Off-the-grid dynamic super-resolution for fluorescence microscopy.

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MORPHEME
MORPHOLOGIE ET IMAGES

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Image biological structures at small scales

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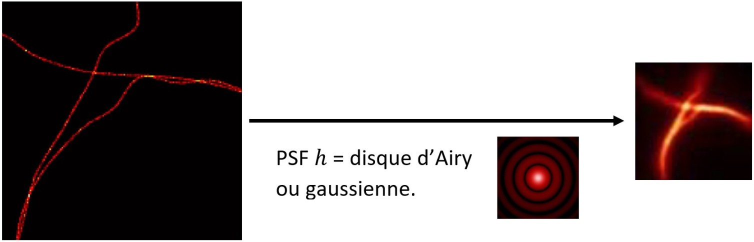

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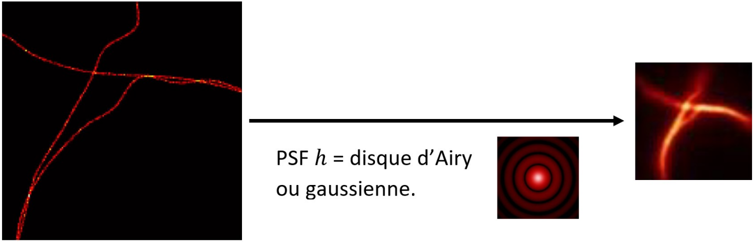

Reconstruction e.g. by fluorescence microscopy SMLM: acquisition stack with few lit fluorophores per image. Drawback: many images ($\approx 1 \times 10^4$, does not allow imaging of living cells).

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SOFI imaging (Super-resolution optical fluctuation imaging).
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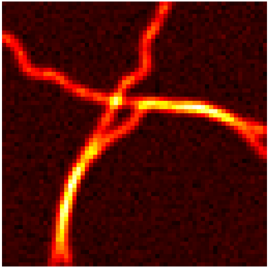

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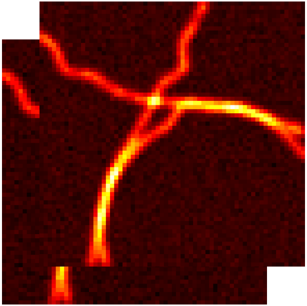

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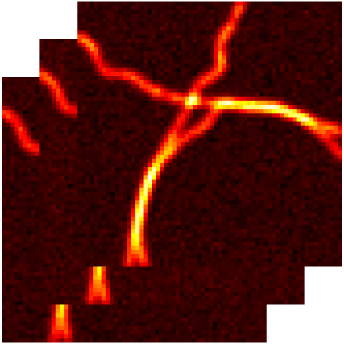

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Acquisition

Reconstruction

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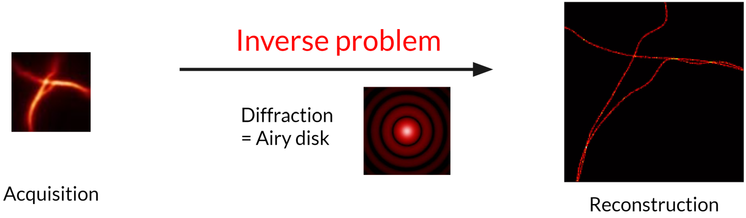

- off-the-grid deconvolution can be understood as the 'limit' of an increasingly fine grid;
- not limited by the fine grid but still limited by the noise.

Link with grid problem

$$\min_{a\in\mathbb{R}^L} \|y - \Phi_L a\|_{\mathcal{H}}^2 + \lambda \|a\|_1 \quad \text{(LASSO)}$$

$$\min_{m\in\mathcal{M}(\mathcal{X})} \|y - \Phi m\|_{\mathcal{H}}^2 + \lambda \|m\|_{\mathrm{TV}} \quad \text{(BLASSO)}$$

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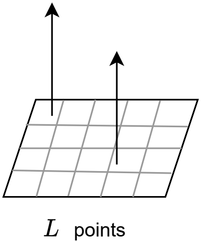

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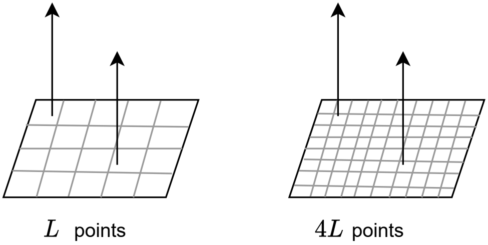

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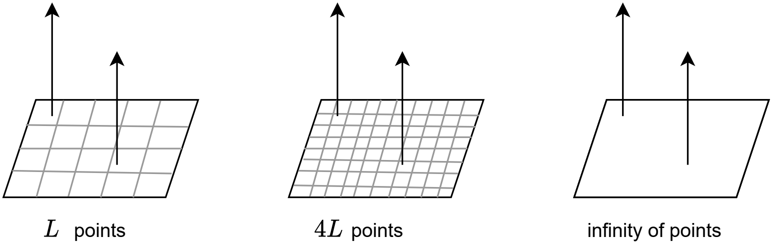

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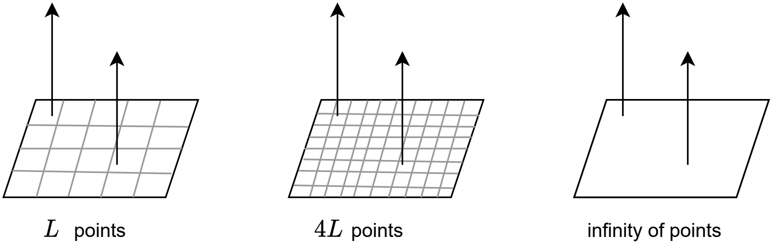

BLASSO is the functiunal limit of the LASSO problem for $L \to +\infty$.

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Off-the-grid case

- not limited by the grid;
- convexity of the functional on an infinite dimensional space;
- existence and uniqueness guarantees;
- recent field of research.

Off-the-grid digest

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- topological dual of $\mathscr{C}_0(\mathcal{X})$ ($= \mathscr{C}(\mathcal{X})^*$ here) for $\langle f, m \rangle = \int_{\mathcal{X}} f \, \mathrm{d}m$. Generalisation of $\mathrm{L}^1(\mathcal{X})$ since $\mathrm{L}^1(\mathcal{X}) \hookrightarrow \mathcal{M}(\mathcal{X})$;

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- Banach for the TV-norm: $m \in \mathcal{M}(\mathcal{X})$,

$$|m|(\mathcal{X}) \stackrel{\text{def.}}{=} \sup \left(\int_{\mathcal{X}} f \, \mathrm{d}m \,\middle|\, f \in \mathscr{C}(\mathcal{X}), \|f\|_{\infty,\mathcal{X}} \leq 1 \right).$$

If $m = \sum_{i=1}^N a_i \delta_{x_i}$ is a discrete measure then $|m|(\mathcal{X}) = \sum_{i=1}^N |a_i|$.

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We call **BLASSO** the optimisation problem [Castro12, Duval15] for $\lambda > 0$:

$$\operatorname*{argmin}_{m \in \mathcal{M}(\mathcal{X})} \frac{1}{2} \|y - \Phi m\|^2_{\mathrm{L}^2(\mathcal{X})} + \lambda |m|(\mathcal{X}) \qquad (\mathcal{P}_\lambda(y))$$

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The optimisation space $\mathcal{M}(\mathcal{X})$ is an infinite dimensional space, reflexive only for weak-* topology: a difficult problem.

Dual certificate

To solve this problem, we have the strong (Fenchel) duality:

$$\eta_\lambda \in \partial|m|(\mathcal{X}) \cap \Phi^* y$$

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Conditions[1] on the dual certificate + on the operator = reconstruction guarantees.

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Numerous other algorithms:

	pros	cons
moments method [Lasserre10]		difficult nD case
conditional gradient [Bredies13]	convergence guarantees	difficult iteration
particle gradient flow [Chizat20]	quick to compute	not robust wrt noise

Illustration of Conic Particle Gradient Flow reconstruction [Chizat20]:

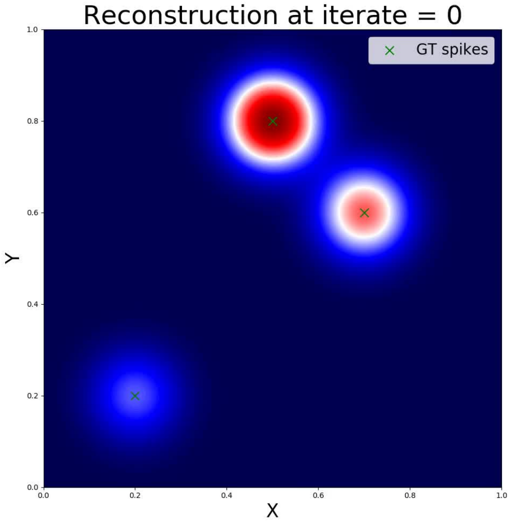
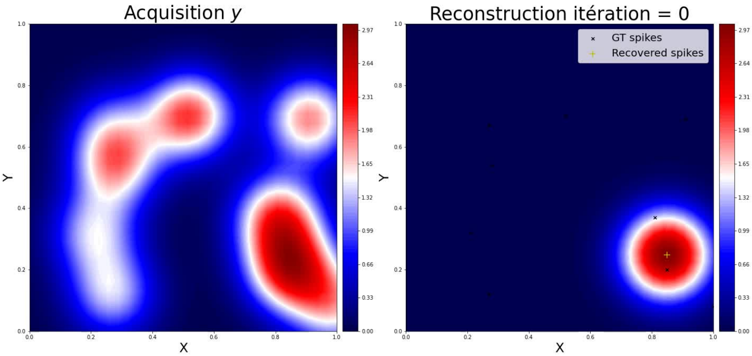


Illustration of Sliding Frank-Wolfe [Denoyelle19] iterative reconstruction:



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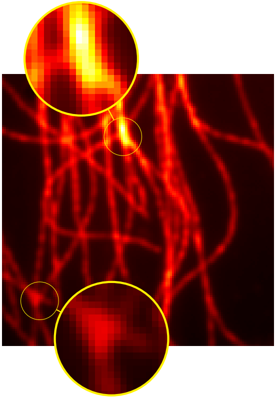

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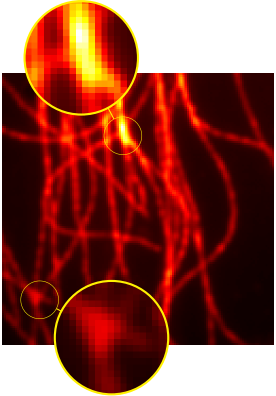

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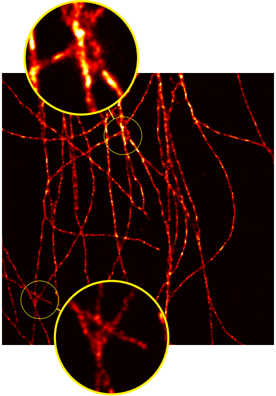

Off-the-grid SFW

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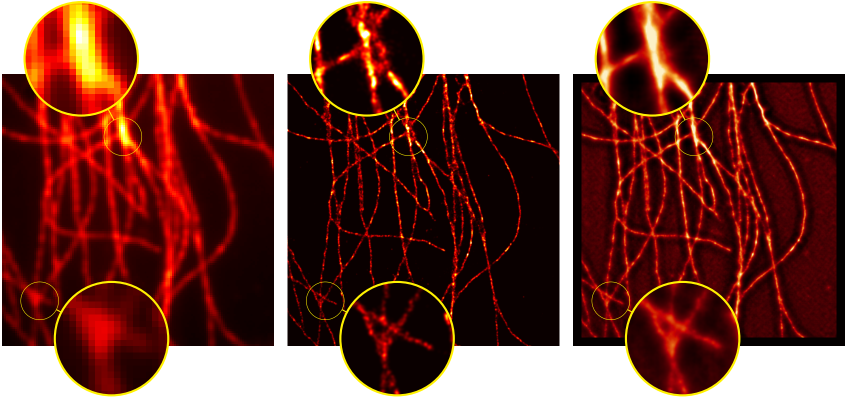

Mean of stack — Off-the-grid SFW — SRRF [Culley18]

Dynamic off-the-grid

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- we aim to reconstruct the *dynamic* measure:

$$t \mapsto \mu(t) \overset{\text{def.}}{=} \sum_{i=1}^{N} a_i(t)\delta_{x_i} \in \mathrm{L}^2(0, T; \mathcal{M}(\mathcal{X}))$$

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Cumulants are a tool to reconstruct the positions x_i. Example : temporal mean $\bar{y} \stackrel{\text{def.}}{=} \frac{1}{T} \int_0^T y(\cdot, t)\, \mathrm{d}t$. One have $\Phi m_{a,x} = \bar{y}$ where $m_{a,x} \stackrel{\text{def.}}{=} \sum_{i=1}^{N} \bar{a}_i \delta_{x_i}$ and $\bar{a}_i$ is the mean of $a_i(\cdot)$.

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&= \dots \quad \text{(independence of fluctuations [Dertinger10])} \\
&= \sum_{i=1}^{N} \underbrace{M_i}_{a_i \text{ variance}} \; h(u-x_i)h(v-x_i) \\
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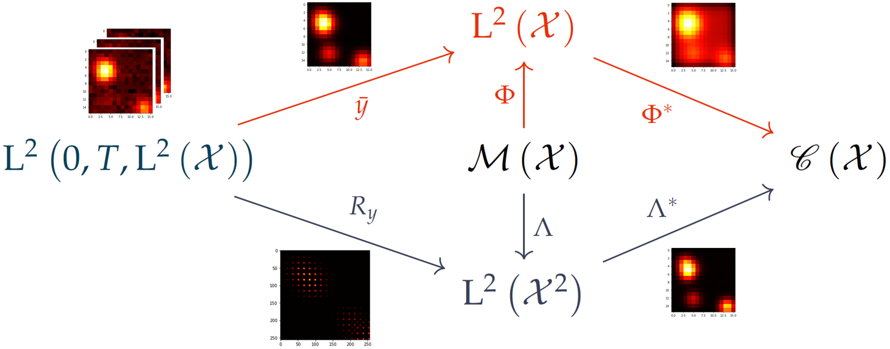
$m_{M,x} \overset{\text{def.}}{=} \sum_{i=1}^{N} M_i \delta_{x_i}$ shares the same positions as $\mu = \sum_{i=1}^{N} a_i(t)\delta_{x_i}$, we call $\Lambda : \mathcal{M}(\mathcal{X}) \to \mathrm{L}^2(\mathcal{X}^2)$ this « covariance operator ».

Quantities digest



Legend: dynamic part, temporal mean part $\bar{y}$ and covariance R_y.

BLASSO on cumulants

Let $\lambda > 0$,
covariance problem writes down:

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while mean reconstruction is:

$$\operatorname*{argmin}_{m \in \mathcal{M}(\mathcal{X})} S_\lambda(m) \stackrel{\text{def.}}{=} \frac{1}{2} \| \bar{y} - \Phi(m) \|^2_{\mathrm{L}^2(\mathcal{X})} + \lambda |m|(\mathcal{X}) \qquad (\mathcal{P}_\lambda(\bar{y}))$$

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Let $\Delta \overset{\text{def.}}{=} \min_{i \neq j} \left| x_i - x_j \right|$ be the *minimum* separation distance

Proposition

Support of a ***real*** *Radon measure in noiseless setting is reconstructed:*

- *for* $(\mathcal{P}_\lambda(\bar{y}))$ *if* $\Delta \gtrsim 1{,}1\sigma$ *[Bendory16] ;*
- *for* $(\mathcal{Q}_\lambda(y))$ *if* $\Delta \gtrsim 1{,}1\sigma/\sqrt{2}$*:* ***better!*** *.*

Numerical results 1D

Implementation in an OOP module in `python`:

- to use Radon measures, certificates, optimisation algorithm, ($\mathcal{Q}_\lambda(y)$) et ($\mathcal{P}_\lambda(\bar{y})$);
- written in `PyTorch` + CUDA (GPU);
- question of quality metrics. L^2 distance is not suitable, we prefer the *flat metric* (or Kantorovitch-Rubinstein metric).

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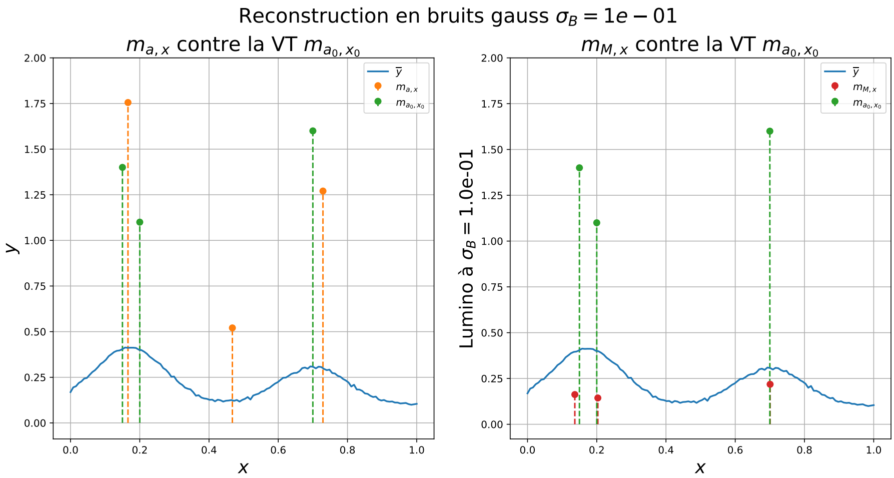
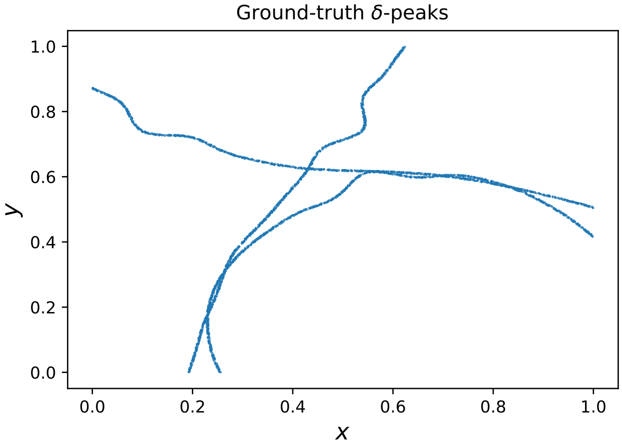


Figure 1: $\mathcal{W}_1(m_{a_0,x_0}, m_{a,x}) \approx 1 \times 10^{-1}$ et $\mathcal{W}_1(m_{a_0,x_0}, m_{M,x}) \approx 5 \times 10^{-3}$.

Numerical 2D results SOFItool

Test on 2D tubulins from ISBI challenge 2016:

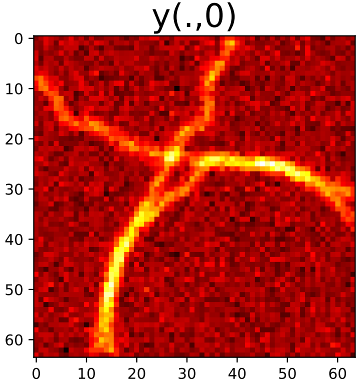
- stack of 1000 acquisitions 64×64 simulated by SOFItool;
- 8700 emitters scattered along the tubulins; **high** background noise + Poisson noise at 4 + Gaussian noise at 1×10^{-2}. SNR $\approx$ 10 db.



Numerical 2D results SOFItool

Test on 2D tubulins from ISBI challenge 2016:

- stack of 1000 acquisitions 64×64 simulated by SOFItool;
- 8700 emitters scattered along the tubulins; **high** background noise + Poisson noise at 4 + Gaussian noise at 1×10^{-2}. SNR $\approx$ 10 db.



Numerical 2D results SOFItool

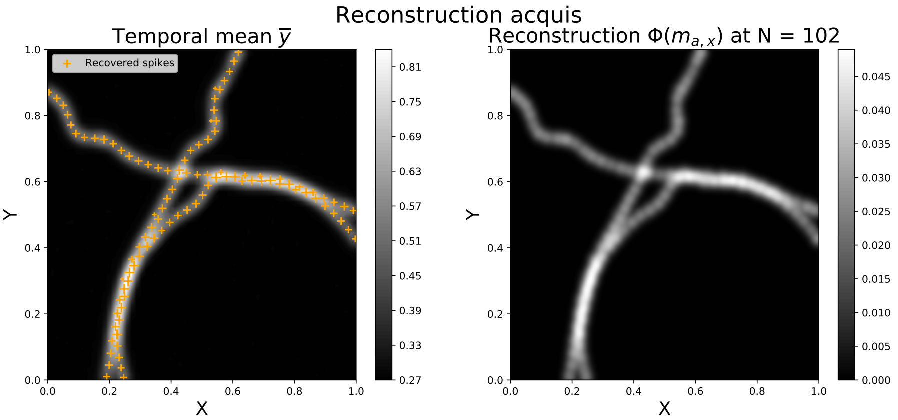


Figure 2: Reconstruction by $(\mathcal{P}_\lambda(\bar{y}))$.

Numerical 2D results SOFItool

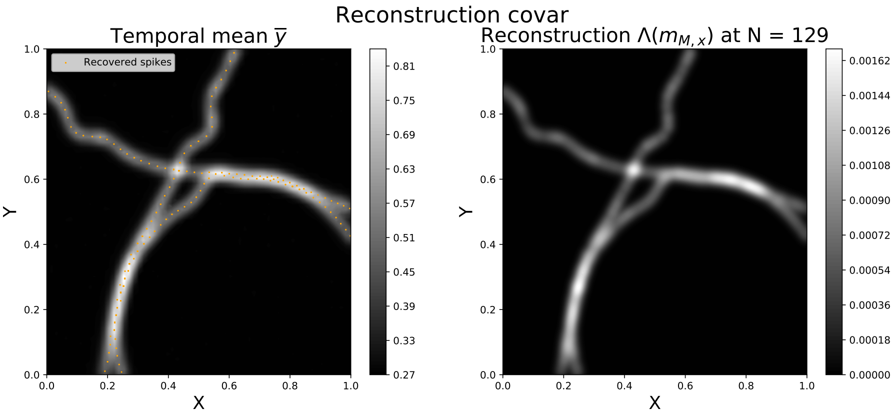


Figure 2: Reconstruction by $(\mathcal{Q}_\lambda(y))$.

Numerical 2D results SOFItool

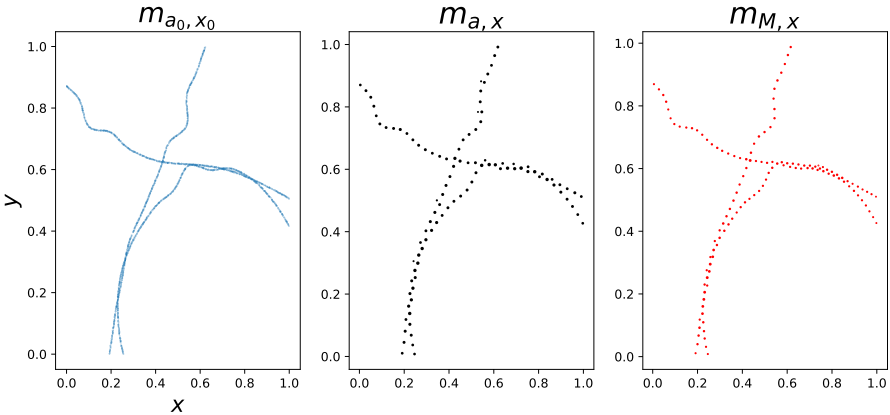


Figure 2: Comparison between ground-truth and solutions of both $(\mathcal{P}_\lambda(\bar{y}))$ and $(\mathcal{Q}_\lambda(y))$.

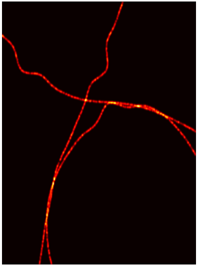


Figure 3: Ground-truth

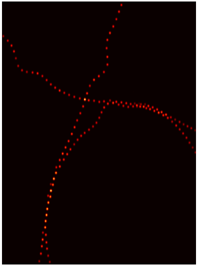


Figure 4: $(\mathcal{Q}_\lambda(y))$

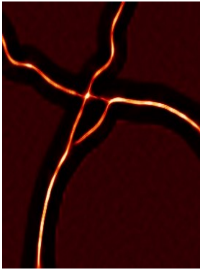


Figure 5: Grid: SRRF [Culley18]

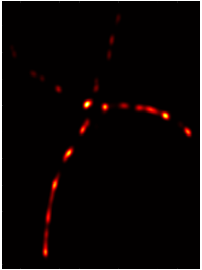


Figure 6: Grid: SPARCOM [Solomon18]

Conclusion

Take home statements

- off-the-grid methods squeeze all the 'information' out the acquisition y: no discretisation drawback;
- strong results for existence and uniqueness of BLASSO solution;
- only one efficient numerical algorithm: Sliding Frank-Wolfe;

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- off-the-grid methods squeeze all the 'information' out the acquisition y: no discretisation drawback;
- strong results for existence and uniqueness of BLASSO solution;
- only one efficient numerical algorithm: Sliding Frank-Wolfe;

Outlook

- results only for sparse spike problem with known forward operator at the moment: extendable to other imagery problems? (Obviously yes, gridless compressed sensing, etc.)
- theory only suited for spikes: what about other source structures?
- quite costly numerical algorithms: learning approaches?

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Sliding Frank-Wolfe

Algorithm 1: *Sliding Frank-Wolfe.*

Entrées: Acquisition $y \in \mathcal{H}$, nombre d'itérations K, $\lambda > 0$

Initialisation : $m^{[0]} = 0$ $N^{[k]} = 0$

for *Récurrence pour l'étape k,* $0 \leq k \leq K$ **do**

Pour $m^{[k]} = \sum_{i=1}^{N^{[k]}} a_i^{[k]} \delta_{x_i^{[k]}}$ telle que $a_i^{[k]} \in \mathbb{R}$, $x_i^{[k]} \in \mathcal{X}$, trouver $x_*^{[k]} \in \mathcal{X}$ tel que :

$$x_*^{[k]} \in \underset{x \in \mathcal{X}}{\operatorname{argmax}} \left| \eta^{[k]}(x) \right| \qquad \text{où} \quad \eta^{[k]}(x) \stackrel{\text{def.}}{=} \frac{1}{\lambda} \Phi^*(\Phi m^{[k]} - y),$$

if $\left| \eta^{[k]}(x_*^{[k]}) \right| < 1$ **then**

$m^{[k]}$ est la solution du BLASSO. Stop.

else

Calculer $m^{[k+1/2]} = \sum_{i=1}^{N^{[k]}} a_i^{[k+1/2]} \delta_{x_i^{[k+1/2]}} + a_{N^{[k]}+1}^{[k+1/2]} \delta_*^{[k+1/2]}$ telle que :

$$a_i^{[k+1/2]} \in \underset{a \in \mathbb{R}^{N^{[k]}+1}}{\operatorname{argmin}} \frac{1}{2} \|y - \Phi_{x^{[k+1/2]}}(a)\|_{\mathcal{H}}^2 + \lambda \|a\|_1$$

$$\text{pour} \quad x^{[k+1/2]} \stackrel{\text{def.}}{=} \left(x_1^{[k]}, \ldots, x_{N^{[k]}}^{[k]}, x_*^{[k]} \right).$$

Calculer $m^{[k+1]} = \sum_{i=1}^{N^{[k+1]}} a_i^{[k+1]} \delta_{x_i^{[k+1]}}$ telle que :

$$(a_i^{[k+1]}, x_i^{[k+1]}) \in \underset{(a,x) \in R}{\operatorname{argmax}} \frac{1}{2} \|y - \Phi_{x^{[k+1/2]}}(a)\|_{\mathcal{H}}^2 + \lambda \|a\|_1$$

end

end

Sortie: Mesure discrète $m^{[k]}$ pour k l'itération d'arrêt.

Choice of λ

λ is the only tuning parameter in BLASSO: it drives the number N of reconstructed spikes.

How do we choose it?

- Cross-validation.
- Homotopy algorithm.
- experimental choice.