Optimal transport regularization of dynamic inverse problems

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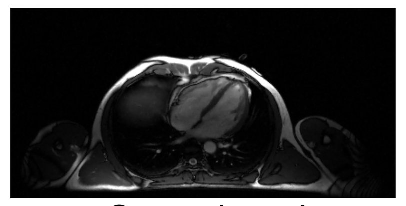
Joint work with K. Bredies, M. Carioni and F. Romero

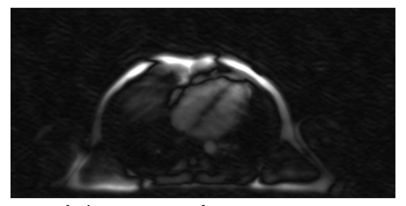
KB, SF are funded by FWF/CDG Grant PIR 27 and FWF Grant P 29192. MC is funded by the Royal Society Fellowship NIF-R1-192048

Motivation: Motion-Aware Reconstruction

Motion on sub-acquisition time-scales $\rightsquigarrow$ **artefacts** in reconstructed images
Example: Heart-lung imaging , High-resolution imaging
Workarounds: anaesthetics, breath-holding, gating
Drawbacks: assumes periodicity, low-resolution
Objectives:

- Robust reconstruction method via **Dynamic OT**
- Enforce **sparse** time-continuous reconstructions
- Numerical Algorithm based on **extremal points**


Ground truth


No regularization

Dynamic Inverse Problem

- **Data**: time dependent curve $t \mapsto f_t \in H_t$ with $\{H_t\}_t$ family of Hilbert spaces
- **Unknown:** curve of measures $t \mapsto \rho_t \in \mathcal{M}(\Omega)$, with $\Omega \subset \mathbb{R}^d$ bounded
- **Forward operators:** linear continuous operators $K_t^* \colon \mathcal{M}(\Omega) \to H_t$

Inverse Problem: given $t \mapsto f_t$, find a curve of measures $t \mapsto \rho_t \in \mathcal{M}(\Omega)$ s.t.

$$K_t^* \rho_t = f_t \quad \text{for a.e.} \quad t \in (0,1)\,. \tag{1}$$

Assumptions: very weak time-regularity for $\{H_t\}_t$ and K_t^*
Example. (K_t^*, H_t) can model Fourier transform with time-varying mask

Dynamic Optimal Transport

Static OT: transport a probability measure ρ_0 into ρ_1 while minimizing a cost

$$\mathbf{T} \in \arg\min \left\{ \int_\Omega |T(x) - x|^2 \, d\rho_0(x) : \; T \colon \Omega \to \Omega, \; T_{\#}\rho_0 = \rho_1 \right\}$$

Benamou-Brenier. The optimal transport $\mathbf{T}$ can be computed by solving

$$\min_{(\rho_t, v_t)} \frac{1}{2} \int_0^1 \int_\Omega |v_t(x)|^2 \, d\rho_t(x) \quad s.t. \quad \partial_t \rho_t + \operatorname{div}(v_t \rho_t) = 0 \tag{2}$$

- $t \mapsto \rho_t$ unknown mass trajectory s.t. $\rho_{t=0} = \rho_0$ and $\rho_{t=1} = \rho_1$
- $v_t(x) \colon [0,1] \times \Omega \to \mathbb{R}^d$ velocity field advecting the mass ρ_t

Note. Introducing the momentum $m_t := v_t \rho_t$ problem (2) becomes **convex** and the continuity equation **linear**

References

[1] K. Bredies, M. Carioni, S. Fanzon. "A superposition principle for the inhomogeneous continuity equation with Hellinger-Kantorovich-regular coefficients". Comm in PDE 47(10), 2022

[2] K. Bredies, M. Carioni, S. Fanzon, F. Romero. "A generalized conditional gradient method for dynamic inverse problems with optimal transport regularization". Found Comut Math, 2022

[3] K. Bredies, M. Carioni, S. Fanzon, F. Romero. "On the extremal points of the ball of the Benamou-Brenier energy". Bull London Math Soc 53(), 2021

[4] K. Bredies, S. Fanzon. "An optimal transport approach for solving dynamic inverse problems in spaces of measures". ESAIM: M2AN 54(6), 2020

Future Research. The theory in [4] works also with unbalanced optimal transport regularizers:

$$J(\rho, m, \mu) := \int_X \left|\frac{dm}{d\rho}\right|^2 + \left|\frac{d\mu}{d\rho}\right|^2 \, d\rho(t,x) + \alpha \, \|\rho\|_{\mathcal{M}(X)} \quad \text{s.t.} \quad \partial_t \rho + \operatorname{div}(m) = \mu \quad \text{in} \quad X \tag{6}$$

The extremal points of (6) are curves $t \mapsto h(t)\delta_{\gamma(t)}$, where the weight h can vanish [1]. We could then develop numerical methods for dynamic inverse problems regularized via unbalanced OT

Variational Regularization

- Time-space domain $X := (0,1) \times \Omega$, measures $\mathcal{M} := \mathcal{M}(X) \times \mathcal{M}(X; \mathbb{R}^d)$
- Continuity equation solutions

$$\mathcal{D} := \{(\rho, m) \in \mathcal{M} : \; \partial_t \rho + \operatorname{div}(m) = 0 \;\text{ in }\; X\}$$

- Convex optimal transport regularizer over $\mathcal{M}$, based on (2)

$$J_{\alpha,\beta}(\rho, m) := \frac{\beta}{2} \int_X \left|\frac{dm}{d\rho}\right|^2 d\rho(t,x) \; + \; \alpha \, \|\rho\|_{\mathcal{M}(X)} + \mathcal{X}_{\mathcal{D}}(\rho, m)$$

- $\alpha > 0$ promotes sparsity, while $\beta > 0$ penalizes speed
- $J_{\alpha,\beta}(\rho, m) < \infty \implies \rho = dt \otimes \rho_t$, $m = v\rho$ with $v \colon X \to \mathbb{R}^d$ measurable and $t \mapsto \rho_t \in \mathcal{M}^+(\Omega)$ narrowly continuous

OT Regularization: Let $(t \mapsto f_t) \in L^2_H$. We regularize (1) via

$$\min_{(\rho,m) \in \mathcal{M}} T_{\alpha,\beta}(\rho, m) := \frac{1}{2} \int_0^1 \|K_t^* \rho_t - f_t\|^2_{H_t} \, dt + J_{\alpha,\beta}(\rho, m) \tag{3}$$

Theorem. ([4]) If $(t \mapsto f_t) \in L^2_H$, problem (3) admits a solution.

Sparsity

Definition. An **atom** in $\mathcal{M}$ is of the form (ρ_γ, m_γ) with $\gamma \in H^1 := H^1([0,1]; \Omega)$,

$$\rho_\gamma := a_\gamma \, dt \otimes \delta_{\gamma(t)}\,, \quad m_\gamma := \dot\gamma(t)\, \rho_\gamma\,, \quad a_\gamma := \left(\frac{\beta}{2} \int_0^1 |\dot\gamma(t)|^2 \, dt + \alpha \right)^{-1}$$

Theorem. ([3]) The **extremal points** of $C_{\alpha,\beta} := \{J_{\alpha,\beta} \le 1\}$ are atoms or $(0,0)$. For finite dimensional data $T_{\alpha,\beta}$ at (3) admits a **sparse minimizer** of the form $\rho = \sum_{i=1}^N c_i \rho_{\gamma_i}$ with $N \in \mathbb{N}$, $c_i > 0$ and $\gamma_i \in H^1$

Generalized Conditional Gradient Method

Find **numerical solutions** to (3) by GCGM applied to $T_{\alpha,\beta}$ with linearized fidelity. The key step consists in finding a **descent direction** around $(\tilde\rho, \tilde m)$ by solving

$$\min_{(\rho,m) \in C_{\alpha,\beta}} - \int_0^1 \langle \rho_t, w_t \rangle \, dt\,, \quad w_t := -K_t(K_t^* \tilde\rho_t - f_t) \in C(\Omega) \tag{4}$$

Theorem. ([2]) Problem (4) admits a solution which is either an **atom** or $(0,0)$. Therefore (4) can be casted in H^1, and is hence numerically feasible (see (5))

Numerical Algorithm

Let $(t \mapsto f_t) \in L^2_H$ be given data. Initialize $\rho^0 := 0$

1. **Insertion:** Given $\rho^n = \sum_{i=1}^N c_i \, \rho_{\gamma_i}$, set $w_t^n := -K_t(K_t^* \tilde\rho_t^n - f_t)$ and find

$$\gamma^* \in \arg\min_{\gamma \in H^1} -a_\gamma \int_0^1 w_t(\gamma(t)) \, dt\,, \qquad \rho^{n+1/2} := \rho^n + c_{N+1} \rho_{\gamma^*} \tag{5}$$

2. **Coefficients Optimization:** Solve the quadratic problem

$$(c_j^*)_j \in \arg\min_{c_j \ge 0} \; T_{\alpha,\beta}(\rho^{n+1/2}, m^{n+1/2})\,, \qquad \rho^{n+1} := \sum_{i=1}^{N+1} c_i^* \, \rho_{\gamma_i}$$

Theorem. ([2]) The sequence (ρ^n, m^n) generated by Algorithm converges weak* to a solution of (3). The convergence rate is of order $O(1/n)$

Undersampled Fourier Measurements

- $\Omega := [0,1]^2$ image frame, $t \mapsto \sigma_t \in \mathcal{M}^+(\mathbb{R}^2)$ frequencies sampling measure
- Fourier transform $\mathfrak{F} \colon \mathcal{M}(\Omega) \to C^\infty(\mathbb{R}^2; \mathbb{C})$
- $H_t := L^2_{\sigma_t}(\mathbb{R}^2; \mathbb{C})$ and $K_t^* \colon \mathcal{M}(\Omega) \to H_t$ defined by $K_t^* \rho := \mathfrak{F}\rho$

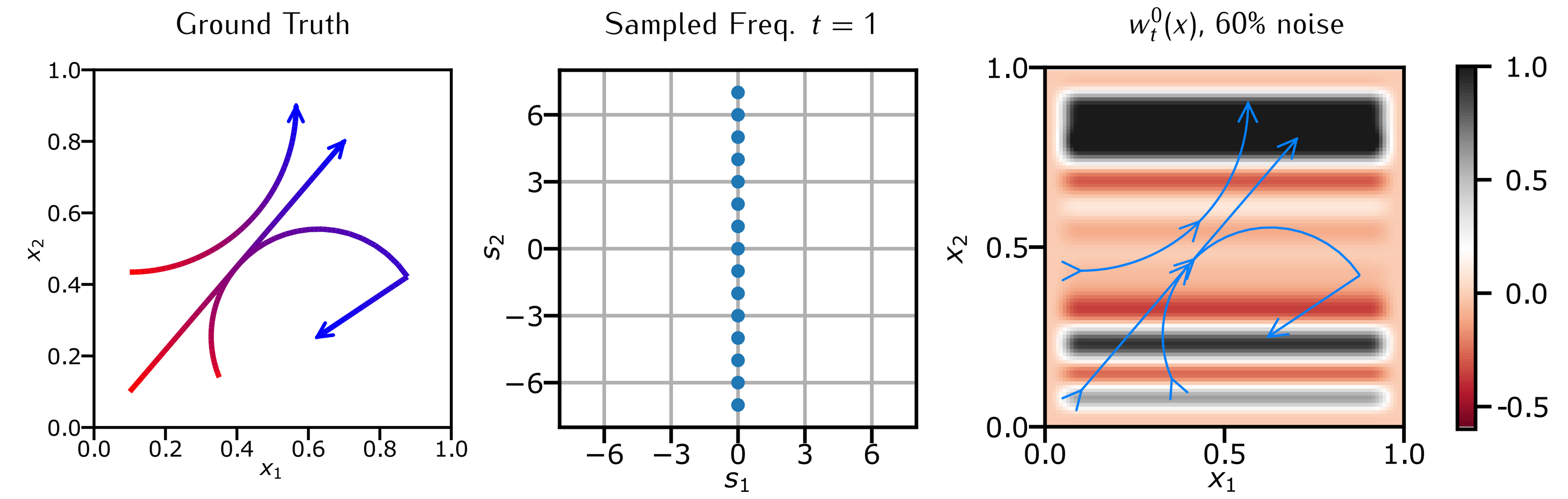
Note. K_t^* corresponds to the Fourier transform undersampled according to σ_t
Time-discrete sampling: Fix T times samples, $t_i := i/T$ for $i = 0, \dots, T$

- At each time t_i sample $n_i \in \mathbb{N}$ frequencies $\{S_{i,1}, \dots, S_{i,n_i}\} \subset \mathbb{R}^2$
- Define $t \mapsto \sigma_t$ so that $\sigma_{t_i} = \sum_{k=1}^{n_i} \delta_{S_{i,k}}$. In this case $H_{t_i} = \mathbb{C}^{n_i}$ and

$$K_{t_i}^* \rho = \left(\int_{\mathbb{R}^2} \exp(-2\pi i x \cdot S_{i,k}) \, d\rho(x) \right)_{k=1}^{n_i} \in \mathbb{C}^{n_i}$$

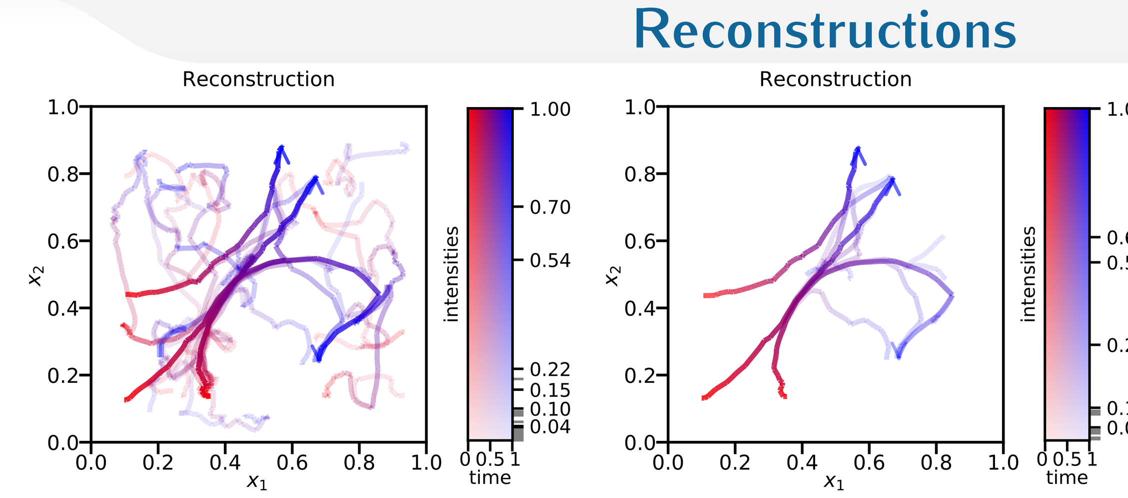
Experiment: Dynamic Spikes Tracking

- $T = 50$, $n_i = 15$ freq. sampled on lines L_i through the origin with angle $\frac{i\pi}{4}$
- **Ground Truth:** $\tilde\rho_t = \delta_{\gamma_1(t)} + \delta_{\gamma_2(t)} + \delta_{\gamma_3(t)}$ as depicted (color=position in time)
- **Synthetic Data:** $f_{t_i} := K_{t_i}^* \tilde\rho_{t_i} + 60\%$ Gaussian Noise
- **Data Visualization:** By plotting the initial dual variable $w_{t_i}^0 := K_{t_i} f_{t_i} \in C(\Omega)$



Warning! At each t_i the inverse problem $K_{t_i}^* \rho = f_{t_i}$ is heavily ill-posed: indeed $K_{t_i}^* \delta_{\hat x} = K_{t_i}^* \delta_{\hat x + \lambda S_i^\perp}$ for $\lambda \in \mathbb{R}$, where $S_i^\perp \in \mathbb{R}^2$ is orthogonal to $L_i \rightsquigarrow$ **Static methods cannot resolve location of $\hat x$**

Reconstructions

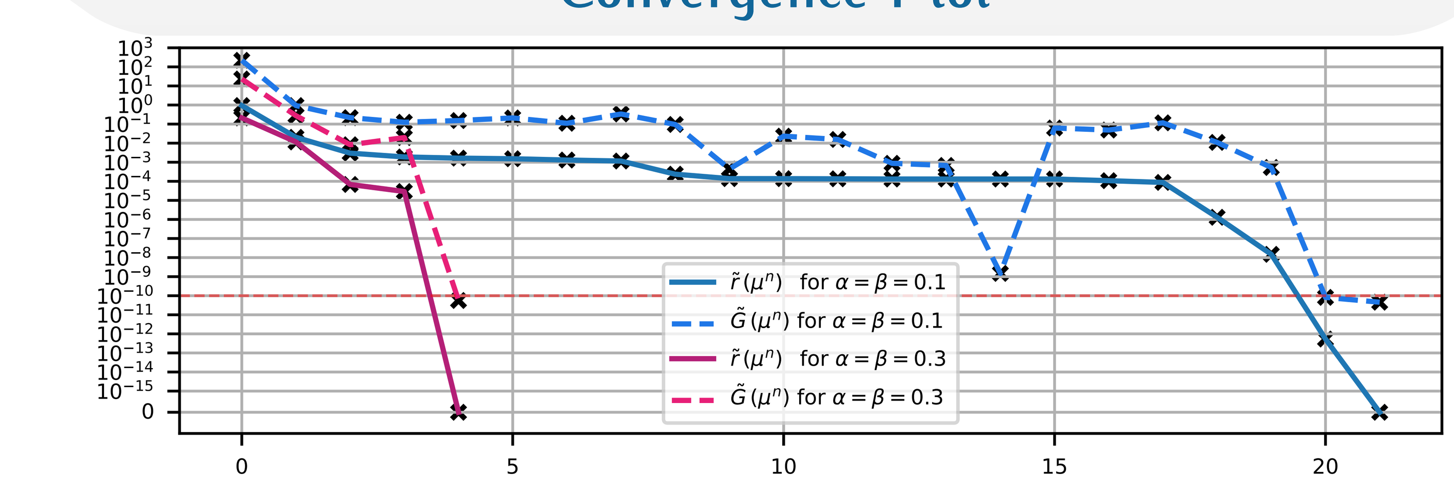


$\alpha = \beta = 0.1$ $\qquad$ $\alpha = \beta = 0.3$

Intensity: weight c_i corresponding to atom δ_{γ_i}

- **Low reg.** $\alpha = \beta = 0.1 \rightsquigarrow$ surge of low-energy artefacts around main trajectories
- **High reg.** $\alpha = \beta = 0.3 \rightsquigarrow$ improved reconstruction

Convergence Plot



Note! Proven sublinear rate of convergence but empirical **linear rate**
As expected, higher regularization results in faster convergence