Bilevel optimization for automated data-driven inverse problem resolution

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(bpascal-fr.github.io)

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

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Mathematics and Image Analysis (MIA'25)

Observation model

$$\boldsymbol{y} \sim \mathcal{B}\left(\boldsymbol{\Phi}\overline{\boldsymbol{x}}\right)$$

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

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Goal: Estimate $\overline{\boldsymbol{x}}$

Inverse problems in signal and image processing

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- ill-conditioned, rank deficient $\boldsymbol{\Phi}$

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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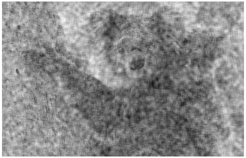
Goal: Estimate $\overline{\boldsymbol{x}}$

- ill-conditioned, rank deficient $\boldsymbol{\Phi}$
- 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

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

- $\mathcal{D}(\boldsymbol{y};\cdot) = -\log \mathbb{P}(\boldsymbol{y}|\cdot)$: negative log-likelihood   Ex: $\mathcal{D}(\boldsymbol{y};\boldsymbol{x}) = \|\boldsymbol{y}-\boldsymbol{x}\|_2^2$

No regularization

$\mathcal{R} = 0$

Variational estimator

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

- $\mathcal{D}(\boldsymbol{y};\cdot) = -\log \mathbb{P}(\boldsymbol{y}|\cdot)$: negative log-likelihood — Ex: $\mathcal{D}(\boldsymbol{y};\boldsymbol{x}) = \|\boldsymbol{y}-\boldsymbol{x}\|_2^2$
- $\mathcal{R}$: regularization term encoding a priori knowledge — Ex: $\mathcal{R}(\boldsymbol{x}) = \|\mathbf{D}_1\boldsymbol{x}\|_q^q$

(Giovannelli & Idier, 2015, *Wiley*)

No regularization

$\mathcal{R} = 0$

Smooth

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

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

Piecewise constant

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

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

Fine-tuning of the regularization parameter

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

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not enough

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not enough

$\lambda = 25$

too regularized

Hyperparameter selection: bilevel optimization

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Oracle-based hyperparameter selection

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

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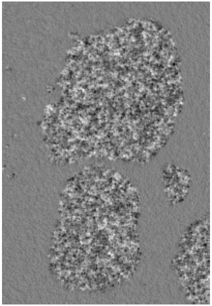
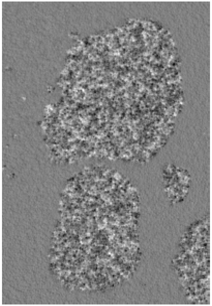
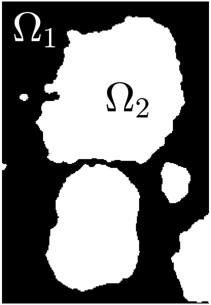
- golden case: $\mathcal{O}(\boldsymbol{y};\lambda) = \|\widehat{\boldsymbol{x}}(\boldsymbol{y};\lambda) - \overline{\boldsymbol{x}}\|^2 \Longrightarrow$ efficient bi-level $(\boldsymbol{x},\lambda)$ minimization
- practical case: ground truth $\overline{\boldsymbol{x}}$ **not available!** $\Longrightarrow$ data-driven $\mathcal{O}(\boldsymbol{y};\lambda)$

Image processing:

Texture segmentation

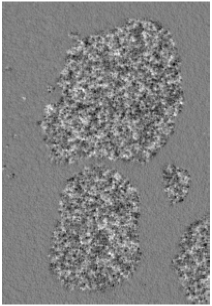


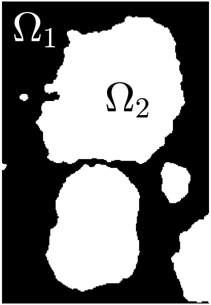




Goal: obtain a partition of the image into K homogeneous textures

$$\Omega = \Omega_1 \bigsqcup \ldots \bigsqcup \Omega_K$$





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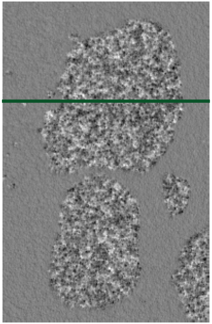
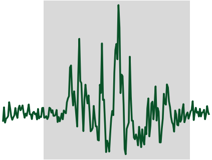
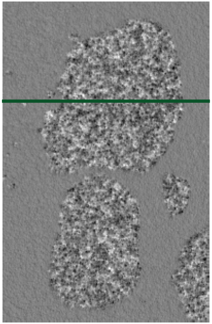
Piecewise monofractal model

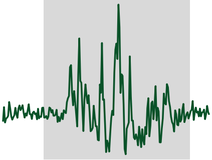




Fractal attributes

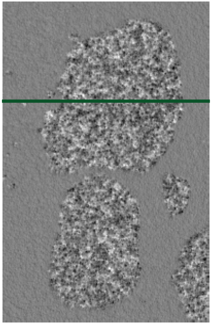
- variance σ^2 *amplitude of variations*

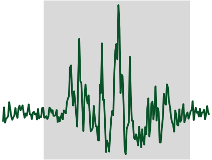




Fractal attributes

- variance σ^2 *amplitude of variations*
- local regularity h *scale invariance*





Fractal attributes

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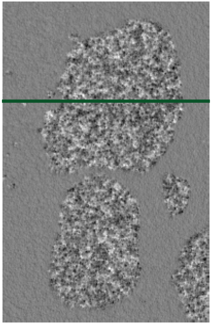
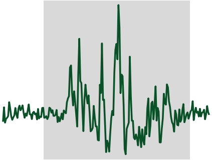
$$|f(x) - f(y)| \leq \sigma(x)|x - y|^{h(x)}$$





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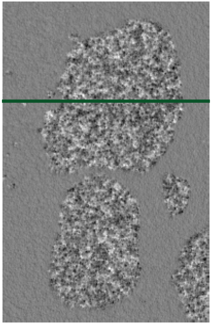
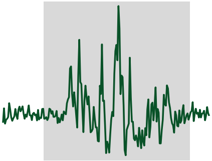
$h(x) \equiv h_1 = 0.9$ $h(x) \equiv h_2 = 0.3$





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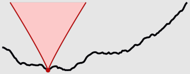

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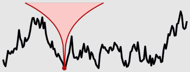

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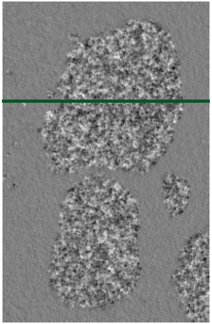

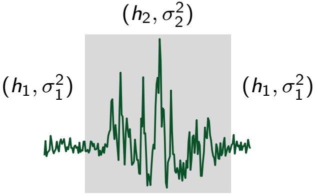

Segmentation

- σ^2 and h piecewise constant

Piecewise monofractal model

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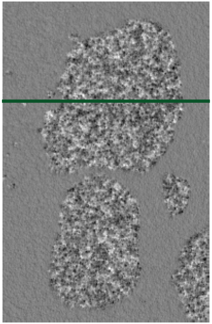
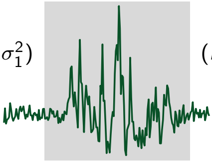
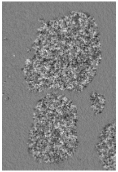




Segmentation

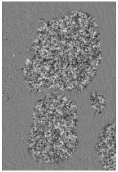
- σ^2 and h piecewise constant
- region Ω_k characterized by (σ_k^2, h_k)

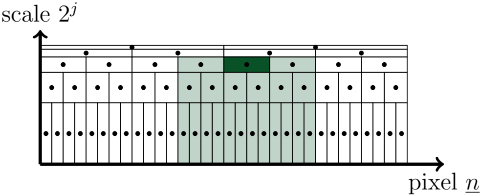
Textured image



Textured image

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





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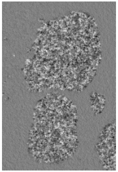
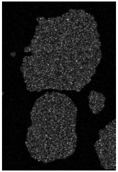


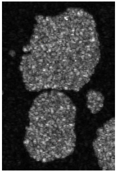
Local maximum of wavelet coefficients: $\mathcal{L}_{a,\cdot}$

Scale

$a = 2^1$

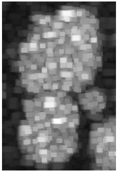


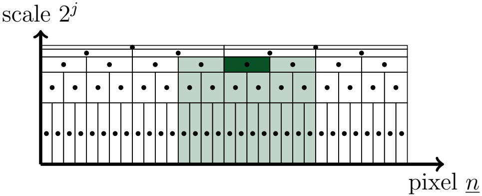
$a = 2^2$



$\ldots$

$a = 2^5$



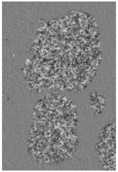


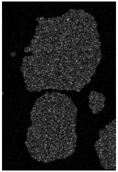
Multiscale analysis

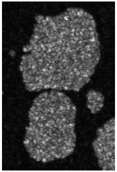
Textured image

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

Scale $a = 2^1$ $\quad a = 2^2$ $\quad \ldots \quad a = 2^5$







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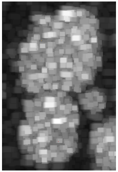
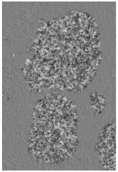


Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

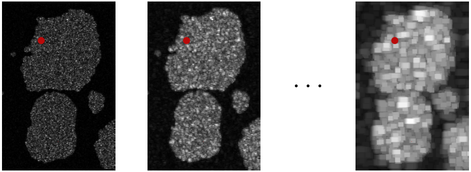
$$\log\left(\mathcal{L}_{a,\cdot}\right) \underset{a\to 0}{\simeq} \log(a) \underset{\text{regularity}}{\boldsymbol{h}} + \underset{\substack{\propto \log(\boldsymbol{\sigma}^2) \\ \text{(variance)}}}{\boldsymbol{v}}$$

Textured image



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

Scale $a = 2^1$ $a = 2^2$ $\dots$ $a = 2^5$



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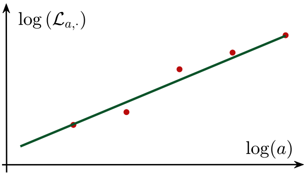

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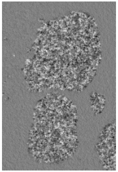

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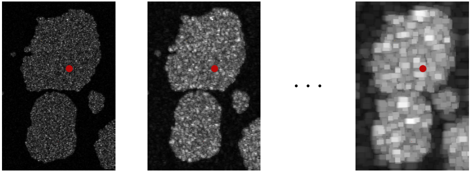

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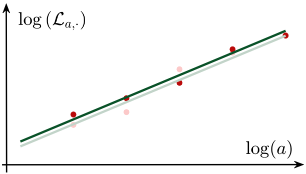

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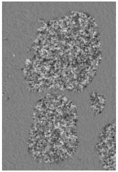

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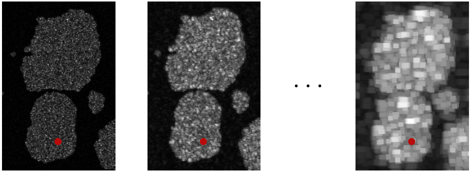

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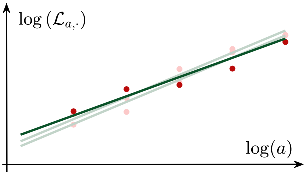

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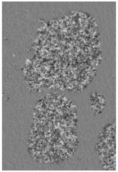

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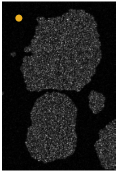
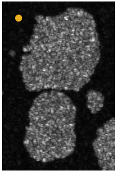
Scale

$a = 2^1$

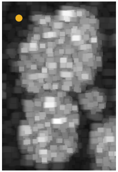


$a = 2^2$



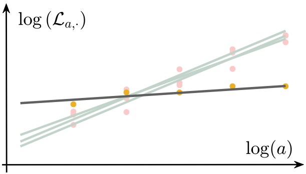
$\cdots$

$a = 2^5$



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

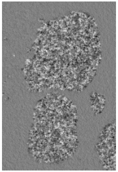
$$\log\left(\mathcal{L}_{a,\cdot}\right) \underset{a\to 0}{\simeq} \log(a) \underbrace{\boldsymbol{h}}_{\text{regularity}} + \underbrace{\boldsymbol{v}}_{\substack{\propto \log(\boldsymbol{\sigma}^2) \\ \text{(variance)}}}$$

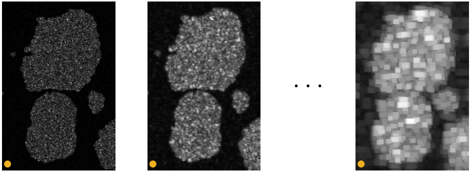


Textured image

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

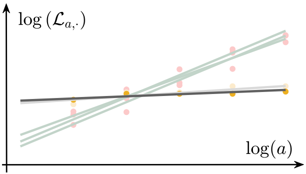
Scale $a = 2^1$ $a = 2^2$ $\dots$ $a = 2^5$





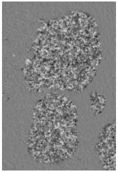
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

$$\log\left(\mathcal{L}_{a,\cdot}\right) \underset{a \to 0}{\simeq} \log(a) \underbrace{\boldsymbol{h}}_{\text{regularity}} + \underbrace{\boldsymbol{v}}_{\substack{\propto \log(\boldsymbol{\sigma}^2) \\ \text{(variance)}}}$$



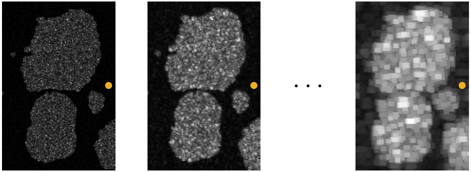
Multiscale analysis

Textured image



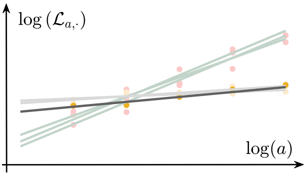
Local maximum of wavelet coefficients: $\mathcal{L}_{a,\cdot}$

Scale $a = 2^1$ $a = 2^2$ … $a = 2^5$



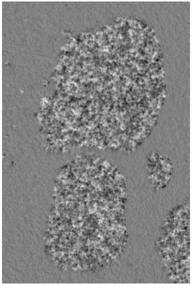
Proposition (Jaffard, 2004, *Proc. Symp. Pure Math.*; Wendt et al., 2009, *Signal Process.*)

$$\log\left(\mathcal{L}_{a,\cdot}\right) \underset{a\to 0}{\simeq} \log(a) \underbrace{\boldsymbol{h}}_{\text{regularity}} + \underbrace{\boldsymbol{v}}_{\substack{\propto \log(\boldsymbol{\sigma}^2) \\ \text{(variance)}}}$$



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

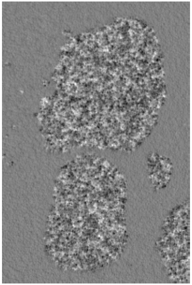
Textured image



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

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

Textured image

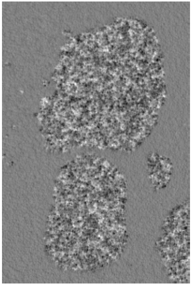


Direct punctual estimation

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

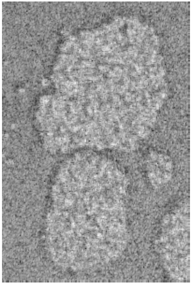
$$\left(\widehat{\boldsymbol{h}}^{\mathrm{LR}}, \widehat{\boldsymbol{v}}^{\mathrm{LR}}\right) = \underset{\boldsymbol{h},\boldsymbol{v}}{\operatorname{argmin}} \sum_{a=a_{\min}}^{a_{\max}} \left\|\log\left(\boldsymbol{\mathcal{L}}_{a,\cdot}\right) - \log(a)\boldsymbol{h} - \boldsymbol{v}\right\|^2$$

Textured image



Local regularity $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

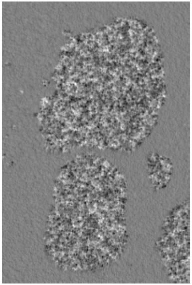
Local power $\widehat{\boldsymbol{v}}^{\mathrm{LR}}$



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

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

Textured image



Local regularity $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

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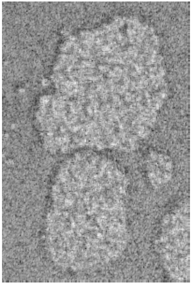
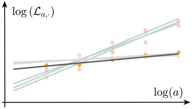


$\longrightarrow$ large estimation variance

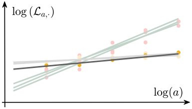
$$\underbrace{\sum_a \|\log \mathcal{L}_{a,.} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2}_{\textbf{Least-Squares}}$$

$\rightarrow$ fidelity to the log-linear model

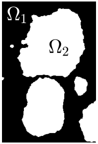


$$\underbrace{\sum_a \|\log \boldsymbol{\mathcal{L}}_{a,.} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2}_{\textbf{Least-Squares}} \quad + \quad \lambda \underbrace{\mathcal{Q}(\mathbf{D}_1\boldsymbol{h}, \mathbf{D}_1\boldsymbol{v}; \alpha)}_{\textbf{Total Variation}}$$

$\rightarrow$ fidelity to the log-linear model

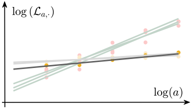


$\rightarrow$ favors piecewise constancy

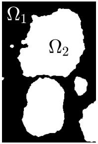


$$\underset{\boldsymbol{h},\boldsymbol{v}}{\text{minimize}} \; \underbrace{\sum_a \|\log \boldsymbol{\mathcal{L}}_{a,.} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2}_{\textbf{Least-Squares}} \; + \; \lambda \, \underbrace{\mathcal{Q}(\mathbf{D}_1\boldsymbol{h}, \mathbf{D}_1\boldsymbol{v}; \alpha)}_{\textbf{Total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

$\rightarrow$ fidelity to the log-linear model

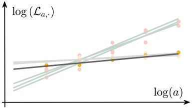


$\rightarrow$ favors piecewise constancy

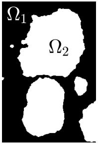


$$\underset{\boldsymbol{h},\boldsymbol{v}}{\text{minimize}} \; \sum_a \underbrace{\|\log \boldsymbol{\mathcal{L}}_{a,.} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2}_{\textbf{Least-Squares}} \; + \; \lambda \, \underbrace{\mathcal{Q}(\mathbf{D}_1 \boldsymbol{h}, \mathbf{D}_1 \boldsymbol{v}; \alpha)}_{\textbf{Total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

$\rightarrow$ fidelity to the log-linear model



$\rightarrow$ favors piecewise constancy

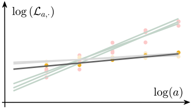


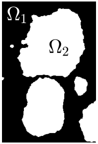
Finite differences $\mathbf{D}_1^{\rightarrow}\boldsymbol{x}$ (horizontal), $\mathbf{D}_1^{\uparrow}\boldsymbol{x}$ (vertical) at each pixel

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

$\rightarrow$ fidelity to the log-linear model

$\rightarrow$ favors piecewise constancy



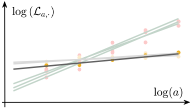


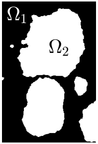
Finite differences $\mathbf{D}_1\boldsymbol{x} = \left[\mathbf{D}_1^{\rightarrow}\boldsymbol{x}, \mathbf{D}_1^{\uparrow}\boldsymbol{x}\right]$

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

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

$$\underset{\boldsymbol{h},\boldsymbol{v}}{\text{minimize}} \; \underbrace{\sum_a \|\log \mathcal{L}_{a,.} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2}_{\substack{\textbf{Least-Squares} \\ \to \text{ fidelity to the log-linear model}}} \; + \; \lambda \underbrace{\mathcal{Q}(\mathbf{D}_1\boldsymbol{h}, \mathbf{D}_1\boldsymbol{v}; \alpha)}_{\substack{\textbf{Total Variation} \\ \to \text{ favors piecewise constancy}}}$$





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

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

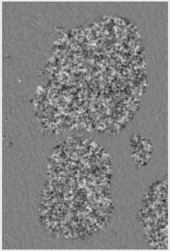
$$\mathcal{Q}_{\mathrm{F}}(\mathbf{D}_1\boldsymbol{h}, \mathbf{D}_1\boldsymbol{v}; \alpha) = \alpha\|\mathbf{D}_1\boldsymbol{h}\|_{2,1} + \|\mathbf{D}_1\boldsymbol{v}\|_{2,1}$$

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

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

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

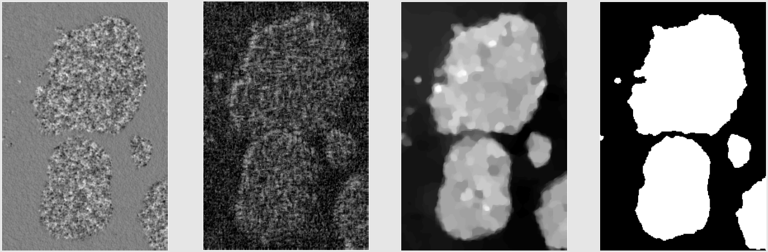
Textured image



Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

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

Textured image | Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$ | Co-localized contours $\widehat{\boldsymbol{h}}^{\mathrm{C}}$ | Threshold estimate† $T\widehat{\boldsymbol{h}}^{\mathrm{C}}$



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

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

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

Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

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

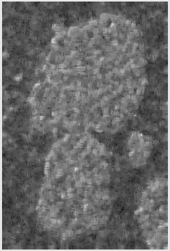
$$\left(\widehat{\boldsymbol{h}}, \widehat{\boldsymbol{v}}\right)(\boldsymbol{\mathcal{L}}; \lambda, \alpha) = \underset{\boldsymbol{h},\boldsymbol{v}}{\operatorname{argmin}} \sum_a \|\log \boldsymbol{\mathcal{L}}_{a,\cdot} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1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

Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

Co-localized contours estimate $\widehat{\boldsymbol{h}}^{\mathrm{C}}$

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

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



too small

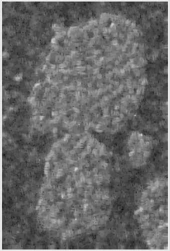
$$\left(\widehat{\boldsymbol{h}}, \widehat{\boldsymbol{v}}\right)(\boldsymbol{\mathcal{L}}; \lambda, \alpha) = \underset{\boldsymbol{h},\boldsymbol{v}}{\operatorname{argmin}} \sum_a \|\log \boldsymbol{\mathcal{L}}_{a,\cdot} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1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

Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$

Co-localized contours estimate $\widehat{\boldsymbol{h}}^{\mathrm{C}}$

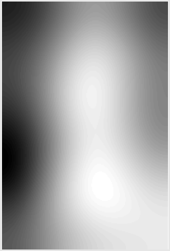
$(\lambda, \alpha) = (0, 0)$

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



too small

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

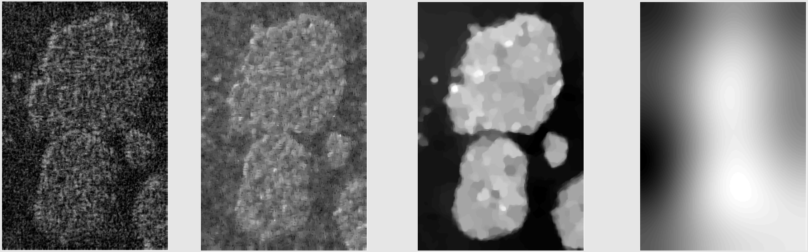


too large

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

Lin. reg. $\widehat{\boldsymbol{h}}^{\mathrm{LR}}$ | Co-localized contours estimate $\widehat{\boldsymbol{h}}^{\mathrm{C}}$

$(\lambda, \alpha) = (0, 0)$ | $(\lambda, \alpha) = (0.5, 0.5)$ | $(\lambda^\dagger, \alpha^\dagger) = (11.5, 0.8)$ | $(\lambda, \alpha) = (500, 500)$



too small | optimal | too large

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

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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

Parameter tuning (Grid search)

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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

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

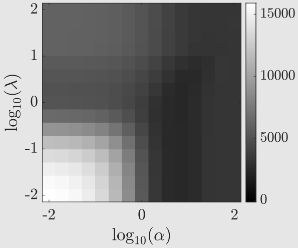
$$\mathcal{R}(\lambda, \alpha) = \left\|\widehat{\boldsymbol{h}}(\boldsymbol{\mathcal{L}}; \lambda, \alpha) - \bar{\boldsymbol{h}}\right\|^2$$

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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

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

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

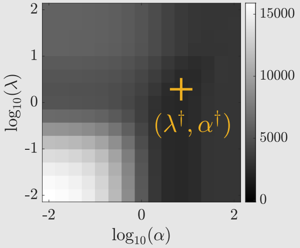


$$\left(\widehat{\boldsymbol{h}}, \widehat{\boldsymbol{v}}\right)(\boldsymbol{\mathcal{L}}; \lambda, \alpha) = \underset{\boldsymbol{h}, \boldsymbol{v}}{\operatorname{argmin}} \sum_{a} \|\log \boldsymbol{\mathcal{L}}_{a,\cdot} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

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

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

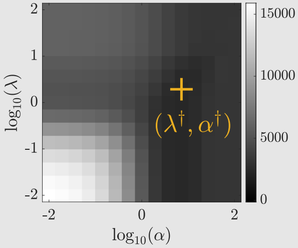


$$\left(\widehat{\boldsymbol{h}}, \widehat{\boldsymbol{v}}\right)(\boldsymbol{\mathcal{L}}; \lambda, \alpha) = \underset{\boldsymbol{h},\boldsymbol{v}}{\operatorname{argmin}} \sum_a \|\log \boldsymbol{\mathcal{L}}_{a,\cdot} - \log(a)\boldsymbol{h} - \boldsymbol{v}\|^2 + \lambda \mathcal{Q}(\mathbf{D}_1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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

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

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



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

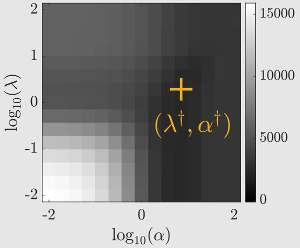
?

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

$\boldsymbol{h}$: *discriminant*, $\boldsymbol{v}$: *auxiliary*

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

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



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

?

Stein Unbiased Risk Estimate
(SURE)

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

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Parametric estimator $(\boldsymbol{y}; \lambda) \mapsto \widehat{\boldsymbol{x}}(\boldsymbol{y}; \lambda)$

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

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

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

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

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

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

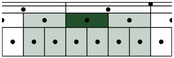
$$\widehat{R}(\boldsymbol{y}; \lambda) \triangleq \|\widehat{\boldsymbol{x}}(\boldsymbol{y}; \lambda) - \boldsymbol{y}\|^2 + 2\rho^2 \operatorname{tr}\left(\partial_{\boldsymbol{y}} \widehat{\boldsymbol{x}}(\boldsymbol{y}; \lambda)\right) - \rho^2 P$$
$$\Longrightarrow R(\lambda) = \mathbb{E}_{\boldsymbol{\zeta}}[\widehat{R}(\boldsymbol{y}; \lambda)].$$

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

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

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

$\boldsymbol{\Phi} : (\boldsymbol{h}, \boldsymbol{v}) \mapsto \{\log(a)\boldsymbol{h} + \boldsymbol{v}\}_a$



$\boldsymbol{\Pi} : (\boldsymbol{h}, \boldsymbol{v}) \mapsto (\boldsymbol{h}, \boldsymbol{0})$

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

Generalized *Stein Unbiased Risk Estimate*

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

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

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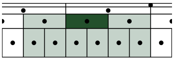


$\boldsymbol{\Pi} : (\boldsymbol{h}, \boldsymbol{v}) \mapsto (\boldsymbol{h}, \mathbf{0})$

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

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

Let $(\boldsymbol{y}; \boldsymbol{\Lambda}) \mapsto \widehat{\boldsymbol{x}}(\boldsymbol{y}; \boldsymbol{\Lambda})$ be an estimator of $\bar{\boldsymbol{x}}$

- weakly differentiable w.r.t. $\boldsymbol{y}$,
- such that $\boldsymbol{\zeta} \mapsto \langle \boldsymbol{\Pi}\widehat{\boldsymbol{x}}(\bar{\boldsymbol{x}} + \boldsymbol{\zeta}; \lambda), \mathbf{A}\boldsymbol{\zeta}\rangle$ is integrable w.r.t. $\mathcal{N}(\mathbf{0}, \boldsymbol{\mathcal{S}})$.

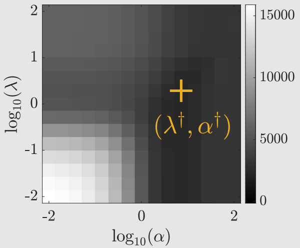
$$\widehat{R}(\boldsymbol{\Lambda}) \triangleq \|\mathbf{A}(\boldsymbol{\Phi}\widehat{\boldsymbol{x}}(\boldsymbol{y}; \boldsymbol{\Lambda}) - \boldsymbol{y})\|^2 + 2\mathrm{tr}\left(\boldsymbol{\mathcal{S}}\mathbf{A}^\top \boldsymbol{\Pi}\partial_{\boldsymbol{y}}\widehat{\boldsymbol{x}}(\boldsymbol{y}; \boldsymbol{\Lambda})\right) - \mathrm{tr}\left(\mathbf{A}\boldsymbol{\mathcal{S}}\mathbf{A}^\top\right)$$

$$\Longrightarrow R_{\boldsymbol{\Pi}}(\boldsymbol{\Lambda}) = \mathbb{E}_{\boldsymbol{\zeta}}[\widehat{R}(\boldsymbol{\Lambda})].$$

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

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

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



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

$$\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{\mathcal{L}}; \lambda, \alpha | \boldsymbol{\mathcal{S}})$$

Parameter tuning (Grid search)

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

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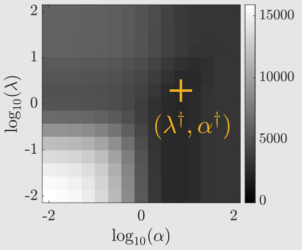

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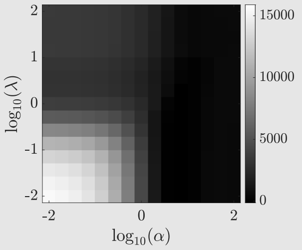

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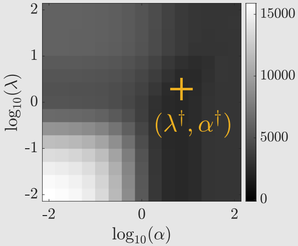

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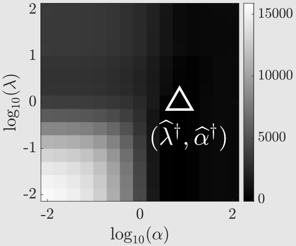

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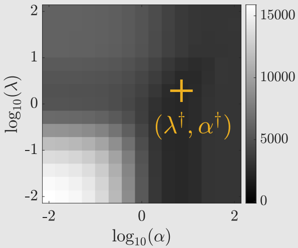

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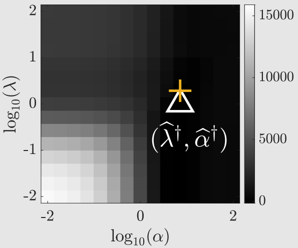

Generalized Finite Difference Monte Carlo SURE

$$\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{y};\boldsymbol{\Lambda}\,|\,\boldsymbol{\mathcal{S}}) =$$
$$\|\mathbf{A}\left(\boldsymbol{\Phi}\widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda}) - \boldsymbol{y}\right)\|^2 + \frac{2}{\nu}\left\langle \boldsymbol{\mathcal{S}}\mathbf{A}^\top \boldsymbol{\Pi}\left(\widehat{\boldsymbol{x}}(\boldsymbol{y}+\nu\boldsymbol{\varepsilon};\boldsymbol{\Lambda}) - \widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda})\right), \boldsymbol{\varepsilon}\right\rangle - \operatorname{tr}\left(\mathbf{A}\boldsymbol{\mathcal{S}}\mathbf{A}^\top\right)$$

Generalized Finite Difference Monte Carlo SUGAR

$$\partial_{\boldsymbol{\Lambda}}\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{y};\boldsymbol{\Lambda}\,|\,\boldsymbol{\mathcal{S}}) = 2\left(\mathbf{A}\boldsymbol{\Phi}\partial_{\boldsymbol{\Lambda}}\widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda})\right)^\top \mathbf{A}\left(\boldsymbol{\Phi}\widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda}) - \boldsymbol{y}\right)$$
$$+ \frac{2}{\nu}\left\langle \boldsymbol{\mathcal{S}}\mathbf{A}^\top \boldsymbol{\Pi}\left(\partial_{\boldsymbol{\Lambda}}\widehat{\boldsymbol{x}}(\boldsymbol{y}+\nu\boldsymbol{\varepsilon};\boldsymbol{\Lambda}) - \partial_{\boldsymbol{\Lambda}}\widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda})\right), \boldsymbol{\varepsilon}\right\rangle$$

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

Let $(\boldsymbol{y};\boldsymbol{\Lambda}) \mapsto \widehat{\boldsymbol{x}}(\boldsymbol{y};\boldsymbol{\Lambda})$ be an estimator of $\bar{\boldsymbol{x}}$

- uniformly-Lipschitz continuous w.r.t. $\boldsymbol{y}$
- such that $\forall \boldsymbol{\Lambda} \in \mathbb{R}^L$, $\widehat{\boldsymbol{x}}(\mathbf{0}_P;\boldsymbol{\Lambda}) = \mathbf{0}_N$,
- uniformly L-Lipschitz continuous w.r.t. $\boldsymbol{\Lambda}$, L independently of $\boldsymbol{y}$. Then

$$\partial_{\boldsymbol{\Lambda}} R_{\boldsymbol{\Pi}}(\boldsymbol{\Lambda}) = \lim_{\nu\to 0}\mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\varepsilon}}\left[\partial_{\boldsymbol{\Lambda}}\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{y};\boldsymbol{\Lambda}\,|\,\boldsymbol{\mathcal{S}})\right]$$

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

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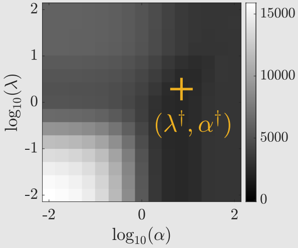
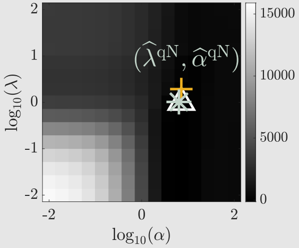


$\bar{\boldsymbol{h}}$: unknown!

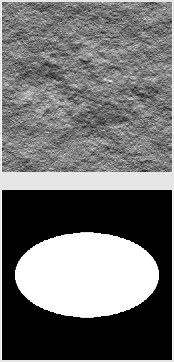
$$\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{\mathcal{L}}; \lambda, \alpha | \boldsymbol{\mathcal{S}})$$



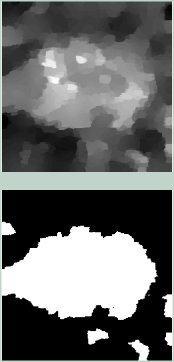
L-BFGS-B quasi-Newton algorithm: $\widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{\mathcal{L}}; \lambda, \alpha | \boldsymbol{\mathcal{S}})$ and $\partial_{\boldsymbol{\Lambda}} \widehat{R}_{\nu,\boldsymbol{\varepsilon}}(\boldsymbol{y}; \boldsymbol{\Lambda} \,|\, \boldsymbol{\mathcal{S}})$

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

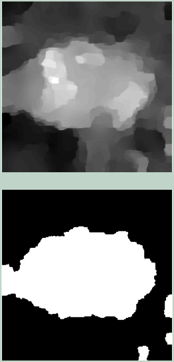
Example



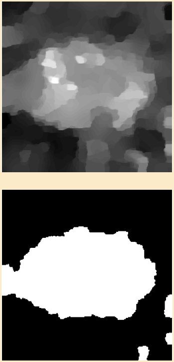
$\widehat{\boldsymbol{h}}^{\mathsf{F}}(\boldsymbol{\mathcal{L}}; \lambda^{\dagger}, \alpha^{\dagger})$
(grid)



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



$\widehat{\boldsymbol{h}}^{\mathsf{F}}(\boldsymbol{\mathcal{L}}; \widehat{\lambda}^{\mathrm{qN}}, \widehat{\alpha}^{\mathrm{qN}})$
(quasi-Newton)

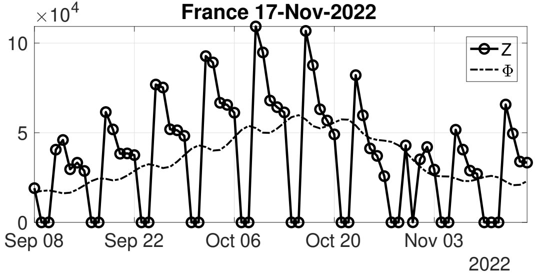


225 calls of the estimator over the grid v.s. **40** for quasi-Newton

Time series analysis:

Epidemiological indicator estimation

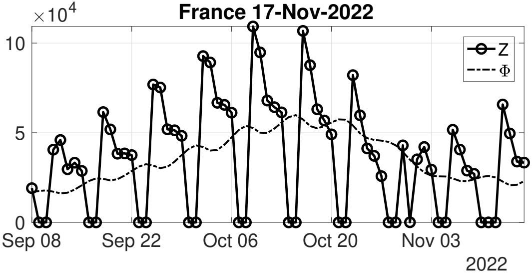
Counts of daily new infections



data from National Health Agencies collected by Johns Hopkins University

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

Counts of daily new infections



data from National Health Agencies collected by Johns Hopkins University

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

Design adapted counter measures and evaluate their effectiveness

$\longrightarrow$ efficient monitoring tools *epidemiological model,*

$\longrightarrow$ robust to low quality of the data *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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Interpretation: at day t

$\mathrm{R}_t > 1$ the virus propagates at exponential speed,

$\mathrm{R}_t < 1$ the epidemic shrinks with an exponential decay,

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$\Longrightarrow$ one single indicator accounting for the overall pandemic mechanism

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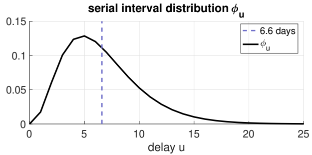
Principle: Z_t new infections at day t

$$\mathbb{E}\left[\mathrm{Z}_t\right] = \mathrm{R}_t \Phi_t, \quad \Phi_t = \sum_{u=1}^{\tau_\Phi} \phi_u \mathrm{Z}_{t-u}$$



with Φ_t global "infectiousness" in the population

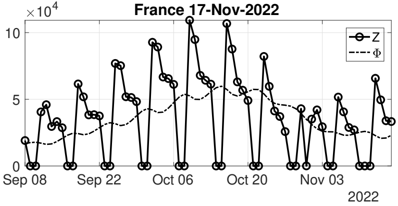
$\{\phi_u\}_{u=1}^{\tau_\Phi}$ distribution of delay between onset of symptoms in primary and secondary cases

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

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

Model: Poisson distribution

$$\mathbb{P}(\mathsf{Z}_t | \mathbf{Z}_{t-\tau_\Phi:t-1}, \mathsf{R}_t) = \frac{(\mathsf{R}_t \Phi_t)^{\mathsf{Z}_t} \mathrm{e}^{-\mathsf{R}_t \Phi_t}}{\mathsf{Z}_t!}$$



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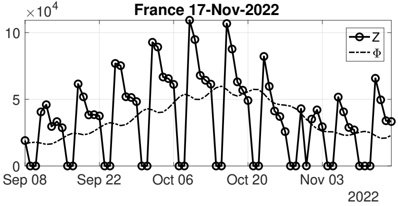

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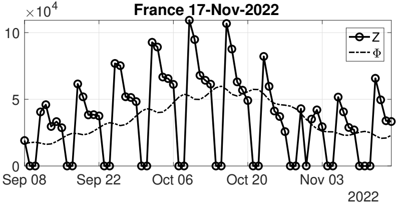
$\Longrightarrow$ At day t: $\quad \mathrm{Z}_t \sim \mathcal{P}(\mathrm{R}_t \Phi_t)$

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



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$\Longrightarrow$ At day t: $\quad \mathrm{Z}_t \sim \mathcal{P}(\mathrm{R}_t \Phi_t)$

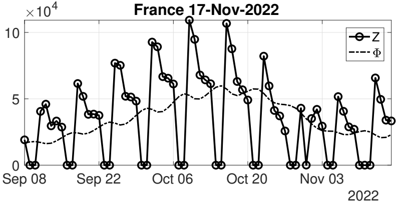
Inverse problem formalism:

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

- $\mathbf{Z} \in \mathbb{N}^T$: reported infection counts,
- $\mathbf{R} = (\mathrm{R}_1, \ldots, \mathrm{R}_T) \in \mathbb{R}_+^T$: daily unknown reproduction number,
- $\boldsymbol{\Phi} = \mathrm{diag}\left(\Phi_1, \ldots, \Phi_T\right)$: linear operator,
- $\mathcal{P}$: data-dependent Poisson noise.

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

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



Model: Poisson distribution

$$\mathbb{P}(Z_t|\mathbf{Z}_{t-\tau_\Phi:t-1}, R_t) = \frac{(R_t\Phi_t)^{Z_t} e^{-R_t\Phi_t}}{Z_t!}$$

Maximum Likelihood Estimate (MLE)

$$\begin{aligned}
&\ln\left(\mathbb{P}(Z_t|\mathbf{Z}_{t-\tau_\Phi:t-1}, R_t)\right) \\
&= Z_t \ln(R_t\Phi_t) - R_t\Phi_t - \ln(Z_t!) \\
&\underset{Z_t \gg 1}{\simeq} Z_t \ln(R_t\Phi_t) - R_t\Phi_t - Z_t\ln(Z_t) + Z_t \\
&\underset{\text{(def.)}}{=} -d_{KL}(Z_t|R_t\Phi_t) \quad \text{(Kullback-Leibler)}
\end{aligned}$$

Pandemic study: modeling at the service of monitoring

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

Model: Poisson distribution

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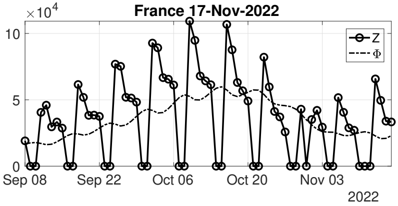

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&\quad \underset{(\text{def.})}{=} -\mathsf{d}_{\mathsf{KL}}(\mathsf{Z}_t | \mathsf{R}_t \Phi_t) \quad (\text{Kullback-Leibler})
\end{aligned}$$

$$\Longrightarrow \widehat{\mathsf{R}}_t^{\mathsf{MLE}} = \mathsf{Z}_t / \Phi_t = \mathsf{Z}_t / \sum_{u=1}^{\tau_\Phi} \phi_u \mathsf{Z}_{t-u}$$

ratio of moving averages

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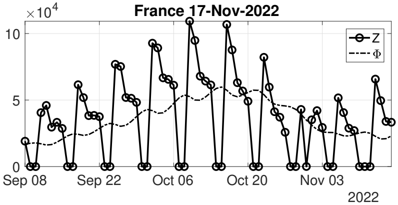

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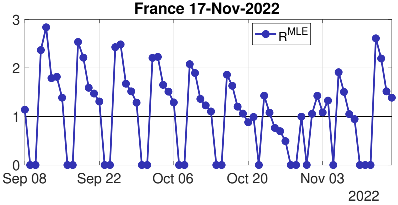

- huge variability along time/ no local trend
- not robust to pseudo-periodicity/ misreported counts

Penalized likelihood: regularization through nonlinear filtering

$$\widehat{\mathbf{R}}^{\mathsf{PKL}} = \underset{\mathbf{R}\in\mathbb{R}_+^T}{\operatorname{argmin}} \sum_{t=1}^{T} \mathsf{d}_{\mathsf{KL}}\left(\mathsf{Z}_t \,|\, \mathsf{R}_t \Phi_t\right) + \lambda \mathcal{R}(\mathbf{R}) \quad \text{(penalized Kullback-Leibler)}$$

with $\mathcal{R}(\mathbf{R})$ favoring some temporal regularity (Abry et al., 2020, *PLOSOne*)

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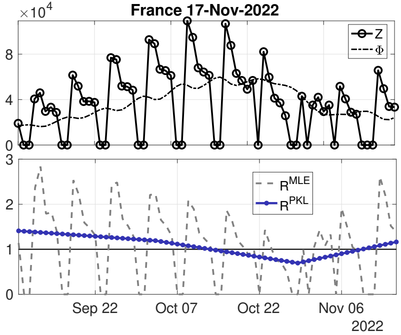
$$\mathcal{R}(\mathbf{R}) = \|\mathbf{D}_2\mathbf{R}\|_1$$

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

2nd order derivative & ℓ_1-norm

$\Longrightarrow$ piecewise linearity



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

Penalized Kullback-Leibler estimator:

$$\widehat{\mathbf{R}}(\mathbf{Z};\lambda) = \operatorname*{argmin}_{\mathbf{R}\in\mathbb{R}_+^T} \sum_{t=1}^{T} \mathrm{d}_{\mathrm{KL}}\left(\mathrm{Z}_t \,|\, \mathrm{R}_t \Phi_t\right) + \lambda \|\mathbf{D}_2\mathbf{R}\|_1$$

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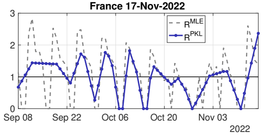
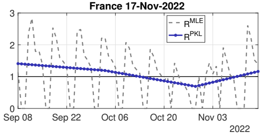
Fine tuning of the regularization parameter:

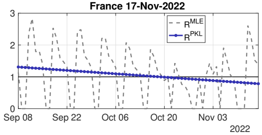
$\lambda = 3.5$



$\boldsymbol{\lambda^\dagger = 50}$



$\lambda = 250$



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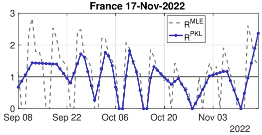

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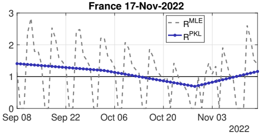

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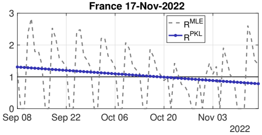

Data-driven oracle minimization

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

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

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Reminder: $\mathbf{Z} \sim \mathcal{P}\left(\boldsymbol{\Phi}\mathbf{R}\right)$

- $\mathbf{Z} \in \mathbb{N}^T$: reported infection counts,
- $\mathbf{R} = (\mathrm{R}_1, \ldots, \mathrm{R}_T) \in \mathbb{R}_+^T$: daily unknown reproduction number,
- $\boldsymbol{\Phi} = \mathrm{diag}\left(\Phi_1, \ldots, \Phi_T\right)$: linear operator,
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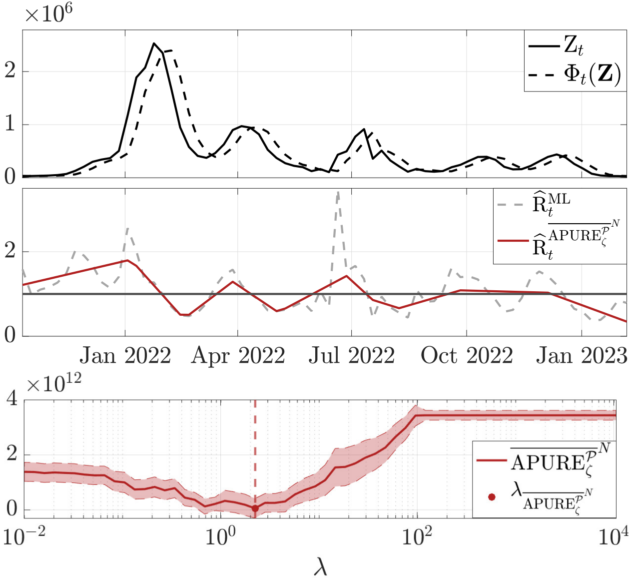
Autoregressive **P**oisson **U**nbiased **R**isk **E**stimate (APURE)



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

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

Inverse problem $\boldsymbol{y} \sim \mathcal{B}\left(\boldsymbol{\Phi}\overline{\boldsymbol{x}}\right)$

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Data-driven parameter selection

$\Longrightarrow$ $\mathcal{O}$: 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.*)

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Extensions and perspectives

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