

Automated data-driven inverse problem resolution:  
Applications in microfluidics and epidemiology

**Barbara Pascal**, [bpascal-fr.github.io](https://github.com/bpascal)

Joint work with Patrice Abry, Nelly Pustelnik, Valérie Vidal, and Samuel Vaiter

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**AI WILD West**, Rennes, France

## Observation model

$$\mathbf{y} \sim \mathcal{B}(\Phi \bar{\mathbf{x}})$$

- $\mathbf{y} \in \mathbb{R}^P$ : degraded observations;
- $\bar{\mathbf{x}} \in \mathbb{R}^N$ : unknown quantity of interest;
- $\Phi : \mathbb{R}^N \rightarrow \mathbb{R}^P$ : known deformation;
- $\mathcal{B}$ : random measurement noise.

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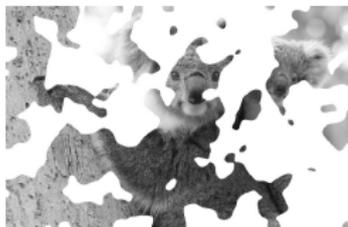
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► ill-conditioned, rank deficient  $\Phi$

Inpainting



(Guillemot et al., 2013, *IEEE Sig. Process. Mag.*)

Super-resolution



(Marquina et al., 2008, *J. Sci. Comput.*)

Deblurring



(Pan, 2016, *IEEE Trans. Pattern Anal. Mach. Intell.*)

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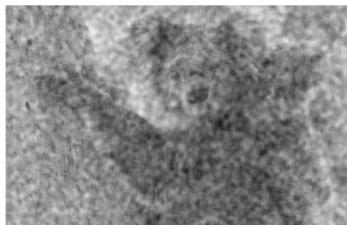
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- ▶ ill-conditioned, rank deficient  $\Phi$
- ▶ correlated, data-dependent  $\mathcal{B}$

Correlated



(Pascal et al., 2021, *J. Math. Imaging Vis.*)

Data-dependent



(Luisier et al., 2010, *IEEE Trans. Image Process.*)

Multiplicative



(Shama, 2016, *Appl. Math. Comput.*)

# The variational framework: penalized log-likelihood

## Variational estimator

$$\hat{\mathbf{x}}(\mathbf{y}; \lambda) \in \underset{\mathbf{x} \in \mathbb{R}^N}{\text{Argmin}} \mathcal{D}(\mathbf{y}, \Phi \mathbf{x})$$

- $\mathcal{D}(\mathbf{y}; \cdot) = -\log \mathbb{P}(\mathbf{y}|\cdot)$ : negative log-likelihood

$$\text{Ex: } \mathcal{D}(\mathbf{y}; \mathbf{x}) = \|\mathbf{y} - \mathbf{x}\|_2^2$$

No regularization



$$\mathcal{R} = 0$$

# The variational framework: penalized log-likelihood

## Variational estimator

$$\hat{\mathbf{x}}(\mathbf{y}; \lambda) \in \underset{\mathbf{x} \in \mathbb{R}^N}{\text{Argmin}} \mathcal{D}(\mathbf{y}, \Phi \mathbf{x}) + \lambda \mathcal{R}(\mathbf{x})$$

- $\mathcal{D}(\mathbf{y}; \cdot) = -\log \mathbb{P}(\mathbf{y}|\cdot)$ : negative log-likelihood
- $\mathcal{R}$ : regularization term encoding a priori knowledge

$$\text{Ex: } \mathcal{D}(\mathbf{y}; \mathbf{x}) = \|\mathbf{y} - \mathbf{x}\|_2^2$$

$$\text{Ex: } \mathcal{R}(\mathbf{x}) = \|\mathbf{D}_1 \mathbf{x}\|_q^q$$

(Giovannelli & Idier, 2015, *Wiley*)

No regularization



$$\mathcal{R} = 0$$

Smooth



$$\mathcal{R}(\mathbf{x}) = \|\mathbf{D}_1 \mathbf{x}\|_2^2$$

(Tikhonov et al., 1977, *Wiley*)

Piecewise constant



$$\mathcal{R}(\mathbf{x}) = \|\mathbf{D}_1 \mathbf{x}\|_1$$

(Rudin et al., 1992, *Physica D*)

## Fine-tuning of the regularization parameter

**Example:**  $\hat{\mathbf{x}}(\mathbf{y}; \lambda) \in \underset{\mathbf{x} \in \mathbb{R}^N}{\text{Argmin}} \|\mathbf{y} - \mathbf{x}\|_2^2 + \lambda \|\mathbf{D}_1 \mathbf{x}\|_2^2$  (Tikhonov)

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too regularized

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# Hyperparameter selection: bilevel optimization

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$$\lambda^\dagger \in \underset{\lambda \in \Lambda}{\text{Argmin}} \mathcal{O}(\mathbf{y}; \lambda)$$

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- golden case:  $\mathcal{O}(\mathbf{y}; \lambda) = \|\hat{\mathbf{x}}(\mathbf{y}; \lambda) - \bar{\mathbf{x}}\|^2 \implies$  efficient bi-level  $(\mathbf{x}, \lambda)$  minimization

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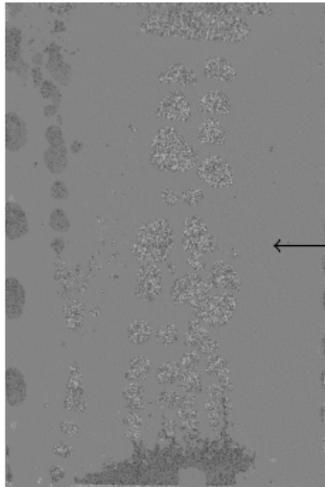
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- practical case: ground truth  $\bar{\mathbf{x}}$  **not available!**  $\implies$  data-driven  $\mathcal{O}(\mathbf{y}; \lambda)$

Image processing:

Texture segmentation

# Multiphase flow through porous media

Laboratoire de Physique, ENS Lyon, V. Vidal, T. Busser, (M. Serres, IFPEN)

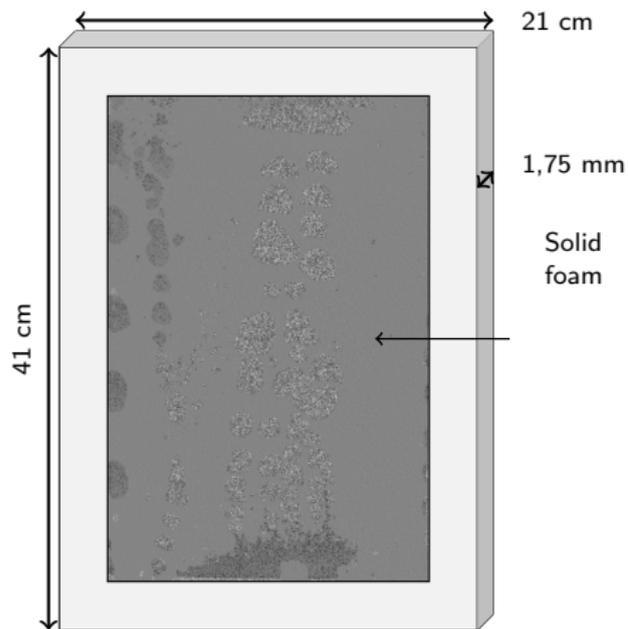


Solid  
foam



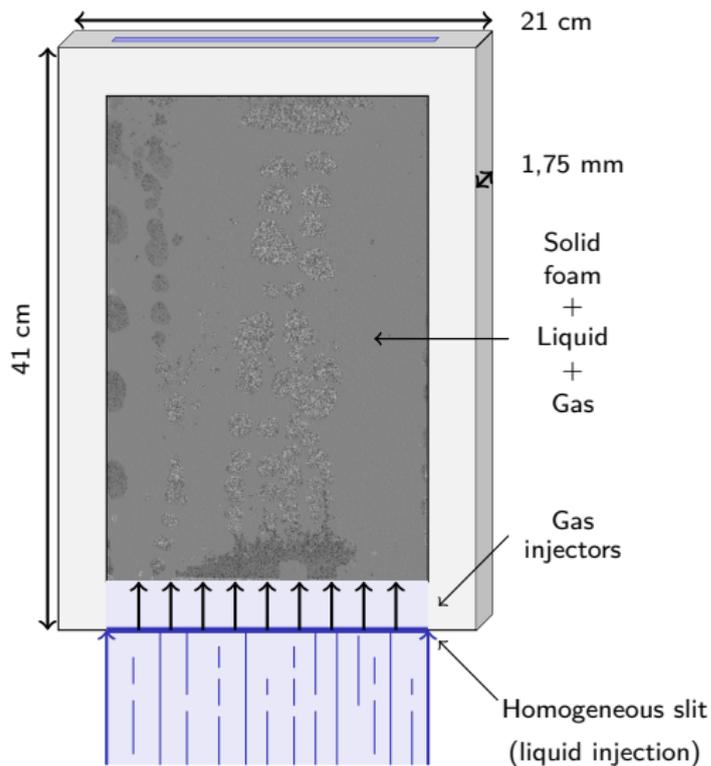
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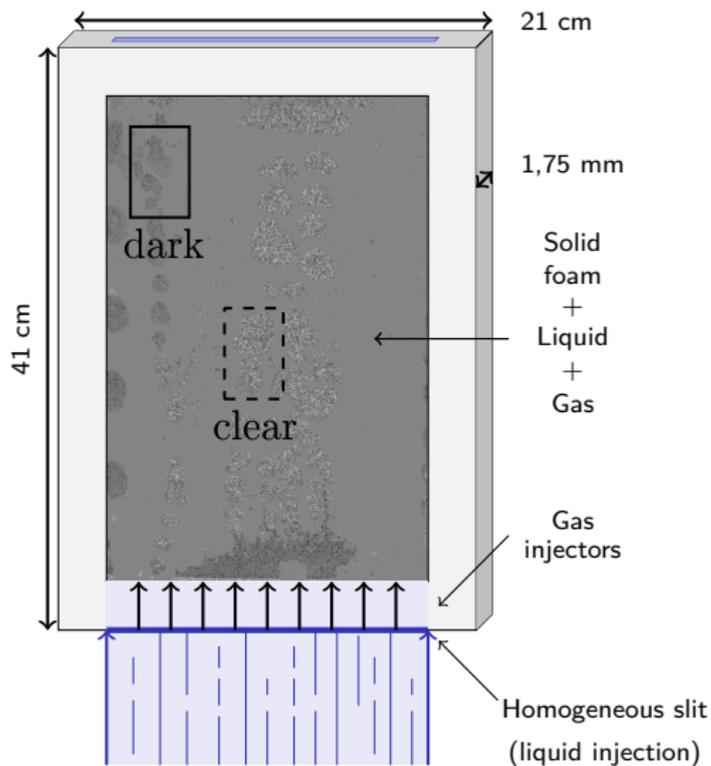
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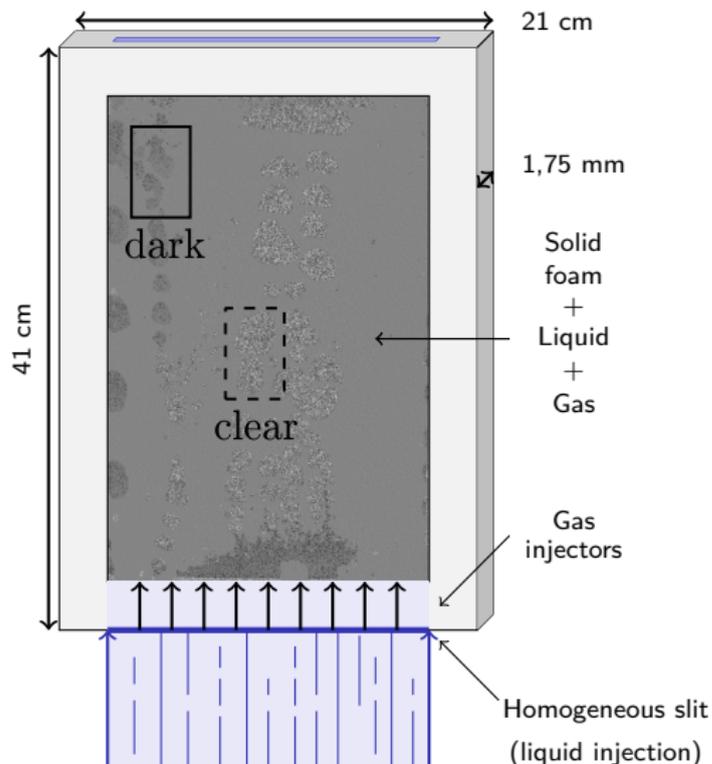
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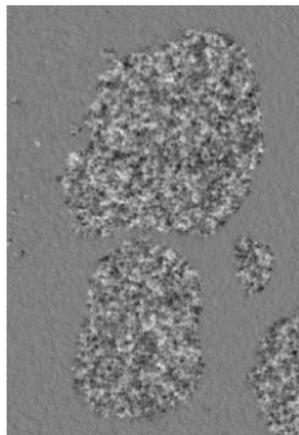


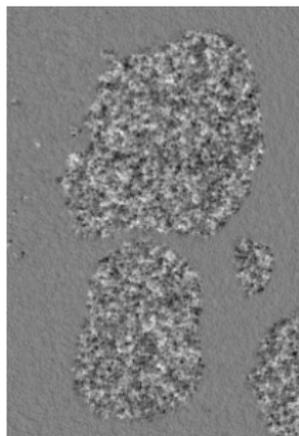
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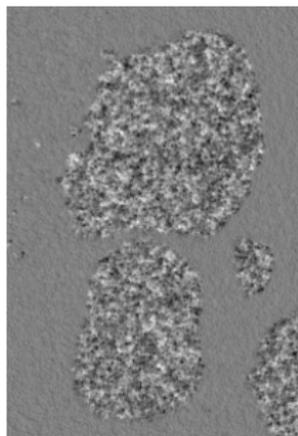
- $1600 \times 1100$  pixels
- video:  $\sim 1000$  images
- phase diagram:  $\sim 10$  flow rates





**Goal:** obtain a partition of the image into  $K$  homogeneous textures

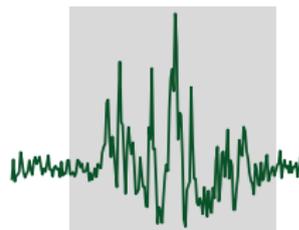
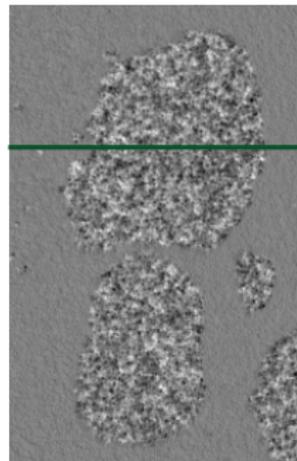
$$\Omega = \Omega_1 \sqcup \dots \sqcup \Omega_K$$



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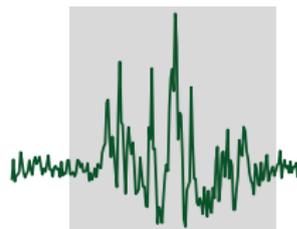
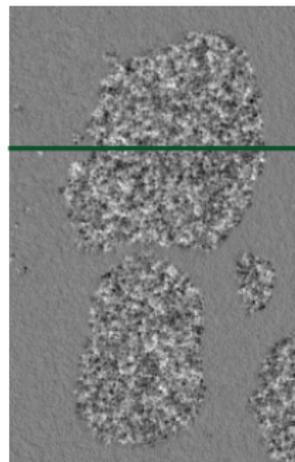
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# Piecewise monofractal model



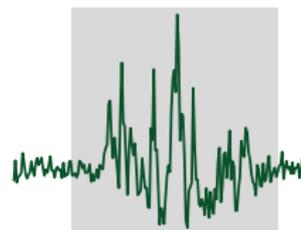
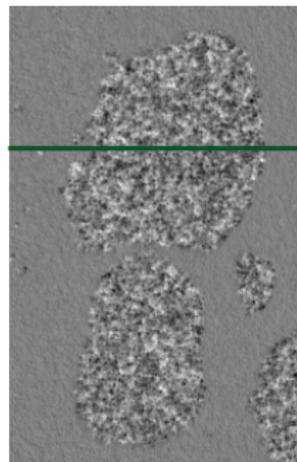
## Fractal attributes

- variance  $\sigma^2$      *amplitude of variations*



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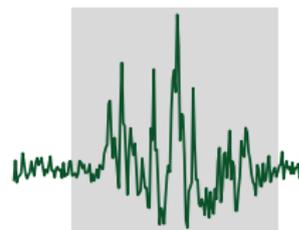
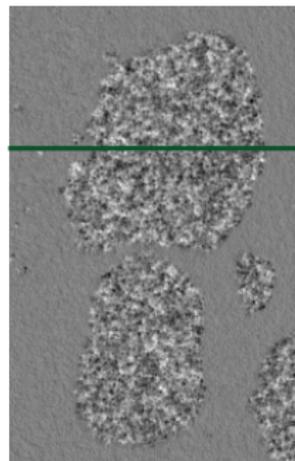
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$$|f(x) - f(y)| \leq \sigma(x)|x - y|^{h(x)}$$



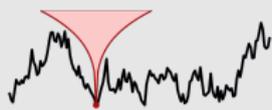
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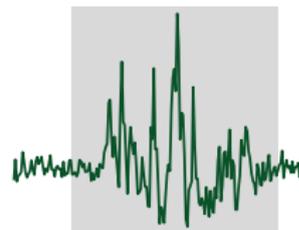
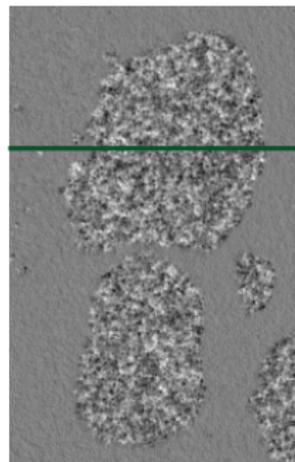
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$$h(x) \equiv h_1 = 0.9$$



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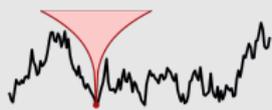
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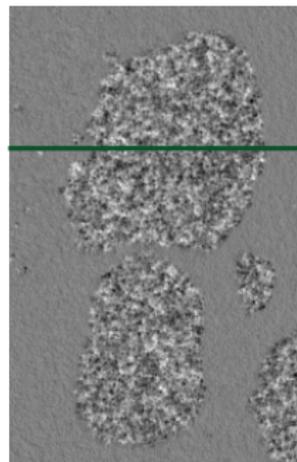
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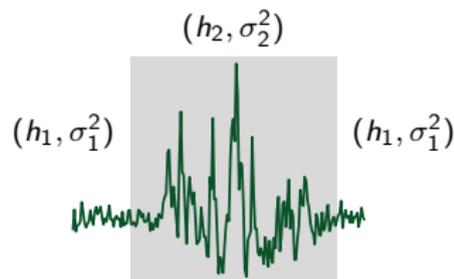


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## Segmentation

- ▶  $\sigma^2$  and  $h$  piecewise constant



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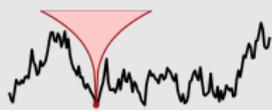
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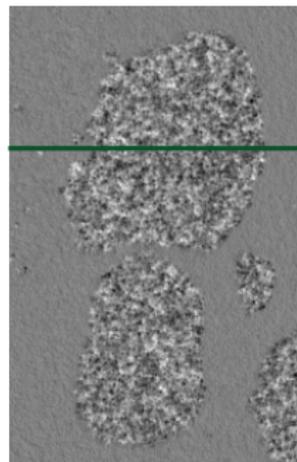
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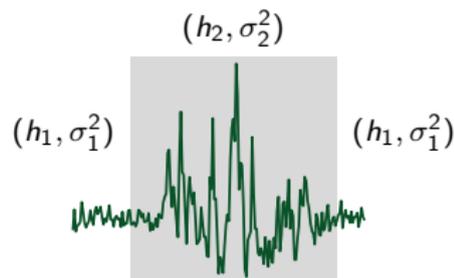


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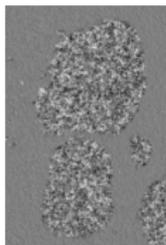


## Segmentation

- ▶  $\sigma^2$  and  $h$  piecewise constant
- ▶ region  $\Omega_k$  characterized by  $(\sigma_k^2, h_k)$



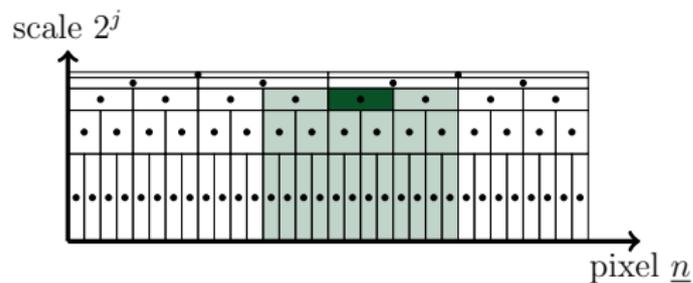
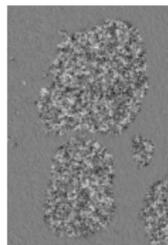
Textured image



# Multiscale analysis

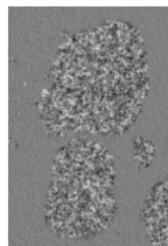
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Local maximum of wavelet coefficients:  $\mathcal{L}_a$ .



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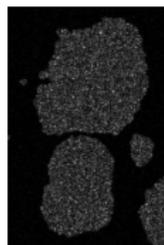
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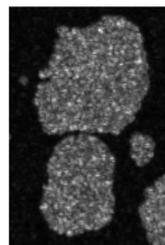
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Scale

$a = 2^1$

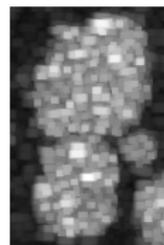


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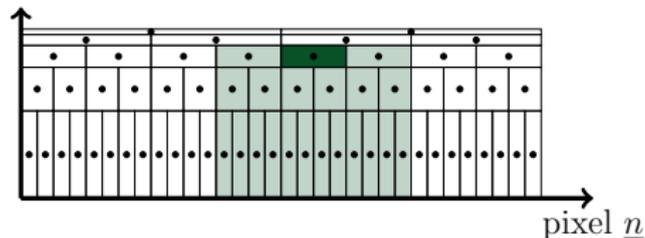


...

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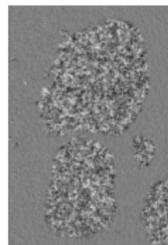


scale  $2^j$



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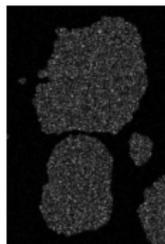
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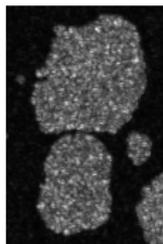
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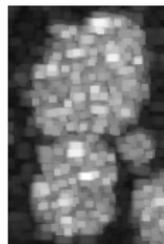


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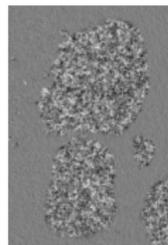


Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

$$\log(\mathcal{L}_{a,\cdot}) \underset{a \rightarrow 0}{\simeq} \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\substack{\propto \log(\sigma^2) \\ \text{(variance)}}}{\mathbf{v}}$$

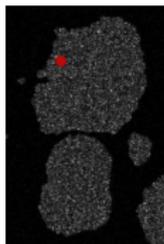
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Textured image

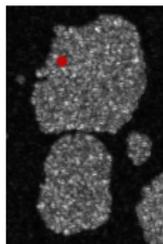


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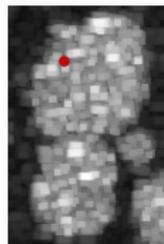


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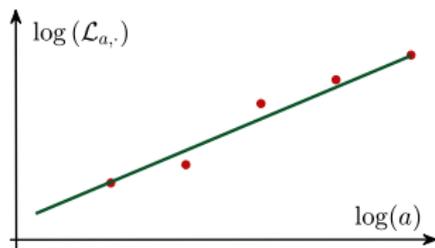
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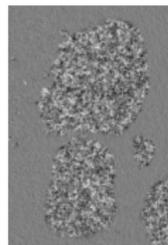
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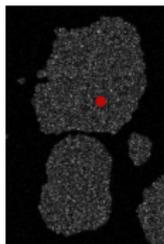
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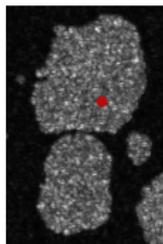
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Local maximum of wavelet coefficients:  $\mathcal{L}_a$ .

$a = 2^1$

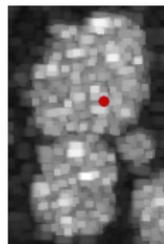


$a = 2^2$



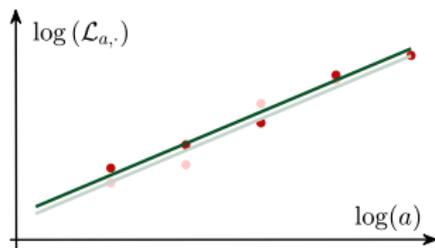
...

$a = 2^5$



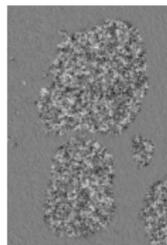
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

$$\log(\mathcal{L}_a) \underset{a \rightarrow 0}{\simeq} \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\substack{\propto \log(\sigma^2) \\ \text{(variance)}}}{\mathbf{v}}$$



# Multiscale analysis

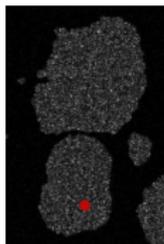
Textured image



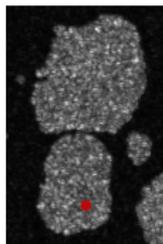
Scale

Local maximum of wavelet coefficients:  $\mathcal{L}_a$ .

$a = 2^1$

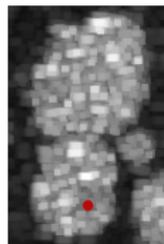


$a = 2^2$



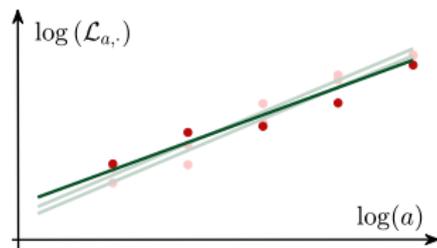
...

$a = 2^5$



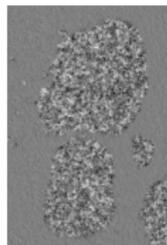
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# Multiscale analysis

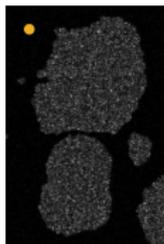
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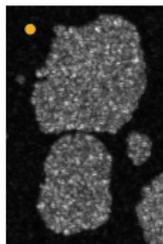
Scale

Local maximum of wavelet coefficients:  $\mathcal{L}_a$ .

$a = 2^1$

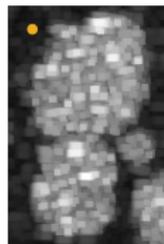


$a = 2^2$



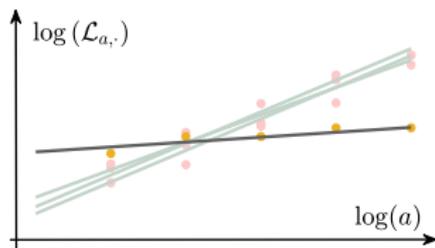
...

$a = 2^5$



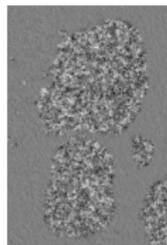
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$$\log(\mathcal{L}_{a,\cdot}) \underset{a \rightarrow 0}{\simeq} \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\substack{\propto \log(\sigma^2) \\ \text{(variance)}}}{\mathbf{v}}$$



# Multiscale analysis

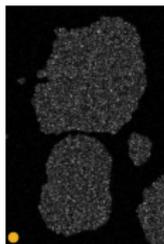
Textured image



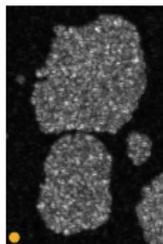
Scale

Local maximum of wavelet coefficients:  $\mathcal{L}_a$ .

$a = 2^1$

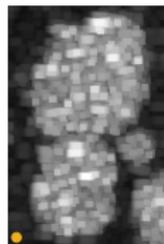


$a = 2^2$



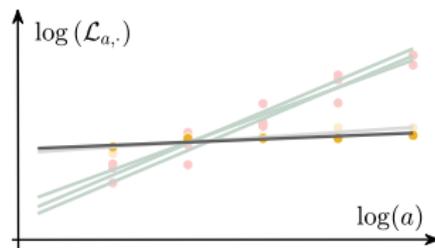
...

$a = 2^5$



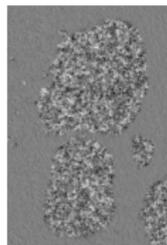
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# Multiscale analysis

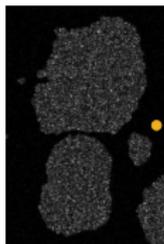
Textured image



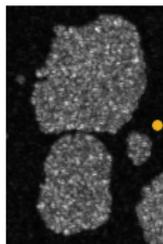
Scale

Local maximum of wavelet coefficients:  $\mathcal{L}_{a,\cdot}$

$a = 2^1$

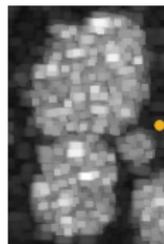


$a = 2^2$



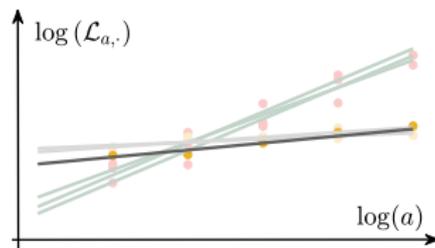
...

$a = 2^5$



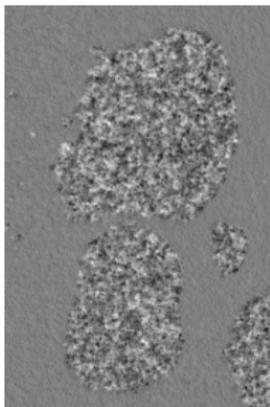
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**Linear regression**      $\log(\mathcal{L}_{a,\cdot}) \simeq \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\propto \log(\sigma^2)}{\mathbf{v}}$

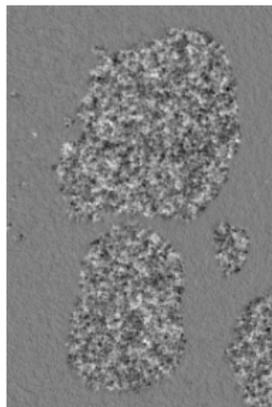
Textured image



**Linear regression**  $\log(\mathcal{L}_{a,\cdot}) \simeq \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\propto \log(\sigma^2)}{\mathbf{v}}$

$$\left( \hat{\mathbf{h}}^{\text{LR}}, \hat{\mathbf{v}}^{\text{LR}} \right) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_{a=a_{\min}}^{a_{\max}} \|\log(\mathcal{L}_{a,\cdot}) - \log(a)\mathbf{h} - \mathbf{v}\|^2$$

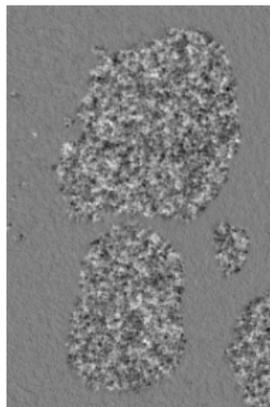
Textured image



**Linear regression**  $\log(\mathcal{L}_{a,\cdot}) \simeq \log(a) \underset{\text{regularity}}{\mathbf{h}} + \underset{\propto \log(\sigma^2)}{\mathbf{v}}$

$$\left(\widehat{\mathbf{h}}^{\text{LR}}, \widehat{\mathbf{v}}^{\text{LR}}\right) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_{a=a_{\min}}^{a_{\max}} \|\log(\mathcal{L}_{a,\cdot}) - \log(a)\mathbf{h} - \mathbf{v}\|^2$$

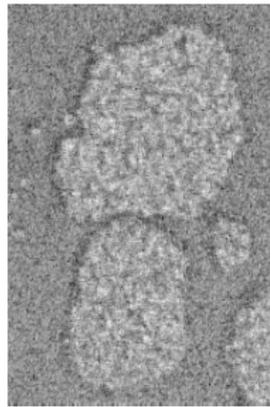
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Local regularity  $\widehat{\mathbf{h}}^{\text{LR}}$



Local power  $\widehat{\mathbf{v}}^{\text{LR}}$

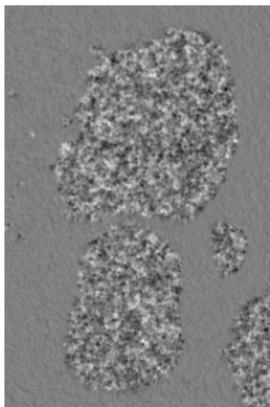


# Direct punctual estimation

**Linear regression**  $\frac{\mathbb{E} \log(\mathcal{L}_{a,\cdot})}{\text{expected value}} = \log(a) \underset{\text{regularity}}{\bar{\mathbf{h}}} + \underset{\propto \log(\sigma^2)}{\bar{\mathbf{v}}}$

$$\left( \hat{\mathbf{h}}^{\text{LR}}, \hat{\mathbf{v}}^{\text{LR}} \right) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_{a=a_{\min}}^{a_{\max}} \|\log(\mathcal{L}_{a,\cdot}) - \log(a)\mathbf{h} - \mathbf{v}\|^2$$

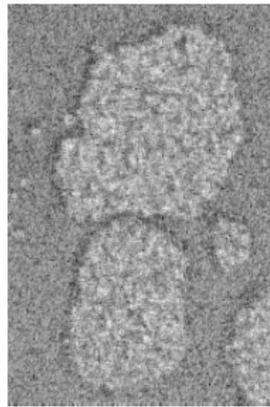
Textured image



Local regularity  $\hat{\mathbf{h}}^{\text{LR}}$



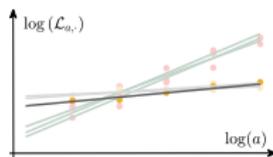
Local power  $\hat{\mathbf{v}}^{\text{LR}}$



→ large estimation variance

$$\sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}}$$

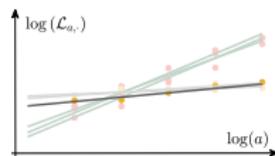
→ fidelity to the log-linear model



# Functionals with either free or co-localized contours

$$\sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}} + \lambda \frac{Q(\mathbf{D}_1\mathbf{h}, \mathbf{D}_1\mathbf{v}; \alpha)}{\text{Total Variation}}$$

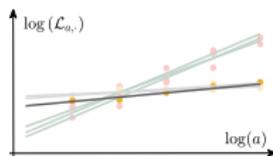
→ fidelity to the log-linear model      → favors piecewise constancy



# Functionals with either free or co-localized contours

$$\underset{h, v}{\text{minimize}} \quad \sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)h - v\|^2}{\text{Least-Squares}} + \lambda \frac{Q(\mathbf{D}_1 h, \mathbf{D}_1 v; \alpha)}{\text{Total Variation}}$$

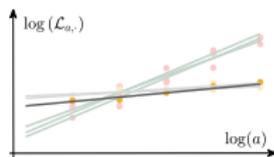
$\rightarrow$  fidelity to the log-linear model  $\rightarrow$  favors piecewise constancy



# Functionals with either free or co-localized contours

$$\underset{h, v}{\text{minimize}} \sum_a \frac{\|\log \mathcal{L}_{a, \cdot} - \log(a) \mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}} + \lambda \frac{Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)}{\text{Total Variation}}$$

$\rightarrow$  fidelity to the log-linear model                       $\rightarrow$  favors piecewise constancy

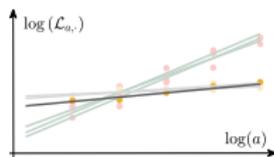


**Finite differences**  $\mathbf{D}_1^{\rightarrow} \mathbf{x}$  (horizontal),  $\mathbf{D}_1^{\uparrow} \mathbf{x}$  (vertical) at each pixel

# Functionals with either free or co-localized contours

$$\underset{\mathbf{h}, \mathbf{v}}{\text{minimize}} \sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}} + \lambda \frac{Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)}{\text{Total Variation}}$$

$\rightarrow$  fidelity to the log-linear model                       $\rightarrow$  favors piecewise constancy



**Finite differences**  $\mathbf{D}_1 \mathbf{x} = [\mathbf{D}_1^{\rightarrow} \mathbf{x}, \mathbf{D}_1^{\uparrow} \mathbf{x}]$

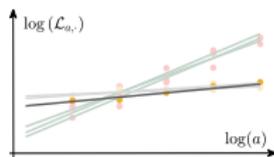
Free:  $\mathbf{h}, \mathbf{v}$  are **independently** piecewise constant

$$Q_F(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha) = \alpha \|\mathbf{D}_1 \mathbf{h}\|_{2,1} + \|\mathbf{D}_1 \mathbf{v}\|_{2,1}$$

# Functionals with either free or co-localized contours

$$\underset{\mathbf{h}, \mathbf{v}}{\text{minimize}} \quad \sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}} + \lambda \frac{\mathcal{Q}(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)}{\text{Total Variation}}$$

$\rightarrow$  fidelity to the log-linear model                       $\rightarrow$  favors piecewise constancy



**Finite differences**  $\mathbf{D}_1 \mathbf{x} = [\mathbf{D}_1^{\rightarrow} \mathbf{x}, \mathbf{D}_1^{\uparrow} \mathbf{x}]$

Free:  $\mathbf{h}, \mathbf{v}$  are **independently** piecewise constant

$$\mathcal{Q}_F(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha) = \alpha \|\mathbf{D}_1 \mathbf{h}\|_{2,1} + \|\mathbf{D}_1 \mathbf{v}\|_{2,1}$$

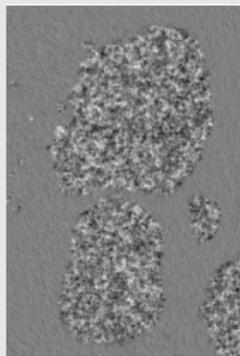
Co-localized:  $\mathbf{h}, \mathbf{v}$  are **concomitantly** piecewise constant

$$\mathcal{Q}_C(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha) = \|[\alpha \mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}]\|_{2,1}$$

## Segmentation *via* iterated thresholding

$$\underset{\mathbf{h}, \mathbf{v}}{\text{minimize}} \quad \sum_a \underbrace{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}_{\text{Least-Squares}} + \lambda \underbrace{Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)}_{\text{Total Variation}}$$

Textured image



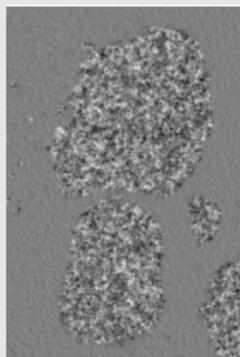
Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$



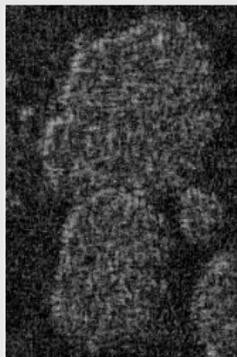
# Segmentation *via* iterated thresholding

$$\underset{\mathbf{h}, \mathbf{v}}{\text{minimize}} \quad \sum_a \frac{\|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2}{\text{Least-Squares}} + \lambda \frac{Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)}{\text{Total Variation}}$$

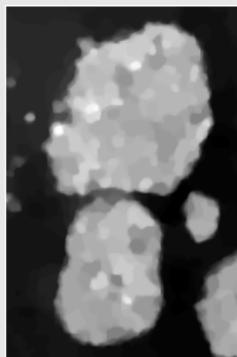
Textured image



Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$



Co-localized  
contours  $\hat{\mathbf{h}}^{\text{C}}$



Threshold  
estimate<sup>†</sup>  $T\hat{\mathbf{h}}^{\text{C}}$



<sup>†</sup>(Cai et al., 2013, *J. Sci. Comput.*)

$$\left(\hat{\mathbf{h}}, \hat{\mathbf{v}}\right) (\mathcal{L}; \lambda, \alpha) = \operatorname{argmin}_{\mathbf{h}, \mathbf{v}} \sum_a \left\| \log \mathcal{L}_{a,\cdot} - \log(a) \mathbf{h} - \mathbf{v} \right\|^2 + \lambda Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

$$(\hat{\mathbf{h}}, \hat{\mathbf{v}})(\mathcal{L}; \lambda, \alpha) = \operatorname{argmin}_{\mathbf{h}, \mathbf{v}} \sum_a \|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2 + \lambda Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$

$(\lambda, \alpha) = (0, 0)$



$$(\hat{\mathbf{h}}, \hat{\mathbf{v}})(\mathcal{L}; \lambda, \alpha) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_a \|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2 + \lambda Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

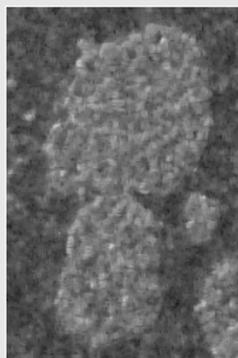
Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$

$(\lambda, \alpha) = (0, 0)$



Co-localized contours estimate  $\hat{\mathbf{h}}^{\text{C}}$

$(\lambda, \alpha) = (0.5, 0.5)$



too small

## Regularization parameters selection

$$(\hat{\mathbf{h}}, \hat{\mathbf{v}})(\mathcal{L}; \lambda, \alpha) = \operatorname{argmin}_{\mathbf{h}, \mathbf{v}} \sum_a \|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2 + \lambda Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

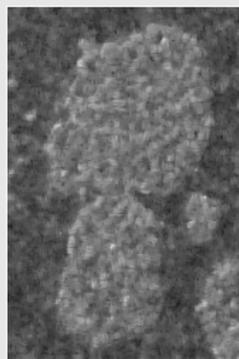
Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$

$(\lambda, \alpha) = (0, 0)$



Co-localized contours estimate  $\hat{\mathbf{h}}^{\text{C}}$

$(\lambda, \alpha) = (0.5, 0.5)$



too small

$(\lambda, \alpha) = (500, 500)$



too large

## Regularization parameters selection

$$(\hat{\mathbf{h}}, \hat{\mathbf{v}})(\mathcal{L}; \lambda, \alpha) = \operatorname{argmin}_{\mathbf{h}, \mathbf{v}} \sum_a \|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2 + \lambda Q(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

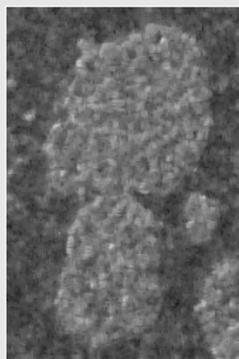
Lin. reg.  $\hat{\mathbf{h}}^{\text{LR}}$

$(\lambda, \alpha) = (0, 0)$



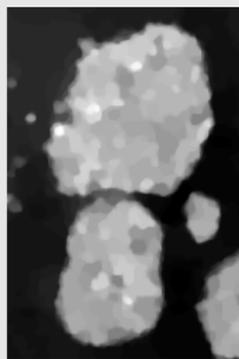
Co-localized contours estimate  $\hat{\mathbf{h}}^{\text{C}}$

$(\lambda, \alpha) = (0.5, 0.5)$



too small

$(\lambda^\dagger, \alpha^\dagger) = (11.5, 0.8)$



optimal

$(\lambda, \alpha) = (500, 500)$



too large

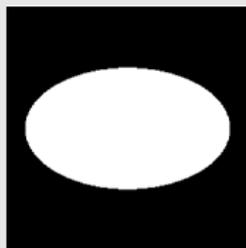
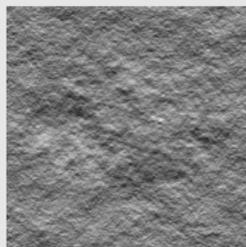
What *optimal* means? How to determine  $\lambda^\dagger$  and  $\alpha^\dagger$ ?

$$\left(\hat{\mathbf{h}}, \hat{\mathbf{v}}\right) (\mathcal{L}; \lambda, \alpha) = \operatorname{argmin}_{\mathbf{h}, \mathbf{v}} \sum_a \|\log \mathcal{L}_{a,\cdot} - \log(a)\mathbf{h} - \mathbf{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

## Parameter tuning (Grid search)

$$\left(\hat{\mathbf{h}}, \hat{\mathbf{v}}\right) (\mathcal{L}; \lambda, \alpha) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_a \|\log \mathcal{L}_{a..} - \log(a) \mathbf{h} - \mathbf{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

Example



## Parameter tuning (Grid search)

$$\left(\hat{\mathbf{h}}, \hat{\mathbf{v}}\right)(\mathcal{L}; \lambda, \alpha) = \underset{\mathbf{h}, \mathbf{v}}{\operatorname{argmin}} \sum_a \left\| \log \mathcal{L}_{a..} - \log(a) \mathbf{h} - \mathbf{v} \right\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1 \mathbf{h}, \mathbf{D}_1 \mathbf{v}; \alpha)$$

$\mathbf{h}$ : discriminant,  $\mathbf{v}$ : auxiliary

$\bar{\mathbf{h}}$ : true regularity

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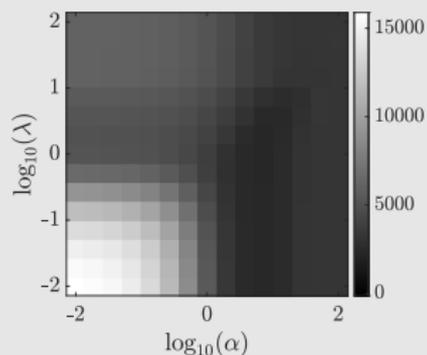
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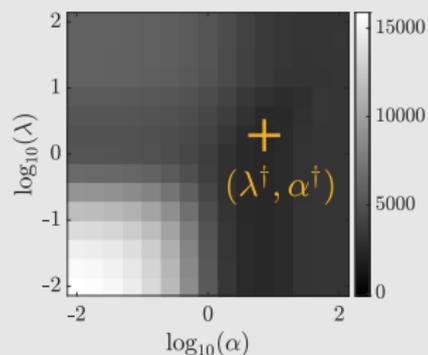
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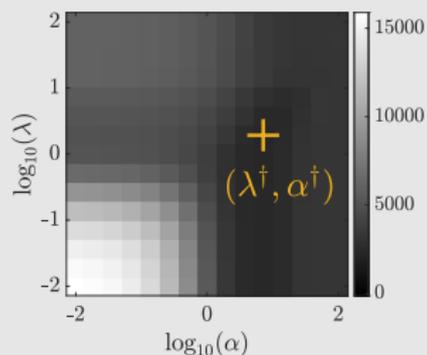
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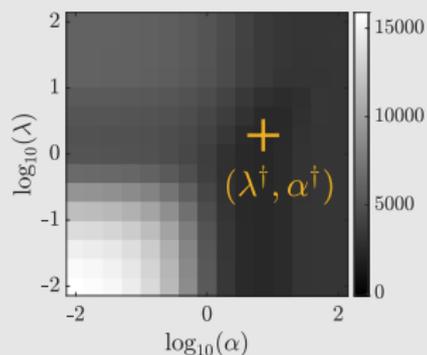
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Stein Unbiased Risk Estimate  
(SURE)

## Stein Unbiased Risk Estimate (Principe)

**Observations**  $\mathbf{y} = \bar{\mathbf{x}} + \boldsymbol{\zeta} \in \mathbb{R}^P$ ,  $\bar{\mathbf{x}}$ : truth and  $\boldsymbol{\zeta} \sim \mathcal{N}(\mathbf{0}, \rho^2 \mathbf{I})$

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**Parametric estimator**  $(\mathbf{y}; \lambda) \mapsto \hat{\mathbf{x}}(\mathbf{y}; \lambda)$

$$\text{Ex. } \hat{\mathbf{x}}(\mathbf{y}; \lambda) = \begin{cases} (\mathbf{I} + \lambda \mathbf{D}^\top \mathbf{D})^{-1} \mathbf{y} & \text{(linear)} \\ \underset{\mathbf{x}}{\operatorname{argmin}} \|\mathbf{y} - \mathbf{x}\|^2 + \lambda \mathcal{Q}(\mathbf{D}\mathbf{x}) & \text{(nonlinear)} \end{cases}$$

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**Theorem** (Stein, 1981, *Ann. Stat.*)

Let  $(\mathbf{y}; \lambda) \mapsto \hat{\mathbf{x}}(\mathbf{y}; \lambda)$  an estimator of  $\bar{\mathbf{x}}$

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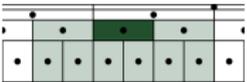
$$\begin{aligned} \hat{R}(\mathbf{y}; \lambda) &\triangleq \|\hat{\mathbf{x}}(\mathbf{y}; \lambda) - \mathbf{y}\|^2 + 2\rho^2 \operatorname{tr}(\partial_{\mathbf{y}} \hat{\mathbf{x}}(\mathbf{y}; \lambda)) - \rho^2 P \\ &\implies R(\lambda) = \mathbb{E}_\zeta [\hat{R}(\mathbf{y}; \lambda)]. \end{aligned}$$

# Generalized Stein Unbiased Risk Estimate

Observations  $\mathbf{y} = \Phi \bar{\mathbf{x}} + \zeta \in \mathbb{R}^P$ ,  $\bar{\mathbf{x}} \in \mathbb{R}^N$ ,  $\Phi : \mathbb{R}^{P \times N}$  and  $\zeta \sim \mathcal{N}(\mathbf{0}, \mathcal{S})$

E.g. the estimators  $\hat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha)$  with free or co-localized contours

$$\log \mathcal{L} = \Phi(\bar{\mathbf{h}}, \bar{\mathbf{v}}) + \zeta \quad \zeta \sim \mathcal{N}(\mathbf{0}, \mathcal{S}) \quad \mathcal{R} = \|\hat{\mathbf{h}} - \bar{\mathbf{h}}\|^2$$

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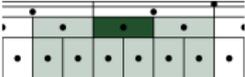
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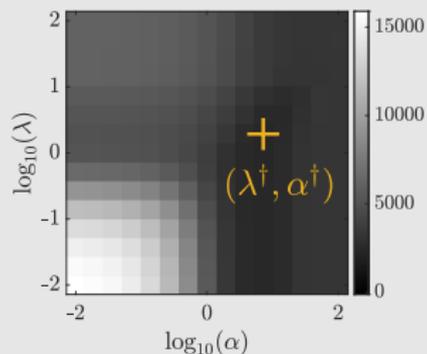
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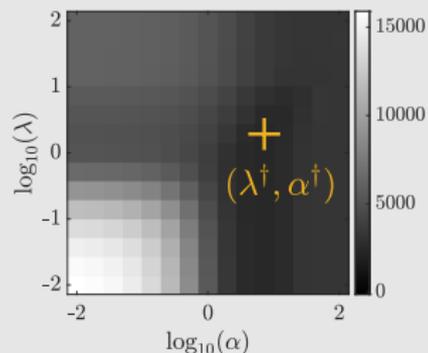
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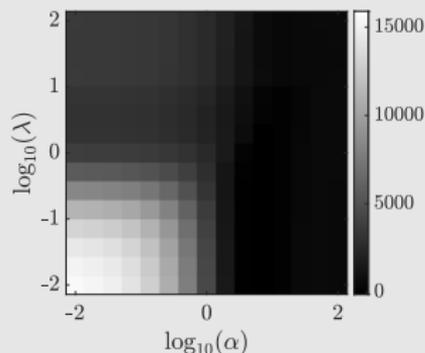
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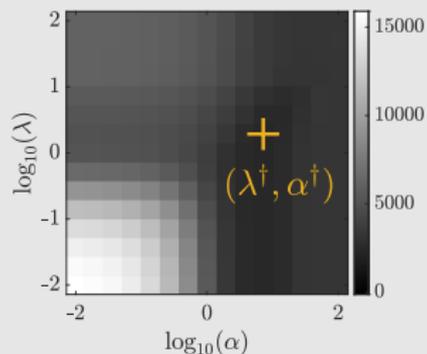


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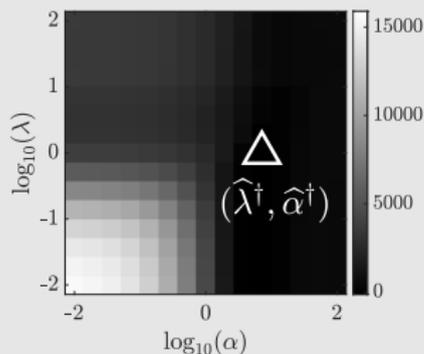
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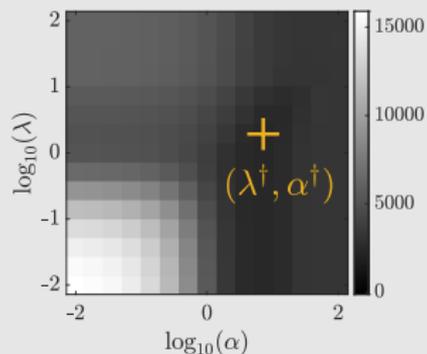


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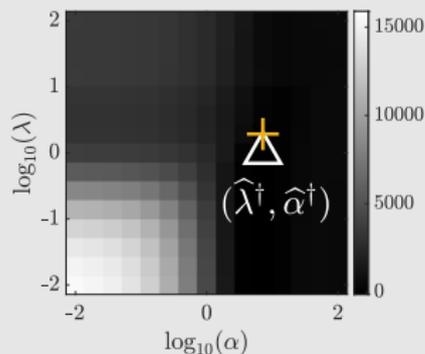
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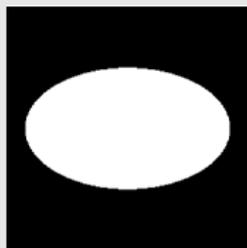
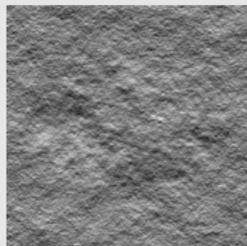
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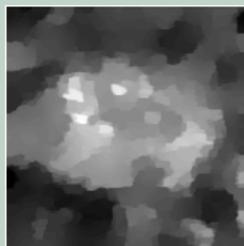
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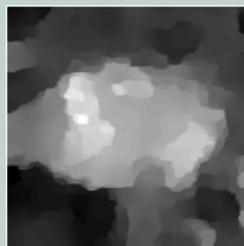
Example



$\hat{\mathbf{h}}^F(\mathcal{L}; \lambda^\dagger, \alpha^\dagger)$   
(grid)

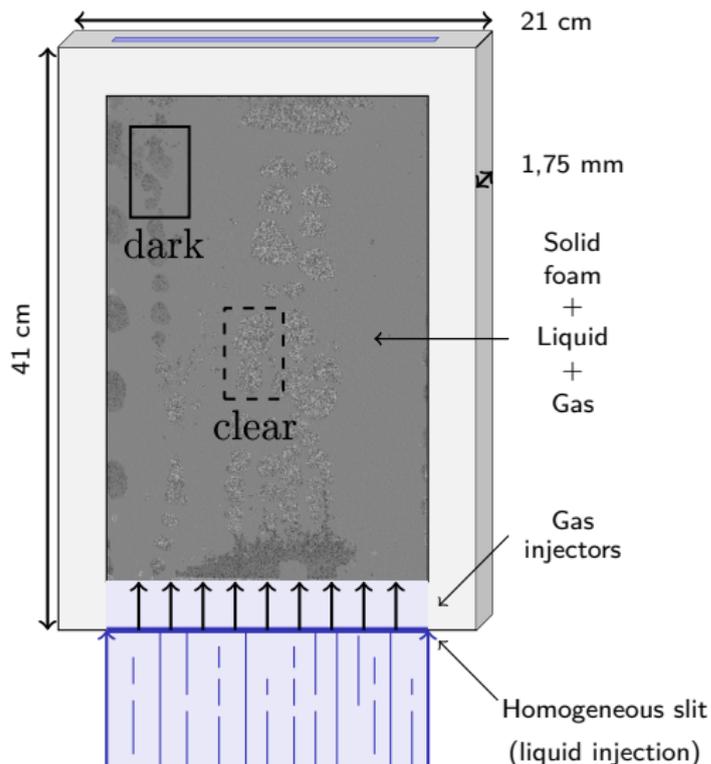


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# Multiphase flow through porous media

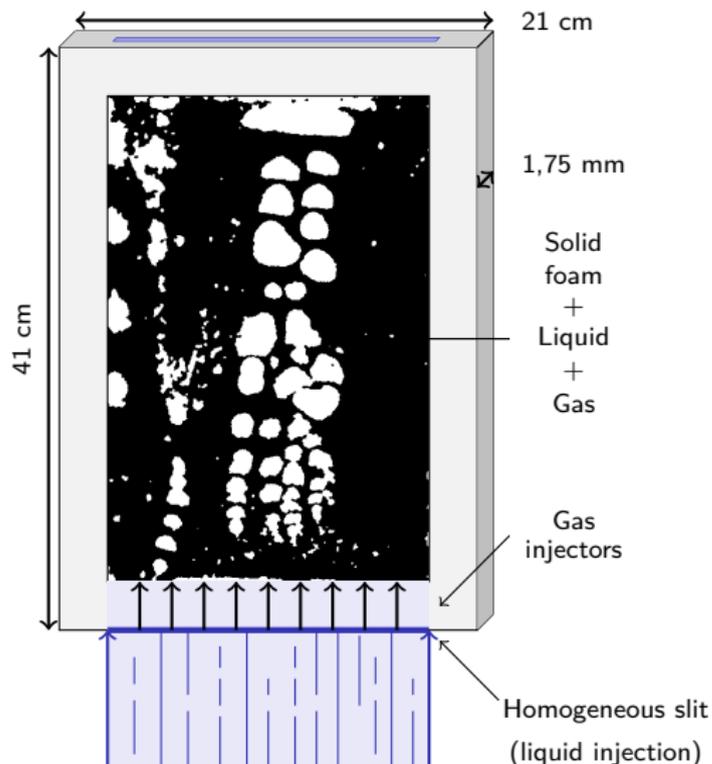
Laboratoire de Physique, ENS Lyon, V. Vidal, T. Busser, (M. Serres, IFPEN)



- 1600 × 1100 pixels
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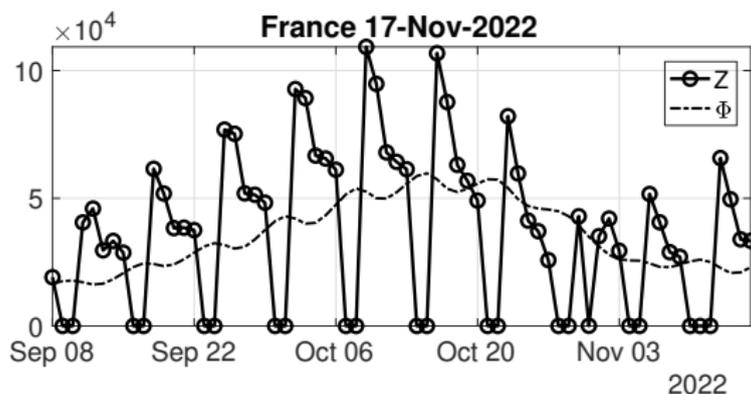


- $1600 \times 1100$  pixels
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Time series analysis:

Epidemiological indicator estimation

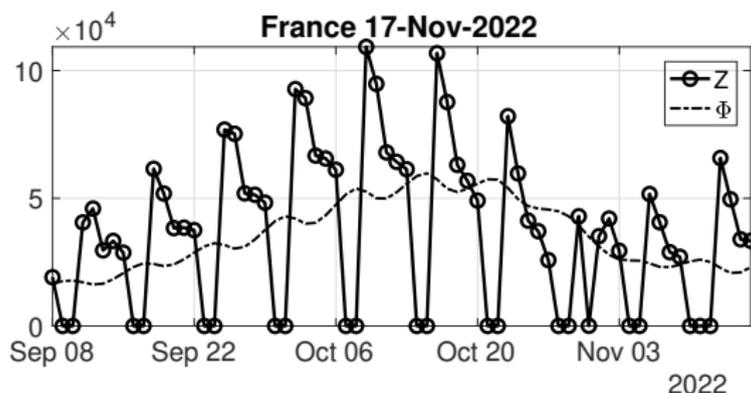
## Counts of daily new infections



data from National Health Agencies collected by Johns Hopkins University

$\implies$  number of cases not informative enough: need to capture the **dynamics**

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Design adapted counter measures and evaluate their effectiveness

→ efficient monitoring tools

→ robust to low quality of the data

*epidemiological model,  
managing erroneous counts.*

## Reproduction number in Cori model

“averaged number of secondary cases generated by a typical infectious individual”

(Cori et al., 2013, *Am. Journal of Epidemiology*; Liu et al., 2018, *PNAS*)

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$R_t > 1$  the virus propagates at exponential speed,

$R_t < 1$  the epidemic shrinks with an exponential decay,

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⇒ one single indicator accounting for the overall pandemic mechanism

# Pandemic study: modeling at the service of monitoring

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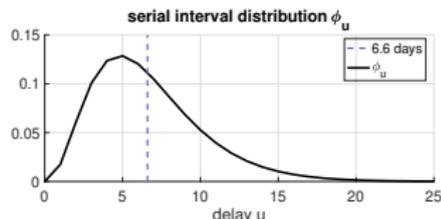
**Principle:**  $Z_t$  new infections at day  $t$

$$\mathbb{E}[Z_t] = R_t \Phi_t, \quad \Phi_t = \sum_{u=1}^{\tau_\Phi} \phi_u Z_{t-u}$$

with  $\Phi_t$  global “infectiousness” in the population

$\{\phi_u\}_{u=1}^{\tau_\Phi}$  distribution of delay between onset of symptoms in primary and secondary cases

Gamma distribution truncated at 25 days, of mean 6.6 days and standard deviation 3.5 days



# Pandemic study: modeling at the service of monitoring

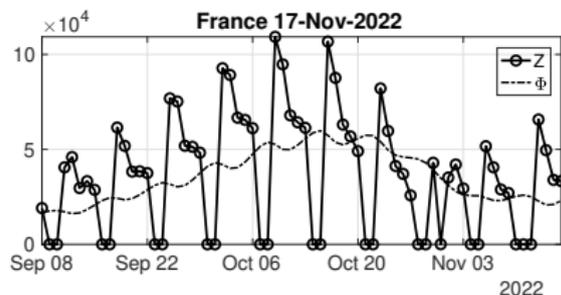
**Data:** daily counts  $\mathbf{Z} = (Z_1, \dots, Z_T)$

**Model:** **scaled** Poisson distribution

$$\frac{Z_t}{\gamma} \mid Z_{t-\tau_\phi}, \dots, Z_{t-1}; R_t \sim \mathcal{P} \left( \frac{R_t \phi_t}{\gamma} \right)$$

$\gamma > 0$  scaling parameter: controls **variance**

(Pascal & Vaiter, 2025, *Signal Process.*)



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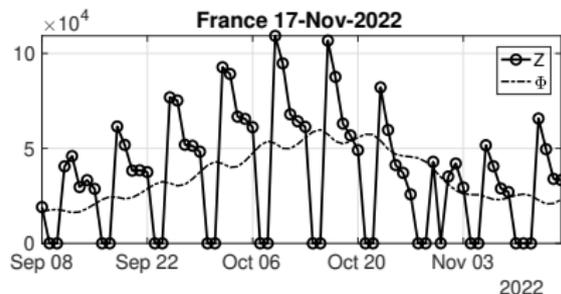
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**Inverse problem formalism:**

$$\frac{\mathbf{Z}}{\gamma} \sim \mathcal{P} \left( \frac{\Phi \mathbf{R}}{\gamma} \right)$$

- $\mathbf{Z} \in \mathbb{N}^T$ : reported infection counts,
- $\mathbf{R} = (R_1, \dots, R_T) \in \mathbb{R}_+^T$ : daily unknown reproduction number,
- $\Phi = \text{diag}(\Phi_1, \dots, \Phi_T)$ : linear operator,
- $\mathcal{P}$ : data-dependent Poisson noise, with scale parameter  $\gamma$

$$\implies \mathcal{D}(\mathbf{Z}, \Phi \mathbf{R}) = -\log \mathbb{P}(\mathbf{Z} | \mathbf{R})$$

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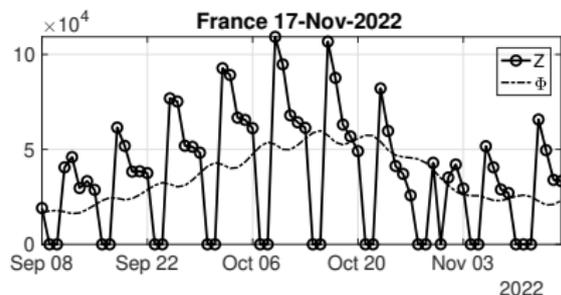
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## Maximum Likelihood Estimate (MLE)

$$\ln (\mathbb{P}(Z_t \mid \mathbf{Z}_{t-\tau_\phi:t-1}, R_t))$$

$$\stackrel{\text{(def.)}}{=} -\frac{1}{\gamma} d_{\text{KL}}(Z_t \mid R_t \phi_t) \quad (\text{Kullback-Leibler})$$

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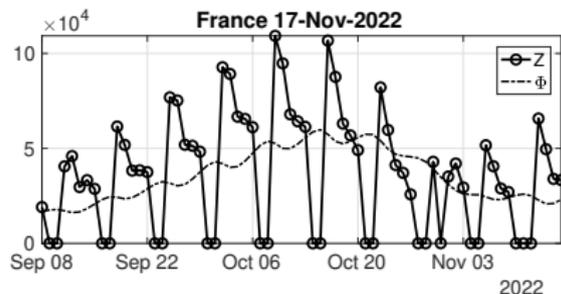
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$$\stackrel{\text{(def.)}}{=} -\frac{1}{\gamma} d_{\text{KL}}(Z_t \mid R_t \phi_t) \quad (\text{Kullback-Leibler})$$

$$\Rightarrow \hat{R}_t^{\text{MLE}} = Z_t / \phi_t = Z_t / \sum_{u=1}^{\tau_\phi} \phi_u Z_{t-u}$$

ratio of moving averages

# Pandemic study: modeling at the service of monitoring

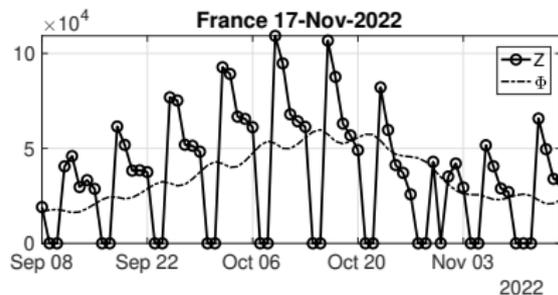
**Data:** daily counts  $\mathbf{Z} = (Z_1, \dots, Z_T)$

**Model:** **scaled** Poisson distribution

$$\frac{Z_t}{\gamma} \mid Z_{t-\tau_\phi}, \dots, Z_{t-1}; R_t \sim \mathcal{P} \left( \frac{R_t \phi_t}{\gamma} \right)$$

$\gamma > 0$  scaling parameter: controls **variance**

(Pascal & Vaiter, 2025, *Signal Process.*)



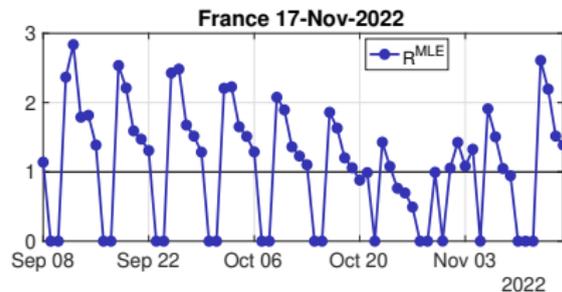
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ratio of moving averages



- huge variability along time / no local trend
- not robust to pseudo-periodicity / misreported counts

Penalized likelihood: regularization through nonlinear filtering

$$\hat{\mathbf{R}}^{\text{PKL}} = \underset{\mathbf{R} \in \mathbb{R}_+^T}{\operatorname{argmin}} \sum_{t=1}^T \frac{1}{\gamma} d_{\text{KL}}(\mathbf{Z}_t | \mathbf{R}_t \Phi_t) + \lambda \mathcal{R}(\mathbf{R}) \quad (\text{penalized Kullback-Leibler})$$

with  $\mathcal{R}(\mathbf{R})$  favoring some temporal regularity

(Abry et al., 2020, *PLoSOne*)

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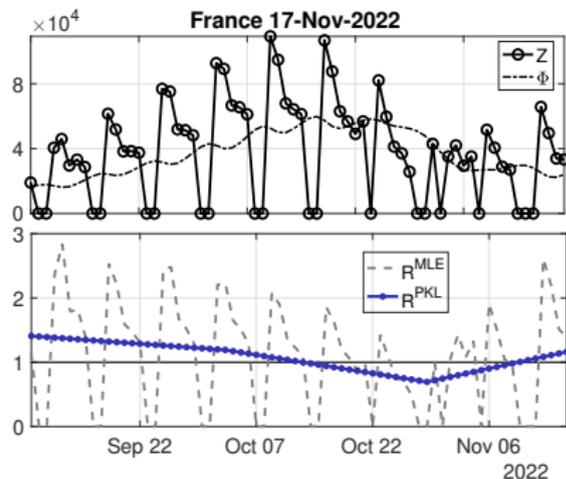
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$$\mathcal{R}(\mathbf{R}) = \|\mathbf{D}_2 \mathbf{R}\|_1$$

$$(\mathbf{D}_2 \mathbf{R})_t = R_{t+1} - 2R_t + R_{t-1}$$

2nd order derivative &  $\ell_1$ -norm

$\Rightarrow$  piecewise linearity



captures global **trend**, **smooth** temporal behavior, **no pseudo-oscillations**

Penalized Kullback-Leibler estimator:

$$\hat{\mathbf{R}}(\mathbf{Z}; \lambda) = \operatorname{argmin}_{\mathbf{R} \in \mathbb{R}_+^T} \sum_{t=1}^T \frac{1}{\gamma} d_{\text{KL}}(Z_t | R_t \Phi_t) + \lambda \|\mathbf{D}_2 \mathbf{R}\|_1$$

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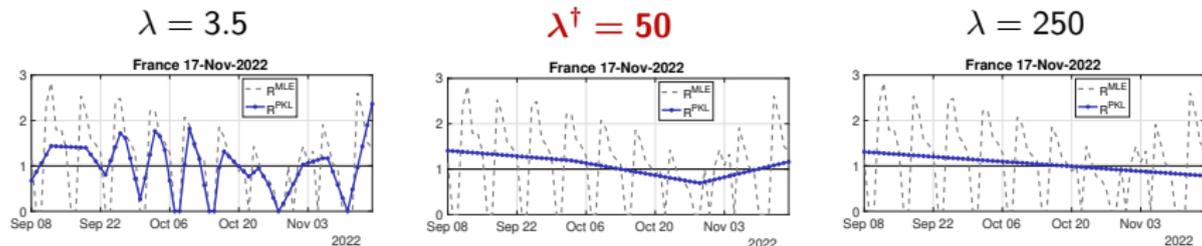
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**Fine tuning of the regularization parameter:**



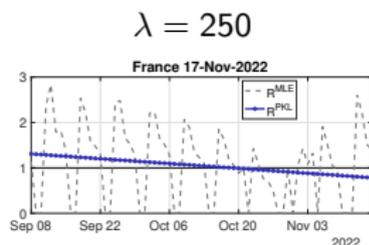
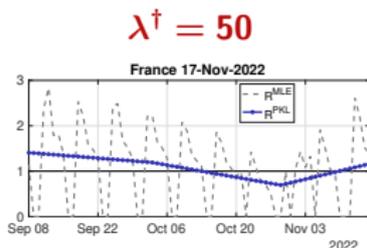
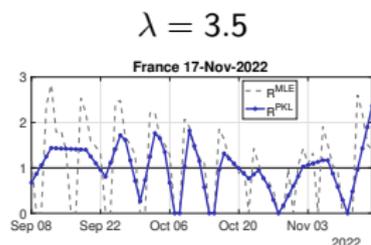
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**Fine tuning of the regularization parameter:**



**Data-driven oracle minimization**

$$\lambda^\dagger \in \underset{\lambda \in \Lambda}{\operatorname{Argmin}} \mathcal{O}(\mathbf{Z}; \lambda)$$

$\Rightarrow$  **Goal:**  $\mathcal{O}$  data-driven proxy for  $\|\hat{\mathbf{R}}(\mathbf{Z}; \lambda) - \bar{\mathbf{R}}\|_2^2$

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**Reminder:**

$$\frac{\mathbf{Z}}{\gamma} \sim \mathcal{P} \left( \frac{\Phi \mathbf{R}}{\gamma} \right)$$

- $\mathbf{Z} \in \mathbb{N}^T$ : reported infection counts,
- $\mathbf{R} = (R_1, \dots, R_T) \in \mathbb{R}_+^T$ : daily unknown reproduction number,
- $\Phi = \text{diag}(\Phi_1, \dots, \Phi_T)$ : linear operator,
- $\mathcal{P}$ : data-dependent Poisson noise, with scale parameter  $\gamma$ .

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### Challenges:

- ▶ **Poisson model: Stein lemma does not apply** (Eldar, 2008, *IEEE Trans. Signal Process.*; Luisier et al., 2010, *IEEE Trans. Image Process.*; Li et al., 2017, *IEEE Trans. Image Process.*)

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- ▶ Nonstationary driven autoregressive model:  $(\Phi\mathbf{R})_t = R_t \sum_{s=1}^{T\Phi} \phi_s \mathbf{Z}_{t-s}$   
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**Autoregressive Poisson Unbiased Risk Estimate (APURE)**

## Model

$$\frac{Z_t}{\gamma} \sim \mathcal{P} \left( \frac{\bar{R}_t \Phi_t(Z_1, \dots, Z_{t-1})}{\gamma} \right)$$

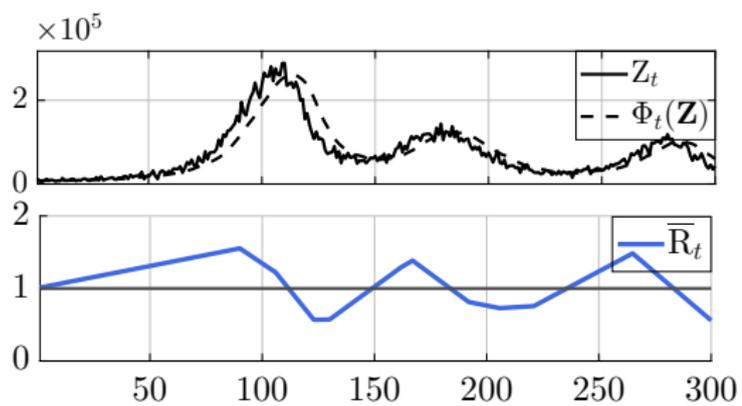
with scale parameter  $\log_{10} \gamma \equiv 3$

# Data-driven hyperparameter selection on synthetic Poisson data

## Model

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## True prediction $\mathcal{P}$ & estimation $\mathcal{E}$ errors

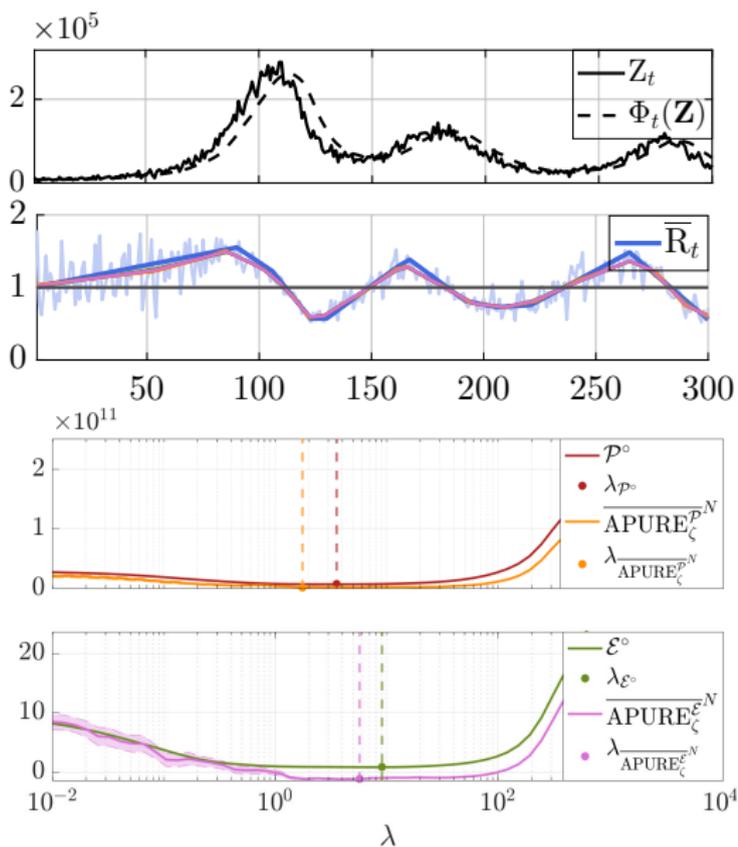
$$\mathcal{P}^\circ(\mathbf{Z}; \theta) = \|\hat{\mathbf{R}}(\mathbf{Z}; \theta) \odot \Phi(\mathbf{Z}) - \bar{\mathbf{R}} \odot \Phi(\mathbf{Z})\|_2^2$$

$$\mathcal{E}^\circ(\mathbf{Z}; \theta) = \|\hat{\mathbf{R}}(\mathbf{Z}; \theta) - \bar{\mathbf{R}}\|_2^2$$

## Unbiased risk estimators

$$\overline{\text{APURE}}_{\zeta}^{\mathcal{P}} = \frac{1}{N} \sum_{n=1}^N \text{APURE}_{\zeta^{(n)}}^{\mathcal{P}}$$

$$\overline{\text{APURE}}_{\zeta}^{\mathcal{E}} = \frac{1}{N} \sum_{n=1}^N \text{APURE}_{\zeta^{(n)}}^{\mathcal{E}}$$



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with scale parameter  $\log_{10} \gamma \equiv 3.5$

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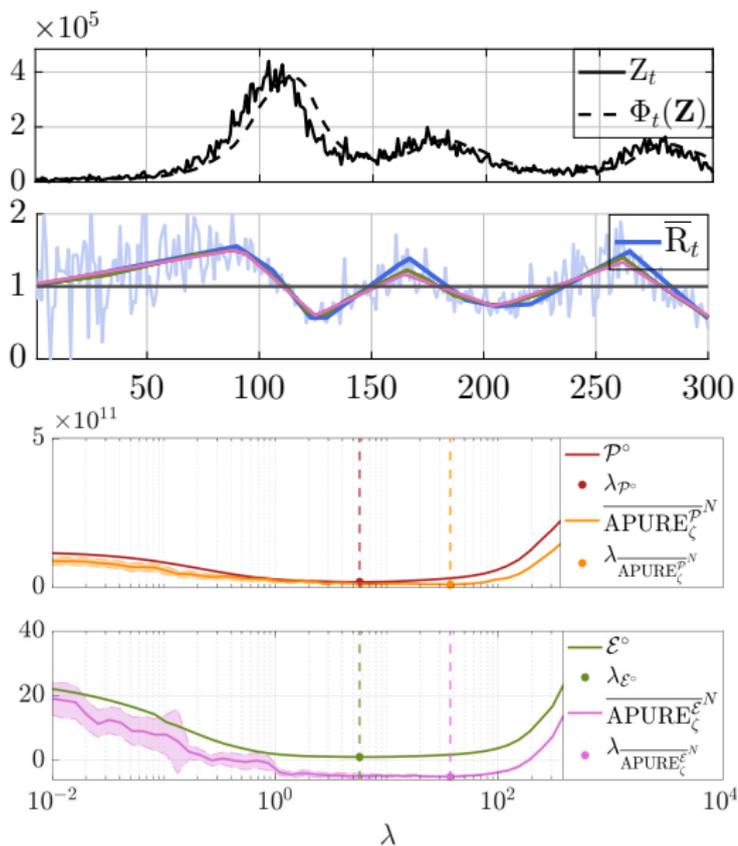
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with scale parameter  $\log_{10} \gamma \equiv 4$

## True prediction $\mathcal{P}$ & estimation $\mathcal{E}$ errors

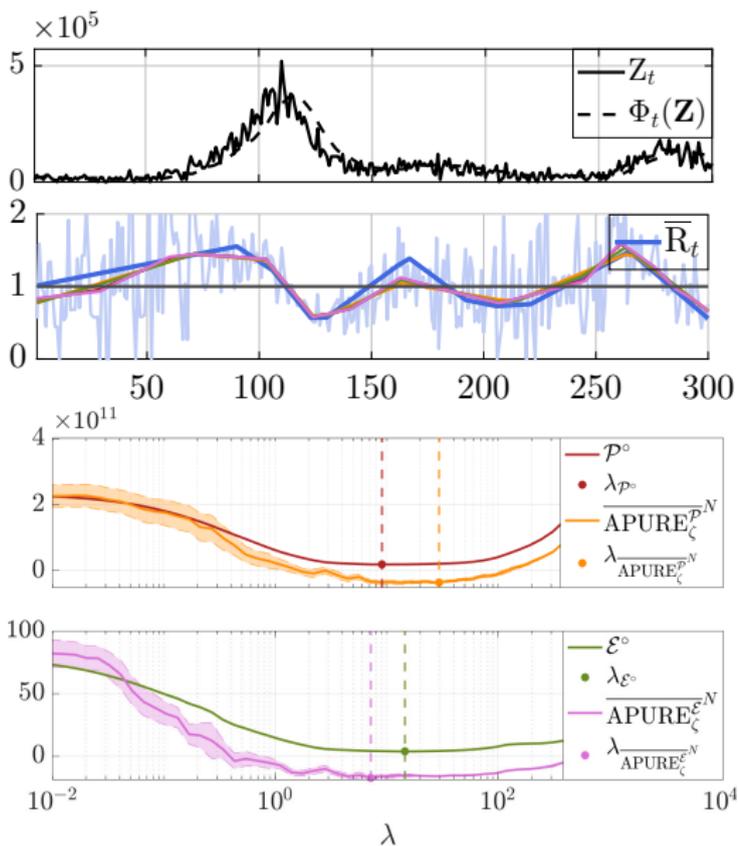
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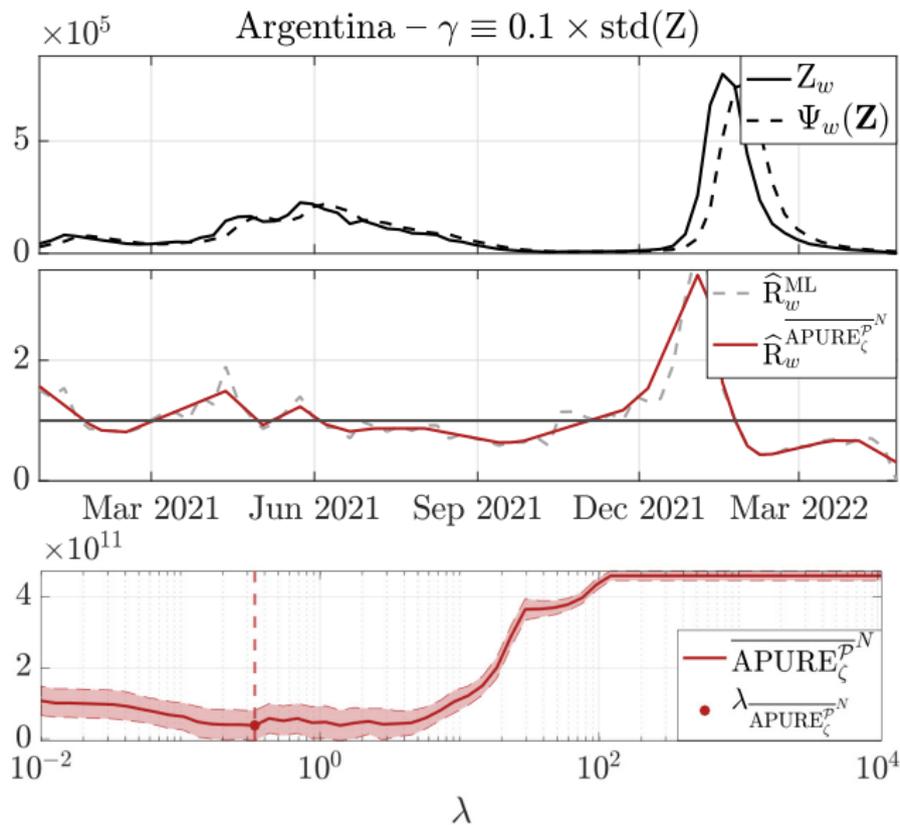
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# Data-driven hyperparameter selection on weekly COVID-19 counts



Pascal & Vaïter, 2024, *Preprint arXiv:2409.14937*

Codes: [github.com/bpascal-fr/APURE-Estim-Epi](https://github.com/bpascal-fr/APURE-Estim-Epi)

**Inverse problem**

$$\mathbf{y} \sim \mathcal{B}(\Phi \bar{\mathbf{x}})$$

$$\lambda^\dagger \in \underset{\lambda \in \Lambda}{\text{Argmin}} \mathcal{O}(\mathbf{y}; \lambda), \quad \text{for} \quad \hat{\mathbf{x}}(\mathbf{y}; \lambda) \in \underset{\mathbf{x} \in \mathbb{R}^N}{\text{Argmin}} \mathcal{D}(\mathbf{y}, \Phi \mathbf{x}) + \lambda \mathcal{R}(\mathbf{x})$$

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## Data-driven parameter selection

$\implies \mathcal{O}$ : Unbiased Risk Estimate (Stein, 1981, *Ann. Stat.*; Eldar, 2008, *IEEE Trans. Signal Process.*; Luisier et al., 2010, *IEEE Trans. Image Process.*; Deledalle et al., 2014, *SIAM J. Imaging Sci.*; Pascal et al., 2021, *J. Math. Imaging Vis.*; Lucas et al., 2023, *Signal, Image Video Process.*)

- ▶ Texture segmentation: additive correlated Gaussian noise;
- ▶ Epidemic monitoring: driven autoregressive data-dependent Poisson noise.

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## Extensions and perspectives

- ▶ Efficient and robust scheme for nonconvex  $\mathcal{R}(\mathbf{x})$ ;
- ▶ Generalization to other noise models: speckle noise in medical imaging;
- ▶ Unsupervised learning for  $\hat{\mathbf{x}}(\mathbf{y}; \lambda) = \mathbf{NN}_\theta(\mathbf{y})$  with loss  $\mathcal{O}(\mathbf{y}; \theta)$ .