

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

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

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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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Goal: Estimate $\bar{\mathbf{x}}$



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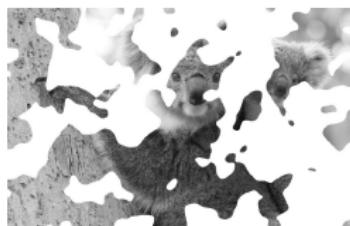
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► ill-conditioned, rank deficient Φ

Inpainting



Super-resolution



Deblurring



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

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

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

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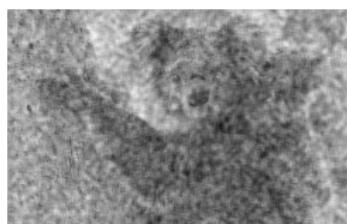
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- ▶ ill-conditioned, rank deficient Φ
- ▶ correlated, data-dependent \mathcal{B}

Correlated



Data-dependent



Multiplicative



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

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

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

The variational framework: penalized log-likelihood

Variational estimator

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

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

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

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

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

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

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)

Hyperparameter selection: bilevel optimization

Fine-tuning of the regularization parameter

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

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not enough

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not enough

$\lambda = 25$



too regularized

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Oracle-based hyperparameter selection

$$\lambda^\dagger \in \operatorname{Argmin}_{\lambda \in \Lambda} \mathcal{O}(y; \lambda)$$

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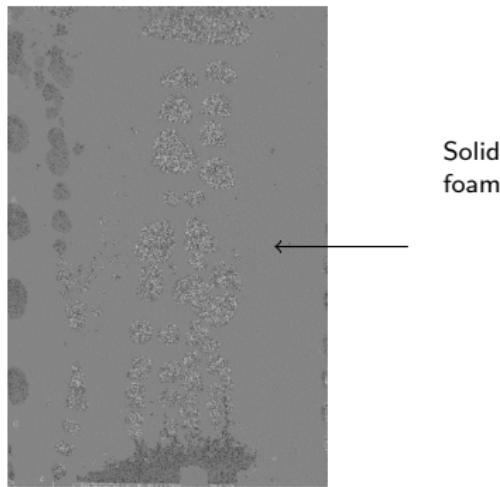
- golden case: $\mathcal{O}(\mathbf{y}; \lambda) = \|\hat{\mathbf{x}}(\mathbf{y}; \lambda) - \bar{\mathbf{x}}\|^2 \implies$ efficient bi-level (\mathbf{x}, λ) minimization
- practical case: ground truth $\bar{\mathbf{x}}$ **not available!** \implies data-driven $\mathcal{O}(\mathbf{y}; \lambda)$

Image processing:

Texture segmentation

Multiphase flow through porous media

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

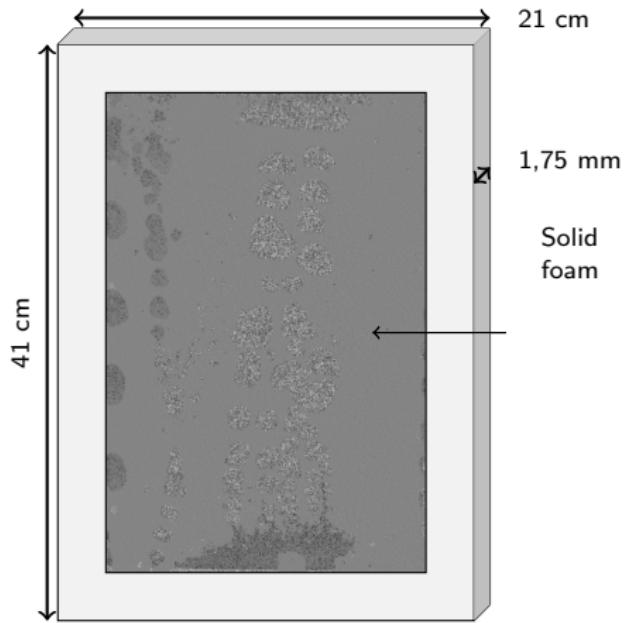


Solid
foam



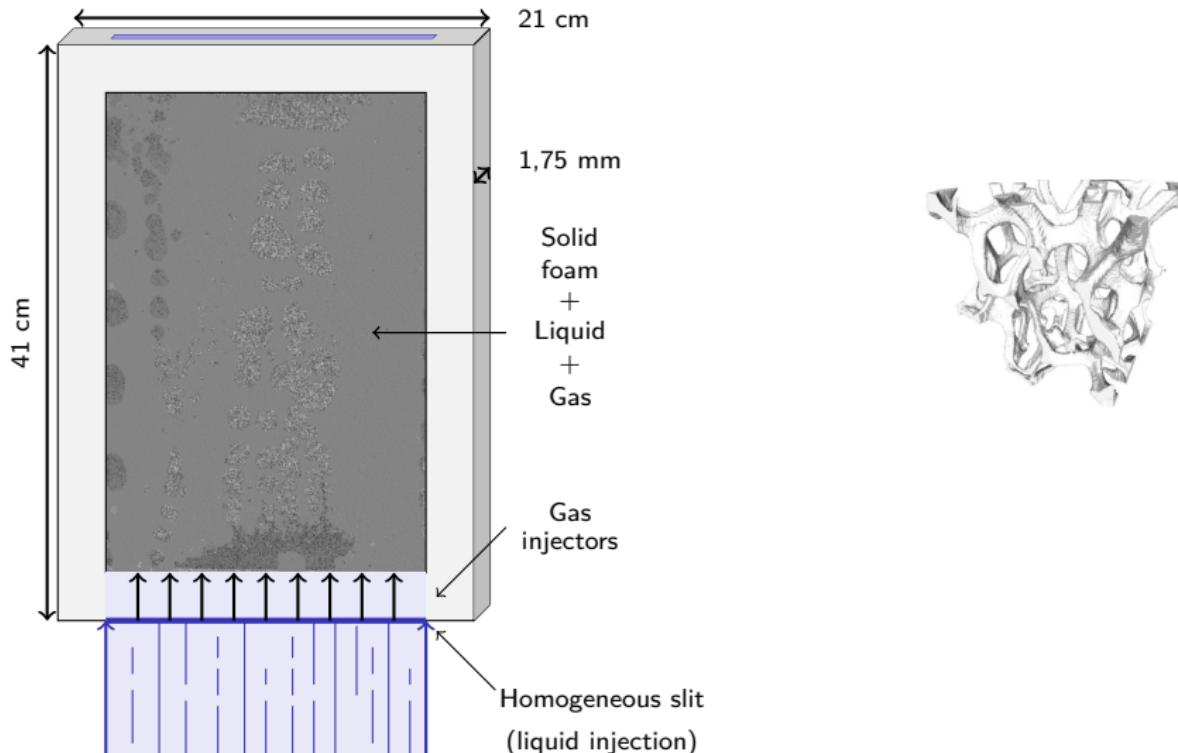
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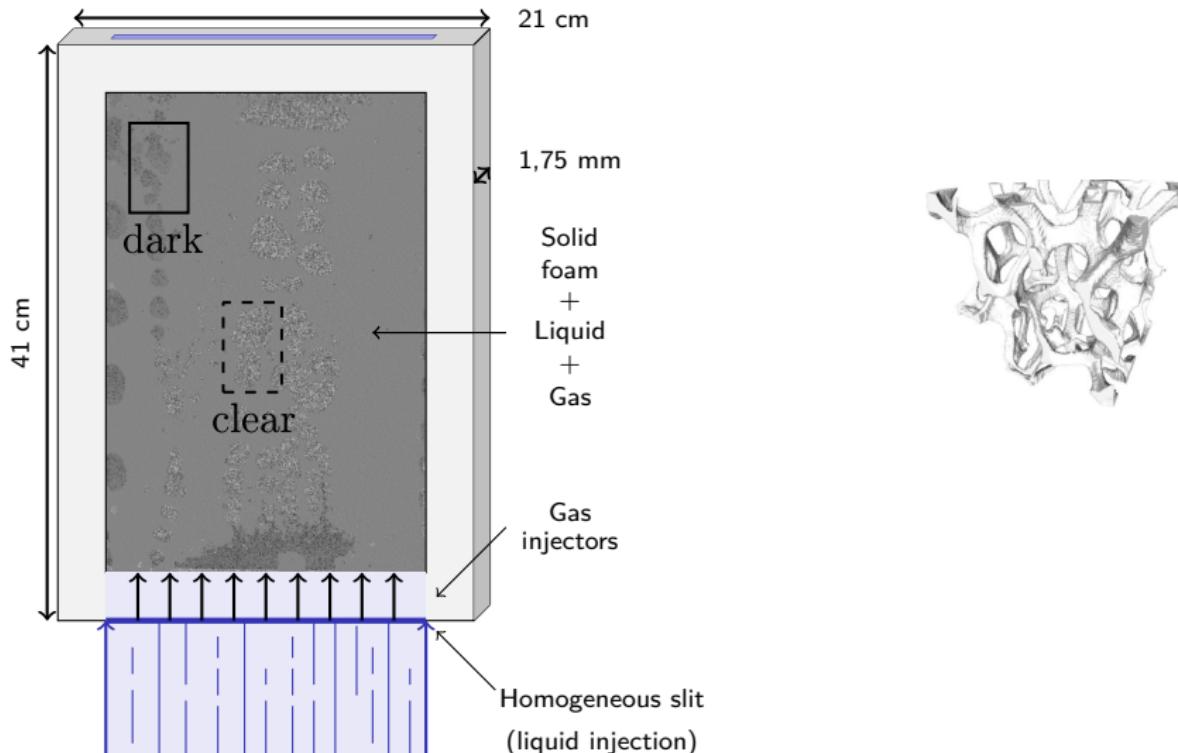
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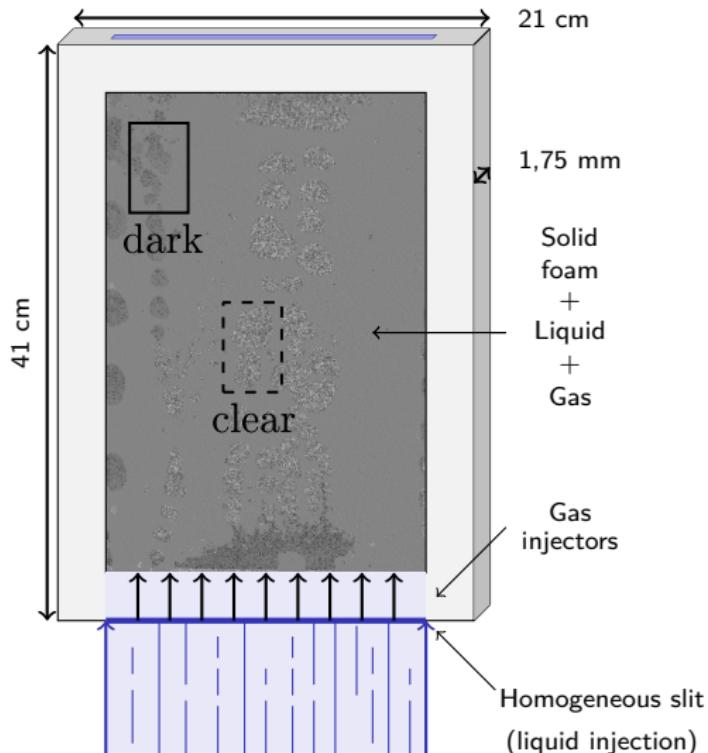
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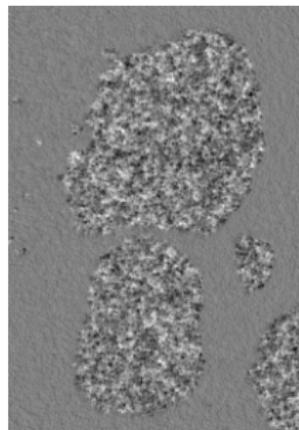
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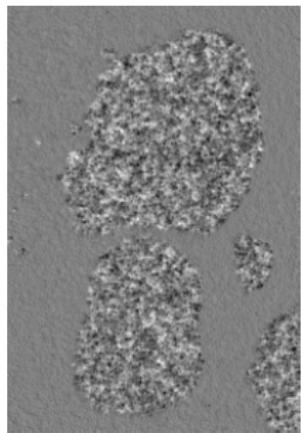


- 1600 × 1100 pixels
- video: ~ 1000 images
- phase diagram: ~ 10 flow rates

Textured image segmentation



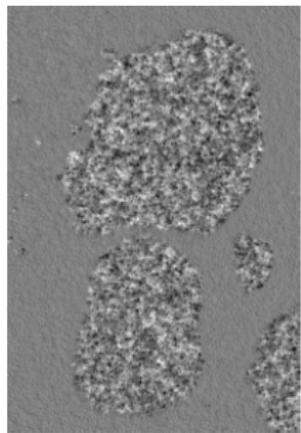
Textured image segmentation



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

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

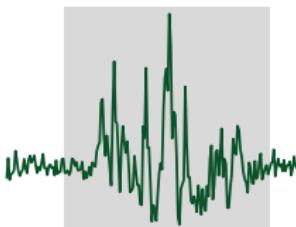
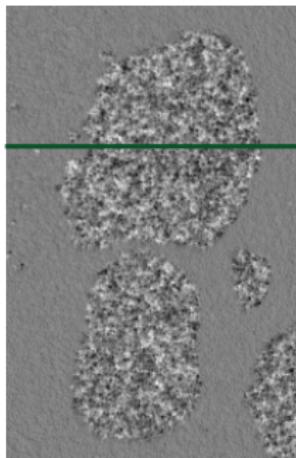
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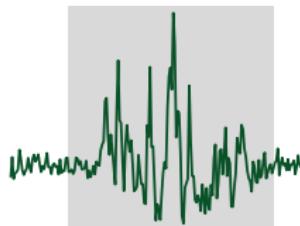
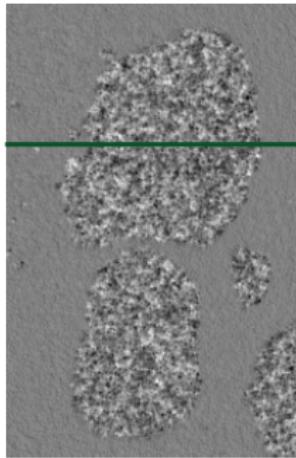
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Piecewise monofractal model



Fractal attributes

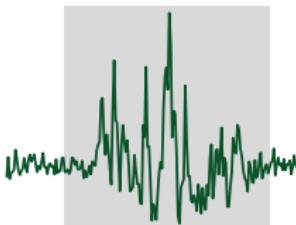
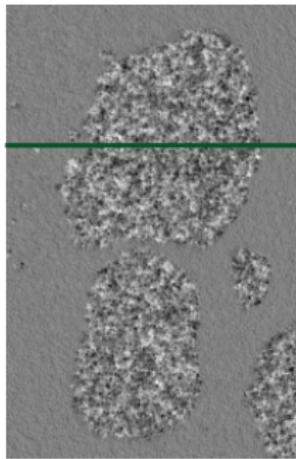
- variance σ^2 *amplitude of variations*



Piecewise monofractal model

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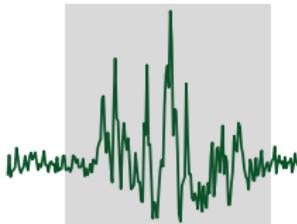
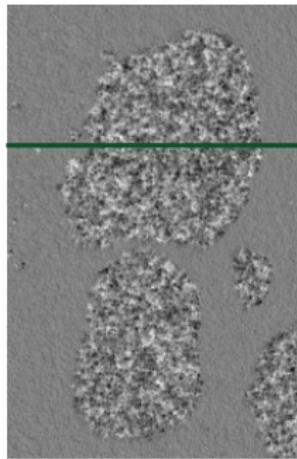
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- local regularity h *scale invariance*



Fractal attributes

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



Piecewise monofractal model

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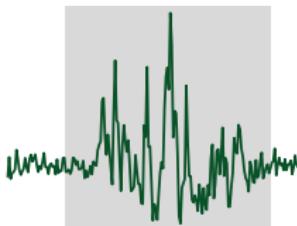
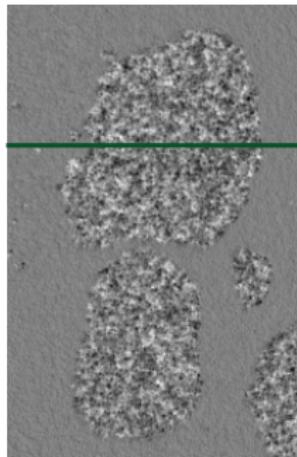
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Piecewise monofractal model

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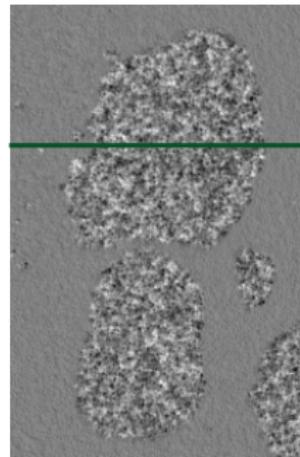
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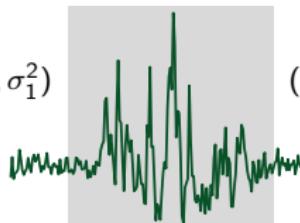
$$h(x) \equiv h_2 = 0.3$$



$$(h_2, \sigma_2^2)$$

$$(h_1, \sigma_1^2)$$

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Segmentation

- σ^2 and h piecewise constant

Piecewise monofractal model

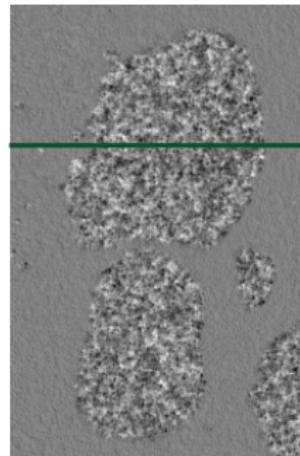
Fractal attributes

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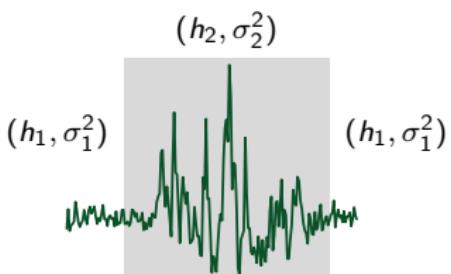


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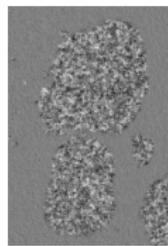
Segmentation

- ▶ σ^2 and h piecewise constant
- ▶ region Ω_k characterized by (σ_k^2, h_k)



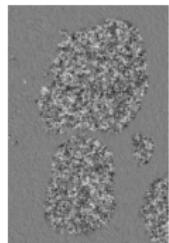
Multiscale analysis

Textured image



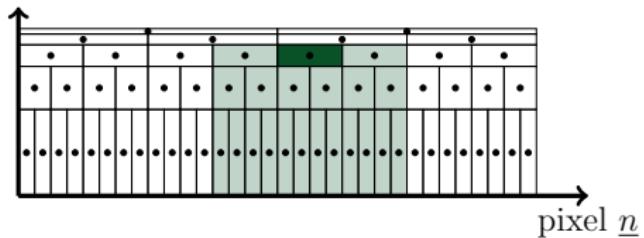
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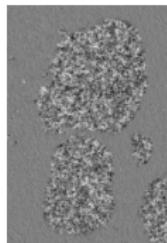
Local maximum of wavelet coefficients: $\mathcal{L}_{a,\cdot}$

scale 2^j



Multiscale analysis

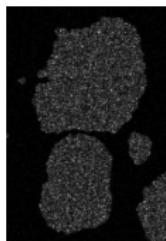
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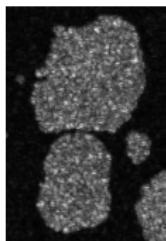
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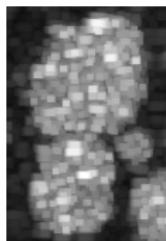
$a = 2^1$



$a = 2^2$

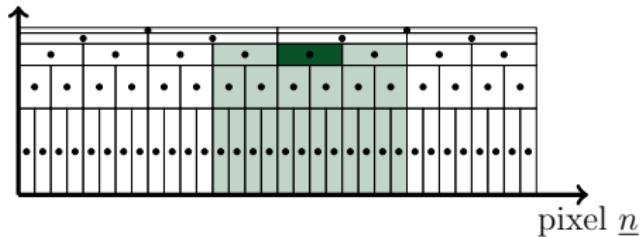


$a = 2^5$



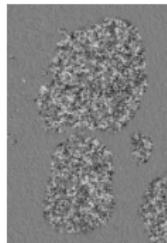
...

scale 2^j



Multiscale analysis

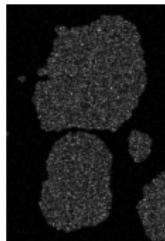
Textured image



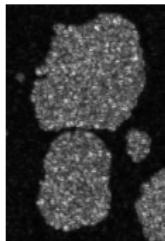
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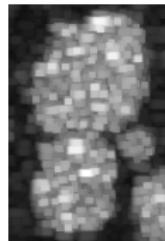


$a = 2^2$



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Proposition (Jaffard, 2004, *Proc. Symp. Pure*

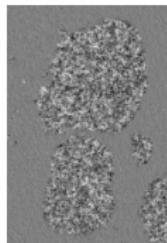
Math.; Wendt et al., 2009, *Signal Process.*)

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

(variance)

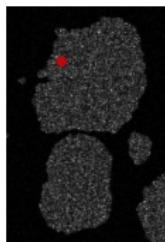
Multiscale analysis

Textured image

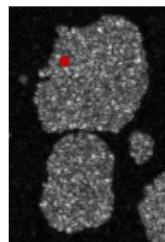


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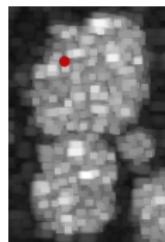


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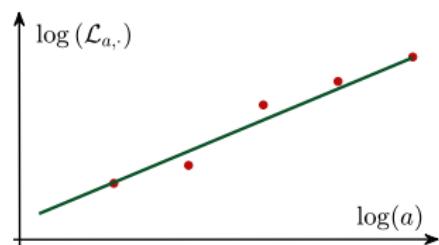
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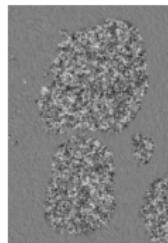
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Multiscale analysis

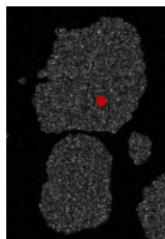
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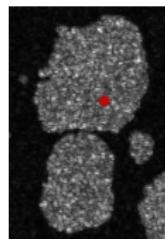
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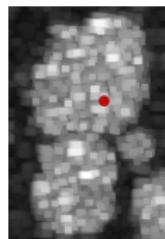
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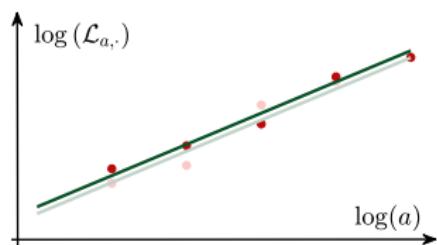
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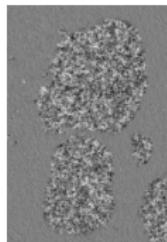
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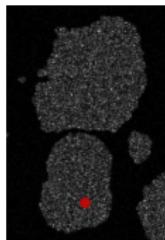
Multiscale analysis

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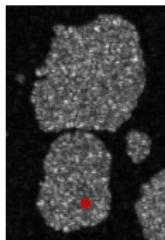


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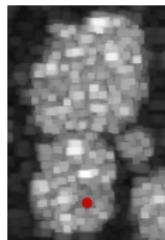
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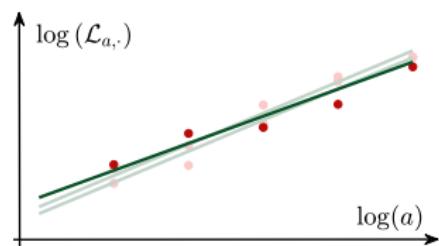
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...

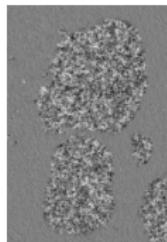
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

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



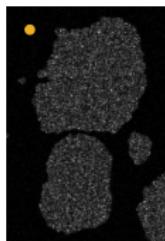
Multiscale analysis

Textured image

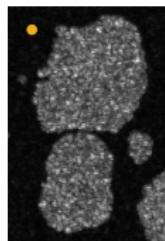


Scale

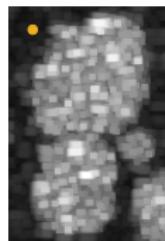
$a = 2^1$



$a = 2^2$



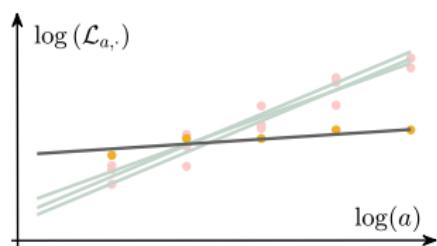
$a = 2^5$



...

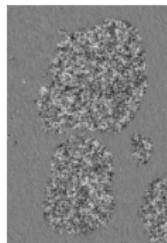
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

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



Multiscale analysis

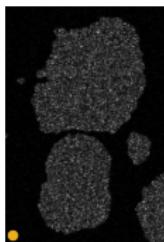
Textured image



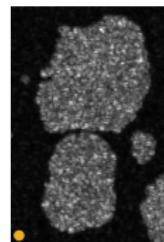
Local maximum of wavelet coefficients: $\mathcal{L}_{a,\cdot}$

Scale

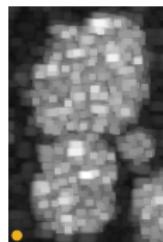
$a = 2^1$



$a = 2^2$



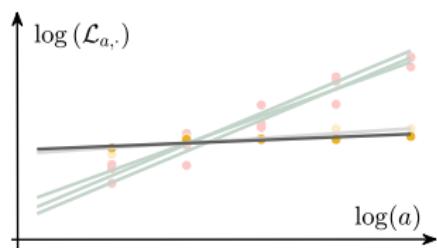
$a = 2^5$



...

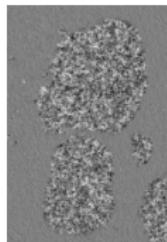
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

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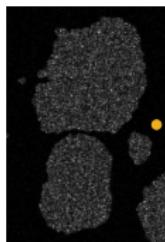
Multiscale analysis

Textured image

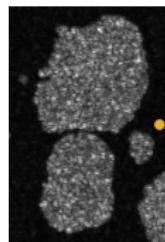


Scale

$a = 2^1$

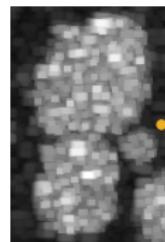


$a = 2^2$



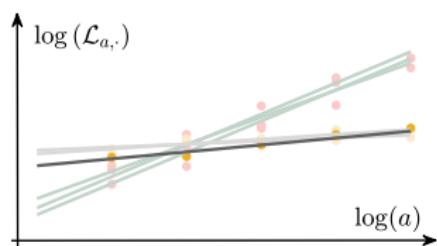
...

$a = 2^5$



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

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

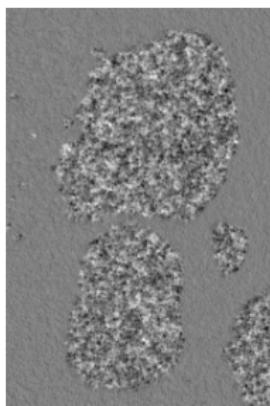


Direct punctual estimation

Linear regression

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

Textured image

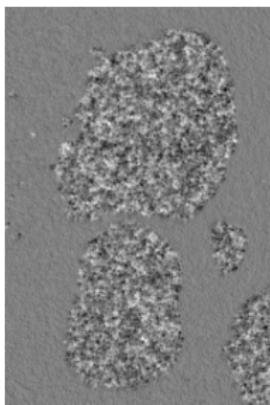


Direct punctual estimation

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

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

Textured image

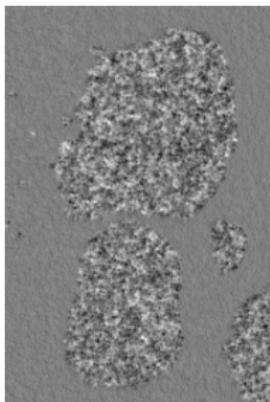


Direct punctual estimation

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

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

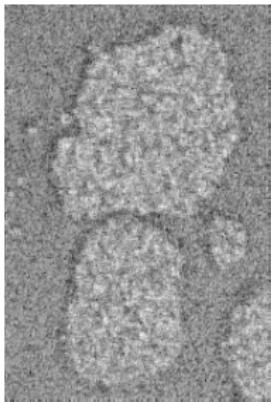
Textured image



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



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



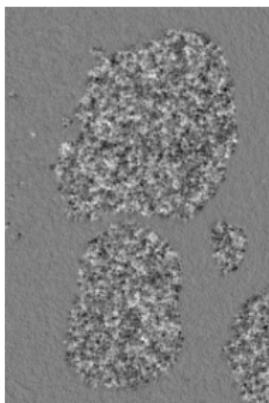
Direct punctual estimation

Linear regression

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

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

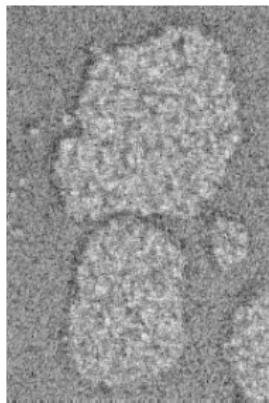
Textured image



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



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

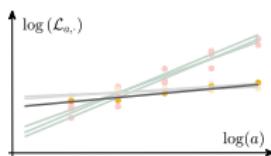


→ large estimation variance

Functionals with either free or co-localized contours

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

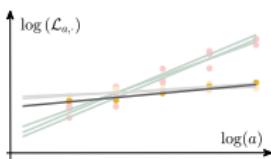
→ fidelity to the log-linear model



Functionals with either free or co-localized contours

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

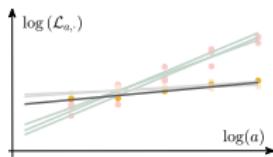
\rightarrow fidelity to the log-linear model
 \rightarrow favors piecewise constancy



Functionals with either free or co-localized contours

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

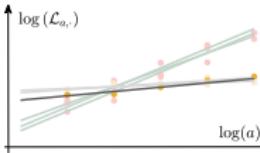
\rightarrow fidelity to the log-linear model
 \rightarrow favors piecewise constancy



Functionals with either free or co-localized contours

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

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

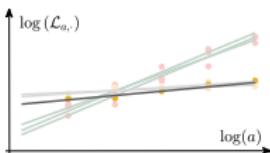


Finite differences $\mathbf{D}_1^\rightarrow \mathbf{x}$ (horizontal), $\mathbf{D}_1^\uparrow \mathbf{x}$ (vertical) at each pixel

Functionals with either free or co-localized contours

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

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



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

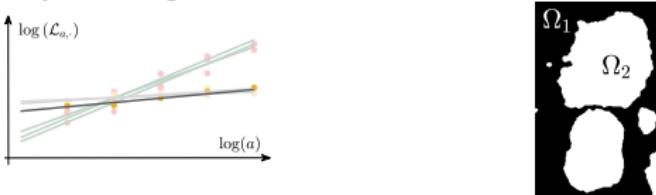
Free: \mathbf{h} , \mathbf{v} are **independently** piecewise constant

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

Functionals with either free or co-localized contours

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

\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

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

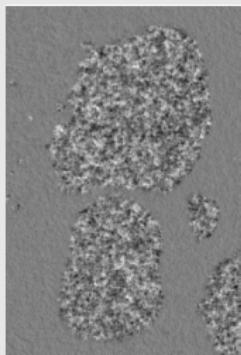
Co-localized: \mathbf{h}, \mathbf{v} are **concomitantly** piecewise constant

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

Segmentation via iterated thresholding

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

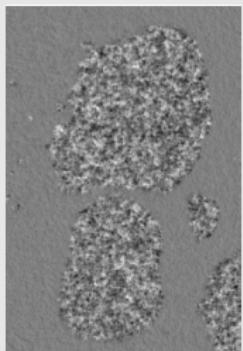
Textured image Lin. reg. $\hat{\mathbf{h}}^{\text{LR}}$



Segmentation via iterated thresholding

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

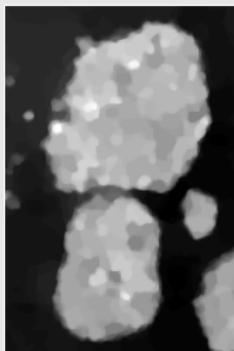
Textured image



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



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



Threshold
estimate[†] $T\hat{\mathbf{h}}^{\text{C}}$



[†](Cai et al., 2013, *J. Sci. Comput.*)

Regularization parameters selection

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

Regularization parameters selection

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

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

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



Regularization parameters selection

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

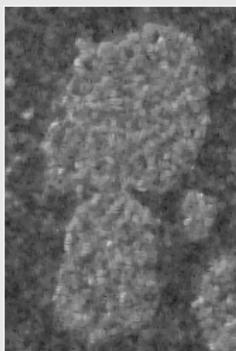
Lin. reg. $\hat{\mathbf{h}}^{\text{LR}}$

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



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

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



too small

Regularization parameters selection

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

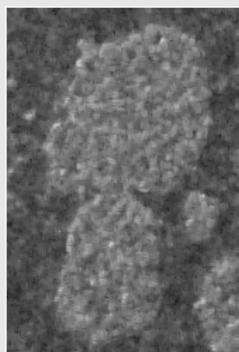
Lin. reg. $\hat{\mathbf{h}}^{\text{LR}}$

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



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

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



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



too small

too large

Regularization parameters selection

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

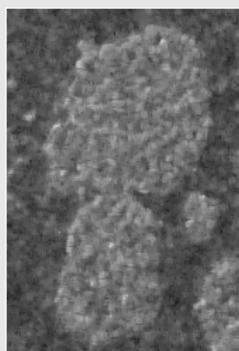
Lin. reg. $\hat{\mathbf{h}}^{\text{LR}}$

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

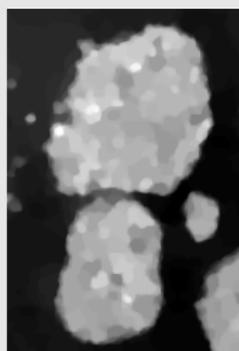


Co-localized contours estimate $\hat{\mathbf{h}}^C$

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



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



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



too small

optimal

too large

What *optimal* means? How to determine λ^\dagger and α^\dagger ?

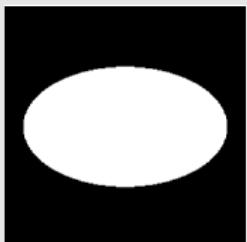
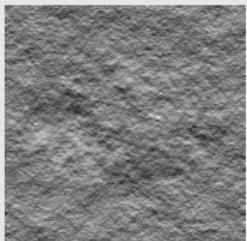
Parameter tuning (Grid search)

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

Parameter tuning (Grid search)

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Example



Parameter tuning (Grid search)

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

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

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

$$\mathcal{R}(\lambda, \alpha) = \left\| \hat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha) - \bar{\mathbf{h}} \right\|^2$$

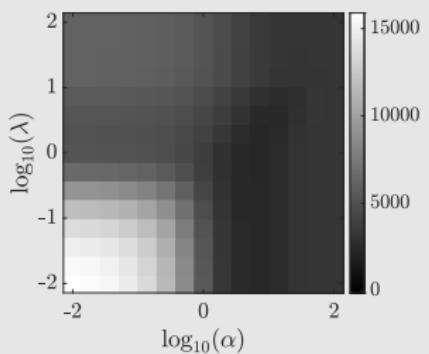
Parameter tuning (Grid search)

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

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

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$$\mathcal{R}(\lambda, \alpha) = \left\| \hat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha) - \bar{\mathbf{h}} \right\|^2$$



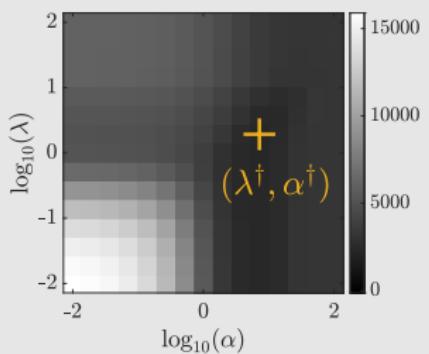
Parameter tuning (Grid search)

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

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

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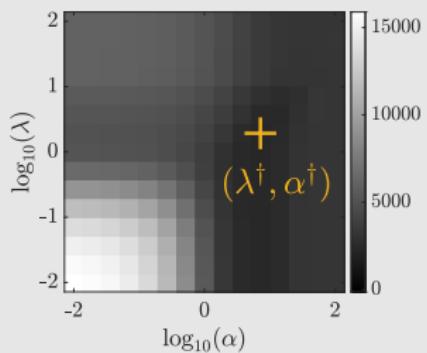
Parameter tuning (Grid search)

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

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

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

$$\mathcal{R}(\lambda, \alpha) = \left\| \hat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha) - \bar{\mathbf{h}} \right\|^2$$



$\bar{\mathbf{h}}$: unknown!

?

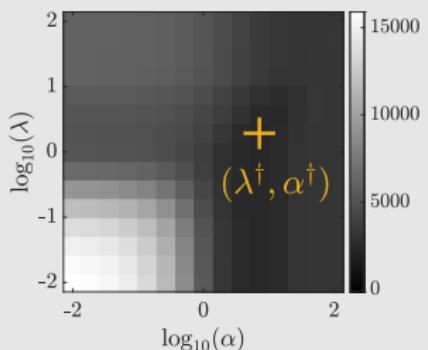
Parameter tuning (Grid search)

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

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

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

$$\mathcal{R}(\lambda, \alpha) = \left\| \widehat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha) - \bar{\mathbf{h}} \right\|^2$$



$\bar{\mathbf{h}}$: unknown!

?

Stein Unbiased Risk Estimate
(SURE)

Stein Unbiased Risk Estimate (Principle)

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

Stein Unbiased Risk Estimate (Principe)

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

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

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Quadratic error $R(\lambda) \triangleq \mathbb{E}_{\boldsymbol{\zeta}} \|\hat{\mathbf{x}}(\mathbf{y}; \lambda) - \bar{\mathbf{x}}\|^2 \stackrel{?}{=} \mathbb{E}_{\boldsymbol{\zeta}} \widehat{R}(\mathbf{y}; \lambda)$ bar x unknown

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

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

- weakly differentiable w.r.t. \mathbf{y} ,
- such that $\boldsymbol{\zeta} \mapsto \langle \hat{\mathbf{x}}(\bar{\mathbf{x}} + \boldsymbol{\zeta}; \lambda), \boldsymbol{\zeta} \rangle$ is integrable w.r.t. $\mathcal{N}(\mathbf{0}, \rho^2 \mathbf{I})$.

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

Generalized Stein Unbiased Risk Estimate

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

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

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

$$\Phi : (\mathbf{h}, \mathbf{v}) \mapsto \{\log(a)\mathbf{h} + \mathbf{v}\}_a \quad \text{and} \quad \Pi : (\mathbf{h}, \mathbf{v}) \mapsto (\mathbf{h}, \mathbf{0})$$

$$\text{Projected estimation error} \quad R_{\Pi}(\Lambda) \triangleq \mathbb{E}_{\zeta} \|\Pi \hat{x}(y; \Lambda) - \Pi \bar{x}\|^2$$

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

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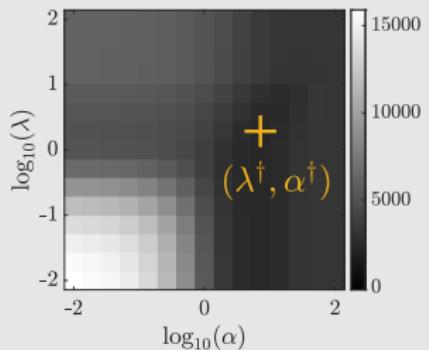
$$\begin{aligned} \hat{R}(\Lambda) &\triangleq \|\mathbf{A}(\Phi \hat{\mathbf{x}}(\mathbf{y}; \Lambda) - \mathbf{y})\|^2 + 2\text{tr} \left(\mathcal{S} \mathbf{A}^\top \Pi \partial_{\mathbf{y}} \hat{\mathbf{x}}(\mathbf{y}; \Lambda) \right) - \text{tr} \left(\mathbf{A} \mathcal{S} \mathbf{A}^\top \right) \\ &\implies R_{\Pi}(\Lambda) = \mathbb{E}_{\zeta} [\hat{R}(\Lambda)]. \end{aligned}$$

Parameter tuning (Grid search)

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

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

$$\mathcal{R}(\lambda, \alpha) = \left\| \widehat{\mathbf{h}}(\mathcal{L}; \lambda, \alpha) - \bar{\mathbf{h}} \right\|^2$$



$\bar{\mathbf{h}}$: unknown!

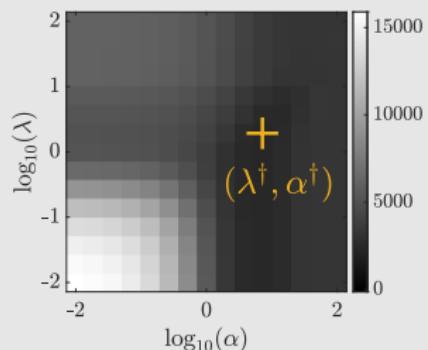
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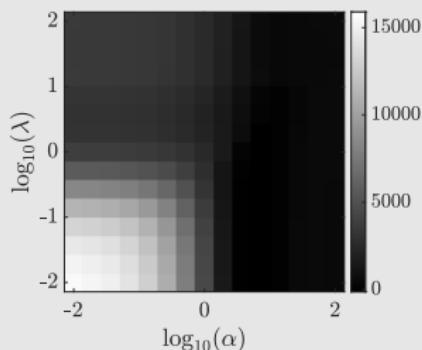
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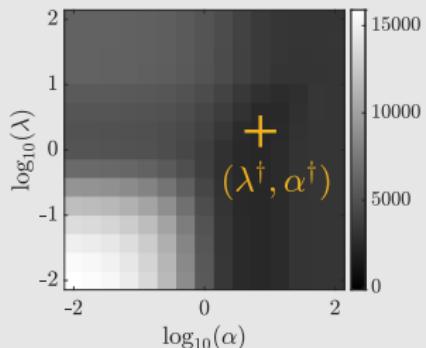


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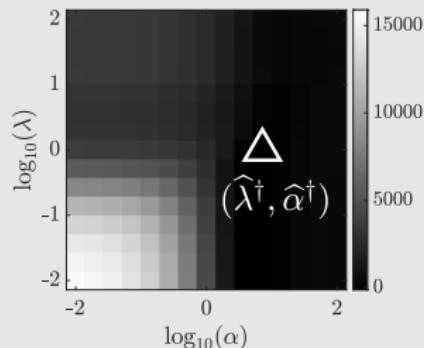
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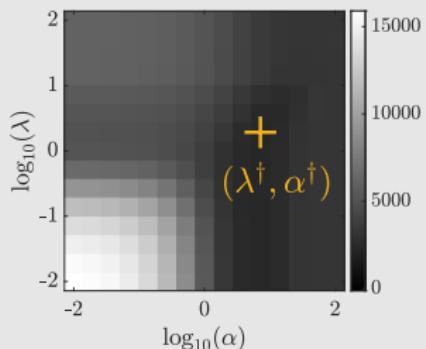


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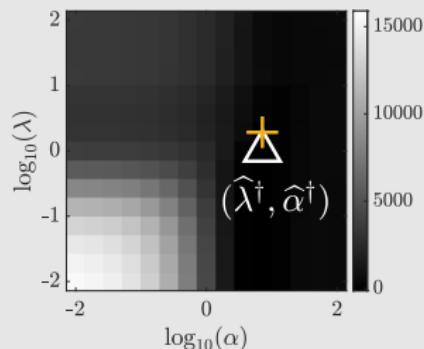
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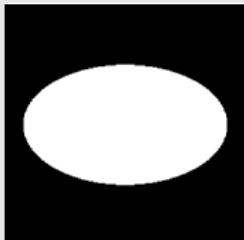
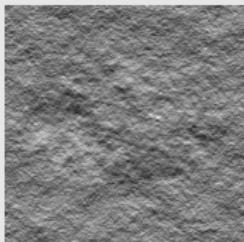
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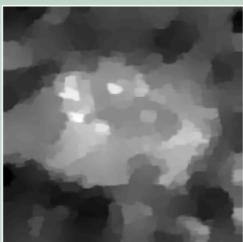
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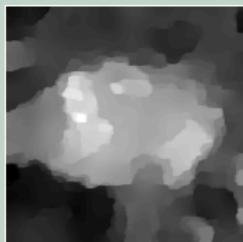
Example



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

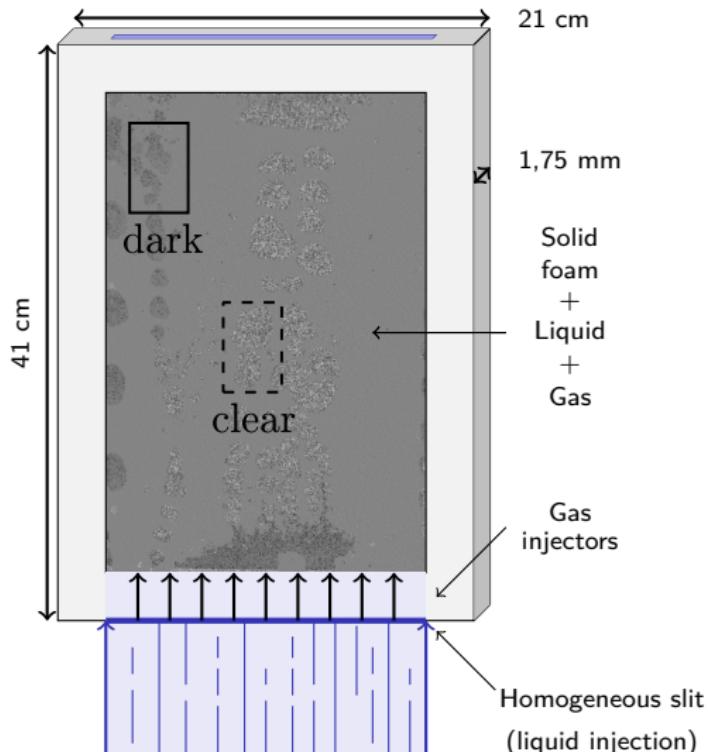


$\widehat{\mathbf{h}}^F(\mathcal{L}; \widehat{\lambda}^\dagger, \widehat{\alpha}^\dagger)$
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Multiphase flow through porous media

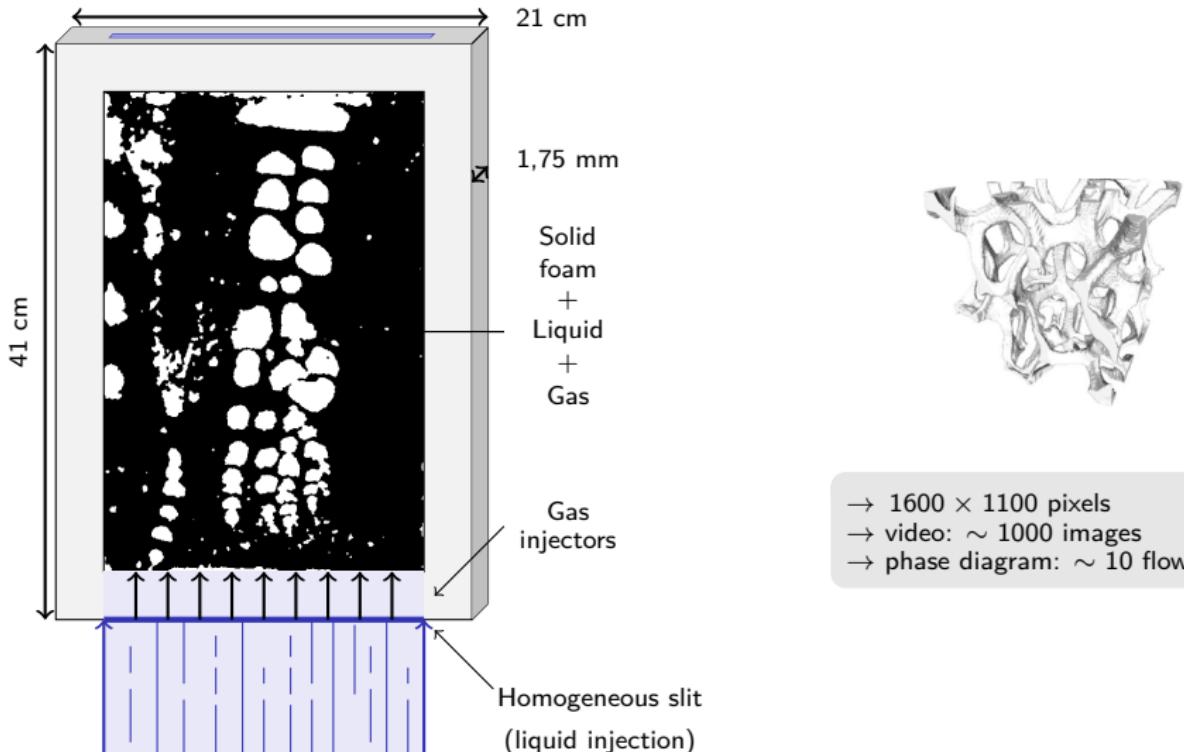
Laboratoire de Physique, ENS Lyon, V. Vidal, T. Busser, (M. Serres, IFPEN)



- 1600 × 1100 pixels
- video: ~ 1000 images
- phase diagram: ~ 10 flow rates

Multiphase flow through porous media

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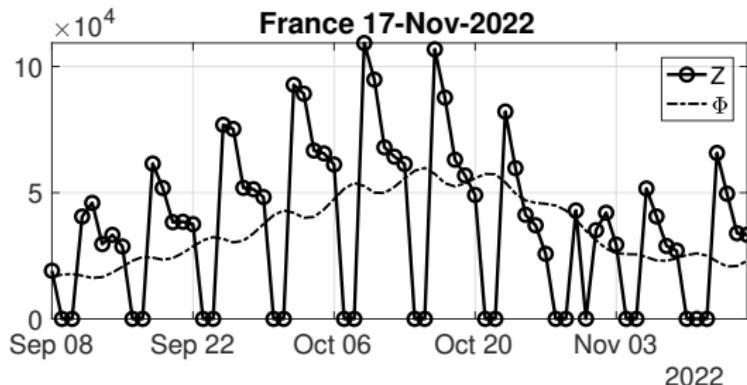


Time series analysis:

Epidemiological indicator estimation

Epidemic propagation: modeling at the service of monitoring

Counts of daily new infections

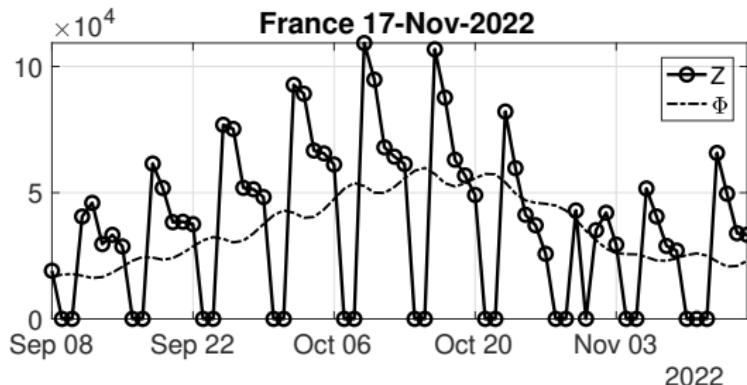


data from National Health Agencies collected by Johns Hopkins University

⇒ number of cases not informative enough: need to capture the **dynamics**

Epidemic propagation: modeling at the service of monitoring

Counts of daily new infections



data from National Health Agencies collected by Johns Hopkins University

⇒ number of cases not informative enough: need to capture the **dynamics**

Design adapted counter measures and evaluate their effectiveness

→ efficient monitoring tools

epidemiological model,

→ robust to low quality of the data

managing erroneous counts.

Pandemic study: modeling at the service of monitoring

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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Interpretation: at day t

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

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

$R_t = 1$ the epidemic is stable.

⇒ one single indicator accounting for the overall pandemic mechanism

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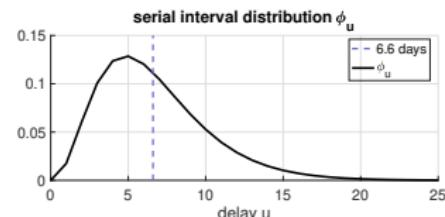
⇒ one single indicator accounting for the overall pandemic mechanism

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 Φ_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

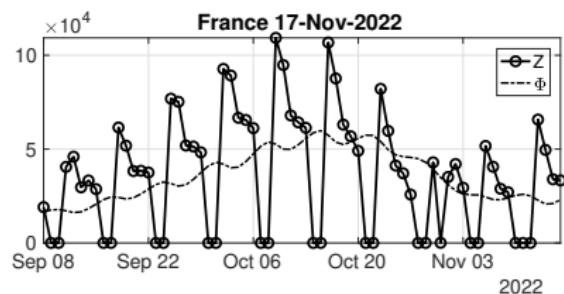
Data: daily counts $\mathbf{Z} = (Z_1, \dots, Z_T)$

Model: **scaled** Poisson distribution

$$\frac{Z_t}{\gamma} | Z_{t-\tau_\Phi}, \dots, Z_{t-1}; R_t \sim \mathcal{P}\left(\frac{R_t \Phi_t}{\gamma}\right)$$

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

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



Pandemic study: modeling at the service of monitoring

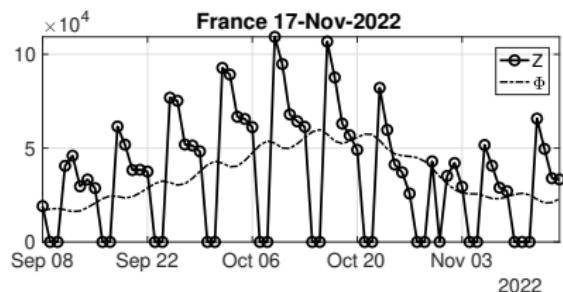
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Inverse problem formalism:

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

- $\mathbf{Z} \in \mathbb{N}^T$: 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 γ

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

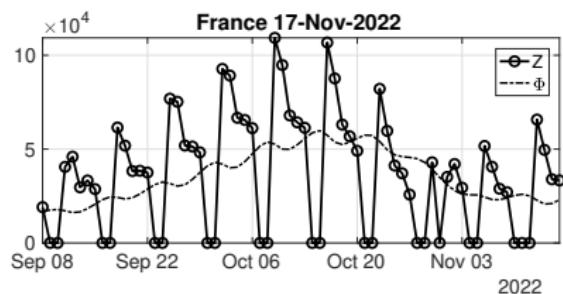
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Maximum Likelihood Estimate (MLE)

$$\ln (\mathbb{P}(Z_t | \mathbf{Z}_{t-\tau_\Phi:t-1}, R_t)) \\ \stackrel{\text{(def.)}}{=} -\frac{1}{\gamma} d_{KL}(Z_t | R_t \Phi_t) \quad (\text{Kullback-Leibler})$$

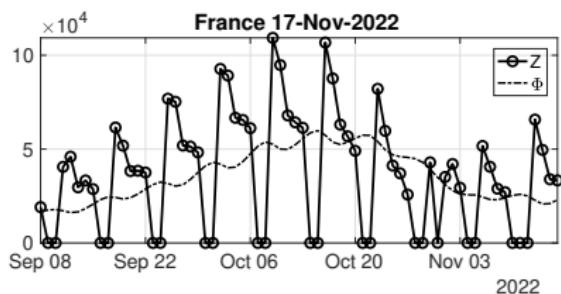
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$$\implies \hat{R}_t^{\text{MLE}} = Z_t / \Phi_t = Z_t / \sum_{u=1}^{\tau_\Phi} \phi_u Z_{t-u}$$

ratio of moving averages

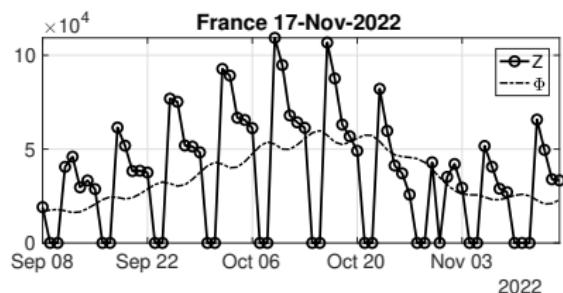
Pandemic study: modeling at the service of monitoring

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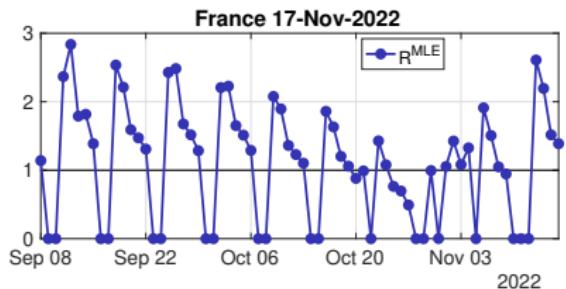
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$$\ln(\mathbb{P}(Z_t | Z_{t-\tau_\Phi:t-1}, R_t))$$

$$= -\frac{1}{\gamma} d_{KL}(Z_t | R_t \Phi_t) \quad (\text{Kullback-Leibler})$$

$$\implies \hat{R}_t^{\text{MLE}} = Z_t / \Phi_t = Z_t / \sum_{u=1}^{\tau_\Phi} \phi_u Z_{t-u}$$

ratio of moving averages



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

Penalized likelihood: regularization through nonlinear filtering

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

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

(Abry et al., 2020, *PLOS One*)

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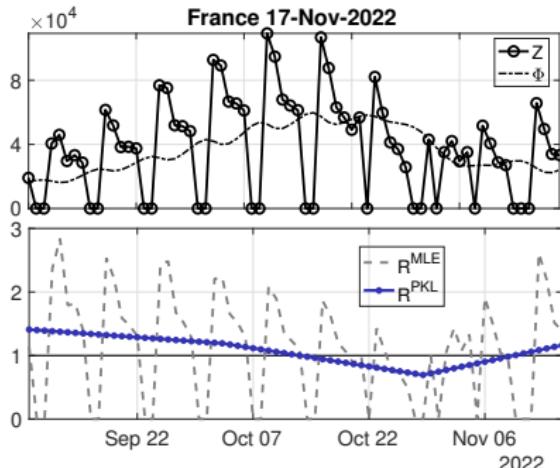
(Abry et al., 2020, *PLOS One*)

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

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

2nd order derivative & ℓ_1 -norm

⇒ piecewise linearity



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

Penalized Kullback-Leibler estimator:

$$\widehat{\mathbf{R}}(\mathbf{Z}; \lambda) = \underset{\mathbf{R} \in \mathbb{R}_+^T}{\operatorname{argmin}} \sum_{t=1}^T \frac{1}{\gamma} d_{KL} (\mathbf{Z}_t | \mathbf{R}_t \boldsymbol{\Phi}_t) + \lambda \|\mathbf{D}_2 \mathbf{R}\|_1$$

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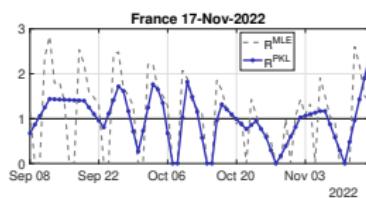
$$\widehat{\mathbf{R}}(\mathbf{Z}; \lambda) = \operatorname{argmin}_{\mathbf{R} \in \mathbb{R}_+^T} \sum_{t=1}^T \frac{1}{\gamma} d_{KL} (\mathbf{Z}_t | \mathbf{R}_t \Phi_t) + \lambda \|\mathbf{D}_2 \mathbf{R}\|_1$$

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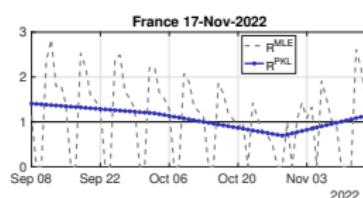
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Fine tuning of the regularization parameter:

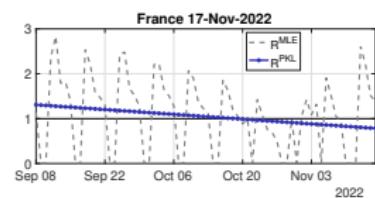
$$\lambda = 3.5$$



$$\lambda^\dagger = 50$$



$$\lambda = 250$$



Penalized Kullback-Leibler estimator:

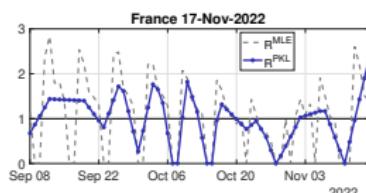
$$\widehat{\mathbf{R}}(\mathbf{Z}; \lambda) = \operatorname{argmin}_{\mathbf{R} \in \mathbb{R}_+^T} \sum_{t=1}^T \frac{1}{\gamma} d_{KL} (\mathbf{Z}_t | \mathbf{R}_t \Phi_t) + \lambda \|\mathbf{D}_2 \mathbf{R}\|_1$$

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

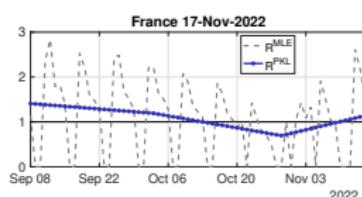
(Abry et al., 2020, *PLOS One*)

Fine tuning of the regularization parameter:

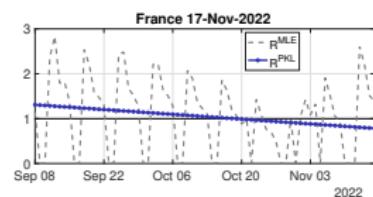
$$\lambda = 3.5$$



$$\lambda^\dagger = 50$$



$$\lambda = 250$$



Data-driven oracle minimization

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

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

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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,
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Autoregressive Poisson Unbiased Risk Estimate (APURE)

Model

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

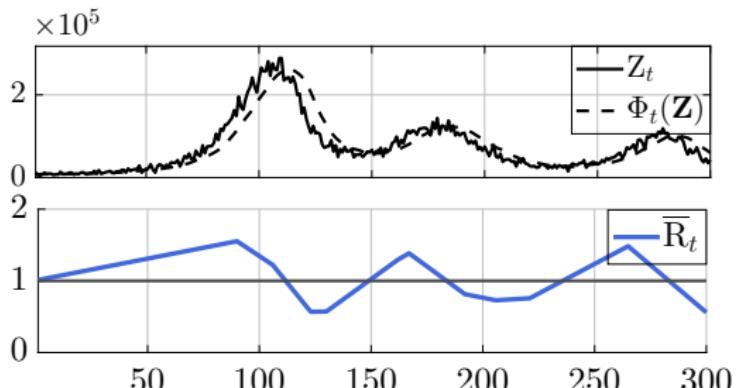
with scale parameter $\log_{10} \gamma \equiv 3$

Data-driven hyperparameter selection on synthetic Poisson data

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

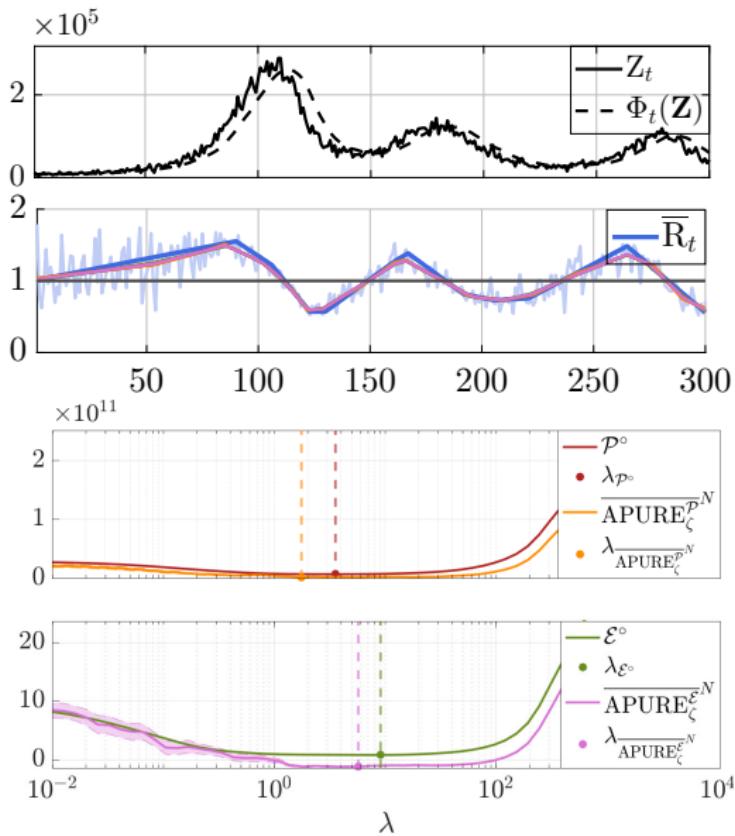
$$\mathcal{P}^\circ(Z; \theta) = \|\hat{R}(Z; \theta) \odot \Phi(Z) - \bar{R} \odot \Phi(Z)\|_2^2$$

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

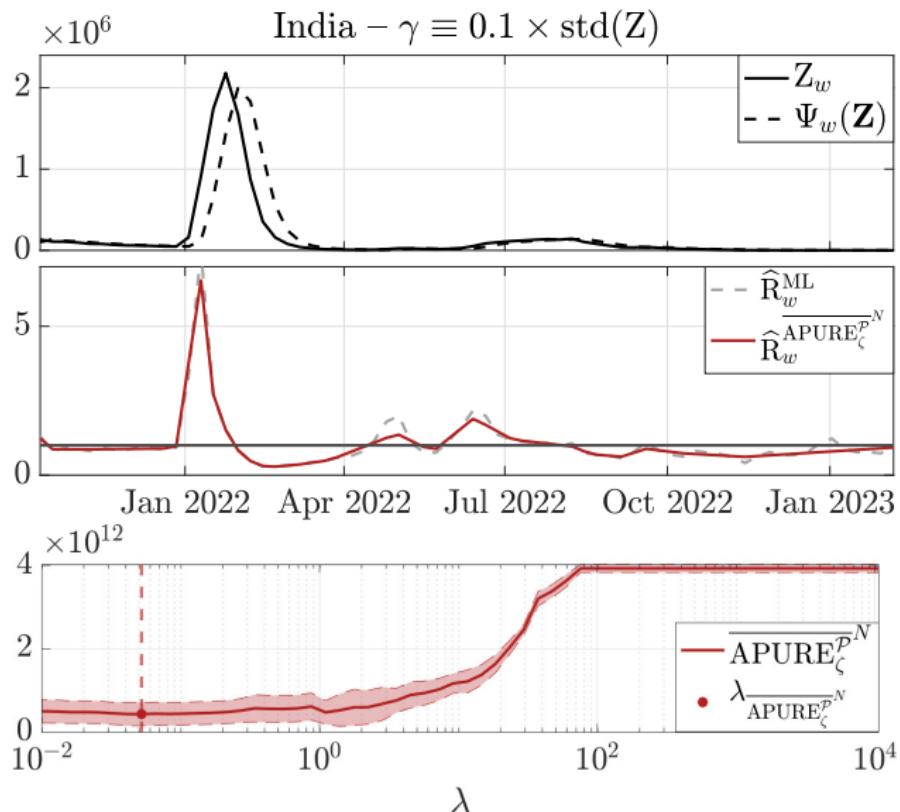
Unbiased risk estimators

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

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



Data-driven hyperparameter selection on weekly COVID-19 counts



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

Codes: github.com/bpascal-fr/APURE-Estim-Epi

Conclusion and perspectives

Inverse problem

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

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⇒ \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;
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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 $\mathcal{O}(\mathbf{y}; \theta)$.