A generalized conditional gradient method for dynamic inverse problems with optimal transport regularization

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Workshop 5: Inverse Problems on Large Scales

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Motivation

Motion-aware tomographic reconstruction

Motion on sub-acquisition time scales $\rightsquigarrow$ artefacts in reconstructed images

- Imaging of the lung or heart (motion cannot be suppressed)
- High-resolution imaging (sub-millimeter motion poses problems)

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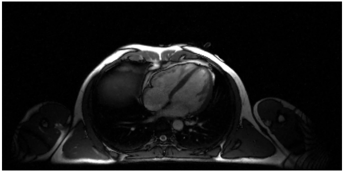

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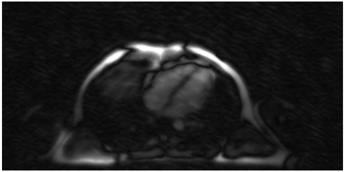

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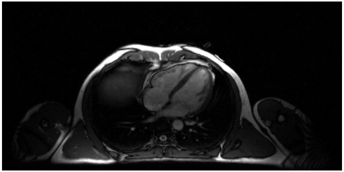

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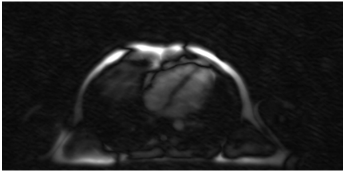

Unregularized reconstruction

$\rightsquigarrow$ **Increase resolution via optimal-transport regularization**

Sparse superresolution

Static problem

- Solve $\mathfrak{F}u = f \quad \text{on} \quad \Sigma$
- $\mathfrak{F}$ Fourier transform, $\Sigma \subset \mathbb{R}^d$ finite set
- Sparsity assumption: $u = \sum_{i=1}^{N} c_i \delta_{x_i}$

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Radon-norm regularization

- Solve variational problem in space of Radon measures
$$\min_{u \in \mathcal{M}(\Omega)} \|u\|_{\mathcal{M}} \quad \text{subject to} \quad \mathfrak{F}u = f \quad \text{on} \quad \Sigma$$
- Relaxed/regularized version (noisy data)
$$\min_{u \in \mathcal{M}(\Omega)} \frac{1}{2}\|\mathfrak{F}u - f\|_{\Sigma,2}^2 + \alpha\|u\|_{\mathcal{M}}$$

[Candès/Fernandez-Granda '13] and many more

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$\rightsquigarrow$ **Study a dynamic version of this approach**

Outline

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1 Peak recovery for static inverse problems
- A successive peak insertion and thresholding algorithm

2 Peak tracking for dynamic inverse problems
- Dynamic optimal-transport formulations and energies
- Regularization of dynamic inverse problems
- Extremal points of the Benamou–Brenier energy

3 A curve insertion and evolution algorithm
- Convergence analysis and numerical example

4 Conclusions and perspectives

Tikhonov functional in Radon space

Tikhonov regularization *[B./Pikkarainen '13]*

$$u_\alpha^\delta \in \operatorname*{arg\,min}_{u \in \mathcal{M}(\Omega)} \frac{\|A^* u - f^\delta\|_H^2}{2} + \alpha \|u\|_{\mathcal{M}}$$

Setting

- H Hilbert space
- Ω sep. locally compact space
- $\mathcal{M}(\Omega) = \mathcal{C}_0(\Omega)^*$
  space of signed Radon measures
- $A \in \mathcal{L}\big(H, \mathcal{C}_0(\Omega)\big)$
  predual forward model
  (B weak*-cont. $\Leftrightarrow$ $B = A^*$)

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Theorem

There exists a minimizer.

Proof:

Direct method for weak*-convergence in $\mathcal{M}(\Omega)$ □

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- Case $\Omega \subset \mathbb{R}^d$ open
  $\rightsquigarrow$ *[Scherzer/Walch '08]*

Optimality conditions

Original problem

$$\min_{u \in \mathcal{M}(\Omega)} \frac{\|A^* u - f^\delta\|_H^2}{2} + \alpha \|\mu\|_{\mathcal{M}}$$

Predual problem

$$\min_{v \in H} \frac{\|v - f^\delta\|_H^2}{2} + I_{\{\|Av\|_\infty \le \alpha\}}(v)$$

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$$\begin{cases} \|A(A^* u^* - f^\delta)\|_\infty \leq \alpha \\ \operatorname{supp} u^* \subset \{|A(A^* u^* - f^\delta)| = \alpha\} \\ u^* \leq 0 \text{ on } \{A(A^* u^* - f^\delta) = \alpha\} \\ u^* \geq 0 \text{ on } \{A(A^* u^* - f^\delta) = -\alpha\} \end{cases}$$

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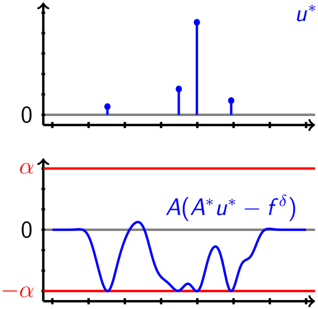

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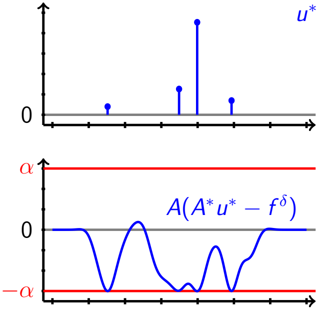

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$\rightsquigarrow$ **Sparse solutions possible**

Stability and regularization properties

Standard result

- $u^\dagger$ unique minimum-norm solution, $f^\dagger = A^* u^\dagger$
- $\|f^\dagger - f^\delta\|_H \leq \delta$, $\dfrac{\delta^2}{\alpha} \to 0$

Then: $u_\alpha^\delta \rightharpoonup^* u^\dagger$.

Remark

Minimum-norm solution $u^\dagger$ non-unique

$\Rightarrow$ $u_\alpha^\delta \rightharpoonup^* u^*$ subsequentially

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Convergence rate

- There exists a $h \in H$ with

$\langle u^\dagger, Ah \rangle = \|u^\dagger\|_{\mathcal{M}}$, $\|Ah\|_\infty = 1$

- Parameter choice $\alpha \sim \delta$

Then: $D(u_\alpha^\delta, u^\dagger) = \mathcal{O}(\delta)$

- D Bregman distance w.r.t. Radon-norm and Ah
- Bases on *[Burger/Osher '04]*

Remark

In general weaker than weak*-convergence.

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Example: Sparse deconvolution

Minimization problem

$$\min_{u \in \mathcal{M}(\Omega - \Omega')} \frac{1}{2} \int_\Omega |u * k - f^\delta|^2 \, dx + \alpha \|u\|_{\mathcal{M}}$$

- $k \in L^2(\Omega')$
- $f^\delta \in L^2(\Omega)$

Predual operator

$Aw = w * \bar{k}, \ \ \bar{k}(x) = k(-x)$

- $A : L^2(\Omega) \to \mathcal{C}_0(\Omega - \Omega')$ linear and continuous
- $A^* : \mathcal{M}(\Omega - \Omega') \to L^2(\Omega)$ convolution + restriction

Applications

- Finding peaks/isotopes in noisy mass-spectrometry data
- Detection of stars in ground-based telescope images

Numerical minimization

Aim

- Produce sparse iterates $\rightsquigarrow u^n = \sum_i v_i^n \delta_{x_i^n}$

Algorithm

1. Set $u_0 = 0$, $M_0 = \|f^\delta\|_H^2/(2\alpha)$
2. Compute $w^n = -A(A^* u^n - f^\delta)$, find a maximum x^* of the function $|w^n|$
3. Set $\nu^n = \alpha^{-1} M_0 w^n(x^*) \delta_{x^*}$ if $|w^n(x^*)| > \alpha$, $\nu = 0$ else
4. Compute convex combination $u^{n+1/2} = u^n + s_n(\nu^n - u^n)$, $s_n \in [0, 1]$ appropriate
5. Perform soft-thresholding step on the coefficients of $u^{n+1/2}$ analogous to *[DDD '04]* $\rightsquigarrow$ next iterate u^{n+1}

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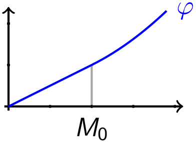
$\rightsquigarrow$ **Successive peak insertion and thresholding (SPInAT)**

Properties of the algorithm

Peak insertion

- Amounts to generalized conditional gradient method on

$$\min_{u \in \mathcal{M}(\Omega)} \frac{\|A^* u - f^\delta\|_H^2}{2} + \varphi(\|u\|_{\mathcal{M}})$$



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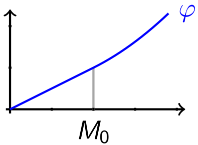

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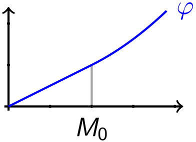

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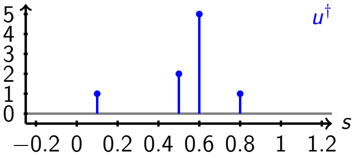
Soft thresholding

- Eliminates "superfluous" peaks
- Decreases functional values $\Rightarrow$ combined method converges

Numerical example



1D Deconvolution

$$\min_{u \in \mathcal{M}(\Omega)} \frac{1}{2}\|u * k - f^\delta\|_H^2 + \alpha\|\mu\|_{\mathcal{M}}$$

- H discrete space, k cubic B-spline

$\rightsquigarrow$ $\mathcal{M}(\Omega)$ **is not discretized**

Additional tweaks

- Merge peaks if functional value decreases
- Gradient flow w.r.t. peak positions

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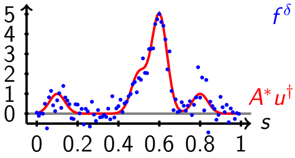

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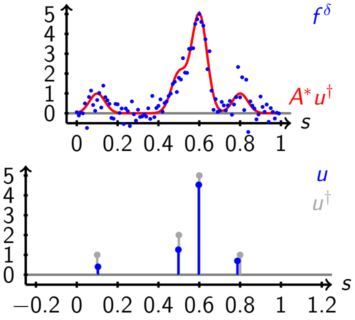

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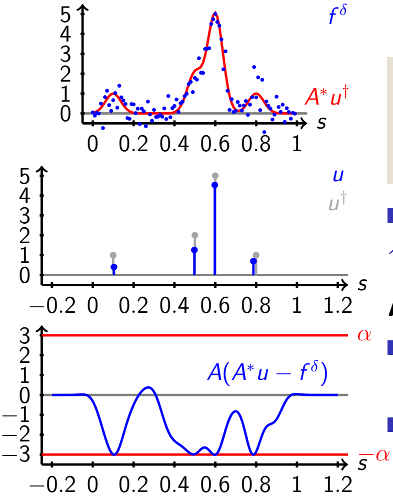

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Static optimal transport

Situation

- $\Omega \subset \mathbf{R}^d$ bounded domain, $\rho_0, \rho_1 \in \mathcal{P}(\Omega)$
- $T : \Omega \to \Omega$ measurable, $\rho_1 = T_{\#}\rho_0$

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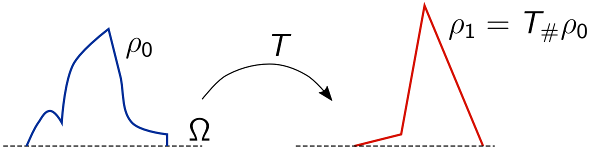

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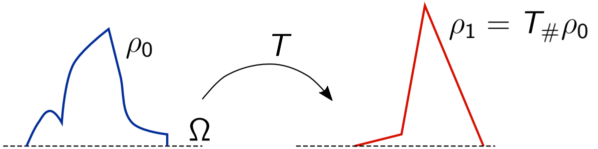

Goal

- Move ρ_0 to ρ_1 in an optimal way
- Cost of moving mass from x to y: $\quad c(x, y) = \frac{1}{2}|x - y|^2$

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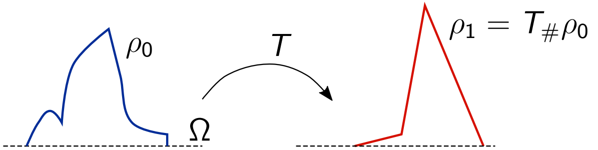

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Optimal transport

Solve $\displaystyle\min_{T:\Omega\to\Omega} \frac{1}{2} \int_\Omega |T(x) - x|^2 \, d\rho_0(x)$ subject to $T_\# \rho_0 = \rho_1$

Dynamic optimal transport

Idea

Introduce a time variable $t \in [0, 1]$ and consider evolution of ρ_t

- Time-dependent probability measures

$$t \mapsto \rho_t \in \mathcal{P}(\Omega) \quad \text{for} \quad t \in [0, 1]$$

- Velocity field advecting ρ_t

$$v_t \colon [0, 1] \times \Omega \to \mathbf{R}^d$$

- (ρ_t, v_t) solves the continuity equation with initial conditions

$$\begin{cases} \partial_t \rho_t + \operatorname{div}(\rho_t v_t) = 0 \\ \text{Initial data } \rho_0, \text{ final data } \rho_1 \end{cases} \qquad \text{(CE-IC)}$$

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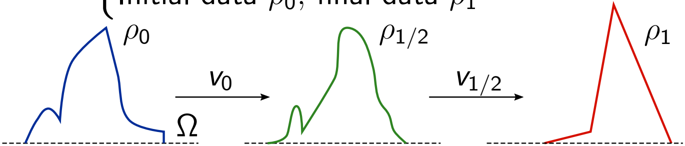

Dynamic optimal transport

Theorem *[Benamou/Brenier '00]*

$$\min_{\substack{(\rho_t, v_t) \\ \text{solving (CE-IC)}}} \int_0^1 \int_\Omega |v_t(x)|^2 \, \rho_t(x) dx \, dt = \min_{\substack{T:\,\Omega\to\Omega \\ T_\# \rho_0 = \rho_1}} \int_\Omega |T(x) - x|^2 \, \rho_0(x) \, dx$$

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Advantages of the dynamic formulation

- By introducing $m_t = \rho_t v_t$, we have the convex energy

$$\int_0^1 \int_\Omega |v_t(x)|^2 \rho_t(x)\, dx\, dt = \int_0^1 \int_\Omega \frac{|m_t(x)|^2}{\rho_t(x)}\, dx\, dt$$

- The continuity equation becomes linear

$$\partial_t \rho_t + \operatorname{div} m_t = 0$$

- Full trajectory ρ_t is known and v_t can be recovered from m_t

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Unbalanced optimal transport

Consider a triple (ρ_t, v_t, g_t) with

- $t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ mass density (not probability measures)
- $v_t \colon (0,1) \times \overline{\Omega} \to \mathbf{R}^d$ velocity field, $g_t \colon (0,1) \times \overline{\Omega} \to \mathbf{R}$ growth rate

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Unbalanced dynamic optimal transport

For $\delta \in (0, \infty]$, solve

$$\min_{\substack{(\rho_t, v_t, g_t) \\ \text{solving (CE-IC*)}}} \int_0^1 \int_{\overline{\Omega}} |v_t(x)|^2 + \delta^2 |g_t(x)|^2 \, d\rho_t(x) \, \mathrm{d}t$$

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- See *[Chizat et al. '18]*, *[Liero/Mielke/Savaré '18]*

Unbalanced optimal transport energy

Definition

- Let $X = (0,1) \times \overline{\Omega}$
- For $(\rho, m, \mu) \in \mathcal{M}(X) \times \mathcal{M}(X)^d \times \mathcal{M}(X)$, let

$$B_\delta(\rho, m, \mu) = \int_X \Psi\left(\frac{d\rho}{d\lambda}, \frac{dm}{d\lambda}, \frac{d\mu}{d\lambda}\right)\, d\lambda$$

where $\lambda \in \mathcal{M}^+(X)$ is such that $\rho, m, \mu \ll \lambda$ and

$$\Psi(t,x,y) = \frac{|x|^2 + \delta^2 y^2}{2t} \quad \text{if} \quad t > 0, \quad \Psi = \infty \text{ else}$$

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- Generalizes

$$\frac{1}{2}\int_0^1 \int_{\overline{\Omega}} \frac{|m|^2}{\rho} + \delta^2 \frac{\mu^2}{\rho} \,\mathrm{d}x \,\mathrm{d}t$$

for functions $\rho : X \to [0,\infty)$, $m : X \to \mathbb{R}^d$, $\mu : X \to \mathbb{R}$ to arbitrary Radon measures

Unbalanced optimal transport energy

Proposition *[B./Fanzon '20]*

- The functional B_δ is proper, convex, weak* lower semi-continuous and 1-homogeneous

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- If $B_\delta(\rho, m, \mu) < \infty$ and $\partial_t \rho + \operatorname{div} m = \mu$, then
  - $\rho = dt \otimes \rho_t$ for a weak*-continuous curve $t \mapsto \rho_t \in \mathcal{M}^+(\overline{\Omega})$
  - $m = \rho v_t$ for some velocity field $v_t \colon (0,1) \times \overline{\Omega} \to \mathbf{R}^d$
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$$B_\delta(\rho, m, \mu) = \frac{1}{2} \int_0^1 \int_{\overline{\Omega}} |v_t(x)|^2 + \delta^2 |g_t(x)|^2 \, d\rho_t(x) \, dt$$

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$\rightsquigarrow$ **Use as an energy for Tikhonov regularization**

Dynamic inverse problem

General setting

- $\Omega \subset \mathbf{R}^d$ bounded open domain, $d \geq 1$
- For $t \in [0,1]$ assume given
  - H_t Hilbert space (measurement space)
  - $K_t^* : \mathcal{M}(\overline{\Omega}) \to H_t$ linear continuous operator (forward operator)

$\rightsquigarrow$ time dependence allows for spatial undersampling

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Inverse problem

Given some data $\{f_t\}_{t\in[0,1]}$ with $f_t \in H_t$, find a curve of measures $t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ such that

$$K_t^* \rho_t = f_t \qquad \text{for a.e.} \quad t \in [0,1]\,. \tag{P}$$

Tikhonov regularization

Inverse problem

Solve $\quad K_t^* \rho_t = f_t \quad \text{in} \quad H_t \quad \text{for a.e. } t \in [0, 1]$

Tikhonov regularized problem

$$\min_{(\rho,m,\mu)\in\mathcal{M}(X)^{d+2}} \underbrace{\frac{1}{2}\int_0^1 \|K_t^*\rho_t - f_t\|_{H_t}^2 \, dt}_{\text{fidelty term}} + \underbrace{\alpha B_\delta(\rho, m, \mu)}_{\text{optimal-transport term}} + \underbrace{\beta\|\rho\|_{\mathcal{M}}}_{\text{total-variation term}}$$

$$\text{subject to} \quad \partial_t \rho + \operatorname{div} m = \mu \qquad \text{(CE)}$$

- Regularization parameters $\alpha > 0$, $\beta > 0$

Tikhonov regularization

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Solve $\qquad K_t^* \rho_t = f_t \quad \text{in} \quad H_t \quad \text{for a.e. } t \in [0,1]$

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- Regularization parameters $\alpha > 0$, $\beta > 0$

- (CE) ensures $\rho = \mathrm{d}t \otimes \rho_t$ and $m, \mu \ll \rho$
- $m = v_t\rho_t \rightsquigarrow$ motion, $\mu = g_t\rho_t \rightsquigarrow$ contrast changes

Dynamic data spaces

Assumption (H)

The spaces H_t vary in a "measurable" way w.r.t $t \in [0,1]$

- $\exists$ Banach space D and $i_t\colon D \to H_t$ linear continuous
- $i_t(D) \subset H_t$ dense, $\sup_t \|i_t\| \leq C$
- for each $\varphi, \psi \in D$ the map $t \mapsto \langle i_t\varphi, i_t\psi \rangle_{H_t}$ is Lebesgue measurable

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- A map $\varphi \colon [0,1] \to D$ is a step function if

$$\varphi_t = \sum_{j=1}^{N} \chi_{E_j}(t)\,\varphi_j \quad \text{for } \varphi_j \in D,\ E_j \subset [0,1] \text{ measurable}$$

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- A map $f \colon [0,1] \to \cup_t H_t$ with $f_t \in H_t$ is strongly measurable if $\exists\ \varphi^n \colon [0,1] \to D$ step functions s.t.

$$\lim_{n\to\infty} \|i_t\varphi_t^n - f_t\|_{H_t} = 0 \quad \text{for a.e.} \quad t \in [0,1]$$

Dynamic data spaces

Definition $L_H^2 = \Big\{ f : [0,1] \to \cup_t H_t \;\Big|\; f_t \in H_t,$

$$f \text{ strongly measurable }, \int_0^1 \|f_t\|_{H_t}^2 \,\mathrm{d}t < \infty \Big\}$$

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Definition $L^2_H = \left\{ f\colon [0,1] \to \cup_t H_t \;\middle|\; f_t \in H_t, \right.$
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Theorem *[B./Fanzon '20]*

The space L^2_H is Hilbert with the scalar product

$$\langle f, g \rangle_{L^2_H} = \int_0^1 \langle f_t, g_t \rangle_{H_t} \,\mathrm{d}t$$

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- For $i_t^* f_t : [0, T] \to D^*$, there exists the Gelfand integral

$$\langle I(f), \varphi\rangle_{D^* \times D} = \int_0^1 \langle i_t^* f_t, \varphi\rangle_{D^*, D} \,\mathrm{d}t \qquad \text{for all } \varphi \in D$$

- In general, $i_t^* f_t$ is not Bochner-strongly measurable

Forward operators

Assumption (K)

The operators $K_t^*\colon \mathcal{M}(\overline{\Omega}) \to H_t$ satisfy

- K_t^* linear continuous and weak*-to-weak continuous
- $\sup_t \|K_t^*\| \leq C$
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$t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ weak* continuous $\Rightarrow$ $t \mapsto K_t^* \rho_t$ is in L_H^2

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Tikhonov functional

Let $f \in L_H^2$ given data. For $(\rho, m, \mu) \in \mathcal{M}(X)^{d+2}$ set

$$T_{\alpha,\beta}(\rho, m, \mu) = \frac{1}{2}\int_0^1 \|K_t^*\rho_t - f_t\|_{H_t}^2 \,\mathrm{d}t + \alpha B_\delta(\rho, m, \mu) + \beta\|\rho\|_{\mathcal{M}}$$

if $\partial_t\rho + \operatorname{div} m = \mu$, and $T_{\alpha,\beta}(\rho, m, \mu) = \infty$ else

Existence and stability

Assume **(H)**-**(K)**.

Theorem *[B./Fanzon '20]*

$$\min_{(\rho,m,\mu)\in\mathcal{M}(X)^{d+2}} T_{\alpha,\beta}(\rho, m, \mu) \qquad \text{(Tikh)}$$

admits a solution for $f \in L^2_H$.

- If K_t^* is injective for a.e. t, then the solution is unique.

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Theorem *[B./Fanzon '20]*

- $\{f^n\}$ noisy data such that $f^n \to f^\dagger$ strongly in L^2_H
- $K_t^* \rho_t^\dagger = f_t^\dagger$ for a.e. $t \in [0,1]$
- (ρ^n, m^n, μ^n) be a solution to (Tikh) with data f^n and $\alpha_n, \beta_n \to 0$ suitably

Then: $$(\rho^n, m^n, \mu^n) \overset{*}{\rightharpoonup} (\rho^\dagger, m^\dagger, \mu^\dagger) \ \text{ in } \ \mathcal{M}(X)^{d+2}$$

Application to undersampled MRI

- $\Omega = (-1,1)^2$ image domain, $t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ proton density
- $H_t = L^2_{\sigma_t}(\mathbf{R}^2, \mathbf{C}^N)$ with $\sigma_t \in \mathcal{M}^+(\mathbf{R}^2)$ sampling measures

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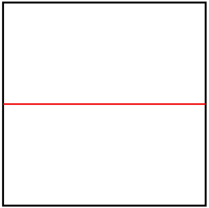

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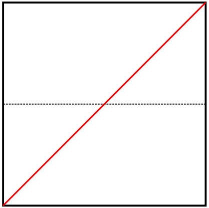

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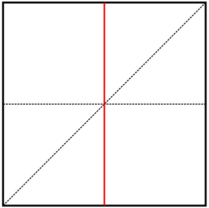

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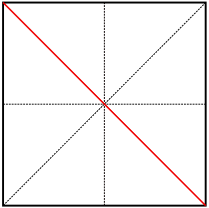

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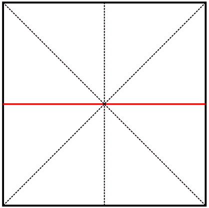

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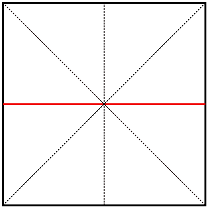

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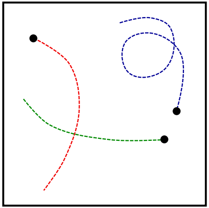

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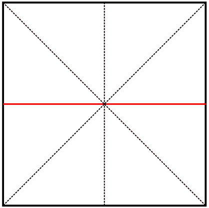

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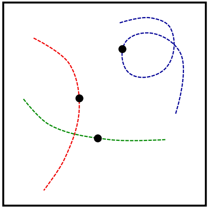

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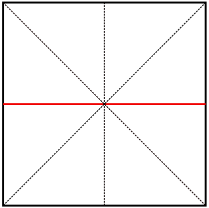

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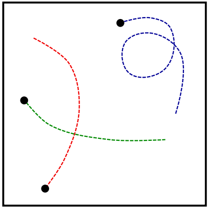

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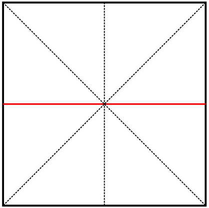
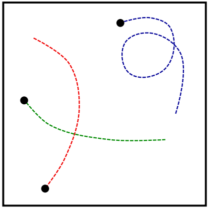
Application to undersampled MRI

- $\Omega = (-1,1)^2$ image domain, $t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ proton density
- $H_t = L^2_{\sigma_t}(\mathbf{R}^2, \mathbf{C}^N)$ with $\sigma_t \in \mathcal{M}^+(\mathbf{R}^2)$ sampling measures



$\sigma_t = \mathcal{H}^1 \llcorner L_t$



$\sigma_t = \mathcal{H}^0 \llcorner P_t$

- $K_t^* : \mathcal{M}(\overline{\Omega}) \to H_t$ masked Fourier transform

$$K_t^* \rho = (\mathfrak{F}(c_1\rho), \ldots, \mathfrak{F}(c_N\rho))$$

with $c_j \in C_0(\mathbf{R}^2; \mathbf{C})$ coil sensitivities (accounting for phase inhomogeneities)

Application to undersampled MRI

Assumption (M)

Assume that the family $\sigma_t \in \mathcal{M}^+(\mathbf{R}^2)$ satisfies

- $\sup_t \|\sigma_t\| \leq C$
- for each $\varphi \in C_0(\mathbf{R}^2, \mathbf{C})$ the map $t \mapsto \int_{\mathbf{R}^2} \varphi(x) \, d\sigma_t(x)$ is measurable

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Theorem *[B./Fanzon '19]*

Assume **(M)**. Let $\alpha, \beta > 0$, $\delta \in (0, \infty]$, $f \in L^2_H$, $c \in C_0(\mathbf{R}^2, \mathbf{C}^N)$. Then,

$$\min_{\substack{(\rho,m,\mu)\in\mathcal{M}(X)^4 \\ \partial_t\rho + \operatorname{div} m = \mu}} \frac{1}{2}\sum_{j=1}^{N}\int_0^1 \|\mathfrak{F}(c_j\rho_t) - f_t\|^2_{L^2_{\sigma_t}}\, dt + \alpha B_\delta(\rho, m, \mu) + \beta\|\rho\|$$

admits a solution

Special case: Benamou–Brenier energy

- Assume $\delta = \infty \rightsquigarrow$ Benamou–Brenier energy

Definition

- For $(\rho, m) \in \mathcal{M}(X) \times \mathcal{M}(X)^d$, let

$$B(\rho, m) = \int_X \Psi\left(\frac{d\rho}{d\lambda}, \frac{dm}{d\lambda}\right) \, d\lambda$$

where $\lambda \in \mathcal{M}^+(X)$ is such that $\rho, m \ll \lambda$ and

$$\Psi(t, x) = \frac{|x|^2}{2t} \quad \text{if} \quad t > 0, \quad \Psi = \infty \text{ else}$$

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Benamou–Brenier regularizer

Let $\alpha, \beta > 0$. For $(\rho, m) \in \mathcal{M}(X) \times \mathcal{M}(X)^d$ we set

$$J_{\alpha,\beta}(\rho, m) = \begin{cases} \alpha B(\rho, m) + \beta \|\rho\|_{\mathcal{M}(X)} & \text{if } \partial_t \rho + \operatorname{div} m = 0 \\ \infty & \text{otherwise} \end{cases}$$

Extremal points of $J_{\alpha,\beta}$

Goal

- Determine the extremal points of $J_{\alpha,\beta}$-balls
- Consider the closed, convex unit ball of $J_{\alpha,\beta}$

$$C = \{(\rho, m) \in \mathcal{M}(X) \times \mathcal{M}(X)^d \mid J_{\alpha,\beta}(\rho, m) \leq 1\}$$

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Theorem *[B./Carioni/Fanzon/Romero '21]*

The extremal points of C are characterized by

$$\mathrm{Extr}(C) = \{(0,0)\} \cup \mathcal{C}$$

where $\mathcal{C} = \{(\rho_\gamma, m_\gamma) \,|\, \gamma \in \mathrm{AC}^2([0,1]; \overline{\Omega})\}$

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Sparsity for finite-dimensional data

Fix $N \geq 1$ times $0 < t_1 < t_2 < \cdots < t_N < 1$, let

- H_i finite-dimensional Hilbert space, $\mathcal{H} = \bigtimes_{i=1}^{N} H_i$
- $K_i^* : \mathcal{M}(\overline{\Omega}) \to H_i$ linear and weak*-continuous

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- For $(f_1, \ldots, f_N) \in \mathcal{H}$ find a curve $t \mapsto \rho_t \in \mathcal{M}(\overline{\Omega})$ such that

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Theorem *[B./Carioni/Fanzon/Romero '21]*

$$\min_{(\rho,m)\in\mathcal{M}(X)^{d+1}} \frac{1}{2} \sum_{i=1}^{N} \|K_i \rho_{t_i} - f_i\|_{H_i}^2 + \alpha B(\rho, m) + \beta \|\rho\|_{\mathcal{M}(X)}$$

admits a solution of the form $(\rho^*, m^*) = \sum_{i=1}^{p} c_i \, (\rho_{\gamma_i}, m_{\gamma_i})$

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Proof Also see *[Boyer et al. '19]*, *[B./Carioni '20]*

Further direction: unbalanced OT case

Hellinger–Kantorovich regularizer

Let $\alpha, \beta, \delta > 0$. For $(\rho, m, \mu) \in \mathcal{M}(X)^{d+2}$ we set

$$J_{\alpha,\beta}(\rho, m) = \begin{cases} \alpha B_\delta(\rho, m, \mu) + \beta \|\rho\|_{\mathcal{M}(X)} & \text{if } \partial_t \rho + \operatorname{div} m = \mu \\ \infty & \text{otherwise} \end{cases}$$

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Key ingredients

- Extremal point characterization:
$$\rho = h(t)\,dt \otimes \delta_{\gamma(t)}\,, \quad m = \dot{\gamma}\rho\,, \quad \mu = \frac{\dot{h}}{h}\,\rho$$
- $h\colon [0,1] \to [0,\infty)$, $\gamma\colon [0,1] \to \overline{\Omega}$ satisfy certain regularity properties
- Based on a new superposition principle for $\partial_t \rho + \operatorname{div} m = \mu$

Outline

A conditional gradient method

Consider the equivalent time-continuous problem

$$\min_{(\rho,m)\in\mathcal{M}(X)^{d+1}} \tilde{T}_{\alpha,\beta}(\rho,m)$$

for $$\tilde{T}_{\alpha,\beta}(\rho,m) = \frac{1}{2}\int_0^1 \|K_t^*\rho_t - f_t\|_{H_t}^2 \,\mathrm{d}t + \varphi(J_{\alpha,\beta}(\rho,m))$$

where, e.g., $\varphi(t) = t + \chi_{\{s\leq M_0\}}(t)$, $M_0 = \frac{1}{2}\int_0^1 \|f_t\|_{H_t}^2 \, dt$

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Conditional gradient method

- Linearization of the smooth term around $(\tilde{\rho}, \tilde{m})$

$$\min_{(\rho,m)\in\mathcal{M}(X)^{d+1}} -\int_0^1 \langle \rho_t, w_t\rangle_{\mathcal{M}(\overline{\Omega})\times C(\overline{\Omega})} \, dt + \varphi(J_{\alpha,\beta}(\rho, m))$$

- $w_t = -K_t(K_t^*\tilde{\rho}_t - f_t)$

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Consider the convex unit ball of $J_{\alpha,\beta}$

$$C = \{(\rho, m) \in \mathcal{M}(X)^{d+1} : \ J_{\alpha,\beta}(\rho, m) \leq 1\}$$

and denote by $\mathrm{Extr}(C) = \{0\} \cup \mathcal{C}$ its extremal points

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Theorem *[B./Carioni/Fanzon/Romero '21]*

- Assume **(H)-(K)**, let $f \in L^2_H$, $t \mapsto \tilde{\rho}_t \in \mathcal{M}(\overline{\Omega})$ weak* continuous, set $w_t = -K_t(K_t^* \tilde{\rho}_t - f_t)$

There exists a solution $(\rho^*, m^*) \in \mathrm{Extr}(C)$ to

$$\min_{(\rho,m)\in C} -\int_0^1 \langle \rho_t, w_t \rangle_{\mathcal{M}(\overline{\Omega})\times C(\overline{\Omega})} \, dt$$

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and an $M \geq 0$ such that $(M\rho^*, Mm^*)$ is a solution to

$$\min_{(\rho,m)\in\mathcal{M}(X)^{d+1}} - \int_0^1 \langle \rho_t, w_t \rangle_{\mathcal{M}(\overline{\Omega}), C(\overline{\Omega})} \, dt + \varphi(J_{\alpha,\beta}(\rho, m))$$

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2. **Optimization** Solve the quadratic program

$$\bar c^n = (\bar c_j^n)_j \in \operatorname*{arg\,min}_{c_j^n \geq 0} T_{\alpha,\beta}\Big(\sum_j c_j^n (\rho_{\gamma_j^n}, m_{\gamma_j^n})\Big)$$

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- Set $(\rho^{n+1}, m^{n+1}) = \sum_j \bar{c}_j^n (\rho_{\gamma_j^n}, m_{\gamma_j^n})$

Convergence

- Define functional distance $r(\rho, m) = T_{\alpha,\beta}(\rho, m) - \min T_{\alpha,\beta}$

Theorem *[B./Carioni/Fanzon/Romero '22]*

Let $f \in L^2_H$, $\alpha, \beta > 0$, $\{(\rho^n, m^n)\}$ in $\mathcal{M}(X)^{d+1}$ the sequence in the conditional gradient method. Then,

- $\{(\rho^n, m^n)\}$ is minimizing with $\quad r(\rho^n, m^n) \leq \dfrac{C}{n}$

  where $C > 0$ depends only on f, α, β
- Each weak* accumulation point of $\{(\rho^n, m^n)\}$ is a minimizer for $T_{\alpha,\beta}$

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Faster convergence
Under certain regularity assumptions, R-linear convergence in terms of r, γ_j and c_j can be obtained
[B./Carioni/Fanzon/Walter, in preparation]

Details and additionals tweaks

- Solve the curve insertion problem

$$\gamma_0^n \in \operatorname*{arg\,min}_{\gamma \in \mathrm{AC}^2([0,1];\overline{\Omega})} -\left(\frac{\alpha}{2}\int_0^1 |\dot{\gamma}(t)|^2 \, dt + \beta\right)^{-1} \int_0^1 w_t^n(\gamma(t)) \, dt$$

  via gradient descent with suitable stepsize rule

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Theorem *[B./Carioni/Fanzon/Romero '22]*

Under suitable regularity assumptions, the gradient descent procedure converges subsequentially to stationary points and strongly in $AC^2([0,1];\overline{\Omega})$.

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Theorem *[B./Carioni/Fanzon/Romero '22]*
Under suitable regularity assumptions, the gradient descent procedure converges subsequentially to stationary points and strongly in $\mathrm{AC}^2([0,1];\overline{\Omega})$.

- Multiple starts with suitable initial guess (crossovers, random curves, etc.) to increase chance to obtain global minimizer
- Multiple insertion $\rightsquigarrow$ insert all obtained stationary points

Details and additionals tweaks

- **Alternative** Curve insertion via dynamic programming
  $\rightsquigarrow$ *[Duval/Tovey '21]*

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  $\rightsquigarrow$ *[Duval/Tovey '21]*

- **Sliding step** Perform gradient descent steps for

$$\min_{c_j^n \geq 0,\ \gamma_j^n \in \mathrm{AC}^2([0,1];\overline{\Omega})} T_{\alpha,\beta}\Big(\sum_j c_j^n(\rho_{\gamma_j^n}, m_{\gamma_j^n})\Big)$$

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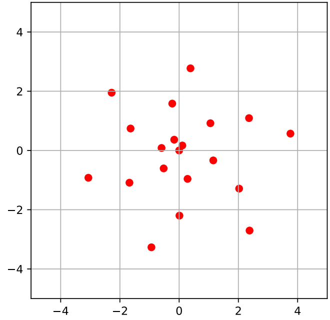
- **Stopping criterion**

$$\left(\frac{\alpha}{2}\int_0^1 |\dot{\gamma}_0^n(t)|^2\,dt + \beta\right)^{-1}\int_0^1 w_t^n(\gamma_0^n(t))\,dt \leq 1$$

  or up to some tolerance

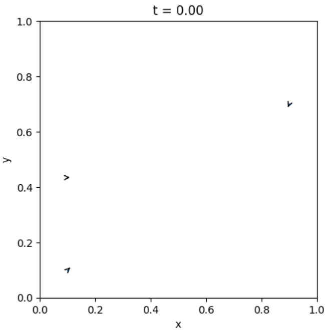
Numerical experiments

- $\Omega = (0,1)^2$, $\sigma = \mathcal{H}^0 \llcorner s$ where $s =$ spiral points in Ω
- $H_t = L^2_\sigma(\mathbf{R}^2, \mathbf{C})$ (time independent)
- $K_t^* : \mathcal{M}(\overline{\Omega}) \to H_t$ masked Fourier transform

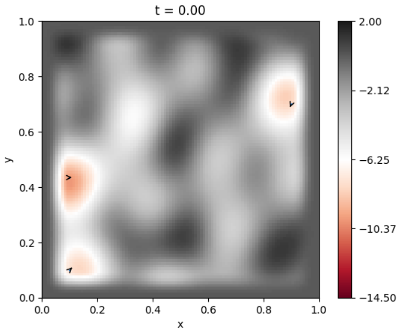


Numerical experiments

A simple example



Ground truth



Backprojected data

Numerical experiments

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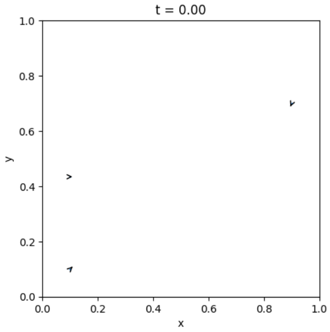

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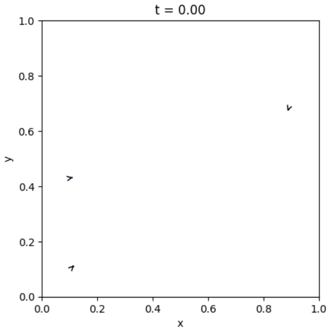

Reconstruction
(thresholded at 0.01)

Numerical experiments

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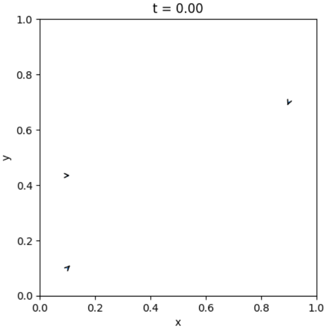
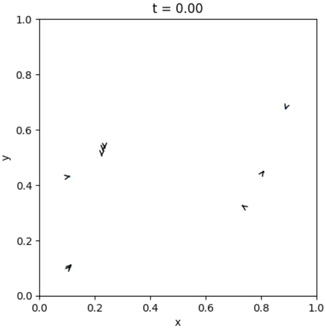
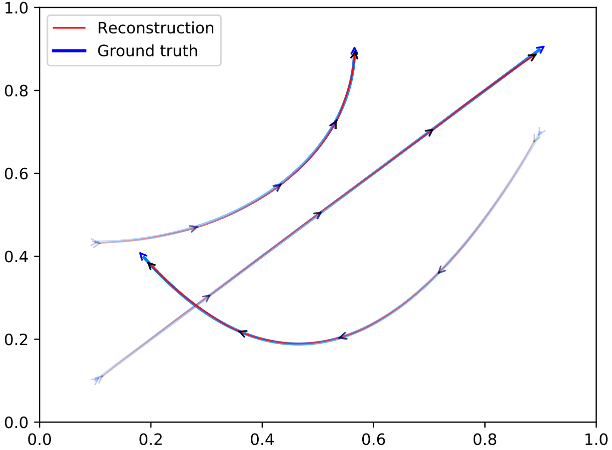


Ground truth



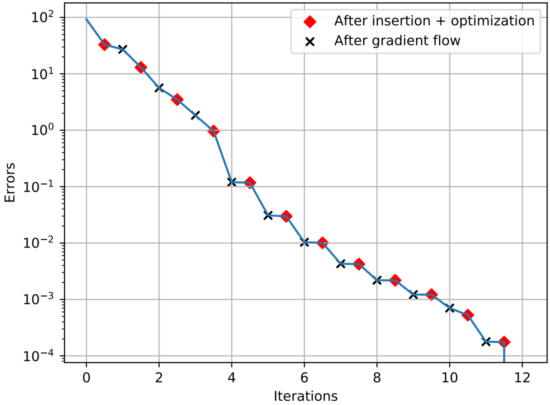
Reconstruction
(no thresholding)

Numerical experiments



Reconstructed trajectories

Numerical experiments

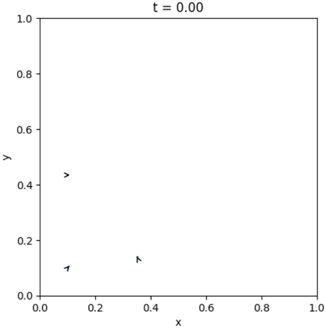


Convergence plot: exhibits linear rate

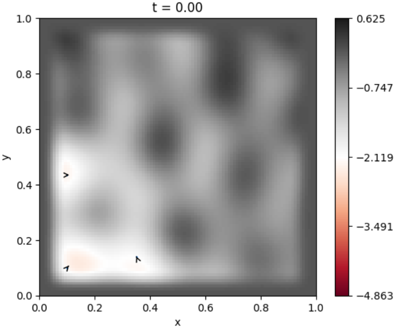
$$\text{Error} = T_{\alpha,\beta}(\rho^n, m^n) - T_{\alpha,\beta}(\rho^{n+1}, m^{n+1})$$

Numerical experiments

A more difficult example



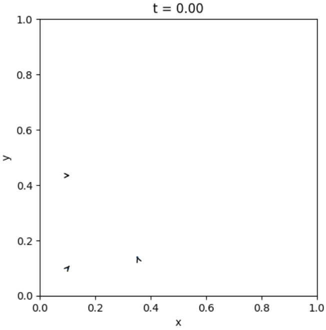
Ground truth



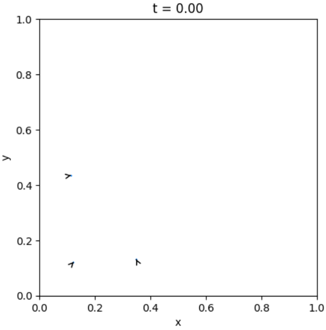
Backprojected data

Numerical experiments

A more difficult example



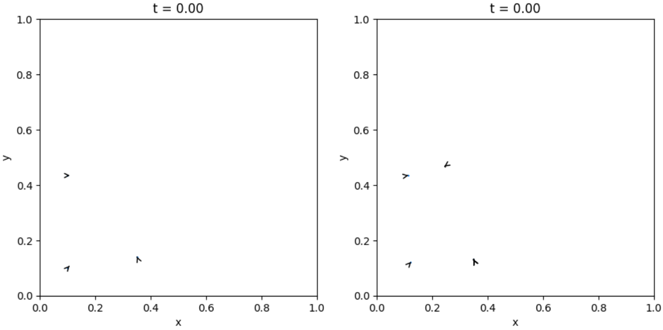
Ground truth



Reconstruction
(thresholded at 0.05)

Numerical experiments

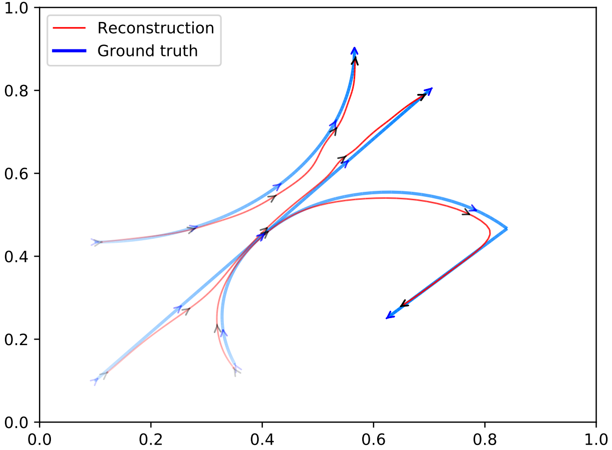
A more difficult example



Ground truth

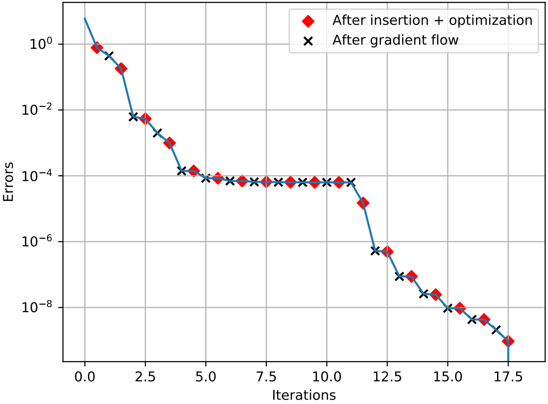
Reconstruction (no thresholding)

Numerical experiments



Reconstructed trajectories

Numerical experiments



Convergence plot: exhibits linear rate

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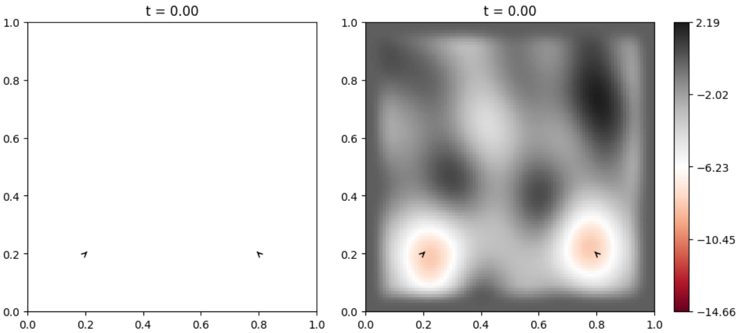
Numerical experiments

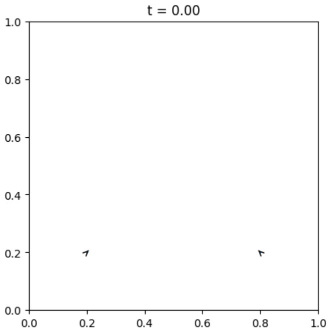
A crossing example



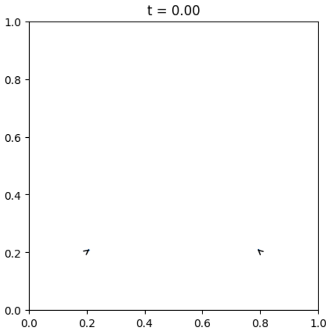
Ground truth　　Backprojected data

Numerical experiments

A crossing example



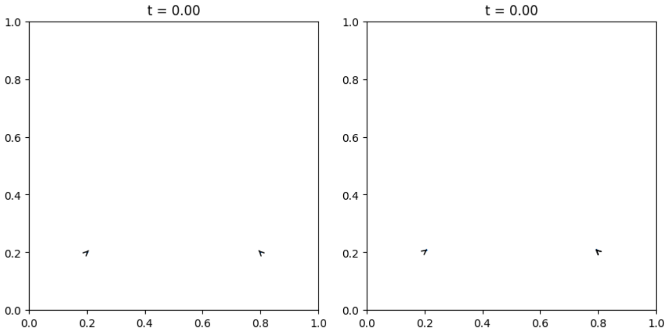
Ground truth



Reconstruction
(thresholded at 0.01)

Numerical experiments

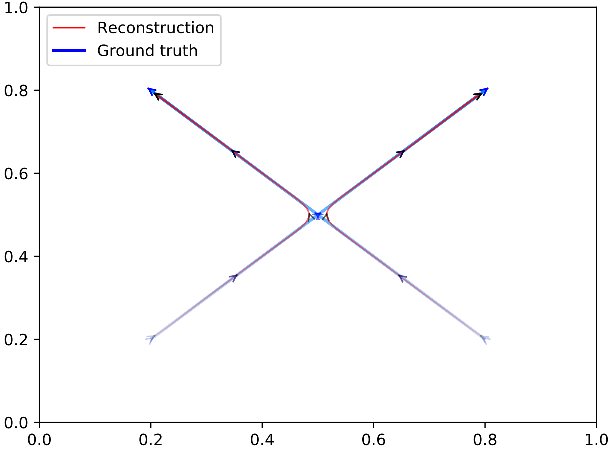
A crossing example



Ground truth

Reconstruction
(no thresholding)

Numerical experiments



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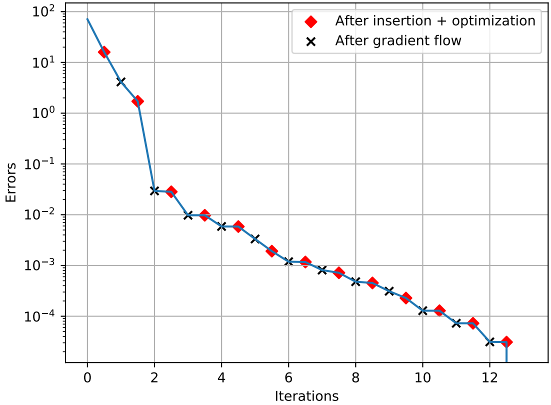
Numerical experiments



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Outline

Conclusions and perspectives

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- Extension to unbalanced transport (extremal points characterization already done) *[B./Carioni/Fanzon '22]*

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