The Microlocal Analysis of some X-ray transforms in Electron Tomography (ET)

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Joint work with Raluca Felea (lines),
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The Model of Electron Tomography (ET)

Intro

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

The X-ray Transform:

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

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

Data Acquisition: Take multiple micrographs (ET images) of a prepared sample of particles by moving the sample in relation to the electron beam.

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- For small fields of view ($\sim$ 300 nm), narrow electron beams travel along lines so the math is known. However, data are from a limited range of directions that image only a small region of interest.
- For larger fields of view ($\sim$ 8,000 nm), the electron beams need to be wider and electrons far from the central axis travel over helix-like curves, not lines [A. Lawrence et al.].

The Admissible Case for Lines in $\mathbb{R}^3$

The model: the X-ray transform over lines

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$$S_{\boldsymbol{x}} = \bigcup \{\ell \in \Xi \,|\, \boldsymbol{x} \in \ell\}$$

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Definition (Cone Condition (Admissible Line Complex))

Ξ satisfies the *Cone Condition* if for all $\ell \in \Xi$ and any two points $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ in ℓ, the cones $S_{\boldsymbol{x}_0}$ and $S_{\boldsymbol{x}_1}$ have the same tangent plane along ℓ.

[Gelfand and coauthors, Guillemin, Greenleaf, Uhlmann, Boman, Q, Finch, Katsevich, Sharafutdinov, and many others]

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They wrote a series of beautiful articles using sophisticated microlocal analysis to understand admissible complexes, Ξ, of geodesics on manifolds.

The associated X-ray transform $\mathcal{P}$ is an elliptic Fourier integral operator associated to a certain canonical relation $\Gamma = (N^*(Z))' \setminus \mathbf{0}$ [Guillemin].

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[GU 1989]: If Γ satisfies a curvature condition, then $\mathcal{P}^*\mathcal{P}$ is a singular Fourier integral operator in $I^{(-1),0}(\Delta, \Gamma_\Sigma)$ where Γ_Σ is a flow-out from the diagonal, Δ.

So, $\mathcal{P}^*\mathcal{P}(f)$ can have added singularities (compared to f) because of Γ_Σ.

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Applications of microlocal analysis in tomography and radar: Ambartsoumian, Antoniano, Cheney, deHoop, Felea, Finch, Greenleaf, Guillemin, Krishnan, Lan, Nolan, Q, Stefanov, Uhlmann, and many others.

Small field of view ET: Lines parallel a curve on S^2

$\theta :]a, b[\to S^2$ a smooth, regular curve. $C = \theta(]a, b[\,)$

For any $x \in \mathbb{R}^3$,

$$S_{\boldsymbol{x}} = \{x + s\theta(t) \,|\, s \in \mathbb{R},\ t \in]a, b[\,\}$$

is a cone and the complex of lines with directions parallel C is admissible.

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Hypothesis (Curvature Conditions)

Let $\theta :]a, b[\to S^2$ be a smooth regular curve. Let $\beta(t) = \theta(t) \times \theta'(t)$. We assume the following curvature conditions

(a) $\forall t \in]a, b[\,,\ \ \theta''(t) \cdot \theta(t) \neq 0.$

(b) $\forall t \in]a, b[\,,\ \ \beta'(t) \neq \mathbf{0}.$

(c) *The curve $t \mapsto \beta(t)$ is simple.*

Examples

Single Axis Tilt ET: This complex is admissible but *does not* satisfy the curvature conditions so [GU 1989] does not apply.

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In the coordinate system of the specimen, conical tilt data are over lines in the complex of lines parallel C_{cone}.

For $\boldsymbol{x} \in \mathbb{R}^3$, $S_{\boldsymbol{x}}$ is the circular cone with vertex $\boldsymbol{x}$ with opening angle α with vertical axis.

This complex satisfies the cone condition and the curvature conditions and [GU 1989] does apply.

Theorem (Microlocal Regularity Theorem [FeQu 2011])

Assume the smooth regular curve $C \subset S^2$ satisfies the curvature conditions, and let $\mathcal{P}$ be the associated X-ray transform with a smooth nowhere zero measure. Let D be the second order derivative on the detector plane in the θ' direction. Then $\mathcal{L} = \mathcal{P}^* D \mathcal{P}$ is in $I^{0,1}(\Delta, \Gamma_\Sigma)$ where
$\Gamma_\Sigma = \{(\boldsymbol{y}, \xi, \boldsymbol{x}, \xi) \big| (\boldsymbol{y}, \xi) \in N^*(S_{\boldsymbol{x}})\}$.
Therefore the wavefront set above $\boldsymbol{x}$

$$\mathrm{WF}(\mathcal{L}(f))_{\boldsymbol{x}} \subset (\mathrm{WF}(f)_{\boldsymbol{x}} \cap \mathcal{V}_{\boldsymbol{x}}) \cup \mathcal{A}(f)_{\boldsymbol{x}}$$

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$\mathcal{A}(f)_{\boldsymbol{x}} = \{(\boldsymbol{x}, \xi) \big| \exists \boldsymbol{y} \in S_{\boldsymbol{x}} \text{ such that } (\boldsymbol{y}, \xi) \in (N^*(S_{\boldsymbol{x}}) \cap \mathrm{WF}(f))\}$.

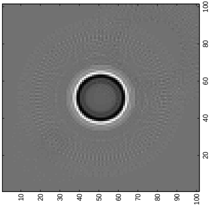
Therefore $\mathcal{L}(f)$ can show visible singularities of f.
However, $\mathcal{L}(f)$ can add *(or mask)* singularities at $\boldsymbol{x}$ coming from other covectors in $\mathrm{WF}(f)$ conormal to $S_{\boldsymbol{x}}$. (Proof uses [GU])

Morals

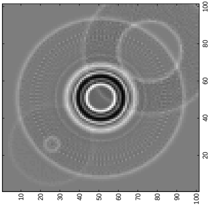
- Since $\mathcal{L} \in I^{0,1}(\Delta, \Gamma_\Sigma)$, the added singularities will be *one degree weaker in Sobolev scale* than if D were an arbitrary differential operator since, in general, $\mathcal{L}$ would be in $I^{1,0}$.
- This algorithm has been tested on electron microscope data for single axis tilt [QO 2008, QSO 2009].

Cross-section of reconstructions from conical tilt data of several balls [QBC 2008]. Note decreased strength of added singularities when using D instead of Δ.

Reconstruction using D



Reconstruction using Δ



Large Field of View ET: The Curvilinear X-ray Transform

The curvilinear paths: For each tilt angle $t \in]a, b[$, electron paths are inverse images of the smooth fiber map

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

$\boldsymbol{y}$ is on the detector plane.

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

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

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

Backprojection Operator: $\mathcal{P}^*_{\boldsymbol{p}} g(\boldsymbol{x}) = \int_{t \in]a,b[} g\left(t, \boldsymbol{p}_t(\boldsymbol{x})\right) dt,$

which is the integral over all curves through $\boldsymbol{x}$ (as $\boldsymbol{x} \in \gamma_{t,\boldsymbol{p}_t(\boldsymbol{x})}$)

If the curve doesn't join up at a and b, one multiplies by a cut off function near the ends of $]a, b[$.

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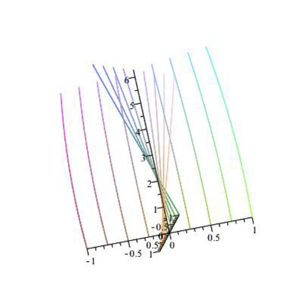
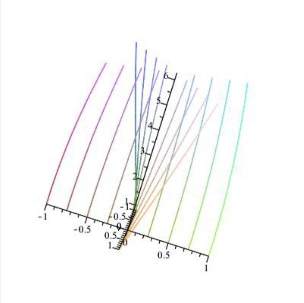
Example (Helical Electron Paths With Pitch 20π)





Single-axis tilt data geometry, multi-axis tilt ET and conical tilt ET over curves fit into our model.

Regularity Assumptions:

($\partial_{\boldsymbol{x}}$ and ∂_t are gradients)

1. For each $t \in]a, b[$, the curves $\gamma_{t,\boldsymbol{y}}$ are smooth, unbounded, and don't intersect. $(\boldsymbol{x}, t) \mapsto \boldsymbol{p}_t(\boldsymbol{x}) \in \mathbb{R}^2$ is a C^∞ map. Fixing t, $\boldsymbol{p}_t$ is a fiber map in $\boldsymbol{x}$ with fibers diffeomorphic to lines. Therefore, $\partial_{\boldsymbol{x}}\boldsymbol{p}_t(\boldsymbol{x})$ has maximal rank (two).
2. Curves move differently at different points as t changes. $\forall (t, \boldsymbol{y}) \in Y$ and $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ in $\gamma_{t,\boldsymbol{y}}$, if $\boldsymbol{x}_1 \neq \boldsymbol{x}_0$, then $\partial_t \boldsymbol{p}_t(\boldsymbol{x}_0) \neq \partial_t \boldsymbol{p}_t(\boldsymbol{x}_1)$.
3. The curves wiggle enough as t changes. The 4×3 matrix $\begin{pmatrix} \partial_{\boldsymbol{x}}\boldsymbol{p}_t(\boldsymbol{x}) \\ \partial_t\partial_{\boldsymbol{x}}\boldsymbol{p}_t(\boldsymbol{x}) \end{pmatrix}$ has maximal rank (three). Geometric Meaning

Our Reconstruction Operator

$\mathcal{L}(f) = \mathcal{P}_{\boldsymbol{p}}^* D \mathcal{P}_{\boldsymbol{p}} f$ where D is a 2^{nd} order PDO

Using the composition calculus of FIO "essentially"

$$\mathcal{L}(f)(\boldsymbol{x}) \sim D' \mathcal{P}_{\boldsymbol{p}}^* \mathcal{P}_{\boldsymbol{p}} f = D' \int_{S_{\boldsymbol{x}}} f \, W dA$$

for some singular weight W and ΨDO D' where

$$S_{\boldsymbol{x}} = \bigcup_{t \in]a,b[} \gamma_{t, \boldsymbol{p}_t(\boldsymbol{x})}$$ is the "cone" of curves through $\boldsymbol{x}$

Our Reconstruction Operator Adds Singularities

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Thus, singularities of f that are normal to $S_{\boldsymbol{x}}$ could appear as **added** singularities in the reconstruction $\mathcal{L}f(\boldsymbol{x})$ (as in the admissible case).

Theorem (Microlocal Regularity Theorem, [QR 2012])

Let $\mathcal{P}_{\boldsymbol{p}}$ satisfy our assumptions. Let $f \in \mathcal{E}'(\mathbb{R}^3)$. Let D be a differential operator on $\mathbb{R}^2$ acting on $\boldsymbol{y}$. Then, the wavefront set at $\boldsymbol{x}$

$$(\mathrm{WF}(\mathcal{L}(f)))_{\boldsymbol{x}} \subset (\mathrm{WF}(f) \cap \mathcal{V}_{\boldsymbol{x}}) \cup \mathcal{A}_{\boldsymbol{x}}$$

Proof uses Hörmander-Sato Lemma. [Stefanov-Uhlmann (magnetic geodesics), Greenleaf and Uhlmann, Guillemin, Krishnan, Palamodov...]

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where $\mathcal{V}_{\boldsymbol{x}}$ is the set of visible singularities (normals to curves through $\boldsymbol{x}$), and $\mathcal{A}_{\boldsymbol{x}}$ is a set of added singularities above $\boldsymbol{x}$ coming from singularities of f that are $\perp$ to $S_{\boldsymbol{x}}$.

- Our algorithm can accurately show visible singularities of f.
- However, any backprojection algorithm can add *(or mask)* singularities to the reconstruction from singularities of f normal to $S_{\boldsymbol{x}}$ at points far from $\boldsymbol{x}$. This is because

▸ $\Pi_L : \mathcal{C} \to T^*(Y)$ is not Injective ▸ Π_L is not an immersion

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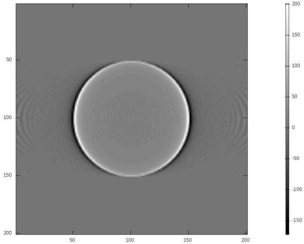
Helical data with Pitch 20π

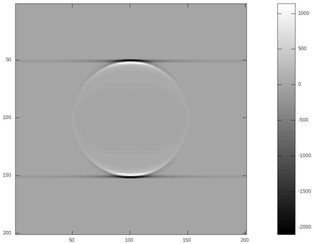
As in the admissible case, the choice of derivative can decrease the effect of the added singularities. However, here, it deceases only *nearby* added singularities!

Reconstruction of one ball. 70 angles in $[0, \pi]$. x_1 axis is vertical.

Derivative in good direction



Derivative $\perp$ good direction



Summary

- **For admissible complexes:**
  - Greenleaf and Uhlmann's theory shows what singularities are added.
  - Choosing the right differential operator can decrease the strength of added singularities. This is behind the improved local algorithms for cone beam CT [Katsevich, Anastasio, Wang] and slant hole SPECT/conical tilt ET [QBC, QÖ]. A first order ΨDO was suggested for cone beam CT in [FLU].

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  - Added singularities are intrinsic to any backprojection algorithm for this data.

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- **For curved paths:**
  - No inversion algorithm exists in general. Our algorithm is local, shows boundaries, and easy to implement.
  - Added singularities are intrinsic to any backprojection algorithm for this data.
  - In general, the good differential operator decreases *nearby* singularities but not all singularities (because far-away added singularities are in directions that don't get annihilated by it).

HAPPY BIRTHDAY, GUNTHER! Thanks for the beautiful math!

Fourier Integral Operators

Z and X are open subsets of $\mathbb{R}^n$:

$$F(f)(\boldsymbol{z}) = \int_{\boldsymbol{x} \in X, \omega \in \mathbb{R}^n} e^{i\phi(\boldsymbol{z}, \boldsymbol{x}, \omega)} p(\boldsymbol{z}, \boldsymbol{x}, \omega) f(\boldsymbol{x}) dx\, d\omega$$

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Canonical Relation:

$\mathcal{C} = \{(\boldsymbol{z}, \partial_{\boldsymbol{z}}\phi(\boldsymbol{z},\boldsymbol{x},\omega); \boldsymbol{x}, -\partial_{\boldsymbol{x}}\phi(\boldsymbol{z},\boldsymbol{x},\omega)) | \partial_\omega\phi(\boldsymbol{z},\boldsymbol{x},\omega) = 0\}$

$$\begin{array}{ccc} & \mathcal{C} & \\ \Pi_L \swarrow & & \searrow \Pi_R \\ Z\times(\mathbb{R}^n\setminus\mathbf{0}) & & X\times(\mathbb{R}^n\setminus\mathbf{0}) \end{array}$$

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WF relation: $\mathrm{WF}(F(f)) \subset \Pi_L\left(\Pi_R^{-1}(\mathrm{WF}(f))\right)$.

What it means: FIO change singularities in specific ways determined by the geometry of $\mathcal{C}$.

Pseudodifferential operators (ΨDOs)

$$P(f)(\boldsymbol{z}) = \int e^{i(\boldsymbol{z}-\boldsymbol{x})\cdot\omega} p(\boldsymbol{z}, \boldsymbol{x}, \omega) f(\boldsymbol{x}) dx\, d\omega$$

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WF relation: $\mathrm{WF}(P(f)) \subset \Pi_L\left(\Pi_R^{-1}(\mathrm{WF}(f))\right) = \mathrm{WF}(f)$.

What it means: ΨDO do not move wavefront set.

Back

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- So, the normal plane doesn't "change" as t is changed infinitesimally.

From data $\mathcal{P}_{\boldsymbol{p}} f$, one sees only covectors conormal to $\gamma_{t,\boldsymbol{p}_t(\boldsymbol{x})}$ at $\boldsymbol{x}$.
Moral: Infinitesimally, one does not see a full three-dimensional set of cotangent vectors at $\boldsymbol{x}$ from the data $(\frown)$.

Theorem (QR 2012)

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

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$$\eta \cdot (\partial_t \boldsymbol{p}_t(\boldsymbol{x}_0) - \partial_t \boldsymbol{p}_t(\boldsymbol{x}_1)) = \boldsymbol{0}. \tag{2}$$

Condition (2) means that η is perpendicular to $\partial_t \boldsymbol{p}_t(\boldsymbol{x}_0) - \partial_t \boldsymbol{p}_t(\boldsymbol{x}_1)$. In all cases, for all $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ in $\gamma_{t, \boldsymbol{p}_t(\boldsymbol{x}_0)}$ there are covectors 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 $\begin{pmatrix} \partial_{\boldsymbol{x}} \boldsymbol{p}_t(\boldsymbol{x}) \\ \partial_t \partial_{\boldsymbol{x}} \boldsymbol{p}_t(\boldsymbol{x}) \end{pmatrix}$ is assumed to have maximal rank (three) and $\partial_{\boldsymbol{x}} \boldsymbol{p}_t$ has maximal rank (two). □

Back

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

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

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

where D operates on the $\boldsymbol{y}$ coordinate.

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