Fourier reconstruction in diffraction tomography with an arbitrarily rotated object
Project EF3-6: Deformation Based Regularization of Inverse Problems in Manifolds

Michael Quellmalz | TU Berlin | MATH+ Spotlight, 2 June 2021
joint work with Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl

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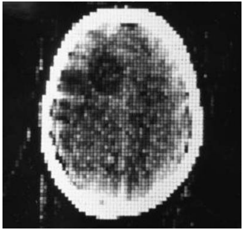
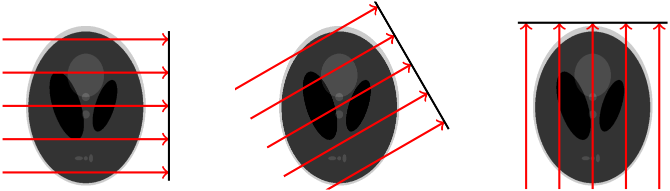
Computerized tomography (CT)



Nobel price in physiology or medicine 1979:
Allan M. Cormack and Godfrey N. Hounsfield
(Image: first clinical CT scan, London 1971)

X-ray images from different directions



Object $f\colon \mathbb{R}^2 \to \mathbb{R}$ [Radon, 1917]

Radon transform $\mathcal{R}f(\ell) = \int_\ell f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \qquad \ell$ line in $\mathbb{R}^2$

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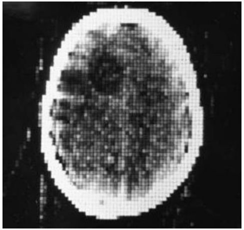

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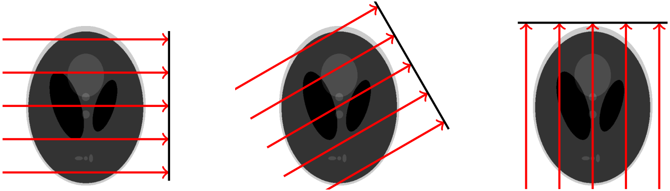

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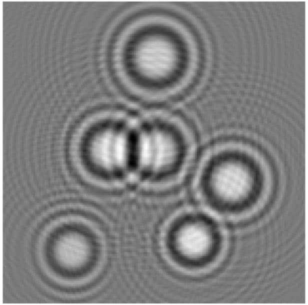
Optical diffraction

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)

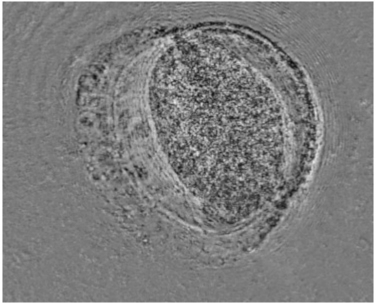


Image with diffraction

Arbitrary rotations

- Sample confinement, such as fixation on a surface or embedding in a gel, has substantial impact on biological cell clusters
- Contact-less tools for 3D manipulation based on optical and acoustical tweezers
  [Kvåle-Løvmo, Pressl, Thalhammer, Ritsch-Marte 2020]
- Drawback: less control about the exact movement

Video of trapped specimen (pollen)
© Medizinische Universität Innsbruck

At first

Assume we know the rotation

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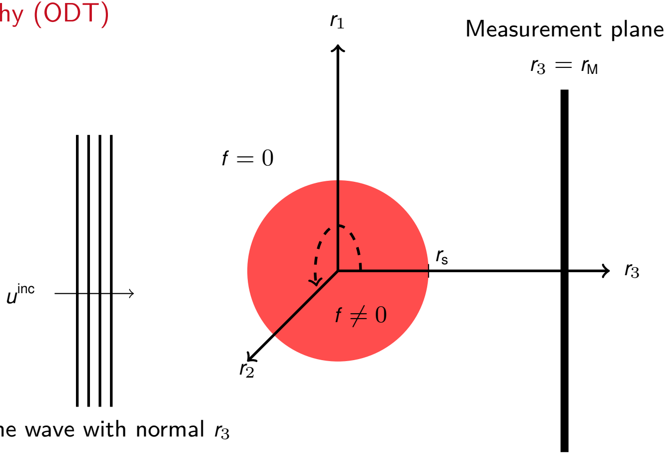
Optical Diffraction Tomography (ODT)



Incident field: Plane wave with normal r_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.
Arxiv prerpint, 2104.07990, 2021.

Modeling of Optical Diffraction Tomography

- We have the scattered field $u(r_1, r_2, r_M)$ at measurement plane $r_3 = r_M$
- We want the scattering potential $f(\boldsymbol{r})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_s} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\text{inc}}(\boldsymbol{r}) = e^{ik_0 r_3}$
- Total field $u^{\text{tot}}(\boldsymbol{r}) = u(\boldsymbol{r}) + u^{\text{inc}}(\boldsymbol{r})$ solves the wave equation

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

- Rearranging yields

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

Born approximation

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

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Fourier diffraction theorem

Theorem

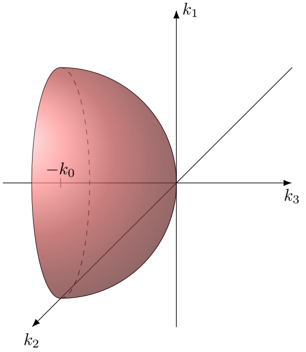
1. scattering potential $f \in L^p$, $p > 1$, where $\operatorname{supp}(f) \subset \mathcal{B}_{r_s}$, $0 < r_s < r_M$,
2. incident field is a plane wave $u^{inc}(\boldsymbol{r}) = e^{ik_0 r_3}$,
3. Born approximation is valid and u satisfies the Sommerfeld condition (u is an outgoing wave),
4. scattered field u is measured at the plane $r_3 = r_M$.

Then

$$\sqrt{\frac{2}{\pi}} \kappa i e^{-i\kappa r_M} \mathcal{F}_{1,2} \underbrace{u(k_1, k_2, r_M)}_{\text{measurements}} = \mathcal{F} f \begin{pmatrix} k_1 \\ k_2 \\ \kappa - k_0 \end{pmatrix}, \quad (k_1, k_2) \in \mathbb{R}^2,$$

where $\kappa := \sqrt{k_0^2 - k_1^2 - k_2^2}$.

[Wolf 1969] [Natterer, Wuebbeling 2001] [Kak, Slaney 2001]



Semisphere of available data in Fourier space

Rotation of the object

Rotation $R_{\boldsymbol{n}(t),\alpha(t)} \in \mathrm{SO}(3)$ around the axis $\boldsymbol{n}(t) \in \mathbb{S}^2$ with angle $\alpha(t)$, $t \in [0, L]$

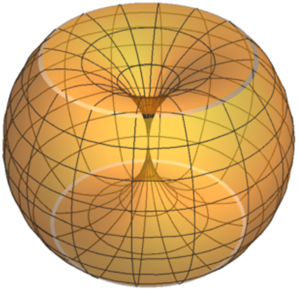
$$\sqrt{\frac{2}{\pi}}\kappa \mathrm{i} e^{-\mathrm{i}\kappa r_\mathrm{M}} \mathcal{F}_{1,2} \underbrace{u_t(k_1, k_2, r_\mathrm{M})}_{\text{measurements}} = \underbrace{\mathcal{F} f \left(R_{\boldsymbol{n}(t),\alpha(t)} \begin{pmatrix} k_1 \\ k_2 \\ \kappa - k_0 \end{pmatrix} \right)}_{=: \, T(k_1, k_2, t)},$$

where $\kappa = \sqrt{k_0^2 - k_1^2 - k_2^2}$

We have $\mathcal{F} f(T(k_1, k_2, t))$ on

$$\mathcal{U} = \{(k_1, k_2, t) : k_1^2 + k_2^2 \le k_0^2, \ t \in [0, L]\}$$

We want $f \colon \mathbb{R}^3 \to \mathbb{C}$ with $\operatorname{supp} f \subset \mathcal{B}_{r_s}$



Set $T(\mathcal{U})$ for full rotation around $\boldsymbol{n} = (1, 0, 0)^T$

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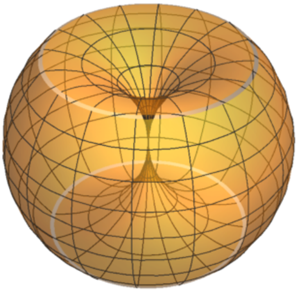

Set $T(\mathcal{U})$ for full rotation around $\boldsymbol{n} = (1, 0, 0)^T$

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Backpropagation

Idea: Compute inverse Fourier transform of $1_{T(\mathcal{U})}\mathcal{F}f$

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

Theorem

Let the rotation axis $\boldsymbol{n} \in C^1([0,L],\mathbb{S}^2)$ and angle $\alpha \in C^1[0,L]$. Then

$$f_{\mathrm{bp}}(\boldsymbol{r}) = (2\pi)^{-\frac{3}{2}} \int_{\mathcal{U}} \mathcal{F}f(T(k_1,k_2,t))\, \mathrm{e}^{\mathrm{i}T(k_1,k_2,t)\cdot\boldsymbol{r}} \frac{|\det \nabla T(k_1,k_2,t)|}{\operatorname{Card} T^{-1}(T(k_1,k_2,t))}\, d(k_1,k_2,t),$$

where

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

where $\boldsymbol{h} := (k_1, k_2, \pm\kappa - k_0)^\top$.

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

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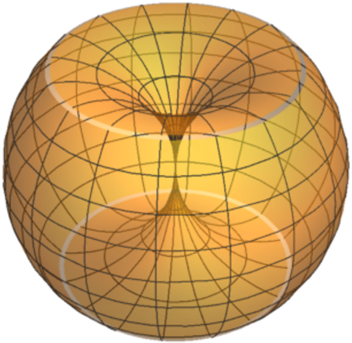
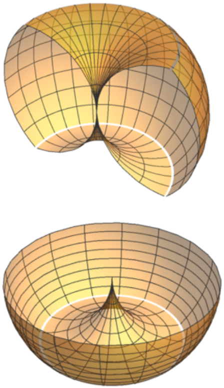
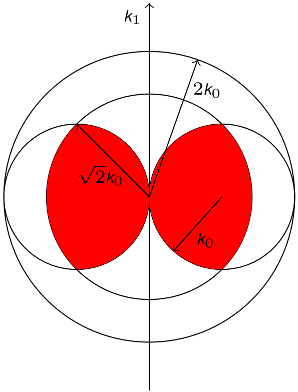
Example: Rotation around the first axis

Backpropagation formula $f_{\mathrm{bp}}^{\pm}(\boldsymbol{r}) = (2\pi)^{-\frac{3}{2}} \int_{\mathcal{U}} \mathcal{F}f(T(k_1,k_2,t))\, \mathrm{e}^{T(k_1,k_2,t)\cdot \boldsymbol{r}}\, \frac{k_0\,|k_2|}{2\kappa}\, \mathrm{d}(k_1,k_2,t)$

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



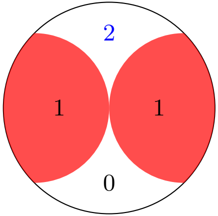




Example: Half rotation

Constant rotation axis $\boldsymbol{n} = (1, 0, 0)^\top$

Restricted angle $\alpha \in [0, \pi]$



$\mathrm{Card}(T^{-1}(\boldsymbol{y}))$ at section $y_1 = 0$

Example: Moving rotation axis

Moving rotation axes $\boldsymbol{n}(t) = (\cos(c\,\sin(t)), \sin(c\,\sin(t)), 0)^\top$, for $c > 0$

Rotation angle $\alpha(t) = t \in [0, 2\pi)$

Then

$$\mathrm{Card}(T^{-1}(\boldsymbol{y})) = \begin{cases} 4 & \text{in a neighborhood of the line segment } \{\boldsymbol{y} = (y_1, 0, 0)^\top : 0 < y_1 < 2k_0 \sin(c)\} \\ 2 & \text{elsewhere on } T(\mathcal{U}). \end{cases}$$

Content

Inversion methods

Approach 1: Inverse NDFT

- Discretize the forward problem $f \mapsto \mathcal{F}f$ as an NDFT (non-uniform discrete Fourier transform)
- Fast algorithm for the NDFT in $\mathcal{O}\left(N^3 \log N\right)$ steps

  [Dutt, Rokhlin 93], [Beylkin 95], [Potts, Steidl, Tasche 01], [Potts, Kunis, Keiner 04+]
- Computation the inverse with conjugate gradient method (CGNE)
- Cost: 2 NDFTs per iteration step
- Suitable for arbitrary rotations

Approach 2: Discrete backpropagation

- Discretize the integral in the backpropagation formula using the values of $\mathcal{F}f$ on $T(\mathcal{U}_N)$
- Cost: 1 NDFT
- Requires the computation of the Crofton symbol $\mathrm{Card}(T^{-1}(T(k_1, k_2, t)))$

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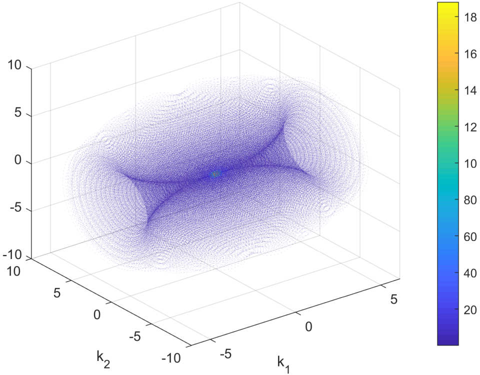
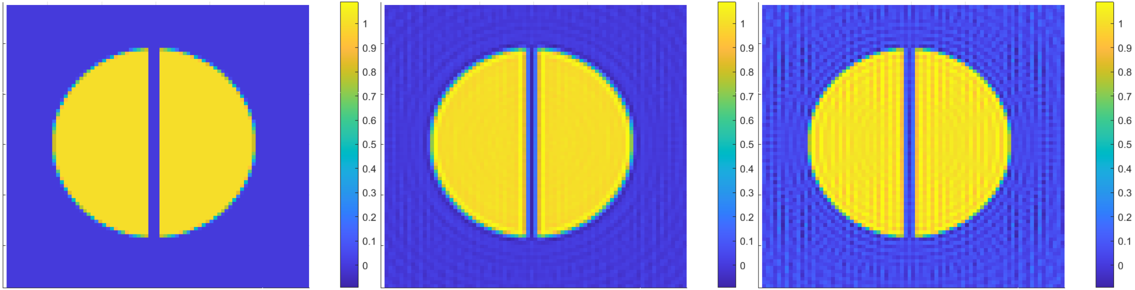
Test setup

- Normalized wavelength $\lambda = 1 \Rightarrow k_0 = \frac{2\pi}{\lambda} = 2\pi$
- Test function f given analytically
- Compute the simulated data $\mathcal{F}f$ with a very fine grid of size $5N$ to avoid the "inverse crime"



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

Numerical test



Test function
slice plot $r_1 = 0$

Inverse NDFT
(PSNR 29.52, SSIM 0.863)

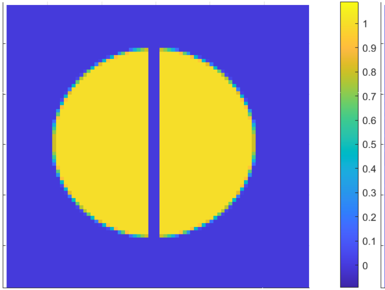
Backpropagation
(PSNR 25.25, SSIM 0.366)

Grid: $80 \times 80 \times 80 = 512\,000$ grid points
$M = 496\,944$ points in Fourier space

Fixed rotation axis $\boldsymbol{n} = (1, 0, 0)^\top$

Computation time: Inverse NDFT: 8.1 sec (with 20 iterations), Backpropagation: 0.4 sec

Numerical test: Rotation around other axis



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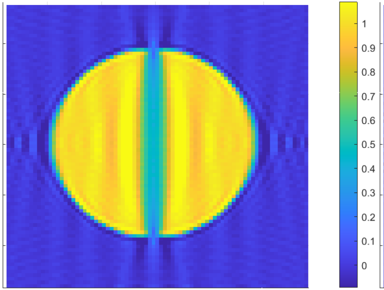
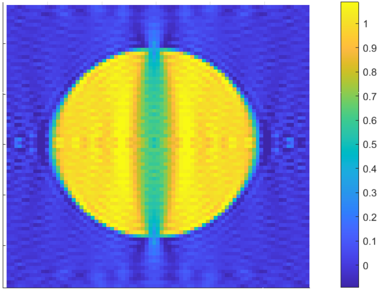


Inverse NDFT
(PSNR 22.94, SSIM 0.658)

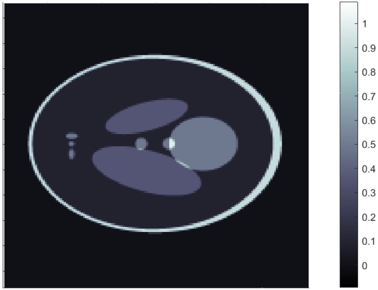


Packpropagation
(PSNR 21.04, SSIM 0.341)

Grid: $80 \times 80 \times 80 = 512\,000$ grid points

Fixed rotation axis $\boldsymbol{n} = (0, 1, 0)^\top$

Numerical test: Shepp–Logan phantom



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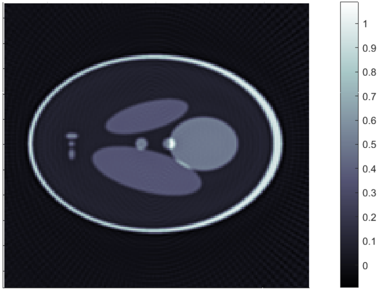
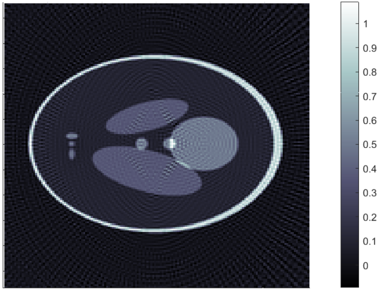


Inverse NDFT
(PSNR 32.56, SSIM 0.892)



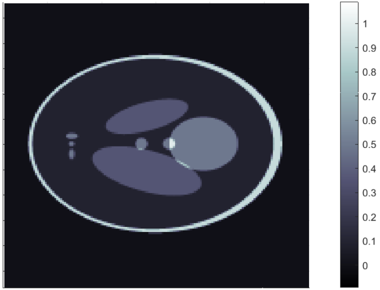
Backpropagation
(PSNR 27.81, SSIM 0.422)

Grid: $160 \times 160 \times 160 = 4\,096\,000$ grid points
$M = 4\,050\,624$ points in Fourier space

Fixed rotation axis $\boldsymbol{n} = (1, 0, 0)^\top$

Computation time: Inverse NDFT: 46 sec (with 20 iterations), Backpropagation: 10 sec

Numerical test: Non-constant rotation axis



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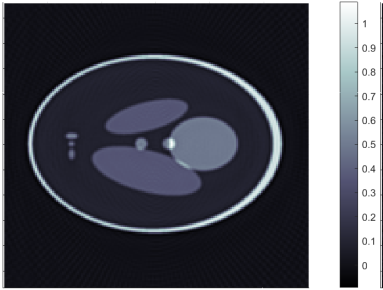
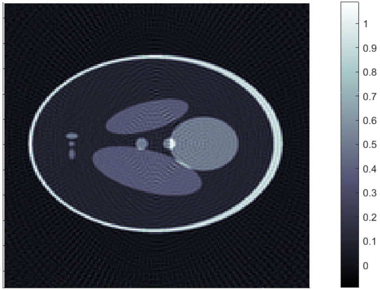


Inverse NDFT
(PSNR 33.62, SSIM 0.934)

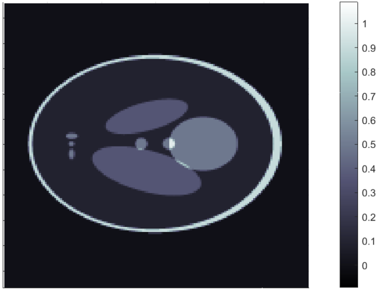


Backpropagation
(PSNR 27.55, SSIM 0.440)

Moving rotation axis

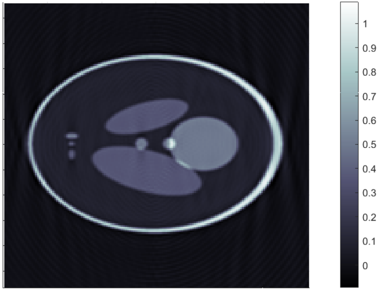
$$\boldsymbol{n}(t) = \left(\cos(\tfrac{\pi}{8}\ \sin(t)), \sin(\tfrac{\pi}{8}\ \sin(t)), 0\right)^\top, \qquad t \in [0, 2\pi]$$

Numerical test: Half rotation



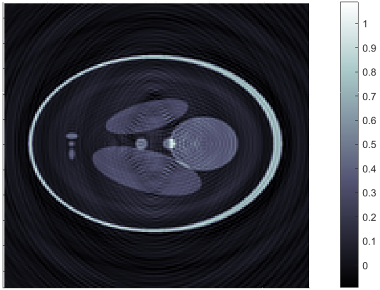
Test function

slice $r_1 = 0$



Inverse NDFT

(PSNR 30.80, SSIM 0.816)



Backpropagation

(PSNR 26.01, SSIM 0.324)

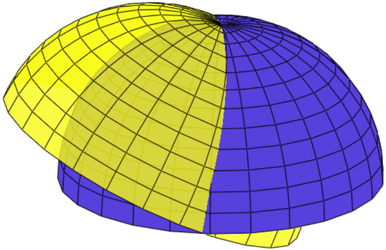
Content

Motion detection

Goal: Estimate the rotation R_t from the measurements u_t at time t

Common circle approach:

- For each t we have the Fourier data $\mathcal{F}f$ on one semisphere
- Two semispheres intersect in a circle (arc), where $\mathcal{F}f$ must agree
- Find the common circle of two semispheres



Conclusion

- Fourier diffraction theorem on $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared two reconstruction method
  - Backpropagation is faster
  - Inverse NFFT is always applicable and shows slightly better results

Future research

- Detection of rotation from data
- Application to real-world data
- Higher order approximations of wave equation
- Measuring only the intensities (phase retrieval)

Thank you for your attention!

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