Electron Microscope Tomography

Todd Quinto

www.tufts.edu/∼equinto
Tufts University

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2. The sample can warp and optical distortions can occur during data acquisition [A. Lawrence, et al.].

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3. For small objects, the electron beams travel along lines.
4. For large electron beams, electrons far from the central axis travel over curves [*ibid.*].

The Model

f is the density or scattering potential of an object
γ is a line or curve over which electrons travel.

The X-ray Transform:

$$\text{ET Data} \sim \mathcal{P}f(\gamma) := \int_{\mathbf{x}\in\gamma} f(\mathbf{x})ds$$

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The Goal: Recover a picture of the object including boundaries, molecule shapes,..., from ET data over a finite number of lines (curves).

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- We will use microlocal analysis to determine which boundaries are visible and develop an algorithm to reconstruct these features.
- This is a regularization method (reconstruct only what's visible).

Linear Electron Paths

Now show reconstructions for small samples ($\sim 100 \times 100$ nm). We use a model that assumes electrons travel over lines, and our ELT algorithm is based on Lambda CT.

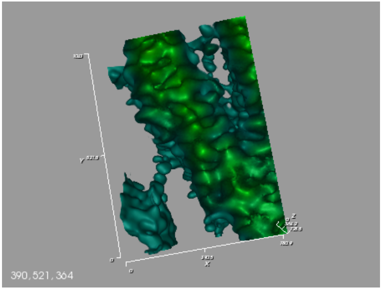
This is joint with Ozan Öktem (Comsol and Royal Institute of Technology, Stockholm) and Ulf Skoglund (Karolinska Institute, Stockholm).

Supported by: NSF, The Wenner Gren Stiftelserna, Tufts, Sidec and the University of Stockholm.

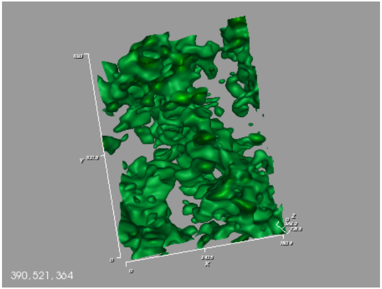
Comparison Using *In Situ* Nephrin [QÖ 2008]

In situ kidney sample, 200 kV TEM single-axis tilt data, uniform sampling, tilt angles every 2° between -60° and 60°, 418 $e^-/$pixel total dose. 70 nm^3 ROI. Data are assumed to be on lines.

ELT reconstruction

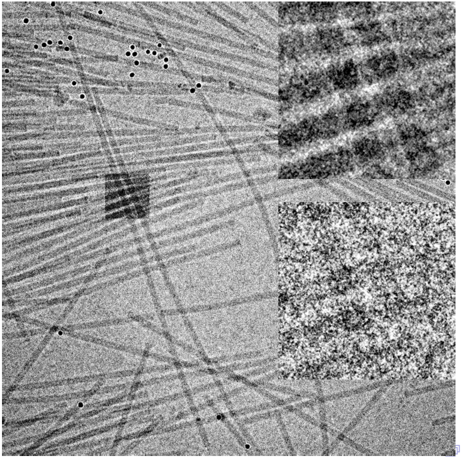


Sidec's original low-pass FBP reconstruction



TMV Data

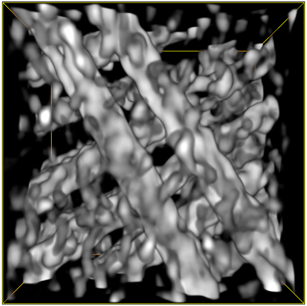
High-dose electron micrograph of Tobacco Mosaic Virus (TMV). The middle inset is the ROI and the two on the right are high-dose (top) and low-dose images of the ROI.



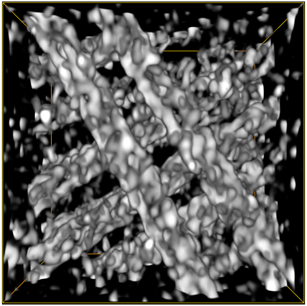
3-D Comparison Using TMV [QSÖ 2009]

*T*MV sample, 300 kV TEM single-axis tilt data, uniform sampling, tilt angles every 2° between $-62°$ and 62°, 407 $e^-/$pixel total dose. 115 nm^3 ROI.

ELT reconstruction



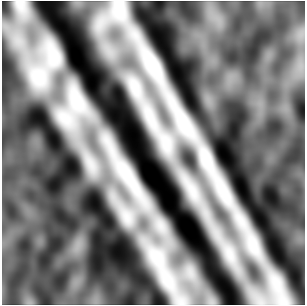
Karolinska's optimized FBP reconstruction



2-D Comparison Using TMV [QSÖ 2009]

*T*MV sample, 300 kV TEM single-axis tilt data, uniform sampling, tilt angles every 2° between $-62°$ and $62°$, 407 $e^-/$pixel total dose. 115 nm $\times$ 115 nm $\times$ 1.15 nm ROI.

ELT reconstruction



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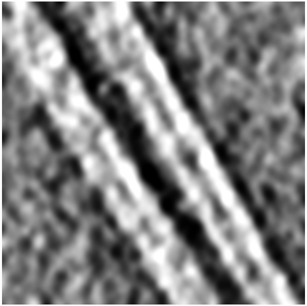


Curvilinear Electron Paths

We now develop a Radon transform that integrates over curves and provide reconstructions on simulated data.

Much integral geometric work has been done for X-ray transforms [Greenleaf and Uhlmann, Cormack, Gelfand et al., Finch, Globevnik, Krishnan, Kuchment, Kunyansky, Kurusa, Palamodov, Romanov, Stefanov ...]

The very new theoretical work is joint with Hans Rullgård.

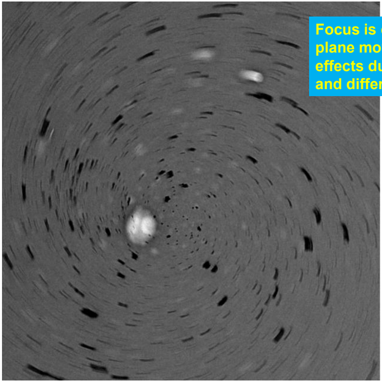
Supported by: NSF and Tufts

In large electron microscopes one can take images of about 8,000 nm square.

In large-field ET the electrons travel over curvilinear paths [A. Lawrence et al.].

NCMIR

Helical Distortions



Focus is changed in steps so focal plane moves through object. Note effects due to Helical trajectories and differential magnification.

The Mathematical Setup

The curvilinear paths: For each angle $\theta \in]a, b[$, the curves are defined by the smooth map (a projection in some global coordinates)

$$\boldsymbol{p}_\theta : \mathbb{R}^3 \to \mathbb{R}^2, \quad \boldsymbol{p}_\theta(\boldsymbol{x}) = \boldsymbol{y}$$

where $\boldsymbol{y}$ is the point on the detector plane and the electron beam through $\boldsymbol{x}$ for tilt θ.

Curves: $(\theta, \boldsymbol{y}) \in Y =]a, b[\times \mathbb{R}^2 \qquad \gamma_{\theta,\boldsymbol{y}} = {\boldsymbol{p}_\theta}^{-1}(\{\boldsymbol{y}\}) \cong$ a line

Curvilinear X-ray Transform: $\mathcal{P}_{\boldsymbol{p}} f(\theta, \boldsymbol{y}) = \int_{\boldsymbol{x} \in \gamma_{\theta,\boldsymbol{y}}} f(x) ds$

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Backprojection Set: $S_{\boldsymbol{x}} = \{(\theta, \boldsymbol{y}) \big| x \in \gamma_{\theta,\boldsymbol{y}}\}$, all curves containing $\boldsymbol{x}$

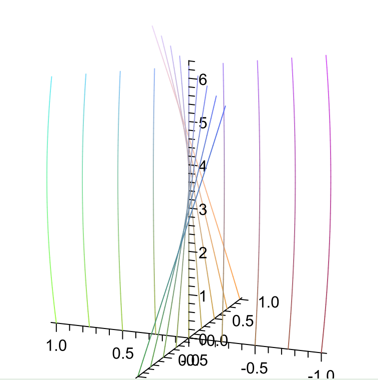
Backprojection Operator:

$$\mathcal{P}_{\boldsymbol{p}}^* g(\boldsymbol{x}) = \int_{(\theta,\boldsymbol{y}) \in S_{\boldsymbol{x}}} g(\theta, \boldsymbol{y}) d\theta = \int_{\theta \in]a,b[} g\left(\theta, \boldsymbol{p}_\theta(\boldsymbol{x})\right) d\theta.$$

If $S_{\boldsymbol{x}}$ cannot be made compact, one cuts off near the ends of $]a,b[$.

Example

Helical electron paths with pitch 20π.



Notation: $\partial_{\boldsymbol{x}}$ is the gradient in $\boldsymbol{x}$ and similarly for $\partial_{\boldsymbol{y}}$ and ∂_θ, $\xi \boldsymbol{dx} = \xi_1 \boldsymbol{dx}_1 + \xi_2 \boldsymbol{dx}_2 + \xi_3 \boldsymbol{dx}_3$ and $\eta \boldsymbol{dy} = \eta_1 \boldsymbol{dy}_1 + \eta_2 \boldsymbol{dy}_2$.

The Mathematical Assumptions

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Our Assumptions:

1. $(\boldsymbol{x}, \theta) \mapsto \boldsymbol{p}_\theta(\boldsymbol{x}) \in \mathbb{R}^2$ is C^∞ and is a fiber map in $\boldsymbol{x}$ with fibers diffeomorphic to lines. So, the matrix $\partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x})$ has maximal rank (two).
2. The maps $Y \ni (\theta, \boldsymbol{y}) \mapsto \gamma_{\theta,\boldsymbol{y}}$ and $\mathbb{R}^3 \ni \boldsymbol{x} \mapsto S_{\boldsymbol{x}}$ are one-to-one.
3. The 4×3 matrix $\begin{pmatrix} \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x}) \\ \partial_\theta \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x}) \end{pmatrix}$ has maximal rank (three).

Geometric Meaning

Wavefront Set

Definition

Let $(\boldsymbol{x}_0, \xi_0 \boldsymbol{dx}) \in T^*(\mathbb{R}^n)$, $\xi_0 \neq 0$. The function ***f* is in C^∞ at $\mathbf{x}_0$ in direction ξ_0** if there is a cut-off function φ near $\boldsymbol{x}_0$ such that

$$\mathcal{F}(\varphi f)(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\boldsymbol{x}\in\mathbb{R}^n} e^{-i\boldsymbol{x}\cdot\xi} \varphi(\boldsymbol{x})\, f(\boldsymbol{x})\, dx \tag{1}$$

is rapidly decreasing in some open cone from the origin, V, containing ξ_0.

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Example

$f = 1$ inside a disk in $\mathbb{R}^2$, $f = 0$ outside. What is $\mathrm{WF}(f)$?

The Microlocal Setup

Set of Points: $\mathbb{R}^3$,

Set of Curves: $Y = \{(\theta, \boldsymbol{y}) \,|\, \boldsymbol{y} \in \mathbb{R}^2, \theta \in]a, b[\}$

Incidence Relation: $Z = \{(\theta, \boldsymbol{y}; \boldsymbol{x}) \in Y \times \mathbb{R}^3 \,|\, \boldsymbol{x} \in \gamma_{\theta,\boldsymbol{y}}\}$ [Gelfand, Helgason]

Double Fibration:

$$\begin{array}{ccc} & Z & \\ {}^{\pi_L}\swarrow & & \searrow^{\pi_R} \\ Y & & \mathbb{R}^3 \end{array}$$

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$$\gamma_{\theta,\boldsymbol{y}} = \pi_R\left(\pi_L^{-1}(\{(\theta, \boldsymbol{y})\})\right) \qquad S_{\boldsymbol{x}} = \pi_L\left(\pi_R^{-1}(\{\boldsymbol{x}\})\right)$$

$\mathcal{P}_{\boldsymbol{p}}$ as a FIO

We prove that $\mathcal{P}_{\boldsymbol{p}}$ is an elliptic Fourier integral operator with canonical relation $\mathcal{C} = (N^*(Z) \setminus \mathbf{0})'$. The properties of the FIO $\mathcal{P}_{\boldsymbol{p}}$ and $\mathcal{P}_{\boldsymbol{p}}^*$ are determined by the microlocal diagram:

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In particular, if Π_L *were* an injective immersion, (the Bolker Assumption) $\mathcal{P}_{\boldsymbol{p}}^*\mathcal{P}_{\boldsymbol{p}}$ *would* be an elliptic ΨDO (in visible directions). The extent to which Π_L doesn't satisfy the Bolker Assumption determines how far $\mathcal{P}_{\boldsymbol{p}}^*\mathcal{P}_{\boldsymbol{p}}$ is from being a standard elliptic ΨDO [Guillemin,.... *Admissible Case:* Greenleaf, Uhlmann, Felea, Finch, Lan, Stefanov,....]

Theorem (QR 2009)

Under our assumptions $\mathcal{P}_{\mathbf{p}}$ is an elliptic Fourier integral operator associated to the canonical relation $\mathcal{C} = (N^*Z \setminus \mathbf{0})'$

$$\mathcal{C} = \{(\theta, \mathbf{p}_\theta(\mathbf{x}), -\eta \cdot \partial_\theta \mathbf{p}_\theta(\mathbf{x})d\theta + \eta \cdot \mathbf{dy}; \mathbf{x}, \eta \cdot \partial_{\mathbf{x}} \mathbf{p}_\theta(\mathbf{x})\mathbf{dx}) \\ \big| \theta \in]a,b[,\ \eta \in \mathbb{R}^2 \setminus \mathbf{0},\ \mathbf{x} \in \mathbb{R}^3\}$$

Π_L *is not injective.* ▸ Injectivity Conditions

Π_L *is an immersion above each $(\theta, \mathbf{y})$ except on a one-dimensional set of covectors.* ▸ Immersion Conditions

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Proof.

$\mathcal{P}_{\boldsymbol{p}}$ has Schwartz kernel I_Z, integration over Z. By results of Guillemin, $\mathcal{C}$ is the canonical relation for I_Z. Π_L and Π_R don't map to the zero section, so $\mathcal{P}_{\boldsymbol{p}}$ is a FIO associated to $\mathcal{C}$. Now, study Π_L. □

Theorem (Microlocal Regularity Theorem, QR 2009)

Let $\mathcal{P}_{\boldsymbol{p}}$ *be a curvilinear Radon transform that satisfies our assumptions. Let* $f \in \mathcal{E}'(\mathbb{R}^3)$. *Let* D *be a pseudodifferential operator on* $\mathbb{R}^2$ *acting on* $\boldsymbol{y}$. *Then,*

$$\mathrm{WF}(\mathcal{P}_{\boldsymbol{p}}(f)) \subset \Pi_L \left(\Pi_R^{-1}\mathrm{WF}(f)\right)$$

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When the Bolker Assumption holds globally enough above a singularity of f, $(\boldsymbol{x_0}, \xi_0 \boldsymbol{dx}) \in \mathrm{WF}(f) \cap \Pi_R(\mathcal{C})$, that singularity will be visible in $\mathcal{P}_{\boldsymbol{p}} f$ and then in $\mathcal{P}_{\boldsymbol{p}}^* D \mathcal{P}_{\boldsymbol{p}} f$ (see [QR 2009] for a description depending on $\operatorname{supp} f$ and the geometry of $\mathcal{C}$).

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- Any backprojection algorithm can add singularities to the reconstruction.
- However, backprojection algorithms can show singularities of f $\longrightarrow$.

What Does It All Mean for ET?

Our algorithm: $\Lambda_p f = \mathcal{P}_{\boldsymbol{p}}^* D \mathcal{P}_{\boldsymbol{p}} f$ where $D = D(\theta, \boldsymbol{x})$ is a second order PDO with symbol zero on images under Π_L of covectors on which Π_L is not an immersion.

Description of $D(\theta, \boldsymbol{x})$

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Description of $D(\theta, \boldsymbol{x})$

- Our choice of D suppresses *some* added singularities.
- For admissible complexes (e.g., for ET on lines) the added singularities are suppressed by this differential operator everywhere (noninjectivity$\equiv$nonimmersion).

What Does It All Mean for ET?

Our algorithm: $\Lambda_p f = \mathcal{P}_{\boldsymbol{p}}^* D \mathcal{P}_{\boldsymbol{p}} f$ where $D = D(\theta, \boldsymbol{x})$ is a second order PDO with symbol zero on images under Π_L of covectors on which Π_L is not an immersion.

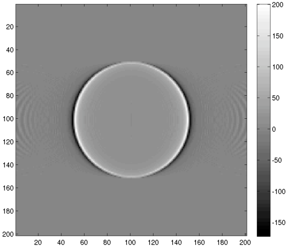
Description of $D(\theta, \boldsymbol{x})$

- Our choice of D suppresses *some* added singularities.
- For admissible complexes (e.g., for ET on lines) the added singularities are suppressed by this differential operator everywhere (noninjectivity≡nonimmersion).
- For nonadmissible complexes, added singularities from far away can show up the reconstruction even if one uses the clever D.

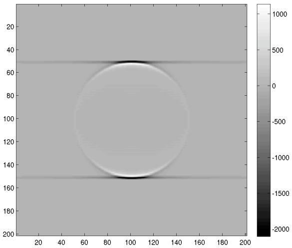
Helix with Pitch 20π, cross-section in xy-plane

One ball of radius 0.5. 70 angles in $[0, \pi]$ and a 201×201 detector grid on $[-1, 1]^2$. x_1 axis is vertical!

Derivative $\perp$ bad direction



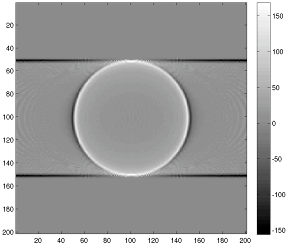
Derivative in bad direction



Helix with Pitch π, cross-section in xy-plane

One ball of radius 0.5. $\theta \in [0, 2\pi]$, full angular data, rotating on the x_1 axis. x_1 axis is vertical!

Derivative $\perp$ bad direction



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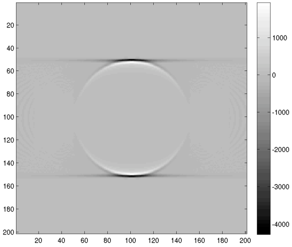

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Thanks for your attention!

Geometric Interpretation of Rank Assumption

If the rank assumption doesn't hold, then $\begin{pmatrix} \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x}) \\ \partial_\theta \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x_0}) \end{pmatrix}$ has rank two.

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So, the tangent plane doesn't "change" as θ is changed infinitesimally.

This means that, infinitesimally, one does not see a full three-dimensional set of cotangent vectors at $\boldsymbol{x}$ from the data as from data $\mathcal{P}_{\boldsymbol{p}} f$, one sees only covectors conormal to $\gamma_{\theta,\boldsymbol{p}_\theta(\boldsymbol{x})}$ at $\boldsymbol{x}$).

Back

Theorem (QR 2009)

Π_L is not injective. Let $(\theta, \boldsymbol{y}) \in Y$ and $\eta \in \mathbb{R}^2 \setminus \boldsymbol{0}$. Covectors in $\mathcal{C}$ map to the same point under Π_L ***iff*** *they are of the form*
$\lambda_j := (\theta, \boldsymbol{p}_\theta(\boldsymbol{x}_j), -\eta \cdot \partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}_j) \boldsymbol{d\theta} + \eta \cdot \boldsymbol{dy}; \boldsymbol{x}_j, \eta \cdot \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x}_j) \boldsymbol{dx})$ *for* $j = 0, 1$, *where*

$$\boldsymbol{p}_\theta(\boldsymbol{x}_0) = \boldsymbol{p}_\theta(\boldsymbol{x}_1) \tag{2}$$

$$\eta \cdot (\partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}_0) - \partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}_1)) = \boldsymbol{0}. \tag{3}$$

Generically, condition (3) will mean that η is perpendicular to $\partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}_0) - \partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}_0)$. In all cases, for all $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ in $\gamma_{\theta, \boldsymbol{p}_\theta(\boldsymbol{x}_0)}$ there are points for which this condition holds.

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Proof.

This follows from the expression for $\Pi_L : \mathcal{C} \to T^* Y$ and that $\begin{pmatrix} \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x}) \\ \partial_{\boldsymbol{x}} \partial_\theta \boldsymbol{p}_\theta(\boldsymbol{x}) \end{pmatrix}$ is assumed to have maximal rank (three) and $\partial_{\boldsymbol{x}} \boldsymbol{p}_\theta$ has maximal rank (two). □

Back

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For each $(\theta, \boldsymbol{y})$ and $\boldsymbol{x} \in \gamma_{\theta,\boldsymbol{y}}$, we choose a unit tangent vector $\boldsymbol{v}$ to $\gamma_{\theta,\boldsymbol{y}}$ at $\boldsymbol{x}$ and we let

$$\eta_0 = \left(\partial_\theta \partial_{\boldsymbol{x}} \boldsymbol{p}_\theta(\boldsymbol{x})\boldsymbol{v}\right)^t \qquad D = D(\theta, \boldsymbol{x}) = \left(\partial_{\eta_0}\right)^2$$

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