol{x_k})\big), & \text{otherwise,} \end{cases}$$

$$\boldsymbol{g}^{(j+1/2)} := \boldsymbol{D}\boldsymbol{f}^{(j+1/2)}$$

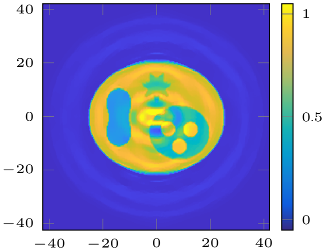
$$\boldsymbol{g}^{(j+1)} := \boldsymbol{d}\,\mathrm{sgn}(\boldsymbol{g}^{(j+1/2)})$$

Output: Approximate scattering potential $\boldsymbol{f}^{(j)}$.

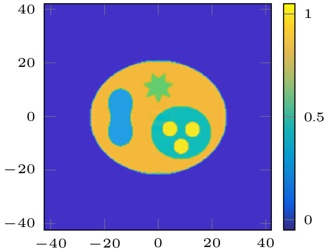
Numerical Phase Retrieval (Exact Data)



(a) HIO/CG reconstruction
$J_{\mathrm{IO}} = 10,\ J_{\mathrm{CG}} = 5$
PSNR 29.52, SSIM 0.713
5 min



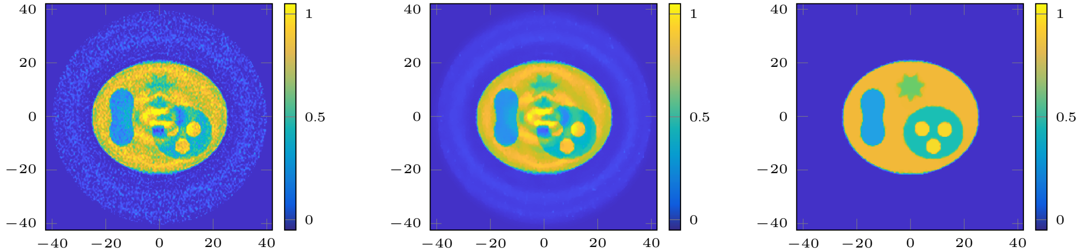
(b) HIO/CG and TVdenoise
$\lambda = 0.02,\ J_{\mathrm{TV}} = 20$
PSNR 29.88, SSIM 0.713
31 sec



(c) HIO/PD with TV
$\lambda{=}0.01,\ J_{\mathrm{IO}}{=}200,\ J_{\mathrm{PD}}{=}5$
PSNR 34.92, SSIM 0.994
3 h 48 min

Figure: Slice of 3D HIO phase retrieval

Numerical phase retrieval (noisy data)



(a) HIO/CG reconstruction
$J_{\mathrm{IO}} = 10$, $J_{\mathrm{CG}} = 5$
PSNR 24.71, SSIM 0.589

(b) HIO/CG and TVd
$\lambda = 0.05$, $J_{\mathrm{PD}} = 20$
PSNR 27.16, SSIM 0.623

(c) HIO/PD with TV
$\lambda{=}0.05$, $J_{\mathrm{IO}}{=}200$, $J_{\mathrm{PD}}{=}5$
PSNR 34.10, SSIM 0.993

Figure: Slice of 3D HIO phase retrieval with 5% Gaussian noise

Computational complexity

- Outer loop with HIO and inner loop with primal-dual (PD)
- Both algorithms often show slow convergence

- Improvements:
- Restart the primal dual with the parameters dual variable from the previous outer step
- Use faster HIO/CG to obtain a starting solution for primal-dual
- Use fast FFT and NFFT algorithms for the Fourier step
- Employ the weights from the backpropagation to the minimization problem

Code available on Github: `https://github.com/michaelquellmalz/FourierODT`

Conclusion

- Fourier diffraction theorem on $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared reconstruction method
  - Backpropagation is faster
  - Inverse NFFT is always applicable and shows slightly better results
- Phase retrieval works well with all-at-once HIO and TV regularization

Future research

- Detection of rotation from data
- Application to real-world data

Thank you for your attention!

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