Off-the-grid curve reconstruction: theory and applications to fluorescence microscopy

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15th September 2023

Morpheme research team
Inria, CNRS, Université Côte d'Azur

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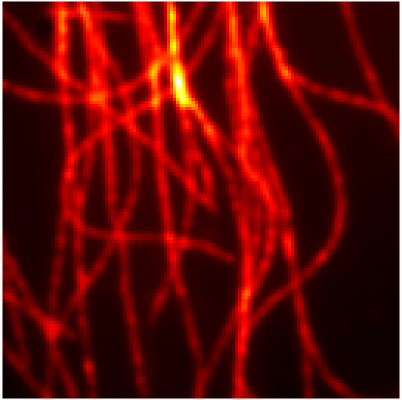
Introduction

How could we recover biological structure from resolution-limited acquisitions?



Microscope acquisition

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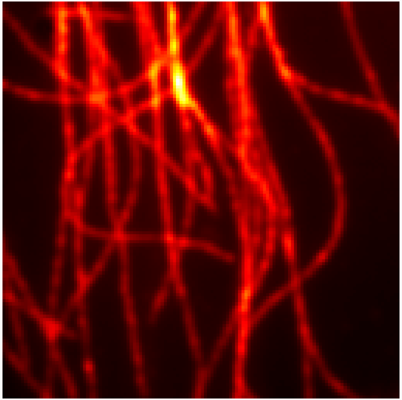

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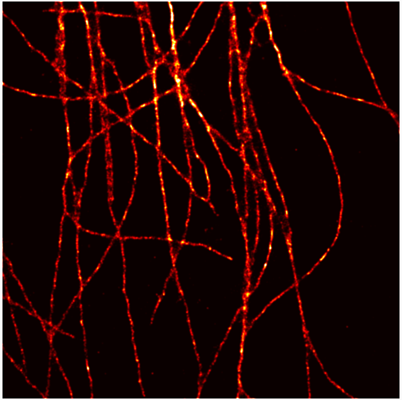
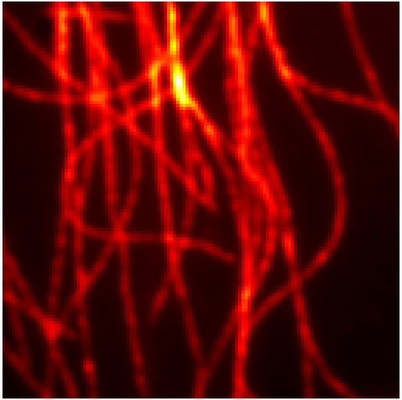


Reconstruction

How could we recover biological structure from resolution-limited acquisitions? This is a case of **inverse problem**.



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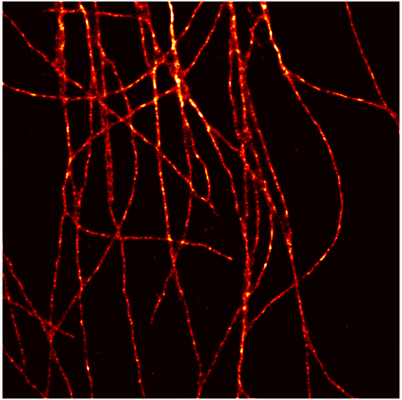

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> *'Can one hear the shape of a drum?'*, Marc Kac (1966)

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Observation

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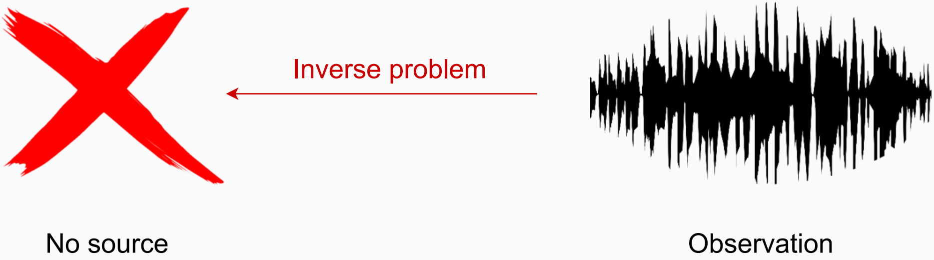

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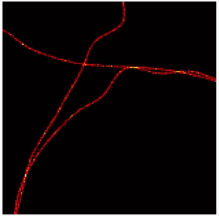

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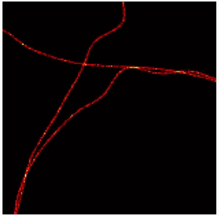

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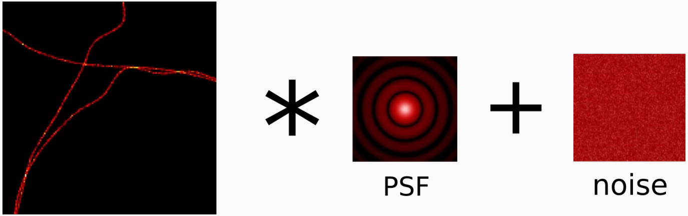

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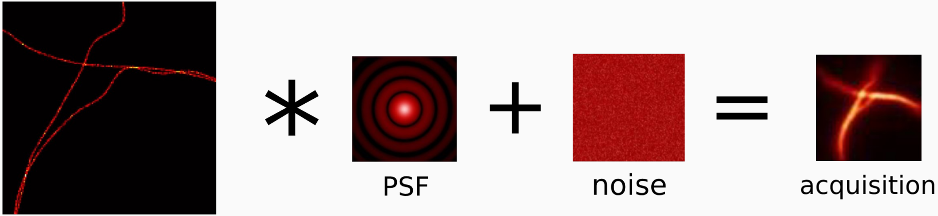

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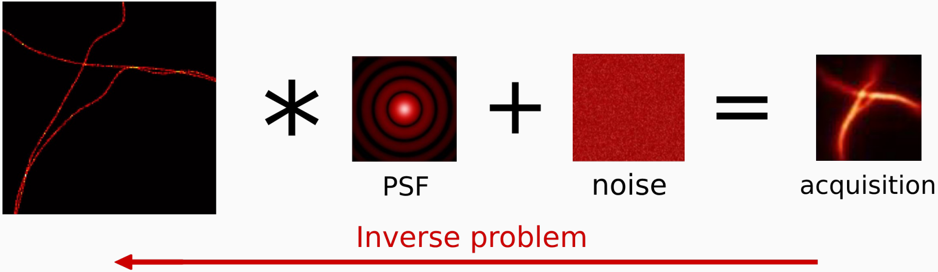

Solve inverse problem through variational approach

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- $R(S)$ regularises the problem (well-posed) and enforces more or less the prior on S w. $\alpha > 0$.

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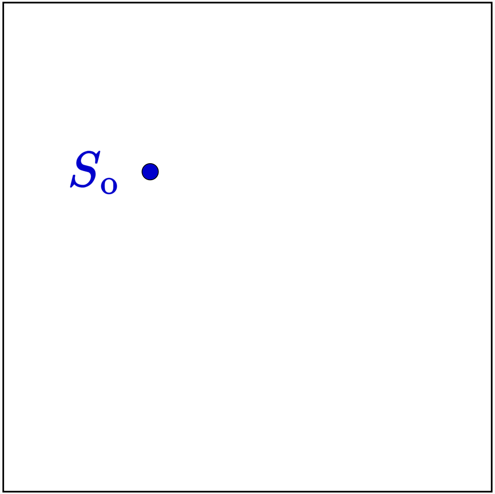

Source to estimate

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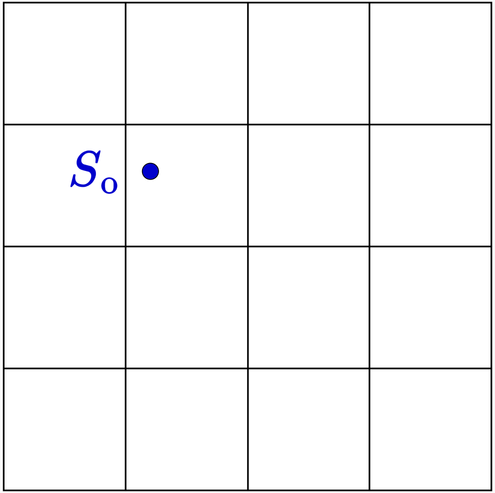
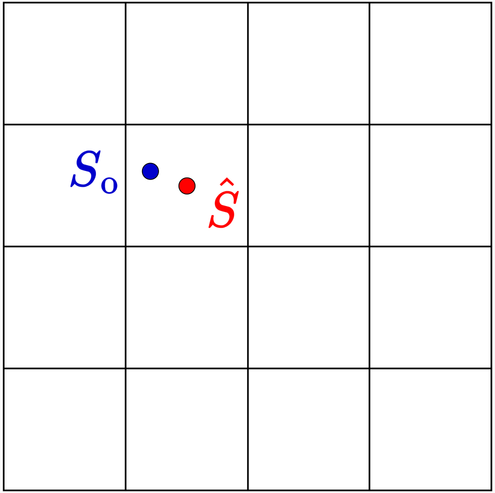


Introducing a grid

Grid or gridless?



Reconstruction $\hat{S}$ on a grid

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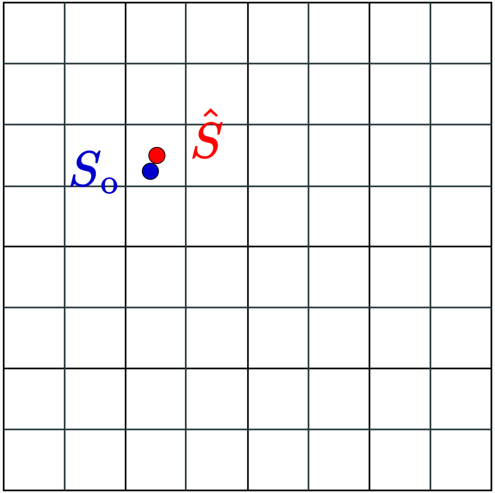

Reconstruction $\hat{S}$ on a finer grid

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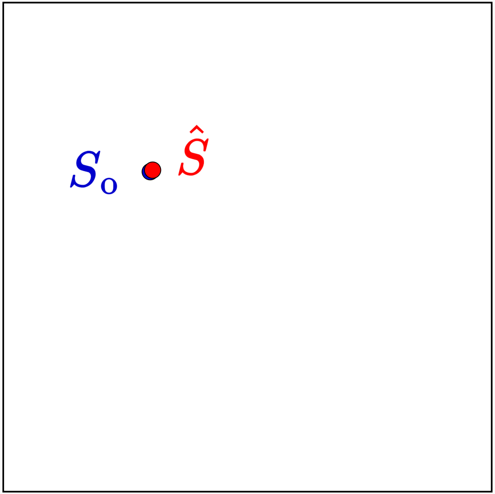

Reconstruction $\hat{S}$ is now **off-the-grid**

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- combinatorial (non-)convex optimisation;
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Off-the-grid

- brings structural prior;
- guarantees (uniqueness, support);
- convex but infinite dimensional;
- young field.

Off-the-grid 101: the sparse spike problem

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Difficult numerical problem: infinite dimensional, non-reflexive. Tackled by greedy algorithm like *Frank-Wolfe* [Frank and Wolfe, 1956] , *etc*.

Some results for spikes reconstruction

Reconstruction by fluorescence microscopy SMLM: acquisition stack with few lit fluorophores per image.

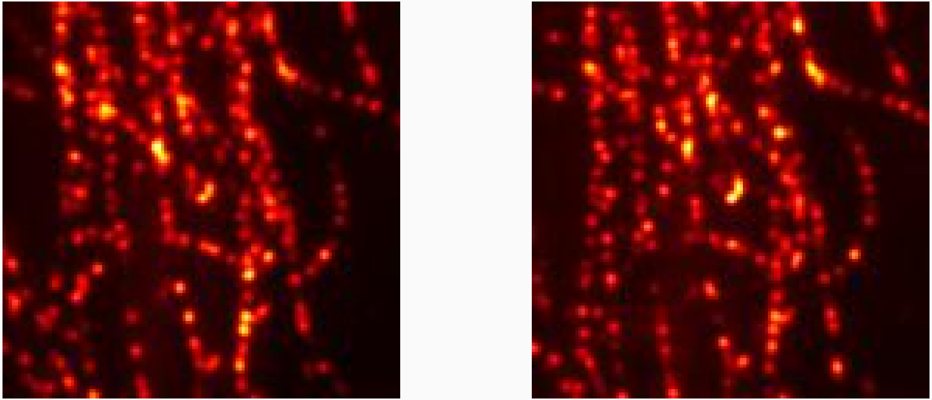
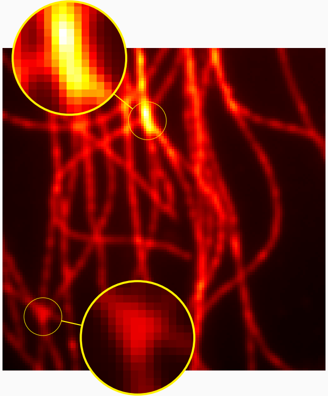


Figure 1: Two excerpts from a SMLM stack

Results on SMLM



Stack mean

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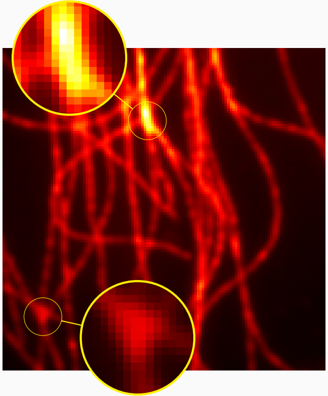

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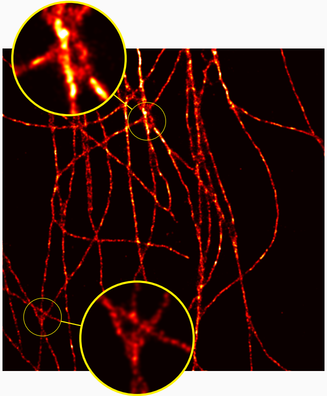

Off-the-grid [Laville et al., 2021]

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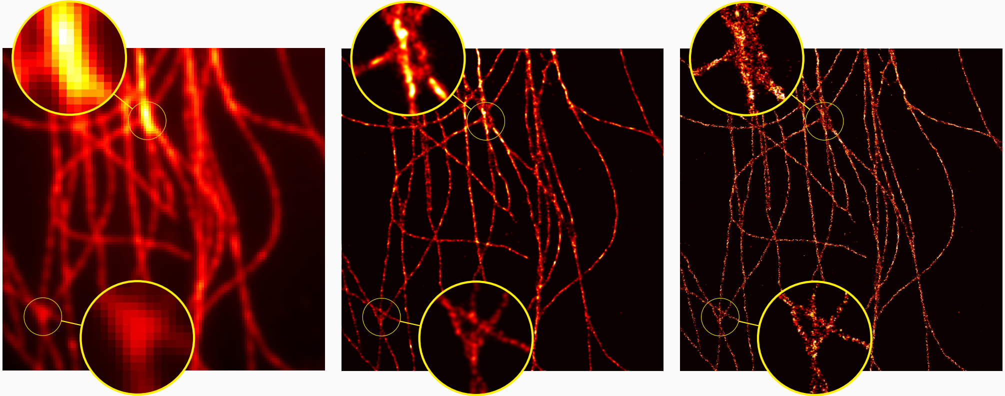

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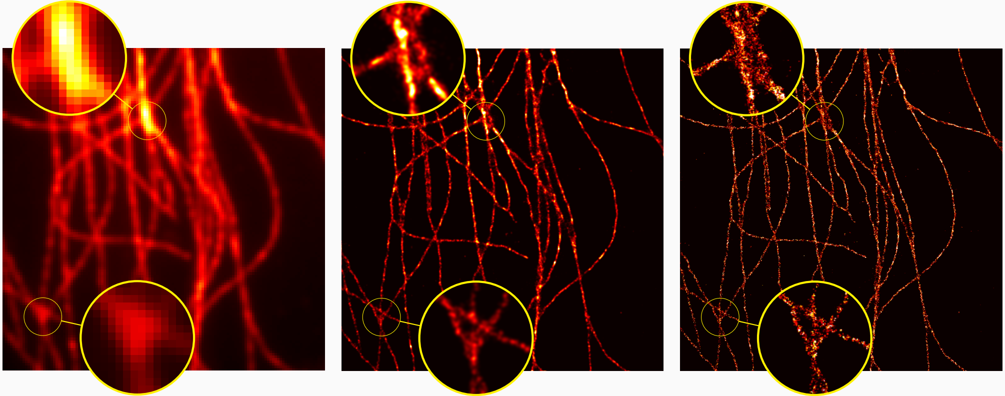

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SMLM drawback: a lot of images, no live-cell imaging.

Off-the-grid covariance spikes reconstruction

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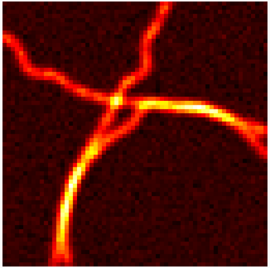

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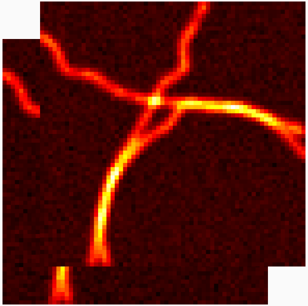

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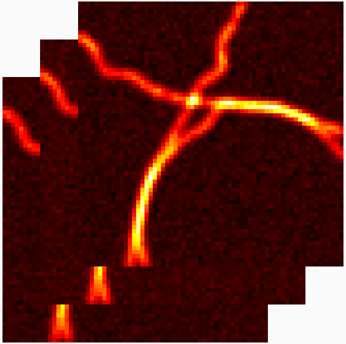

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Moments are a tool to recover the positions x_i.

Example: let the stack mean $\bar{y} \stackrel{\text{def.}}{=} \frac{1}{T}\int_0^T y(\cdot, t)\,\mathrm{d}t$.

Quantities at stake

- acquisition stack i.e. images in $\mathrm{L}^2(\mathcal{X})$ during $[0, T]$;
- $y : [0, T] \to \mathrm{L}^2(\mathcal{X})$ is the SOFI acquisition stack ;
- we aim to reconstruct the *dynamic* measure:

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

generating a.e. $t \in [0, T] : y(t) = \Phi\mu(t)$. In the convolution case for PSF h, $\Phi\mu(t) = \sum_{i=1}^N a_i(t) \int_{\mathcal{X}} h(x - x_i)\,\mathrm{d}x$.

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

Build the variational problem

Let R_y be the spatial covariance, $\forall u, v \in \mathcal{X}$ we yield:

$$R_y(u, v) \stackrel{\text{def.}}{=} \frac{1}{T} \int_0^T \left(y(u, t) - \bar{y}(u)\right) \left(y(v, t) - \bar{y}(v)\right) \, \mathrm{d}t$$

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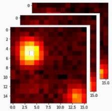
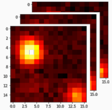
$m_{M,x} \stackrel{\text{def.}}{=} \sum_{i=1}^{N} M_i \delta_{x_i}$ shares the same positions w. $\mu = \sum_{i=1}^{N} a_i(t)\delta_{x_i}$ through Λ.

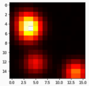
Quantities digest



$$\mathrm{L}^2\left(0, T, \mathrm{L}^2\left(\mathcal{X}\right)\right)$$

Legend: dynamic part, .

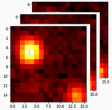


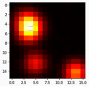


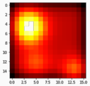
$$
\begin{tikzcd}
 & & L^2(\mathcal{X}) \\
L^2(0,T,L^2(\mathcal{X})) \arrow[urr, "\bar{y}"'] & & \mathcal{M}(\mathcal{X}) \arrow[u, "\Phi"]
\end{tikzcd}
$$

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

Quantities digest







$$
\begin{tikzcd}
& \mathrm{L}^2(\mathcal{X}) \arrow[dr, "\Phi^*"] & \\
\mathrm{L}^2(0, T, \mathrm{L}^2(\mathcal{X})) \arrow[ur, "\bar{y}"] & \mathcal{M}(\mathcal{X}) \arrow[u, "\Phi"] & \mathscr{C}(\mathcal{X})
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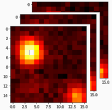

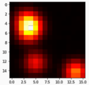

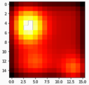

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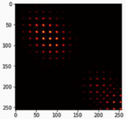

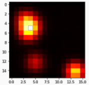

Legend: dynamic part, temporal mean part $\bar{y}$ and covariance R_y.

BLASSO on cumulants

Let $\lambda > 0$,

The energy for covariance-based reconstruction writes down:

$$\underset{m \in \mathcal{M}(\mathcal{X})}{\operatorname{argmin}} \; T_\lambda(m) \stackrel{\text{def.}}{=} \frac{1}{2} \| R_y - \Lambda(m) \|^2_{\mathrm{L}^2(\mathcal{X}^2)} + \lambda |m|(\mathcal{X}). \tag{$\mathcal{Q}_\lambda(y)$}$$

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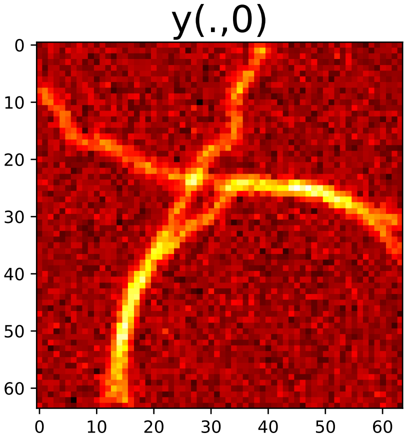
2D numerical results `SOFItool`

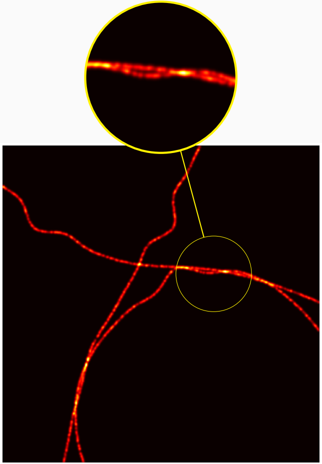
Test on 2D tubulins from ISBI challenge 2016:

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 $\approx 10\,\mathrm{db}$.

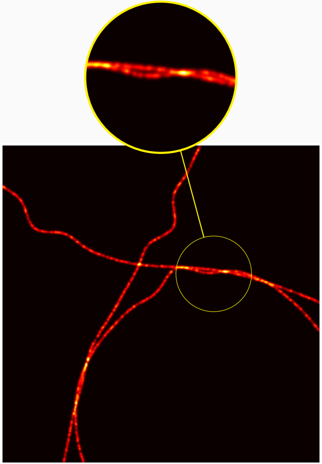


Results



Ground-truth

Results



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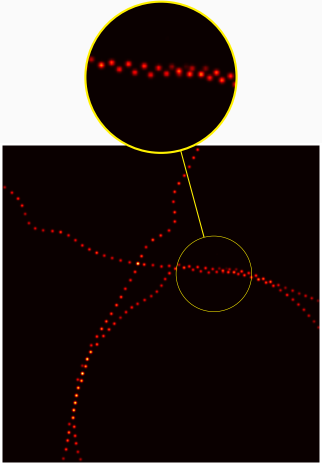

$(\mathcal{Q}_\lambda(y))$ [Laville et al., 2022]

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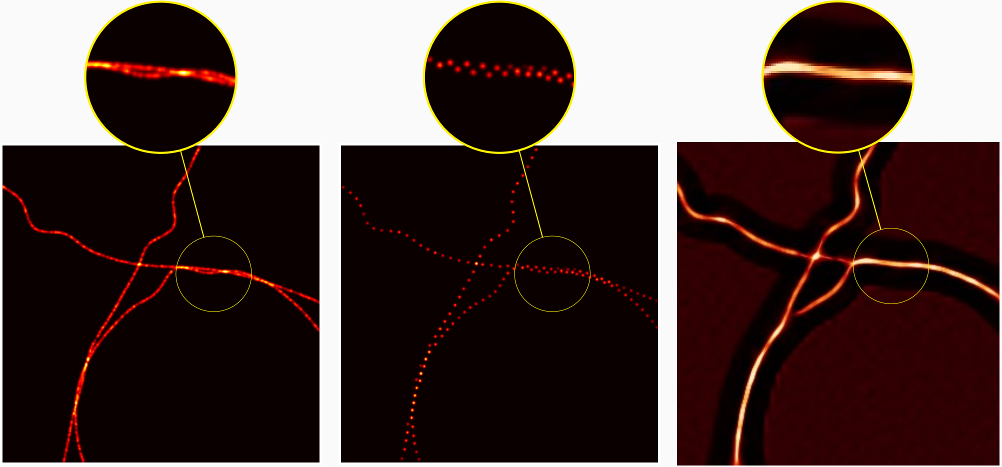

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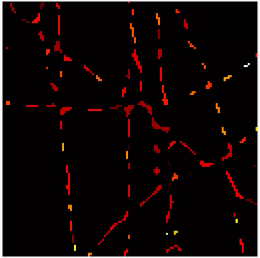
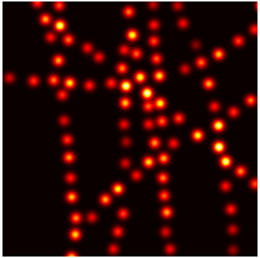
SRRF [Culley et al., 2018]

Partial conclusion



Co$\ell_0$rme [Stergiopoulou et al., 2021]



$(\mathcal{Q}_\lambda(y))$

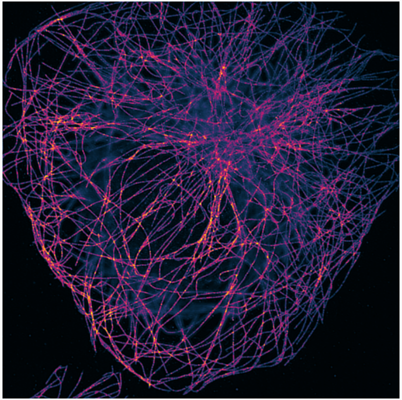
Recap

- a new off-the-grid method for fluctuation microscopy
- the results are a bit dotted, by design.

Practical applications

Biomedical imaging:

- filaments in fluorescence microscopy;



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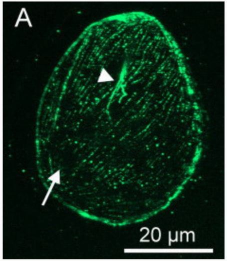

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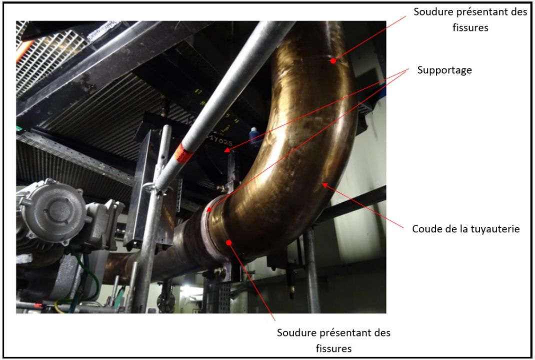
Crackle detection: non-destructive testing on nuclear powerplant pipes, *etc.*



Stress corrosion cracking spotted by *ultrasounds*.

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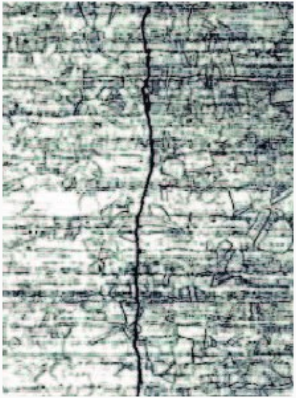

Crackle in the aforementioned pipe.

A new divergence regularisation

2-rectifiable measures reconstruction [de Castro et al., 2021]

- how to model sets measures? Through χ_E where E is a **simple set**, belonging to $\mathrm{BV}(\mathcal{X})$ the set of function of *bounded variation*;

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  One of its minimisers is a sum of level sets χ_E!

Geometry encoded in off-the-grid

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	0D
Geometry	Spikes
Space	$\mathcal{M}\left(\mathcal{X}\right)$
Regulariser	$\left\|\cdot\right\|_{\mathrm{TV}}$

$$\delta_x$$

Geometry encoded in off-the-grid

	0D	2D
Geometry	Spikes	Sets
Space	$\mathcal{M}(\mathcal{X})$	$\mathrm{BV}(\mathcal{X})$
Regulariser	$\|\cdot\|_{\mathrm{TV}}$	$\|\cdot\|_1 + \|\mathrm{D}\cdot\|_{\mathrm{TV}}$

δ_x

χ_E

Geometry encoded in off-the-grid

	0D	1D	2D
Geometry	Spikes	Curves	Sets
Space	$\mathcal{M}(\mathcal{X})$	?	$\mathrm{BV}(\mathcal{X})$
Regulariser	$\lVert\cdot\rVert_{\mathrm{TV}}$	?	$\lVert\cdot\rVert_1 + \lVert \mathrm{D}\cdot\rVert_{\mathrm{TV}}$

δ_x ? χ_E

Desperate times call for desperate measures

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$$\forall \boldsymbol{g} \in \mathbf{C_0}(\boldsymbol{\mathcal{X}})^{\mathbf{2}}, \quad \langle \boldsymbol{\mu}_\gamma, \boldsymbol{g} \rangle_{\boldsymbol{\mathcal{M}}^{\mathbf{2}}} \stackrel{\text{def.}}{=} \int_0^1 \boldsymbol{g}(\gamma(t)) \cdot \dot{\gamma}(t)\,\mathrm{d}t.$$

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- $\operatorname{div} \boldsymbol{\mu}_\gamma = \delta_{\gamma(0)} - \delta_{\gamma(1)}$.

CROC energy

Consider the variational problem we coined *Curves Represented On Charges*:

$$\underset{\boldsymbol{m}\in\mathscr{V}}{\operatorname{argmin}} \frac{1}{2}\|y-\Phi\,\boldsymbol{m}\|_{\mathcal{H}}^2+\alpha\|\boldsymbol{m}\|_{\mathscr{V}}. \tag{CROC}$$

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- $\frac{1}{2}\|y - \Phi\, \boldsymbol{m}\|_{\mathcal{H}}^2$ is the data-term;

CROC energy

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Do curve measures minimise (CROC)?

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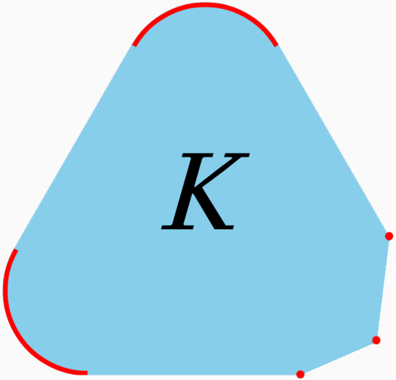

Ext K in red

Link with extreme points: the representer theorem

Let $F : E \to \mathbb{R}^m$, G the data-term, R the regulariser, $\alpha > 0$.

$$F = G + \alpha R$$

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Characterise $\operatorname{Ext} \mathcal{B}_E^1$ of the regulariser $\iff$ outline the structure of a *minimum* of F.

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- If $E = \mathscr{V}$ and $R = \|\cdot\|_{\mathscr{V}}$, then:

$$\mathrm{Ext}(\mathcal{B}_{\mathscr{V}}) = ?$$

Main result

Let the (non-complete) set of curve measures endowed with weak-$*$ topology:

$$\mathfrak{G} \stackrel{\text{def.}}{=} \left\{ \frac{\boldsymbol{\mu_\gamma}}{\|\boldsymbol{\mu_\gamma}\|_{\mathscr{V}}}, \, \gamma \text{ Lipschitz 1-rectifiable simple curve} \right\}.$$

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	0D	1D	2D
Geometry	Spikes	Curves	Sets
Space	$\mathcal{M}(\mathcal{X})$	$\mathscr{V}$	$\mathrm{BV}(\mathcal{X})$
Regulariser	$\lVert\cdot\rVert_{\mathrm{TV}}$	$\lVert\cdot\rVert_{\mathrm{TV}^2} + \lVert \mathrm{div} \cdot\rVert_{\mathrm{TV}}$	$\lVert\cdot\rVert_1 + \lVert \mathrm{D}\cdot\rVert_{\mathrm{TV}}$

Off-the-grid curve numerical reconstruction

General setup in off-the-grid

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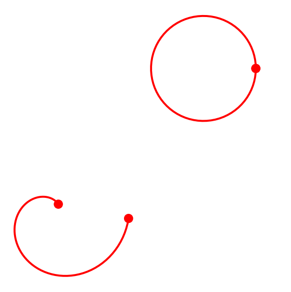
We present the *Charge Sliding Frank-Wolfe* algorithm.

Synthetic problem



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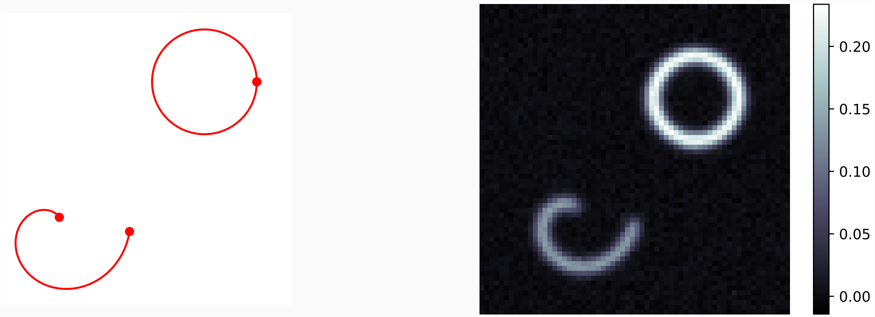

Figure 2: The source and its noisy acquired image I

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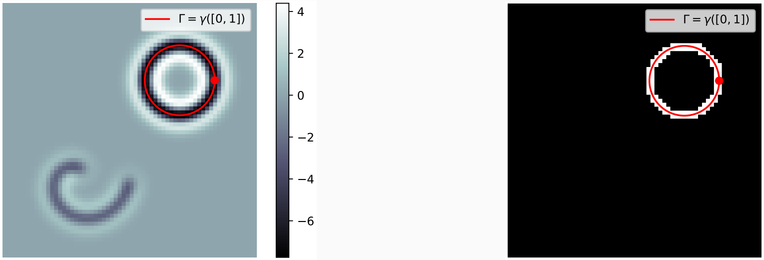

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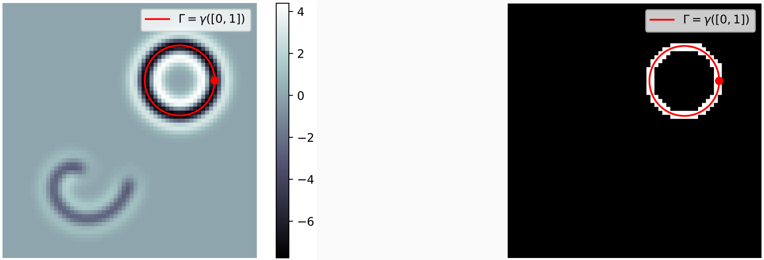

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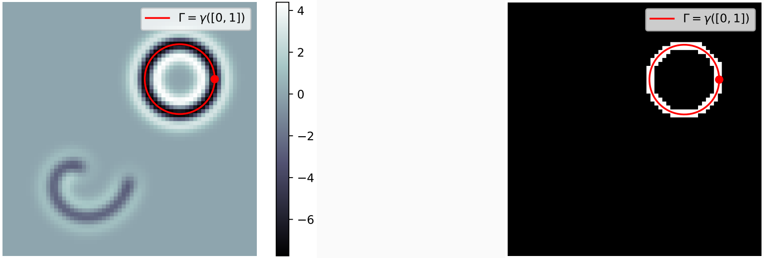

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Amplitude and sliding steps

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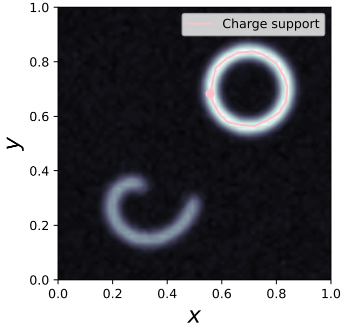

Amplitude optimisation

- we optimise the amplitude a of the new estimated curve;

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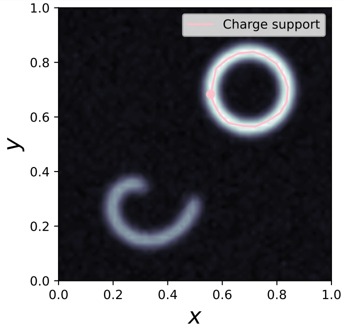

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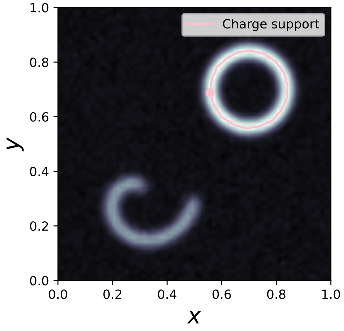

Both amplitude and position optimisation

- we optimise the amplitude a of the new estimated curve;
- we perform a *sliding*: we optimise on both amplitudes a and positions γ.

Recap: iterate the algorithm

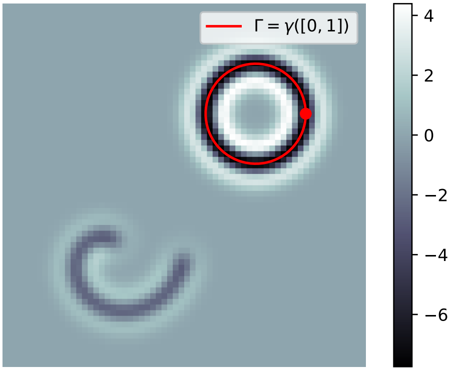

Figure 4: First step of first iteration: certificate and support of new curve estimated

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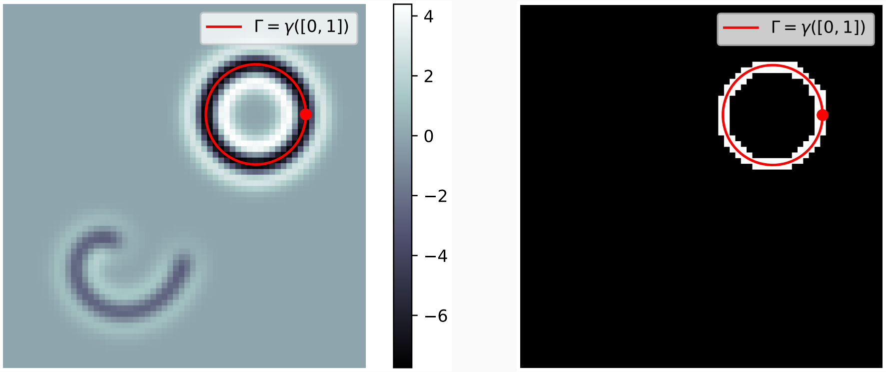

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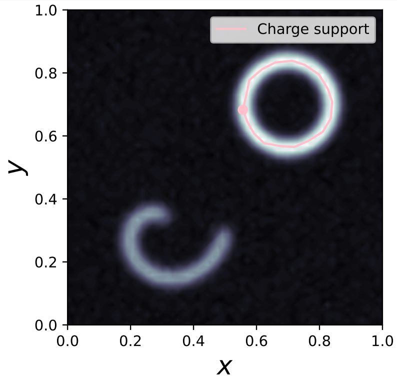

Amplitude optimisation

Figure 4: First iteration: second and third steps

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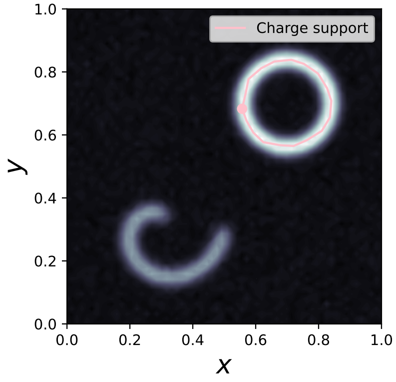

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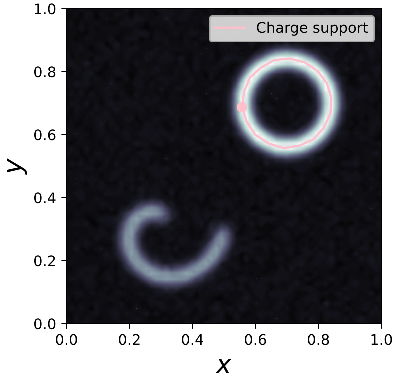

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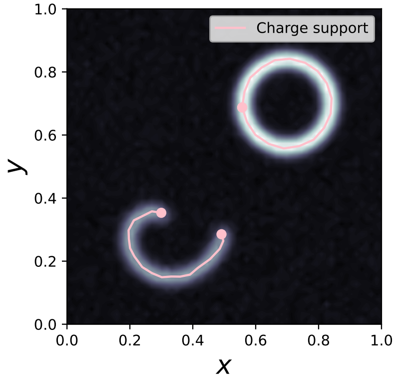

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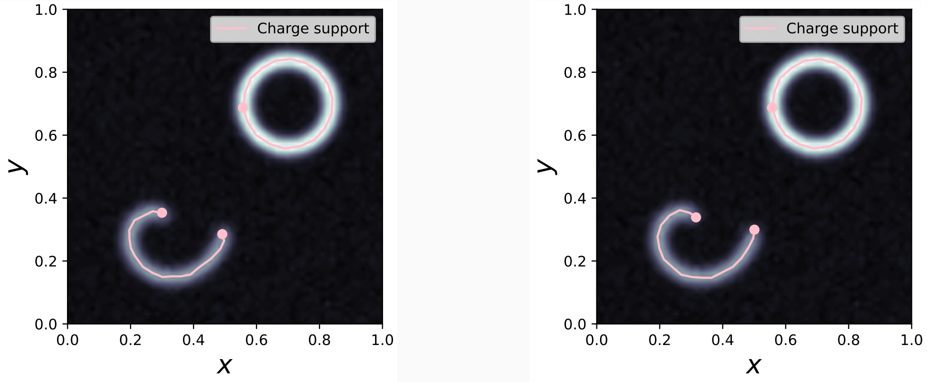

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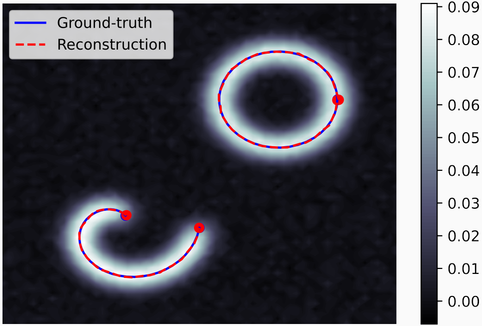

Reconstruction [Laville et al., 2023a].

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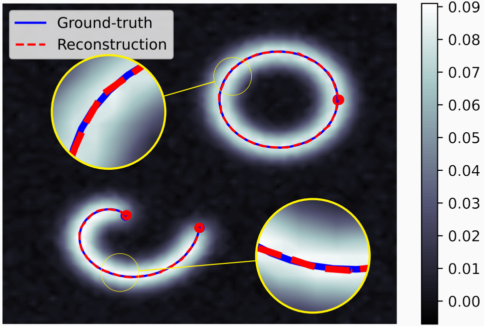

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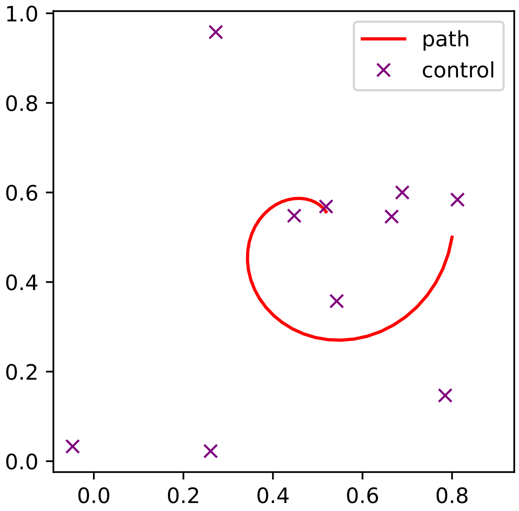

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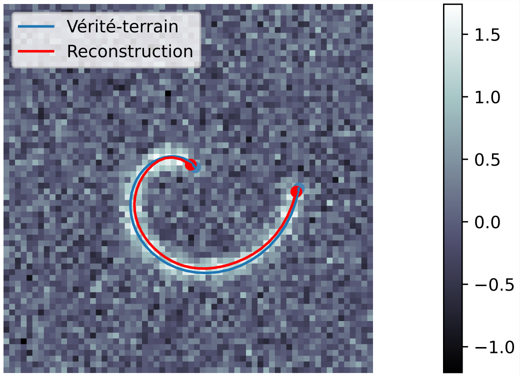
- Pro: always smooth curves. Cons: prone to shortening.



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Still, there is room for improvements:

- define a *scalar* operator, further enabling curve reconstruction in fluctuation microscopy;
- improve the support estimation step;
- tackle the curve crossing issue.

Conclusion

Key points

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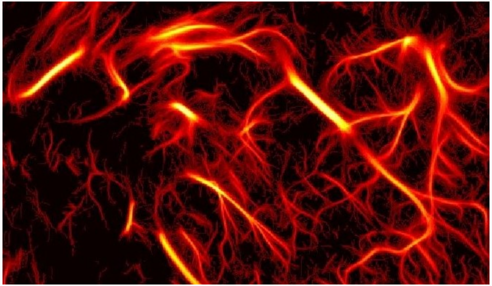
Perspectives

- application on real data images (covariance with Ph.D. Aneva Tsafack, fissures, etc.);



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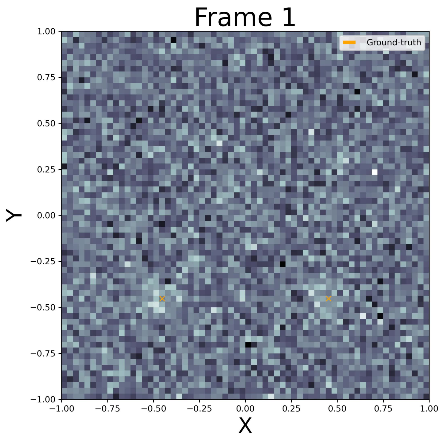

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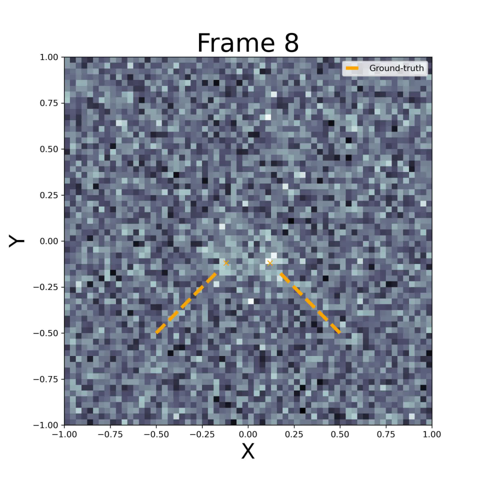

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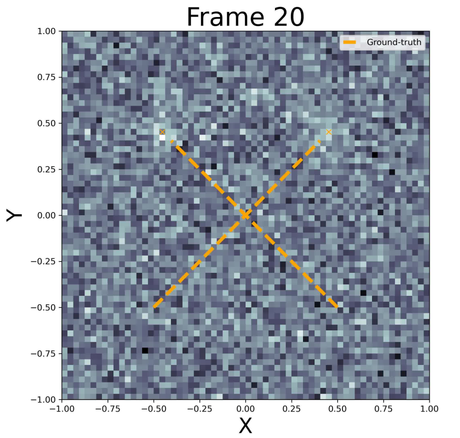

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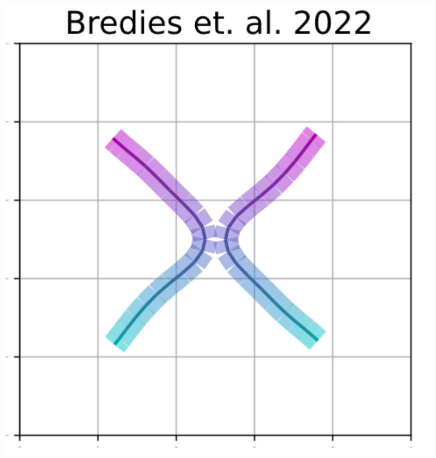

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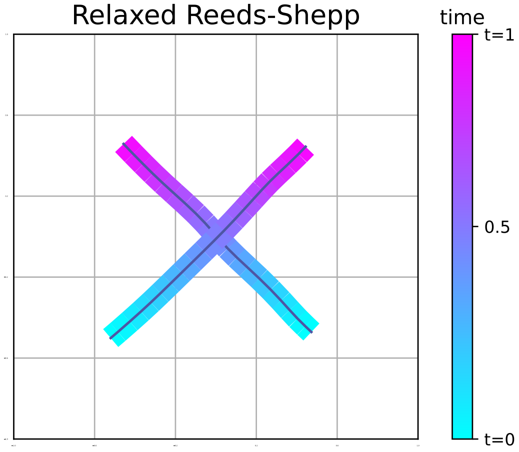

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See our work and papers on

https://www-sop.inria.fr/members/Bastien.Laville/

Proof recipe I

First inclusion:

$$\mathrm{Ext}(\mathcal{B}^1_{\mathscr{V}}) \supset \mathfrak{G}$$

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Let γ a simple Lipschitz curve and μ_γ the measure supported on this curve. By contradiction, let $\boldsymbol{u_1}, \boldsymbol{u_2} \in \mathcal{B}^1_{\mathscr{V}}$ and for $\lambda \in (0,1)$:

$$\frac{\boldsymbol{\mu_\gamma}}{\|\boldsymbol{\mu_\gamma}\|_{\mathscr{V}}} = \lambda \boldsymbol{u_1} + (1-\lambda)\boldsymbol{u_2}.$$

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moreover, each $\boldsymbol{R}$ has *maximal* length implying $\operatorname{spt} \boldsymbol{R} = \operatorname{spt} \mu_\gamma$.

Proof recipe II

$$\operatorname{spt} \boldsymbol{R} = \operatorname{spt} \mu_\gamma.$$

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$$\int_{\mathfrak{G}} \|\boldsymbol{R}\|_{\mathrm{TV}} \,\mathrm{d}\rho(\boldsymbol{R}) < \frac{\|\boldsymbol{\mu}_{\boldsymbol{\gamma}}\|_{\mathrm{TV}}}{\|\boldsymbol{\mu}_{\boldsymbol{\gamma}}\|_{\mathscr{V}}} \underbrace{\rho(\mathfrak{G})}_{=1} = \int_{\mathfrak{G}} \|\boldsymbol{R}\|_{\mathrm{TV}} \,\mathrm{d}\rho(\boldsymbol{R}),$$

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each $\boldsymbol{R}$ is supported on a simple Lipschitz curve $\gamma_{\boldsymbol{R}}$.

Hence, each $\gamma_{\boldsymbol{R}}$ is a reparametrisation of γ yielding $\boldsymbol{R} = \frac{\boldsymbol{\mu}_\gamma}{\|\boldsymbol{\mu}_\gamma\|_{\mathscr{V}}}$, eventually:

$$\boldsymbol{u}_i = \int_{\mathfrak{G}} \boldsymbol{R} \, \mathrm{d}\rho_i = \int_{\mathfrak{G}} \frac{\boldsymbol{\mu}_\gamma}{\|\boldsymbol{\mu}_\gamma\|_{\mathscr{V}}} \, \mathrm{d}\rho_i = \frac{\boldsymbol{\mu}_\gamma}{\|\boldsymbol{\mu}_\gamma\|_{\mathscr{V}}} \underbrace{\rho_i(\mathfrak{G})}_{=1} = \frac{\boldsymbol{\mu}_\gamma}{\|\boldsymbol{\mu}_\gamma\|_{\mathscr{V}}}.$$

Contradiction, then μ_γ is an extreme point.

$\square$

Proof recipe III

Second inclusion:

$$\mathrm{Ext}(\mathcal{B}^1_{\mathscr{V}}) \subset \mathfrak{G}$$

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Let $\boldsymbol{T} \in \mathsf{Ext}(\mathcal{B}^1_{\mathscr{V}})$, then there exists a finite (probability) Borel measure ρ s.t.:

$$\boldsymbol{T} = \int_{\mathfrak{G}} \boldsymbol{R} \, \mathrm{d}\rho(\boldsymbol{R}),$$

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either ρ is supported on a singleton of $\mathfrak{G}$, then there exists μ_γ s.t. $\boldsymbol{T} = \dfrac{\boldsymbol{\mu_\gamma}}{\|\boldsymbol{\mu_\gamma}\|_{\mathscr{V}}}$

or there exists a Borel set $A \subset \mathfrak{G}$ with arbitrary $0 < \rho(A) < 1$ and:

$$\rho = |\rho|(A)\left(\frac{1}{|\rho|(A)}\rho \llcorner A\right) + |\rho|(A^c)\left(\frac{1}{|\rho|(A^c)}\rho \llcorner A^c\right).$$

Proof recipe IV

Then,

$$\boldsymbol{T} = |\rho|(A)\underbrace{\left[\int_{\mathfrak{G}} \frac{1}{|\rho|(A)}\boldsymbol{R}\,\mathrm{d}(\rho \llcorner A)(\boldsymbol{R})\right]}_{\overset{\text{def.}}{=}\boldsymbol{u_1}} + |\rho|(A^c)\underbrace{\left[\int_{\mathfrak{G}} \frac{1}{|\rho|(A^c)}\boldsymbol{R}\,\mathrm{d}(\rho \llcorner A^c)(\boldsymbol{R})\right]}_{\overset{\text{def.}}{=}\boldsymbol{u_2}}$$

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A is chosen (up to a neighbourhood) as a convex set, hence $\boldsymbol{u_1} = \int_A \boldsymbol{R}\,\mathrm{d}\rho(\boldsymbol{R})$ belongs to A, while conversely $\boldsymbol{u_2} \in A^c$, thus $\boldsymbol{u_1} \neq \boldsymbol{u_2}$.

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A **is chosen (up to a neighbourhood) as a convex set, hence** $\boldsymbol{u_1} = \int_A \boldsymbol{R}\,\mathrm{d}\rho(\boldsymbol{R})$ **belongs to** A**, while conversely** $\boldsymbol{u_2} \in A^c$**, thus** $\boldsymbol{u_1} \neq \boldsymbol{u_2}$**. Eventually, thanks to Smirnov's decomposition:**

$$\begin{aligned} \|\boldsymbol{u_1}\|_{\mathscr{V}} &\leq \int_{\mathfrak{G}} \frac{1}{|\rho|(A)} \underbrace{\|\boldsymbol{R}\|_{\mathscr{V}}}_{=1} \mathrm{d}(\rho \llcorner A)(\boldsymbol{R}) \\ &\leq \frac{|\rho|(A)}{|\rho|(A)} = 1. \end{aligned}$$

Proof recipe V

Then $\boldsymbol{u_1}, \boldsymbol{u_2} \in \mathcal{B}^1_{\mathscr{V}}$ while $\boldsymbol{u_1} \neq \boldsymbol{u_2}$, thus reaching a non-trivial convex combination:

$$\boldsymbol{T} = \lambda \boldsymbol{u_1} + (1 - \lambda) \boldsymbol{u_2},$$

Proof recipe V

Then $\boldsymbol{u_1}, \boldsymbol{u_2} \in \mathcal{B}^1_{\mathscr{V}}$ while $\boldsymbol{u_1} \neq \boldsymbol{u_2}$, thus reaching a non-trivial convex combination:

$$\boldsymbol{T} = \lambda \boldsymbol{u_1} + (1 - \lambda)\boldsymbol{u_2},$$

thereby reaching a contradiction, and therefore concluding the proof.

$\square$