Abelian and non-Abelian X-ray transforms: mapping properties and Bayesian inversion

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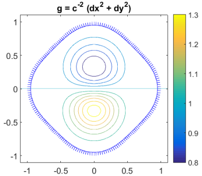
UCI International Zoom Inverse Problems seminar
August 6, 2020

Outline

The geodesic X-ray transform



(M, g), ∂M strictly convex.

$\partial_+ SM$: "inward" boundary ('fan-beam').

Geodesics: $\gamma_{x,v}(t)$.

Geodesic X-ray transform of f:

$$If(x, v) = \int_0^{\tau(x,v)} f(\gamma_{x,v}(t))\, dt, \qquad (x, v) \in \partial_+ SM = \mathbb{S}^1 \times \left(-\frac{\pi}{2}, \frac{\pi}{2}\right).$$

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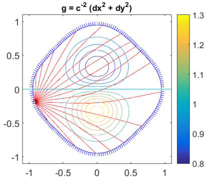

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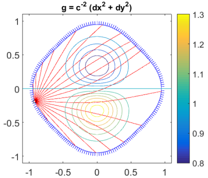

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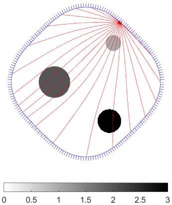
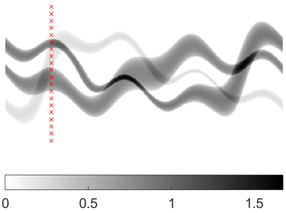


$\overset{I}{\mapsto}$



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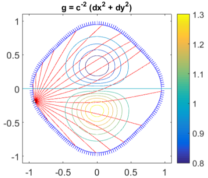

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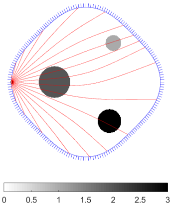
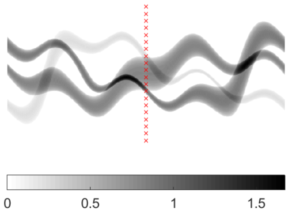
$f(x)$  $\overset{I}{\mapsto}$ 

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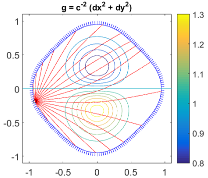

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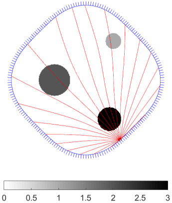
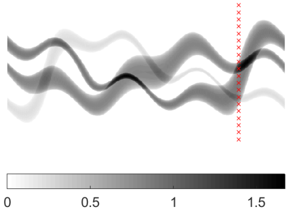
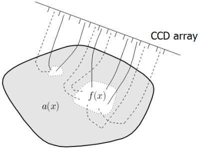
$f(x)$ 

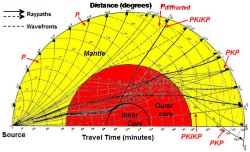
$\overset{I}{\mapsto}$ 

Goal: recover f from If.

Applications of geodesic X-ray transform

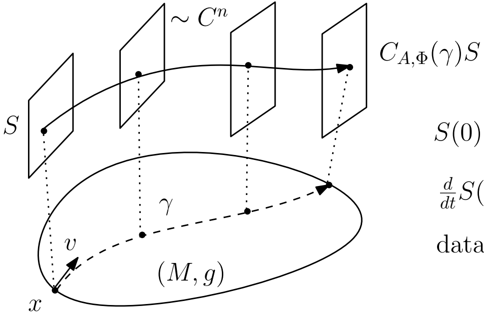
1. Radon transform and X-ray CT
2. SPECT and tomography in media with variable index of refraction
3. Seismology and travel-time tomography.





The non-abelian X-ray transform

$E = M \times \mathbb{C}^n$ trivial bundle over (M, g) a simple Riem. surface
A: hermitian connection on E (= matrix of one-forms)
Φ: skew-hermitian Higgs field ($\Phi : M \to \mathfrak{u}(n)$)



$S(0) = S$

$\frac{d}{dt}S(t) + (A_{\gamma(t)}(\dot\gamma(t)) + \Phi_{\gamma(t)})S(t) = 0$

data: $S(\ell(\gamma)) = C_{A,\Phi}(\gamma)S$

Inverse problem:

- to recover (A, Φ) from $C_{A,\Phi}$ modulo natural obstruction.
- if $A \equiv 0$: to recover Φ from C_Φ.

Vertgeim, Eskin, Novikov, Paternain-Salo-Uhlmann

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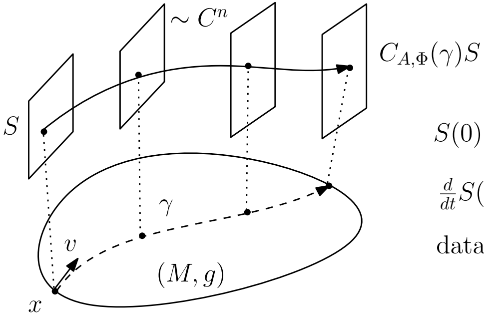

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Applications of non-abelian X-ray transform

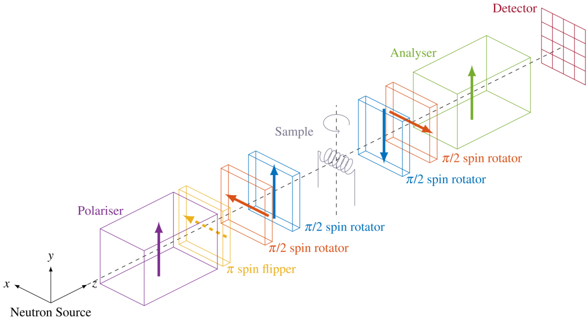
Problem (Polarimetric Neutron Tomography)

To recover a magnetic field from neutron spin-in to spin-out map ("scattering data" of the magnetic field).

While a neutron's trajectory $\gamma(t)$ is unaffected by a magnetic field B, its **spin** S evolves according to

$$\dot{S}(t) = B(t) \times S(t).$$

$B \leftrightarrow \mathfrak{so}(3)$-valued Higgs field.



Src: Sales et al, "3D Polarimetric Neutron Tomography of Magnetic Fields", 2017.

Bayesian approach to noisy inversion 1/2

We consider the problem of recovering a matrix field Φ_0 from

$$Y_j = C_{\Phi_0}(\gamma_j) + \varepsilon_j, \qquad \varepsilon_j \sim \mathcal{N}(0, \sigma^2), \qquad 1 \le j \le N.$$

where $\{\gamma_j\}_{j=1}^N$ are chosen uniformly at random in fan-beam coordinates. Denote $D_N = \{(\gamma_j, Y_j)\}_{1 \le j \le N}$ the data set.

Given a prior model for Φ and a noise model, Bayes' formula gives the proba. density of the posterior random variable $\Phi|D_N$:

$$P(\Phi|D_N) = \frac{P(D_N|\Phi)P(\Phi)}{P(D_N)} \quad \propto \quad \overbrace{P(D_N|\Phi)}^{\text{likelihood}} \cdot \overbrace{P(\Phi)}^{\text{prior}}$$

With a Gaussian prior and Gaussian noise model, one may arrive at the log-posterior distribution:

$$-\log \Pi(\Phi|D_N) = \frac{1}{\sigma^2} \sum_{j=1}^N |Y_j - C_\Phi(\gamma_j)|_F^2 + \|\Phi\|_{H^\alpha}^2 + C.$$

Note: Not gaussian since $\Phi \mapsto C_\Phi$ is non-linear.

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Bayesian approach to noisy inversion 2/2

Rather than looking at the entire posterior object $\Phi|D_N$, consider ONE of its moments $\langle \Phi, \psi \rangle | D_N$, where ψ is a 'test' field.

Important questions:

1. What relevant estimators $\widehat{\Psi}_N$ of $\langle \Phi_0, \psi \rangle$ can we extract from this posterior distribution ? Examples: mean and MAP, when they exist.
2. Are they easily computable ?
3. Consistency: does $\widehat{\Psi}_N \to \langle \Phi_0, \Psi \rangle$ as $N \to \infty$ in any sense ?
4. UQ: does the posterior density "contract" about $\widehat{\Psi}_N$ so one can get confidence/credible sets ?

Outline

Main messages of this talk

1. Making UQ statements for inverse problems requires a refined understanding of mapping properties of the forward and/or the 'normal' (linearized) operator.
2. For X-ray problems on manifolds with boundary, these mapping properties (the natural Hilbert scales involved and their Fréchet limits) are highly sensitive to the choice of certain weights.
3. Said choice of weights can come from: theoretical tractability ("choose the easiest one !") or noise model ("choose the practical one !").

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Main results 1/3

Theorem (M', 2019, arXiv preprint 1910.13691)

On M the Euclidean disk, if $I_0 \colon L^2(M) \to L^2(\partial_+ SM)$ is the X-ray transform with adjoint I_0^*, we have

$$I_0^* I_0 \colon C^\infty(M) \xrightarrow{\cong} C^\infty(M), \quad I_0^* I_0 \colon \widetilde{H}^s(M) \xrightarrow{\cong} \widetilde{H}^{s+1}(M), \quad s \geq 0,$$

where $\widetilde{H}^s := D(\mathcal{L}^s)$ upon defining

$$\mathcal{L} = -\left((1-\rho^2)\partial_\rho^2 + (\rho^{-1} - 3\rho)\partial_\rho + \rho^{-2}\partial_\omega^2\right) + 1.$$

- The L^2 topology on $\partial_+ SM$ is not the usual, 'symplectic' one.
- Generalizations to special cases of simple surfaces also exist.

Main results 2/3

Theorem (M'-Nickl-Paternain, 2020, arXiv preprint 2007.15892)

On M the Euclidean disk, let $\Theta \in C_c^\infty(M, \mathfrak{so}(n))$, and let the attenuated X-ray transform

$$I_\Theta \colon L^2(M, \mathbb{C}^n) \to L^2(\partial_+ SM, \mathbb{C}^n).$$

Then $I_\Theta^* I_\Theta$ is an isomorphism

$$C^\infty(M, \mathbb{C}^n) \xrightarrow{\cong} C^\infty(M, \mathbb{C}^n), \quad \widetilde{H}^s(M, \mathbb{C}^n) \xrightarrow{\cong} \widetilde{H}^{s+1}(M, \mathbb{C}^n), \quad s \geq 0.$$

- based on setting up a suitable Fredholm setting, using the $\widetilde{H}^s$ scale and $\Theta \equiv 0$ as reference case.

Main result 3/3 - application to UQ

Consider the problem of recovering $\Phi_0 \in C_c^\infty(M, \mathfrak{so}(n))$ from

$$Y_j = C_{\Phi_0}(\gamma_j) + \varepsilon_j, \qquad \varepsilon_j \sim \mathcal{N}(0, \sigma^2), \qquad 1 \le j \le N.$$

As above, let $D_N := \{\gamma_j, Y_j\}_{j=1}^N$, and choose a prior among a flexible class and a test field $\psi \in C^\infty(M, \mathfrak{so}(n))$. Denote $\widehat{\Phi}_N$ the posterior mean (from [M.-Nickl-Paternain, CPAM '20], it exists and converges to Φ_0 as $N \to \infty$).

Theorem (M.-Nickl-Paternain, 2020, arXiv preprint 2007.15892)

We have as $N \to \infty$ and in $P_{\Phi_0}^N$-probability, the weak convergence

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- I_{Θ_0} is an attenuated X-ray transform where Θ_0 depends on Φ_0, related to the linearization of the map $\Phi \mapsto C_\Phi$ at Φ_0.

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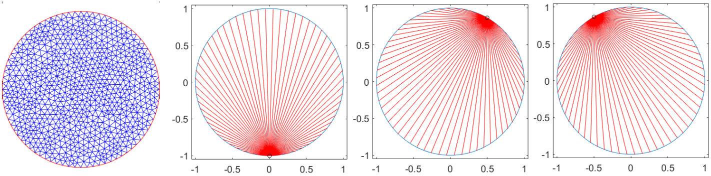
M: Euclidean unit disk.

Unstructured mesh with 886 nodes.



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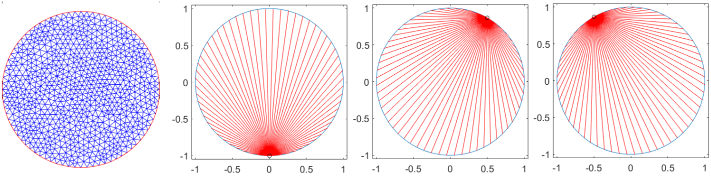
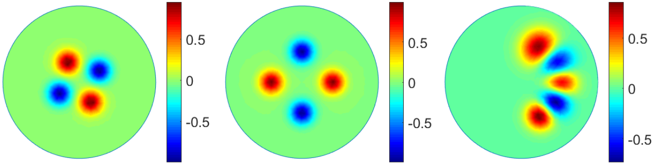


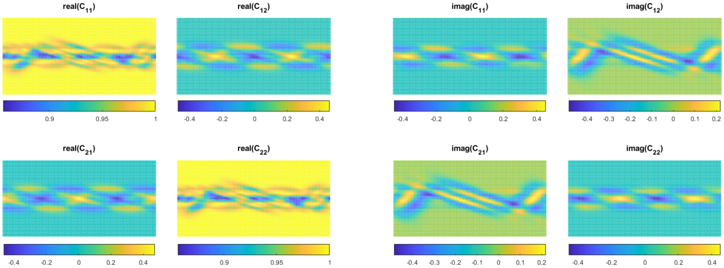
Magnetic field (3 components):



(made $\mathfrak{su}(2)$-valued via $\mathbb{R}^3 \ni (a, b, c) \mapsto \frac{1}{2}\begin{bmatrix} ia & b+ic \\ -b+ic & -ia \end{bmatrix}$)

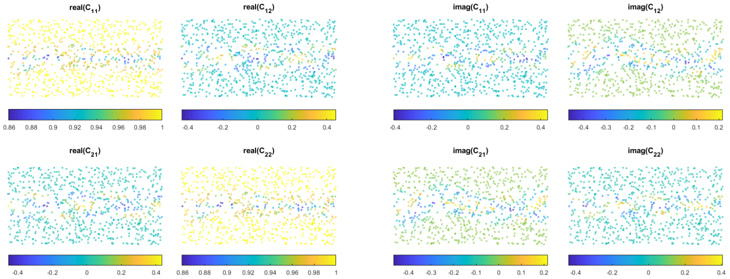
Forward data + sampling

Noiseless



Forward data + sampling

Noiseless, randomly sampled ($N = 800$)



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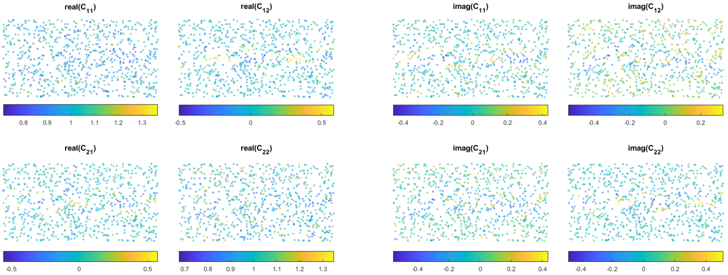
Noisy ($\sigma = 0.1$), randomly sampled ($N = 800$)



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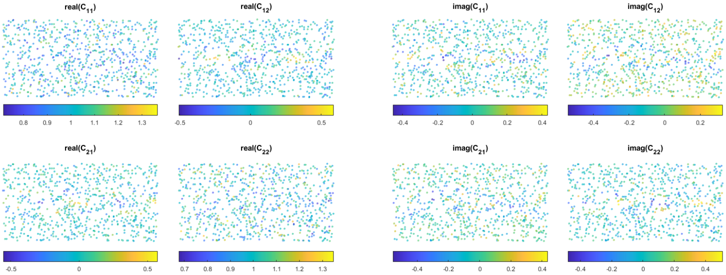
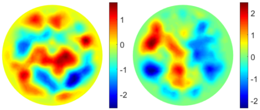


Prior (Matérn) parameters: $\nu = 3$, $\ell = 0.2$. Samples:



Computation of the posterior mean by MCMC

We compute a family of posterior draws using **preconditioned Crank-Nicolson** [Cotter, Stuart, Roberts & White '13].

Fix $\delta \in (0, 1/2)$, $\Phi_0 = 0$, and for $n = 0 : N_s$ do:

1. Draw $\Psi \sim \Pi$ and set $p_n = \sqrt{1-2\delta}\ \Phi_n + \sqrt{2\delta}\ \Psi$.
2. With $\ell(\Phi) = \frac{1}{\sigma^2} \sum_{j=1}^N |Y - C_\Phi(\gamma_j)|_F^2$ the log-likelihood,

$$\text{set} \quad \Phi_{n+1} = \begin{cases} p_n & \text{with proba. } 1 \wedge \exp(\ell(\Phi_n) - \ell(p_n)), \\ \Phi_n & \text{otherwise.} \end{cases}$$

⊗ Visualize $\widehat{\Phi} = \frac{1}{N_s} \sum_{n=1}^{N_s} \Phi_n$ and histograms of moments.

- One can show that $\{\Phi_n\}_n$ forms a Markov chain with unique invariant measure $\Pi(\cdot|(Y_i, x_i)_{i=1}^N)$.
- No inversion required, only forward solves !
- [Hairer-Stuart-Vollmer '14] prove non-asymptotic mixing $Law(\Phi_n) \to \Pi(\cdot|Y)$ under conditions on $\ell(\Phi)$ that do not require convexity.

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1. Draw $\Psi \sim \Pi$ and set $p_n = \sqrt{1-2\delta}\ \Phi_n + \sqrt{2\delta}\ \Psi$.
2. With $\ell(\Phi) = \frac{1}{\sigma^2} \sum_{j=1}^N |Y - C_\Phi(\gamma_j)|_F^2$ the log-likelihood,

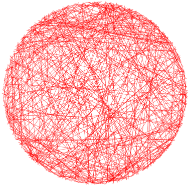
$$\text{set} \quad \Phi_{n+1} = \begin{cases} p_n & \text{with proba. } 1 \wedge \exp(\ell(\Phi_n) - \ell(p_n)), \\ \Phi_n & \text{otherwise.} \end{cases}$$

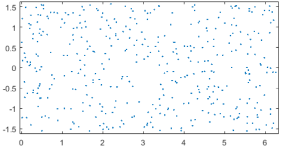
⊗ Visualize $\widehat{\Phi} = \frac{1}{N_s} \sum_{n=1}^{N_s} \Phi_n$ and histograms of moments.

- One can show that $\{\Phi_n\}_n$ forms a Markov chain with unique invariant measure $\Pi(\cdot|(Y_i, x_i)_{i=1}^N)$.
- No inversion required, only forward solves !
- [Hairer-Stuart-Vollmer '14] prove non-asymptotic mixing $Law(\Phi_n) \to \Pi(\cdot|Y)$ under conditions on $\ell(\Phi)$ that do not require convexity.

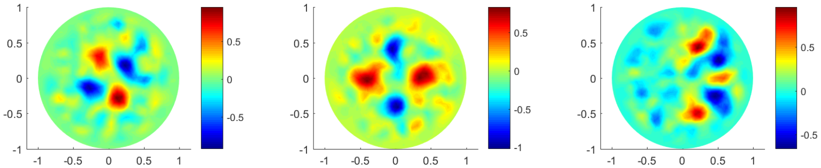
Illustration of consistency - posterior mean

$$N = 400,\ \sigma = 0.05,\ \delta = 2.5 \cdot 10^{-5}$$





MCMC sample average over 10^5 iterations



truth:

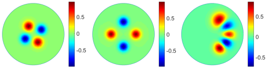
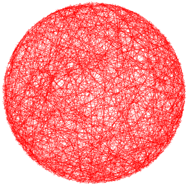
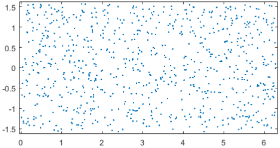


Illustration of consistency - posterior mean

$N = 800$, $\sigma = 0.05$, $\delta = 2.5 \cdot 10^{-5}$





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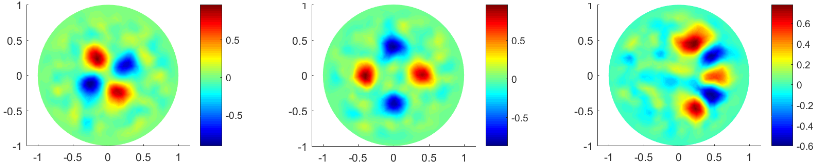

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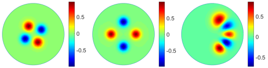
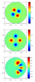
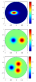
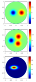
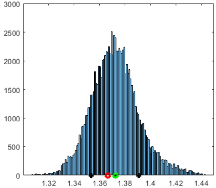
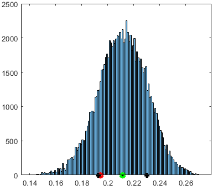


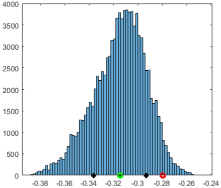
Illustration of approximate normality - histograms

$\langle \Phi,$  $\rangle$, $\langle \Phi,$  $\rangle$, $\langle \Phi,$  $\rangle$

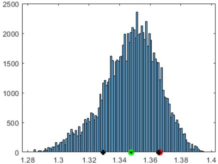
$N = 600, \quad 10^6$ iterations

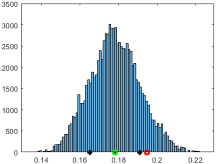


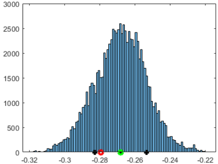




$N = 1000, \quad 10^6$ iterations







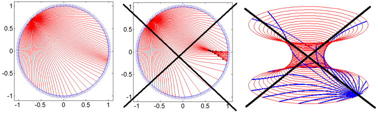
Outline

1. Introduction
2. Main results
3. A numerical illustration
4. Elements of proof: mapping properties of unattenuated X-ray
   - The 'classical' functional setting $L^2(M) \to L^2_\mu(\partial_+ SM)$
   - The Euclidean disk: setting $L^2(\mathbb{D}) \to L^2(\partial_+ S\mathbb{D})$
5. Elements of proof: mapping properties of attenuated X-ray

Outline

The case of simple surfaces

Simple $= \partial M$ stricly convex + no conjugate points + no geodesic of infinite length.



Recovery of f from If is injective [Mukh. '75], ill-posed of order 1/2 in that one may derive the stability estimate

$$\|f\|_{L^2(M)} \le C\|I^\sharp If\|_{H^1(\widetilde{M})}, \quad (I^\sharp : L^2(M) - L^2_\mu(\partial_+ SM) \text{ adjoint})$$

where $\widetilde{M}$ is a simple extension of M. [Stef.-Uhl. '04]

Question: Can one obtain mapping properties of $I^\sharp I$ that do not require an extension ?

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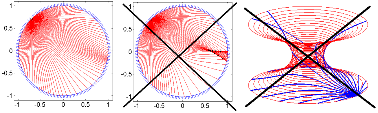

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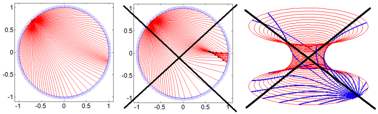

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Extendibility property

In the $L^2(M) \to L^2_\mu(\partial_+ SM)$ setting, the normal operator looks like

$$I^\sharp I f(x) = 2 \int_{S_x} \int_0^{\tau(x,v)} f(\gamma_{x,v}(t))\, dt\, dS(v).$$

If $\widetilde{M}$ is a simple extension of M, one could define $\widetilde{I^\sharp I}$ similarly, and notice that

$$r_M \circ \widetilde{I^\sharp I} \circ e_M = I^\sharp I.$$

Moreover, $\widetilde{I^\sharp I} \in \Psi^{-1}_{ell}(\widetilde{M})$ and satisfies a $-1/2$ transmission condition at ∂M, a symmetry condition on its full symbol expansion relating $\sigma(x, \nu_x)$ and $\sigma(x, -\nu_x)$ at every point $x \in \partial M$. [Boutet de Monvel, Hörmander, Grubb]

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Mapping properties of $I^* I$

Theorem (M.-Nickl-Paternain, AoS '19)

The map $I^\sharp I$ is an isomorphism in the settings below:

$$(i)\ I^\sharp I : d^{-1/2} C^\infty(M) \to C^\infty(M), \qquad d(x) = dist(x, \partial M)$$

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$H^{\mu(s)}(M)$: Hörmander μ-transmission spaces.
$\cap_s H^{\mu(s)}(M) = d^\mu C^\infty(M)$.

Proof of (i) (sketch):

1. $I^\sharp I$ is Fredholm. Uses the μ-transmission property for ΨDOs.
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- ⊕ It's sharp and does not require extension.
- ⊕ Classical Sobolev scales cannot be used everywhere.
- ⊖ The Hörmander transmission spaces aren't great to work with (not clear what $I(H^{-1/2(s)}(M))$ looks like)
- ⊖ Cannot iterate because the smooth spaces don't match ! (E.g.: what is $I^*I(C^\infty(M))$ or $I^*I(H^s(M))$?)

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Hunch: change the weight on the co-domain because in fact, $I: L^2(M) \to L^2(\partial_+ SM)$ is bounded. It is also **the** functional setting where the SVD is known in the Euclidean disk !

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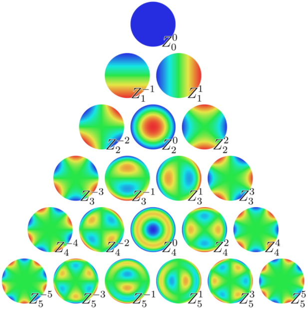
Outline

The Euclidean disk

The SVD has been long known [Cormack, Maass, Louis...].

Zernike polynomials:
$Z_{n,k}$, $n \in \mathbb{N}_0$, $0 \le k \le n$.



Uniquely defined through:

- $Z_{n,0} = z^n$.
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- $Z_{n,k}|_{\partial M}(e^{i\beta}) = e^{i(n-2k)\beta}$.

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[Kazantzev-Bukhgeym '07]

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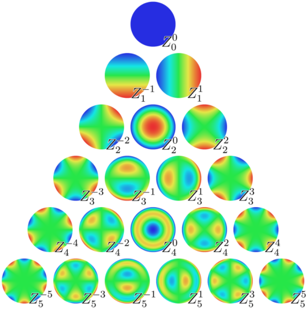

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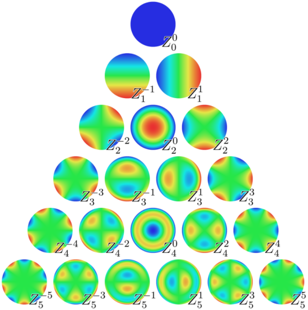

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Euclidean disk: less known facts (see [M. '19])

Denote I^* the adjoint in this setting ($I^* = I^\sharp \frac{1}{\mu}$). Let $T = \partial_\beta - \partial_\alpha$ and $\mathcal{L} := -((1-\rho^2)\partial_\rho^2 + (1/\rho - 3\rho)\partial_\rho + 1/\rho^2 \partial_\omega^2) + 1$. Facts:

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- The appropriate smoothness is w.r.t $\{\mathcal{L}\}$, whose ellipticity degenerates in a prescribed way at the boundary.
- $\widetilde{H}^1(\mathbb{D}) \supsetneq H^1(\mathbb{D})$.

Euclidean disk: on the data side [M. '19]

The relation $I \circ \mathcal{L} = (-T^2) \circ I$ indicates that smoothness in $\mathcal{L}$ translates into smoothness along $(-T^2)$.

Define $H^{1/2}_{T,+}(\partial_+ SM) = \{w \in L^2_+, (-T^2)^{k/2} w \in L^2_+\}$ to obtain

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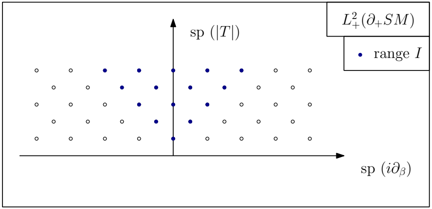

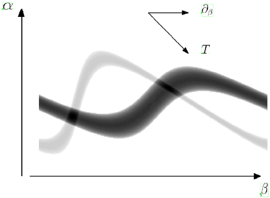

Similar anisotropic scales constructed in [Natterer, Assylbekov-Stefanov '19, Paternain-Salo '19]

There also exists a projection operator onto range(I).

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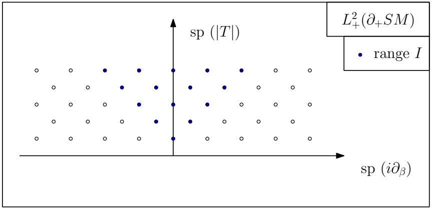

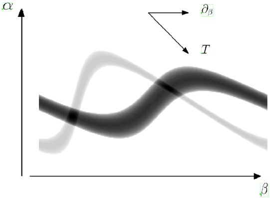

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How far do these results generalize ?

The results above are sensitive to both the geometry and the boundary. In [Mishra-M. '19], [M. '19]: generalizations to geodesic disks of constant curvature, modeled over

$$M_{R,\kappa} = (\mathbb{D}_R, (1+\kappa|z|^2)^{-2}|dz|^2), \qquad R^2|\kappa| < 1.$$

Results: On $M_{R,\kappa}$, there is a weight function w such that $I_0 \colon L^2(M_{R,\kappa}, w) \to L^2(\partial_+ SM_{R,\kappa})$ satisfies:

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Outline

Recalls

Let (M, g) be a simple Riemannian surface with geodesic vector field X, and $\Theta \in C^\infty(M, \mathfrak{u}(n))$ a 'Higgs field'. We define the attenuated X-ray transform $I_\Theta : L^2(M, \mathbb{C}^n) \to L^2_{\mu/\tau}(\partial_+ SM, \mathbb{C}^n)$ as

$$I_\Theta f = u|_{\partial_+ SM},$$

where $u\colon SM \to \mathbb{C}^n$ solves the transport equation

$$Xu + \Theta u = -f \quad (SM), \qquad u|_{\partial_- SM} = 0.$$

Most recent results on the problem of recovering f from $I_\Theta f$ (case $n \geq 2$):

- Injectivity: [Paternain-Salo-Uhlmann '12].
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Main theorems

Theorem (M'-Nickl-Paternain, 2020, arXiv preprint 2007.15892)

Let (M,g) a convex, non-trapping manifold with $\Theta \in C^\infty(M, \mathbb{C}^{n\times n})$. Then the operator $I_\Theta^* I_\Theta$ maps $C^\infty(M,\mathbb{C}^n)$ into itself.

Obtaining the converse mapping property currently requires strong assumptions on the background geometry + compact support.

Theorem (M'-Nickl-Paternain, 2020, arXiv preprint 2007.15892)

On M the Euclidean disk, let $\Theta \in C_c^\infty(M, \mathfrak{u}(n))$, and let the attenuated X-ray transform

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Then $I_\Theta^* I_\Theta$ is an isomorphism

$$C^\infty(M,\mathbb{C}^n) \xrightarrow{\cong} C^\infty(M,\mathbb{C}^n), \quad \widetilde{H}^s(M,\mathbb{C}^n) \xrightarrow{\cong} \widetilde{H}^{s+1}(M,\mathbb{C}^n), \quad s \geq 0.$$

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Elements of proof - forward mapping properties

Elements of proof - isomorphism properties

Conclusion

On the geodesic X-ray transform on the Euclidean disk (. . . and constant curvature disks)

1. Functional relations, link with degenerate elliptic operators.
2. Sharp mapping properties of I^*I and I, SVD of I for a special choice of weights on M and $\partial_+ SM$.
3. Mapping properties for attenuated X-ray transforms with compactly supported attenuation.
4. Consequences for statistical inversions: Bernstein-vonMises theorems on asymptotic posterior normality.

Perspectives:

- how far can we take 1-2 on simple surfaces ?
- higher dimensions ?
- case with non-trivial connections ?

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