Proximal schemes for the estimation of the reproduction number of Covid19:

From convex optimization to Monte Carlo sampling

ACM Seminar

Heriot-Watt University

June 13, 2025

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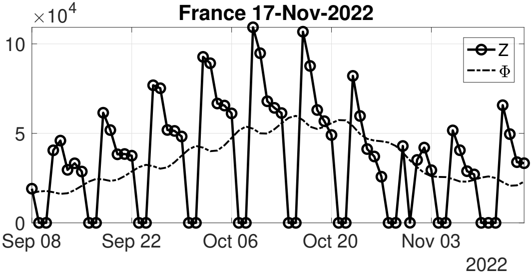
Joint work with P. Abry, N. Pustelnik, S. Roux, R. Gribonval, P. Flandrin;
G. Fort, H. Artigas; Juliana Du

Outline

- Pandemic study: modeling at the service of monitoring
- Reproduction number estimation from minimization of penalized likelihood
- Bayesian framework for credibility interval estimation
- Summary and recent works

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**

Pandemic study: modeling at the service of monitoring

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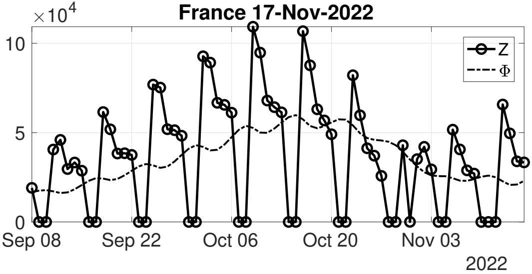

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$\Longrightarrow$ number of cases not informative enough: need to capture the **dynamics**

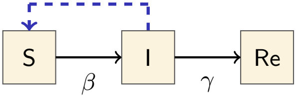
Design adapted counter measures and evaluate their effectiveness

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

$\longrightarrow$ robust to low quality of the data *managing erroneous counts,*

$\longrightarrow$ accompanied by reliable confidence level *credibility intervals.*

Susceptible-Infected-Recovered (SIR), among *compartmental models*



– ODE: $\frac{\mathrm{d}\mathsf{S}_t}{\mathrm{d}t} = -\beta \mathsf{S}_t \mathsf{I}_t$, $\frac{\mathrm{d}\mathsf{I}_t}{\mathrm{d}t} = \beta \mathsf{S}_t \mathsf{I}_t - \gamma \mathsf{I}_t$, $\frac{\mathrm{d}\mathsf{Re}_t}{\mathrm{d}t} = \gamma \mathsf{I}_t$

– Stochastic model: likelihood maximization to infer β, γ

Pandemic study: modeling at the service of monitoring

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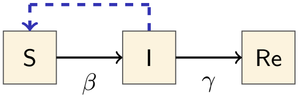

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– Stochastic model: likelihood maximization to infer β, γ

Limitations:

- refinement needed to get socially realistic model
- quadratic increase of the number of parameters
- Bayesian framework: heavy computational burden
- need consolidated and accurate datasets

✗ not adapted to real-time monitoring of Covid19 pandemic

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,

$\mathrm{R}_t = 1$ the epidemic is stable.

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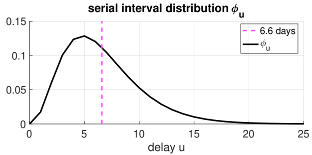
Principle: Z_t new infections at day t

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

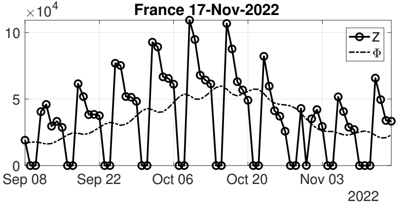


with Φ_t global "infectiousness" in the population

$\{\phi_u\}_{u=1}^{\tau_\Phi}$ 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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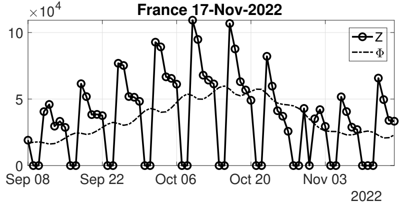

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Maximum Likelihood Estimate (MLE)

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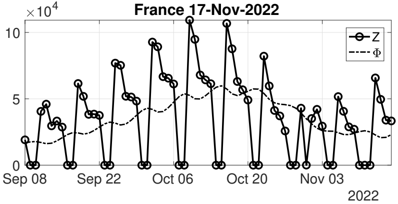

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$$\Longrightarrow \widehat{R}_t^{\text{MLE}} = Z_t / \Phi_t = Z_t / \sum_{u=1}^{\tau_\Phi} \phi_u Z_{t-u}$$

ratio of moving averages

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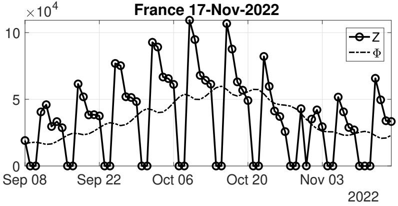

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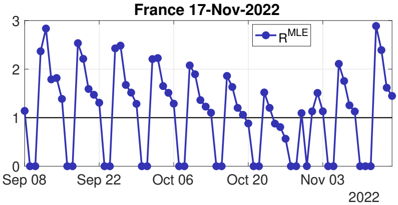


– huge variability along time/ no local trend

– not robust to pseudo-periodicity/ misreported counts

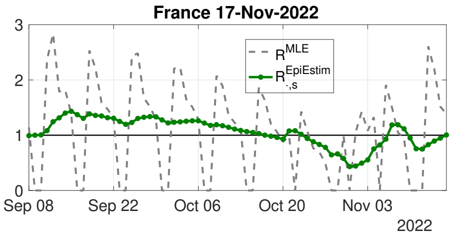
State-of-the-art: smooth regularization over a temporal window

$$\widehat{\mathrm{R}}_{t,s}^{\mathrm{EpiEstim}}, \text{ with } s = 7 \text{ days}$$

(Cori et al., 2013, *Am. Journal of Epidemiology*)

EpiEstim: Estimate Time Varying Reproduction Numbers from Epidemic Curves

Tools to quantify transmissibility throughout an epidemic from the analysis of time series of incidence as described in Cori et al. (2013)



(re-implemented in Matlab following Cori et al., 2013, *Am. Journal of Epidemiology*)

$\Longrightarrow$ smoother than naive MLE but hampered by low quality data and dependent on s

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Solution 1: regularization through nonlinear filtering

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

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

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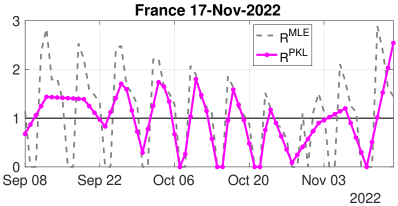
$$\mathcal{P}(\mathbf{R}) = \|\mathbf{D}_2\mathbf{R}\|_1$$

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

2nd order derivative & ℓ_1-norm

$\Longrightarrow$ piecewise linearity

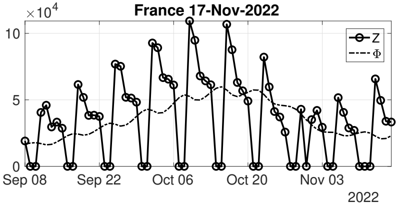


captures global **trend**, more **regular** than MLE, but **pseudo-oscillations**

New infection counts **Z** are corrupted by

- missing samples,
- non meaningful negative counts,
- retrospected cumulated counts,
- pseudo-seasonality effects.

$\Longrightarrow$ full parametric modeling out of reach



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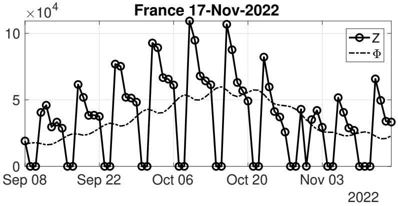

Solution 1': first correct $\mathbf{Z}$, then apply penalized Kullback-Leibler on corrected $\mathbf{Z}^{(C)}$

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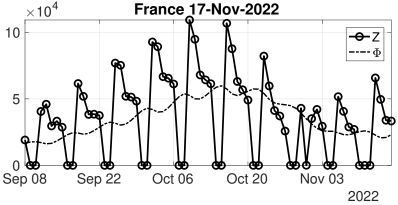

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Solution 2: **one-step** procedure performing jointly

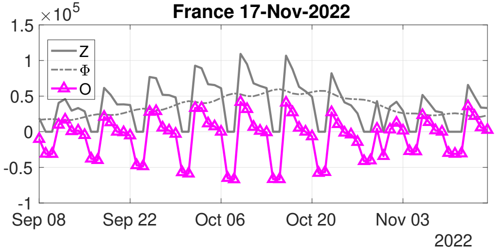
correction of corrupted Z_t & estimation of regularized R_t

(Pascal et al., 2022, *Trans. Sig. Process.*)

Extended Cori Model: additional latent variable O_t accounting for misreport

$$\mathrm{Z}_t \sim \mathrm{Poiss}\left(\mathrm{R}_t\Phi_t + \mathrm{O}_t\right), \quad \mathrm{R}_t\Phi_t + \mathrm{O}_t \geq 0$$

nonzero values of O_t concentrated on specific days (Sundays, day-offs, ...)



Interpretation:

$$\mathrm{Poiss}\left(\mathrm{R}_t\Phi_t + \mathrm{O}_t\right) \sim \begin{cases} \mathrm{Poiss}\left(\mathrm{R}_t\Phi_t\right) + \mathrm{Poiss}\left(\mathrm{O}_t\right) & \text{if } \mathrm{O}_t \geq 0, \\ \mathrm{Poiss}\left(\alpha_t\mathrm{R}_t\Phi_t\right), \ \alpha_t = 1 - \frac{-\mathrm{O}_t}{\mathrm{R}_t\Phi_t} \in [0,1] & \text{if } \mathrm{O}_t < 0. \end{cases}$$

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

Model: corrected Poisson $\quad \mathbb{P}(Z_t | \mathbf{Z}_{t-\tau_\Phi:t-1}, R_t, O_t) = \dfrac{(R_t \Phi_t + O_t)^{Z_t} \mathrm{e}^{-(R_t \Phi_t + O_t)}}{Z_t!}$

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Generalized Penalized Kullback-Leibler

$$(\widehat{\mathbf{R}}, \widehat{\mathbf{O}}) \in \underset{(\mathbf{R},\mathbf{O}) \in \mathbb{R}_+^T \times \mathbb{R}^T}{\operatorname{Argmin}} \sum_{t=1}^{T} \mathrm{d}_{\mathrm{KL}}\left(Z_t \,|\, R_t\Phi_t + O_t\right) + \lambda_{\mathrm{R}} \|\mathbf{D}_2\mathbf{R}\|_1 + \iota_{\geq 0}(\mathbf{R}) + \lambda_{\mathrm{O}} \|\mathbf{O}\|_1$$

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properties of the objective function:

- sum of convex functions composed with linear operators $\Longrightarrow$ globally convex;
- feasible domain: $(\forall t, R_t \geq 0)$ & (if $Z_t > 0, R_t\Phi_t + O_t > 0$, else $R_t\Phi_t + O_t \geq 0$);
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Theorem (Pascal et al., 2022, *Trans. Sig. Process.*)

+ The minimization problem has at least one solution $(\widehat{\mathbf{R}}, \widehat{\mathbf{O}})$.
+ The estimated time-varying Poisson intensity $\widehat{p}_t = \widehat{R}_t \Phi_t + \widehat{O}_t$ is unique.

$$\underset{(\mathbf{R},\mathbf{O})\in\mathbb{R}_+^T\times\mathbb{R}^T}{\text{minimize}} \sum_{t=1}^{T} \mathrm{d}_{\mathrm{KL}}\left(\mathrm{Z}_t \,|\, \mathrm{R}_t\Phi_t + \mathrm{O}_t\right) + \lambda_{\mathrm{R}}\|\mathbf{D}_2\mathbf{R}\|_1 + \iota_{\geq 0}(\mathbf{R}) + \lambda_{\mathrm{O}}\|\mathbf{O}\|_1$$

- each term of the functional is convex;
- ℓ_1-norm and indicative function $\Longrightarrow$ nonsmooth; ✗ gradient descent
- gradient of $\mathrm{p}_t \mapsto \mathrm{d}_{\mathrm{KL}}\left(\mathrm{Z}_t \,|\, \mathrm{p}_t\right)$ is not Lipschitzian; ✗ forward-backward
- linear operator $\mathbf{D}_2 \Longrightarrow$ no explicit form for $\mathrm{prox}_{\|\mathbf{D}_2\cdot\|_1}$ ♣ need splitting

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$$\Longleftrightarrow \underset{(\mathbf{R},\mathbf{O})\in\mathbb{R}_+^T\times\mathbb{R}^T}{\text{minimize}} \quad f(\mathbf{R},\mathbf{O}|\mathbf{Z}) + h(\mathbf{A}(\mathbf{R},\mathbf{O})), \quad \mathbf{A} \text{ linear; } f, h \text{ proximable}$$

$$\mathbf{A}(\mathbf{R},\mathbf{O}) = (\lambda_{\mathrm{R}}\mathbf{D}_2\mathbf{R}, \mathbf{R}, \lambda_{\mathrm{O}}\mathbf{O})\,; \quad h\,(\mathbf{Q}_1,\mathbf{Q}_2,\mathbf{Q}_3) = \|\mathbf{Q}_1\|_1 + \iota_{\geq 0}(\mathbf{Q}_2) + \|\mathbf{Q}_3\|_1$$

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Primal-dual algorithm (Chambolle et al., 2011, *Int. Conf. Comput. Vis.*)

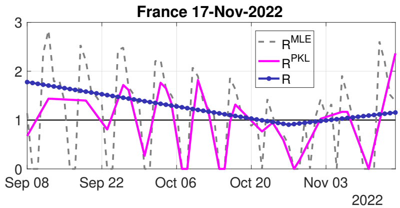
for $k = 1, 2 \ldots$ **do**

$$\mathbf{Q}^{[k+1]} = \mathrm{prox}_{\sigma h^*}(\mathbf{Q}^{[k]} + \sigma\mathbf{A}(\overline{\mathbf{R}}^{[k]}, \overline{\mathbf{O}}^{[k]})) \qquad \text{dual}$$

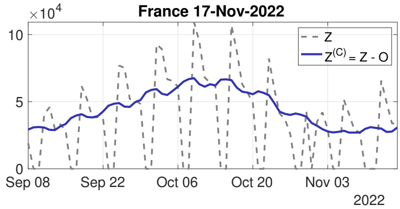
$$(\mathbf{R}^{[k+1]}, \mathbf{O}^{[k+1]}) = \mathrm{prox}_{\tau f(\cdot|\mathbf{Z})}((\mathbf{R}^{[k+1]}, \mathbf{O}^{[k+1]}) - \tau\mathbf{A}^*\mathbf{Q}^{[k+1]}) \qquad \text{primal}$$

$$(\overline{\mathbf{R}}^{[k+1]}, \overline{\mathbf{O}}^{[k+1]}) = 2(\mathbf{R}^{[k+1]}, \mathbf{O}^{[k+1]}) - (\mathbf{R}^{[k]}, \mathbf{O}^{[k]}) \qquad \text{auxiliary}$$

Reproduction number $\widehat{\mathbf{R}}$



Corrected infection counts $\mathbf{Z}^{(C)}$



$\Longrightarrow$ no more pseudo-seasonality, local trends well captured, smooth behavior

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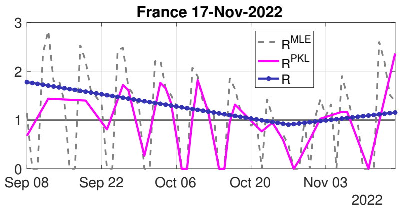

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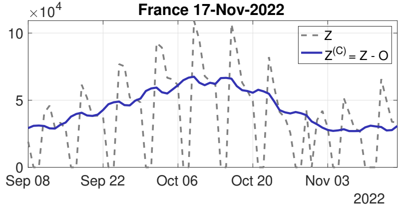

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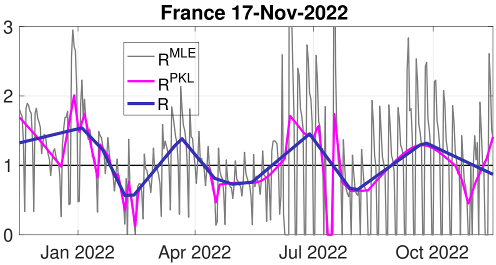

fast numerical scheme: 15 to 30 sec for 70 days to 1 year

New infection counts per county: $\mathbf{Z} = \left\{ \mathrm{Z}_t^{(d)},\, d \in [1, D],\, t \in [1,\, T] \right\}$

$\Rightarrow$ multivariate time-varying reproduction number $\mathrm{R}_t^{(d)}$

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Multivariate extended penalized Kullback-Leibler

$$\left(\widehat{\mathbf{R}}, \widehat{\mathbf{O}}\right) = \underset{(\mathbf{R},\mathbf{O}) \in \mathbb{R}_+^{D \times T} \times \mathbb{R}^{D \times T}}{\operatorname{argmin}} \sum_{d=1}^{D} \sum_{t=1}^{T} \mathsf{d}_{\mathsf{KL}} \left(\mathsf{Z}_t^{(d)} \,\middle|\, \mathsf{R}_t^{(d)} \Phi_t^{(d)} + \mathsf{O}_t^{(d)} \right)$$
$$+ \lambda_{\mathsf{R}} \|\mathbf{D}_2 \mathbf{R}\|_1 + \iota_{\geq 0}(\mathbf{R}) + \lambda_{\text{space}} \|\mathbf{G}\mathbf{R}\|_1 + \lambda_{\mathsf{O}} \|\mathbf{O}\|_1$$

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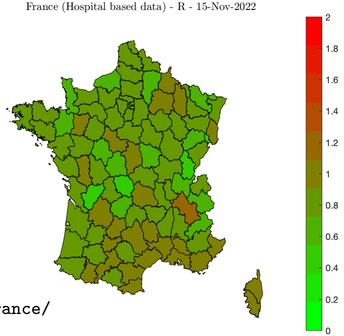
Graph Total Variation

$$\|\mathbf{G}\mathbf{R}\|_1 = \sum_{t=1}^{T} \sum_{d_1 \sim d_2} \left| \mathrm{R}_t^{(d_1)} - \mathrm{R}_t^{(d_2)} \right|$$

sum over neighboring counties

here: $d_1 \sim d_2 \Leftrightarrow$ share terrestrial border

$$\widetilde{\mathbf{A}}(\mathbf{R}, \mathbf{O}) = (\lambda_{\mathrm{R}} \mathbf{D}_2 \mathbf{R}, \mathbf{R}, \lambda_{\text{space}} \mathbf{G}\mathbf{R}, \lambda_{\mathrm{O}} \mathbf{O})$$



http://barthes.enssib.fr/coronavirus/cartes/RFrance/

Pointwise estimate of parameter $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$ from observations $\mathbf{Z}$

$$\underset{\boldsymbol{\theta} \in \mathbb{R}_+^T \times \mathbb{R}^T}{\text{minimize}} \quad f(\boldsymbol{\theta}|\mathbf{Z}) + h(\mathbf{A}\boldsymbol{\theta}) \quad \text{(Pascal et al., 2022, \textit{Trans. Sig. Process.})}$$

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Q: what is the value of R today? **A:** solve the minimization problem and output $\widehat{\mathrm{R}}_T$.

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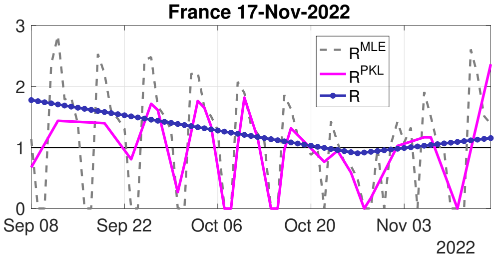

$\widehat{\mathrm{R}}_T = 1.2955$

Bayesian framework for credibility interval estimation

Pointwise estimate of parameter $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$ from observations $\mathbf{Z}$

$$\underset{\boldsymbol{\theta} \in \mathbb{R}_+^T \times \mathbb{R}^T}{\text{minimize}} \quad f(\boldsymbol{\theta}|\mathbf{Z}) + h(\mathbf{A}\boldsymbol{\theta})$$ (Pascal et al., 2022, *Trans. Sig. Process.*)

Bayesian reformulation: interpret $(\widehat{\mathbf{R}}, \widehat{\mathbf{O}})$ as the MAP of

$$\pi(\boldsymbol{\theta}) \propto \exp(-f(\boldsymbol{\theta}|\mathbf{Z}) - h(\mathbf{A}\boldsymbol{\theta}))$$

- $\exp(-f(\boldsymbol{\theta}|\mathbf{Z})) \sim$ likelihood of the observation
- $\exp(-h(\mathbf{A}\boldsymbol{\theta})) \sim$ prior on the parameter of interest

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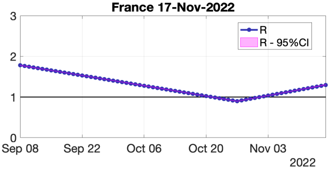
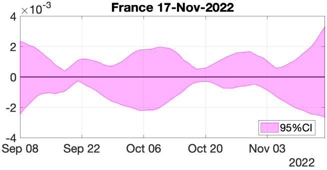
$\Longrightarrow$ instead of focusing on $\widehat{\mathrm{R}}_t$, the **pointwise** MAP, probe π to get

$\mathrm{R}_t \in [\underline{\mathrm{R}}_t, \overline{\mathrm{R}}_t]$ with 95% probability, i.e., **credibility interval** estimates





$$\widehat{\mathrm{R}}_T \in [1.2987, 1.3047]$$

Log-likelihood from Poisson model $\mathcal{D} = \{\boldsymbol{\theta} \,|\, \forall t,\ \ \mathsf{R}_t\Phi_t + \mathsf{O}_t \geq 0,\ \mathsf{R}_t \geq 0\}$

$$f(\boldsymbol{\theta}\,|\mathbf{Z}) := \begin{cases} -\sum_{t=1}^{T}(\mathsf{Z}_t \ln(\mathsf{R}_t\Phi_t + \mathsf{O}_t) - (\mathsf{R}_t\Phi_t + \mathsf{O}_t) + \mathcal{C}(\mathsf{Z}_t)) & \text{if } \boldsymbol{\theta} \in \mathcal{D}, \\ \infty & \text{otherwise,} \end{cases}$$

Bayesian framework for credibility interval estimation

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Prior distribution of $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O}) = (\mathsf{R}_1, \ldots, \mathsf{R}_T, \mathsf{O}_1, \ldots, \mathsf{O}_T) \in (\mathbb{R}_+)^T \times \mathbb{R}^T$

- reproduction number: $\mathsf{R}_t - 2\mathsf{R}_{t-1} + \mathsf{R}_{t-2} \sim \mathrm{Laplace}(\lambda_{\mathsf{R}})$

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$$\Rightarrow g(\boldsymbol{\theta}) = \lambda_{\mathsf{R}} \|\mathbf{D}_2\mathbf{R}\|_1 + \lambda_{\mathsf{O}} \|\mathbf{O}\|_1, \quad \mathbf{D}_2 = \underbrace{\frac{1}{\sqrt{6}} \begin{bmatrix} 1 & -2 & 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & -2 & 1 & 0 & \ldots & 0 \\ \ldots & & & & & & \ldots \\ 0 & \ldots & & & 1 & -2 & 1 \end{bmatrix}}_{\text{Laplacian}}$$

Bayesian framework for credibility interval estimation

Log-likelihood from Poisson model $\mathcal{D} = \{\boldsymbol{\theta} \,|\, \forall t,\;\; \mathsf{R}_t\Phi_t + \mathsf{O}_t \geq 0,\;\; \mathsf{R}_t \geq 0\}$

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Posterior distribution of unknown parameters $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$

$$\pi(\boldsymbol{\theta}) \propto \exp\left(-f(\boldsymbol{\theta}) - g(\boldsymbol{\theta})\right) \mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$$

- f, g convex
- f smooth, g nonsmooth

Purpose: sampling the random variable $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O}) \in \mathbb{R}^{2T}$ according to the posterior[†]

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[†] π is defined up to a normalizing constant

Markov Chain Monte Carlo sampling

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Principle: 1) generate a random sequence $\{\boldsymbol{\theta}^n,\, n \in \mathbb{N}\}$ such that

- $\boldsymbol{\theta}^{n+1}$ only depends on $\boldsymbol{\theta}^n$,
- at convergence, i.e., as $n \to \infty$, $\boldsymbol{\theta}^n \sim \pi$,

2) compute Bayesian estimators, e.g., credibility intervals, on samples $\{\boldsymbol{\theta}^n,\, n \geq N\}$

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Simple and very general approach: *Hastings-Metropolis random walk*

(i) propose a random move according to

$$\boldsymbol{\theta}^{n+\frac{1}{2}} = \boldsymbol{\theta}^n + \sqrt{2\gamma}\Gamma\xi^{n+1}, \quad \xi^{n+1} \sim \mathcal{N}_{2T}(0, \mathrm{I})$$

with γ positive step size, $\Gamma \in \mathbb{R}^{2T\times 2T}$

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(ii) accept: $\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^{n+\frac{1}{2}}$, with probability $1 \wedge \dfrac{\pi(\boldsymbol{\theta}^{n+\frac{1}{2}})}{\pi(\boldsymbol{\theta}^n)}$, or reject: $\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^n$

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Metropolis Adjusted Langevin Algorithm (MALA)

Langevin dynamics: $\boldsymbol{\theta}^{n+\frac{1}{2}} = \mu(\boldsymbol{\theta}^n) + \sqrt{2\gamma}\xi^{n+1}$, (Kent, 1978, *Adv Appl Probab*)

$$\mu(\boldsymbol{\theta}) \text{ adapted to } \pi(\boldsymbol{\theta}) = \exp(-f(\boldsymbol{\theta}) - g(\boldsymbol{\theta}))\mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$$

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Case 1: $g = 0$ and $-\ln \pi = f$ is smooth (Roberts & Tweedie, 1996, *Bernoulli*)

$$\mu(\boldsymbol{\theta}) = \boldsymbol{\theta} - \gamma \Gamma\Gamma^\top \nabla f(\boldsymbol{\theta}) = \boldsymbol{\theta} + \gamma \Gamma\Gamma^\top \nabla \ln \pi(\boldsymbol{\theta})$$

$\Longrightarrow$ move towards areas of higher probability

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Case 2: $-\ln \pi = f + g$ is nonsmooth

$$\mu(\boldsymbol{\theta}) = \operatorname{prox}_{\gamma g}^{\Gamma\Gamma^\top}\left(\boldsymbol{\theta} - \gamma \Gamma\Gamma^\top \nabla f(\boldsymbol{\theta})\right)$$

combining *Langevin* and *proximal*[†] approaches

[†] $\operatorname{prox}_{\gamma g}^{\Gamma\Gamma^\top}(y) = \underset{x\in\mathbb{R}^d}{\operatorname{argmin}} \left(\frac{1}{2}\|x-y\|^2_{\Gamma\Gamma^\top} + \gamma g(x)\right)$: preconditioned proximity operator of g

Posterior density of $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$: $\quad \pi(\boldsymbol{\theta}) \propto \exp\left(-f(\boldsymbol{\theta}) - g(\boldsymbol{\theta})\right) \mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$

- smooth negative log-likelihood

$$\text{if } \boldsymbol{\theta} \in \mathcal{D}, \quad f(\boldsymbol{\theta}) = -\sum_{t=1}^{T} \left(\mathsf{Z}_t \ln \mathsf{p}_t(\boldsymbol{\theta}) - \mathsf{p}_t(\boldsymbol{\theta})\right), \quad \mathsf{p}_t(\boldsymbol{\theta}) = \mathsf{R}_t(\Phi \mathsf{Z})_t + \mathsf{O}_t$$

- nonsmooth convex lower-semicontinuous negative a priori log-distribution

$$g(\boldsymbol{\theta}) = \lambda_{\mathsf{R}} \|\mathbf{D}_2\mathbf{R}\|_1 + \lambda_{\mathsf{O}} \|\mathbf{O}\|_1 = h(\mathbf{A}\boldsymbol{\theta})$$

$\mathbf{A} : \boldsymbol{\theta} \mapsto (\mathbf{D}_2\mathbf{R}, \mathbf{O})$ linear operator, $h(\cdot_1, \cdot_2) = \lambda_{\mathsf{R}} \|\cdot_1\|_1 + \lambda_{\mathsf{O}} \|\cdot_2\|_1$

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Case 3: $-\ln \pi = f + h(\mathbf{A}\cdot)$ (Fort et al., 2022, *preprint*)

closed-form expression of $\mathrm{prox}_{\gamma h}$ but not of $\mathrm{prox}_{\gamma h(\mathbf{A}\cdot)}$

1) extend $\mathbf{A}$ into **invertible** $\overline{\mathbf{A}}$, and h in $\bar{h}$ such that $\bar{h}(\overline{\mathbf{A}}\boldsymbol{\theta}) = h(\mathbf{A}\boldsymbol{\theta})$

2) reason on the **dual** variable $\tilde{\boldsymbol{\theta}} = \overline{\mathbf{A}}\boldsymbol{\theta}$

Proximal-Gradient dual sampler PGdual

Langevin: drift toward higher probability regions

$$\underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmax}} \ln \pi(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\boldsymbol{\theta}) + \bar{h}(\overline{\mathbf{A}}\boldsymbol{\theta}) = \mathbf{A}^{-1} \underset{\tilde{\boldsymbol{\theta}}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\overline{\mathbf{A}}^{-1}\tilde{\boldsymbol{\theta}}) + \bar{h}(\tilde{\boldsymbol{\theta}})$$

Proximal-Gradient dual sampler `PGdual`

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Two strategies to extend $\mathbf{A} = \begin{pmatrix} \mathbf{D}_2 & 0 \\ 0 & \mathbf{I} \end{pmatrix} \in \mathbb{R}^{(2T-1)\times 2T}$ into $\overline{\mathbf{A}} = \begin{pmatrix} \overline{\mathbf{D}} & 0 \\ 0 & \mathbf{I} \end{pmatrix} \in \mathbb{R}^{2T\times 2T}$:

Langevin: drift toward higher probability regions

$$\underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmax}} \ln \pi(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\boldsymbol{\theta}) + \bar{h}(\overline{\mathbf{A}}\boldsymbol{\theta}) = \mathbf{A}^{-1} \underset{\tilde{\boldsymbol{\theta}}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\overline{\mathbf{A}}^{-1}\tilde{\boldsymbol{\theta}}) + \bar{h}(\tilde{\boldsymbol{\theta}})$$

$$\Longrightarrow \quad \mu(\boldsymbol{\theta}) = \underbrace{\overline{\mathbf{A}}^{-1}}_{\text{back to } \boldsymbol{\theta}} \underbrace{\operatorname{prox}_{\gamma\bar{h}}\left(\overline{\mathbf{A}}\boldsymbol{\theta} - \gamma\overline{\mathbf{A}}^{-\top}\nabla f(\boldsymbol{\theta})\right)}_{\text{proximal-gradient on } \tilde{\boldsymbol{\theta}}}$$

Two strategies to extend $\mathbf{A} = \begin{pmatrix} \mathbf{D}_2 & 0 \\ 0 & \mathrm{I} \end{pmatrix} \in \mathbb{R}^{(2T-1)\times 2T}$ into $\overline{\mathbf{A}} = \begin{pmatrix} \overline{\mathbf{D}} & 0 \\ 0 & \mathrm{I} \end{pmatrix} \in \mathbb{R}^{2T\times 2T}$:

Invert

$$\overline{\mathbf{D}}_2 := \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -2/\sqrt{5} & 1/\sqrt{5} & 0 & \cdots & 0 \\ & \mathbf{D}_2 & & & \end{bmatrix}$$

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$$\overline{\mathbf{D}}_2 := \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -2/\sqrt{5} & 1/\sqrt{5} & 0 & \cdots & 0 \\ & \mathbf{D}_2 & & & \end{bmatrix}$$

Ortho

$$\overline{\mathbf{D}}_o := \begin{bmatrix} v_1^\top \\ v_2^\top \\ \mathbf{D}_2 \end{bmatrix} \qquad \begin{gathered} v_1, v_2 \in \mathbb{R}^{2T} \\ v_1 \perp v_2,\ v_1, v_2 \in (\mathbf{D}_2^\top)^\perp \end{gathered}$$

Langevin: drift toward higher probability regions

$$\underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmax}} \ln \pi(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\boldsymbol{\theta}) + \bar{h}(\overline{\mathbf{A}}\boldsymbol{\theta}) = \mathbf{A}^{-1} \underset{\tilde{\boldsymbol{\theta}}\in\mathbb{R}^{2T}}{\operatorname{argmin}}\ f(\overline{\mathbf{A}}^{-1}\tilde{\boldsymbol{\theta}}) + \bar{h}(\tilde{\boldsymbol{\theta}})$$

$$\Longrightarrow \quad \mu(\boldsymbol{\theta}) = \underbrace{\overline{\mathbf{A}}^{-1}}_{\text{back to } \boldsymbol{\theta}} \ \underbrace{\operatorname{prox}_{\gamma\bar{h}}\left(\overline{\mathbf{A}}\boldsymbol{\theta} - \gamma\overline{\mathbf{A}}^{-\top}\nabla f(\boldsymbol{\theta})\right)}_{\text{proximal-gradient on } \tilde{\boldsymbol{\theta}}}$$

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Proposed PGdual **drift terms** on $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$:

reproduction numbers $\mu_{\mathrm{R}}(\boldsymbol{\theta}) = \overline{\mathbf{D}}^{-1} \operatorname{prox}_{\gamma_{\mathrm{R}}\lambda_{\mathrm{R}}\|(\cdot)_{3:T}\|_1}\left(\overline{\mathbf{D}}\,\mathbf{R} - \gamma_{\mathrm{R}}\overline{\mathbf{D}}^{-\top}\nabla_{\mathrm{R}} f(\boldsymbol{\theta})\right)$

outliers $\mu_{\mathrm{O}}(\boldsymbol{\theta}) = \operatorname{prox}_{\gamma_{\mathrm{O}}\lambda_{\mathrm{O}}\|\cdot\|_1}\left(\mathbf{O} - \gamma_{\mathrm{O}}\nabla_{\mathrm{O}} f(\boldsymbol{\theta})\right)$

Data: $\overline{\mathbf{D}} = \overline{\mathbf{D}}_2$ (`Invert`) or $\overline{\mathbf{D}} = \overline{\mathbf{D}}_o$ (`Ortho`)

$\gamma_{\mathrm{R}}, \gamma_{\mathrm{O}} > 0$, $N_{\max} \in \mathbb{N}_\star$, $\boldsymbol{\theta}^0 = (\mathbf{R}^0, \mathbf{O}^0) \in \mathcal{D}$

Result: A $\mathcal{D}$-valued sequence $\{\boldsymbol{\theta}^n = (\mathbf{R}^n, \mathbf{O}^n), n \in 0, \ldots, N_{\max}\}$

for $n = 0, \ldots, N_{\max} - 1$ **do**

Sample $\xi_{\mathrm{R}}^{n+1} \sim \mathcal{N}_T(0, \mathrm{I})$ and $\xi_{\mathrm{O}}^{n+1} \sim \mathcal{N}_T(0, \mathrm{I})$;

Set $\mathbf{R}^{n+\frac{1}{2}} = \mu_{\mathrm{R}}(\boldsymbol{\theta}^n) + \sqrt{2\gamma_{\mathrm{R}}}\,\overline{\mathbf{D}}^{-1}\overline{\mathbf{D}}^{-\top}\,\xi_{\mathrm{R}}^{n+1}$;

$\mathbf{O}^{n+\frac{1}{2}} = \mu_{\mathrm{O}}(\boldsymbol{\theta}^n) + \sqrt{2\gamma_{\mathrm{O}}}\,\xi_{\mathrm{O}}^{n+1}$;

$\boldsymbol{\theta}^{n+\frac{1}{2}} = (\mathbf{R}^{n+\frac{1}{2}}, \mathbf{O}^{n+\frac{1}{2}})$;

Set $\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^{n+\frac{1}{2}}$ with probability

$$1 \wedge \frac{\pi(\boldsymbol{\theta}^{n+\frac{1}{2}})}{\pi(\boldsymbol{\theta}^n)} \frac{q_{\mathrm{R}}(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{\theta}_{\mathrm{R}}^n)}{q_{\mathrm{R}}(\boldsymbol{\theta}^n, \boldsymbol{\theta}_{\mathrm{R}}^{n+\frac{1}{2}})} \frac{q_{\mathrm{O}}(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{\theta}_{\mathrm{O}}^n)}{q_{\mathrm{O}}(\boldsymbol{\theta}^n, \boldsymbol{\theta}_{\mathrm{O}}^{n+\frac{1}{2}})},$$

$q_{\mathrm{R/O}}$: Gaussian kernel stemming from nonsymmetric proposal

and $\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^n$ otherwise.

Algorithm 1: Proximal-Gradient dual: `PGdual Invert` and `PGdual Ortho`

Gaussian proposal: $\theta^{n+\frac{1}{2}} = \mu(\theta^n) + \sqrt{2\gamma}\Gamma\xi^{n+1}$

- random walks: $\mu(\theta) = \theta$

  `RW`: $\Gamma = \mathrm{I}$; `RW Invert`: $\Gamma = \overline{\mathbf{D}}_2^{-1}\overline{\mathbf{D}}_2^{-\top}$; `RW Ortho`: $\Gamma = \overline{\mathbf{D}}_o^{-1}\overline{\mathbf{D}}_o^{-\top}$

- Proximal-Gradient dual: $\mu_{\mathrm{R}}(\theta)$, $\mu_{\mathrm{O}}(\theta)$, $\Gamma = \overline{\mathbf{D}}^{-1}\overline{\mathbf{D}}^{-\top}$

  `PGdual Invert`: $\overline{\mathbf{D}} = \overline{\mathbf{D}}_2$; `PGdual Ortho`: $\overline{\mathbf{D}} = \overline{\mathbf{D}}_o$

Practical settings: $N_{\max} = 10^7$ iterations, 15 independent runs

Comparison of MCMC sampling schemes

Gaussian proposal: $\boldsymbol{\theta}^{n+\frac{1}{2}} = \mu(\boldsymbol{\theta}^n) + \sqrt{2\gamma}\Gamma\xi^{n+1}$

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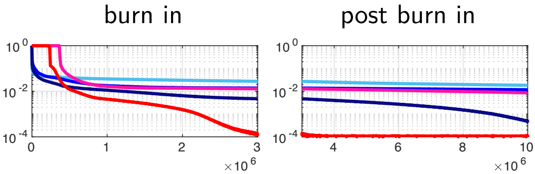
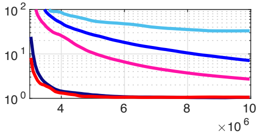
Practical settings: $N_{\max} = 10^7$ iterations, 15 independent runs

log-density



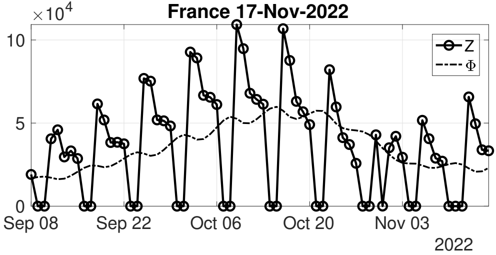
$\left(\ln \pi(\boldsymbol{\theta}^n) - \max \ln \pi\right) / \left(\ln \pi(\boldsymbol{\theta}^0) - \max \ln \pi\right)$

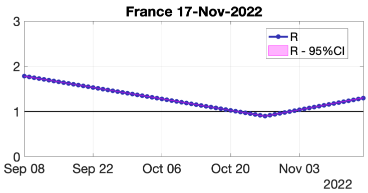
Gelman-Rubin

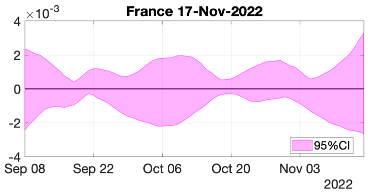


ANOVA-type criterion

Sanitary situation in France







Summary: optimization and sampling to estimate R_t

- Extended Cori model handling erroneous reported counts via a latent variable

$$\mathsf{Z}_t | \mathbf{Z}_{t-\tau_\Phi:t-1}, \mathsf{R}_t, \mathsf{O}_t \sim \mathrm{Poiss}(\mathsf{R}_t \Phi_t + \mathsf{O}_t)$$

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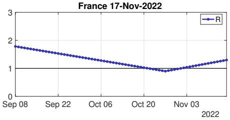
- Estimation of piecewise linear R_t and corrected counts via convex optimization

$$\underset{(\mathbf{R},\mathbf{O})\in\mathbb{R}_+^T\times\mathbb{R}^T}{\mathrm{minimize}} \sum_{t=1}^{T} \mathrm{d}_{\mathrm{KL}}\left(\mathrm{Z}_t \,|\, \mathrm{R}_t\Phi_t + \mathrm{O}_t\right) + \lambda_{\mathrm{R}}\|\mathbf{D}_2\mathbf{R}\|_1 + \iota_{\geq 0}(\mathbf{R}) + \lambda_{\mathrm{O}}\|\mathbf{O}\|_1$$



$\widehat{\mathrm{R}}_T = 1.1959$

(Pascal et al., 2022, *Trans. Sig. Process.*;)

Summary: optimization and sampling to estimate R_t

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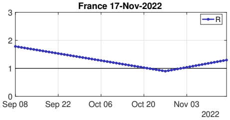
- Bayesian credibility interval estimates via proximal Langevin MCMC samplers



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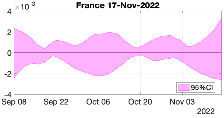
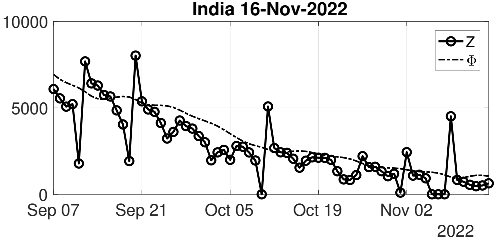


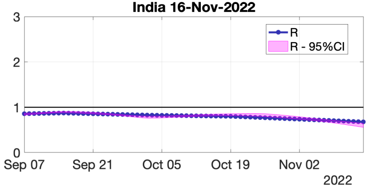
$\widehat{R}_T \in [1.1978, 1.2016]$

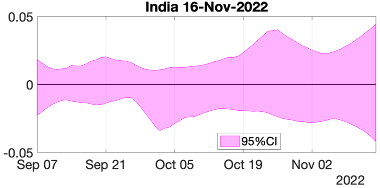
(Pascal et al., 2022, *Trans. Sig. Process.*; Fort et al., 2023, *Trans. Sig. Process.*)

PGdual credibility interval estimation of the reproduction number

Worldwide Covid19 monitoring







Why not United Kingdom?

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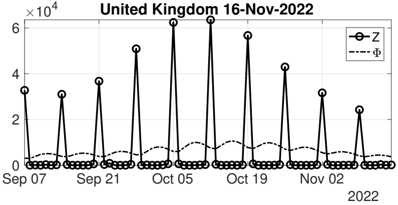
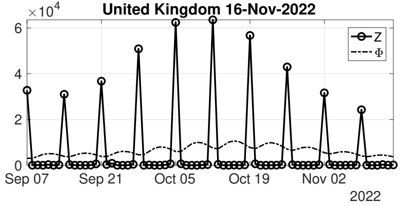


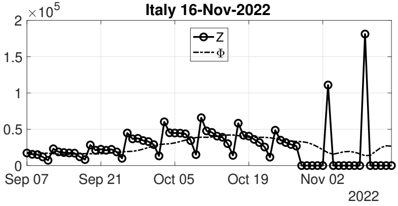
rate of erroneous counts: $6/7$!

Why not United Kingdom?



rate of erroneous counts: $6/7$!

And Italy?

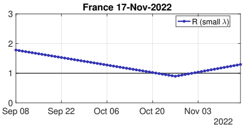


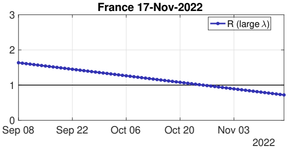
seems to adopt the same reporting rate ...

$\Longrightarrow$ call for new tools, robust to very scarce data

Selection of regularization parameters λ_R, λ_O

$$\underset{(\mathbf{R},\mathbf{O})\in\mathbb{R}_+^T\times\mathbb{R}^T}{\text{minimize}} \sum_{t=1}^{T} \mathrm{d_{KL}}\left(\mathrm{Z}_t \mid \mathrm{R}_t\Phi_t + \mathrm{O}_t\right) + \lambda_\mathrm{R}\|\mathbf{D}_2\mathbf{R}\|_1 + \iota_{\geq 0}(\mathbf{R}) + \lambda_\mathrm{O}\|\mathbf{O}\|_1$$





Reporting on a **weekly** basis: Z_t at week t

$$Z_t \mid Z_1, \ldots, Z_{t-1} \sim \alpha \mathcal{P}\left(\frac{\Phi_t(\mathbf{Z}) R_t}{\alpha}\right)$$

$\Phi_t(\mathbf{Z}) = \sum_{s \geq 1} \varphi_s Z_{t-s}$ with φ the **weekly** serial interval distribution

Pascal & Vaiter, *Preprint arXiv:2409.14937*, 2024
Codes: github.com/bpascal-fr/APURE-Estim-Epi

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Scaling parameter $\alpha > 1$: larger variance of Z_t

$\Longrightarrow$ better accounts for intrinsic variability

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Estimation of R_t from weekly aggregated counts

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

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

Strategy: Unbiased Risk Estimate $\mathbb{E}_{\mathbf{Z}}\left[\mathcal{O}(\mathbf{Z}; \lambda)\right] = \mathbb{E}_{\mathbf{Z}}\left[\|\widehat{\mathbf{R}}(\mathbf{Z}; \lambda) - \overline{\mathbf{R}}\|_2^2\right]$

$$\lambda_{\overline{\mathsf{APURE}_{\zeta}^{\mathcal{P}}}^N} \in \underset{\lambda \in \mathbb{R}_+}{\operatorname{Argmin}} \ \overline{\mathsf{APURE}_{\zeta}^{\mathcal{P}}}^N(\mathbf{Z}; \lambda)$$

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

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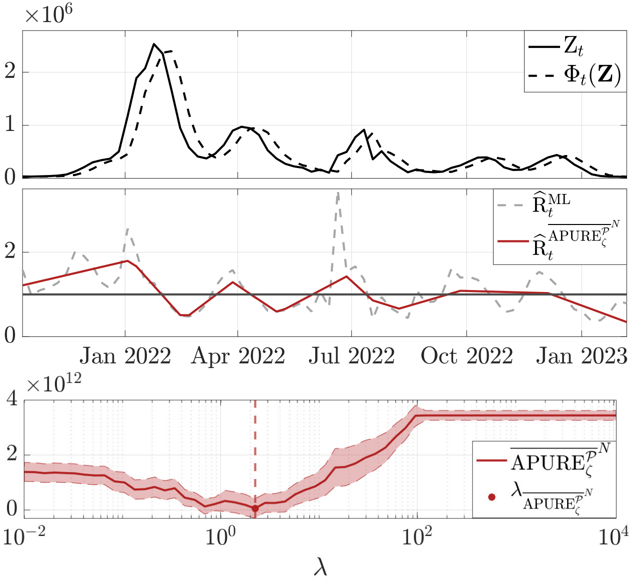
Estimation of R_t from weekly aggregated counts



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

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Prior distribution of $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O}) = (\mathsf{R}_1, \ldots, \mathsf{R}_T, \mathsf{O}_1, \ldots, \mathsf{O}_T) \in (\mathbb{R}_+)^T \times \mathbb{R}^T$

- reproduction number: $\mathsf{R}_t - 2\mathsf{R}_{t-1} + \mathsf{R}_{t-2} \sim \mathrm{Laplace}(\lambda_\mathsf{R})$
- outliers $\mathsf{O}_t \sim \mathrm{Laplace}(\lambda_\mathsf{O})$

Conjugated **Gamma prior** on both λ_R and λ_O: $\Gamma(\alpha_\mathsf{R}, \beta_\mathsf{R})$ and $\Gamma(\alpha_\mathsf{O}, \beta_\mathsf{O})$

`MCMC` **sampler targeting $\pi(\mathbf{R}, \mathbf{O}, \underline{\lambda})$** (Abry et al., 2025, ICASSP)

Data: $\mathbf{Z}, \Phi$; **Parameters:** $(\alpha_\mathsf{R}, \beta_\mathsf{R}, \alpha_\mathsf{O}, \beta_\mathsf{O})$, k_{max}

for $k = 0, \ldots, k_{\max} - 1$ **do**

 # Sample $\mathbf{R}, \mathbf{O}$ *at fixed* $\underline{\lambda}^{(k)}$

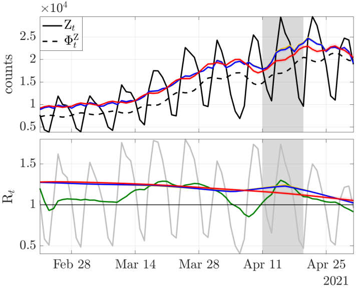
$\mathbf{R}^{(k+1)}, \mathbf{O}^{(k+1)} \sim \mathtt{PGdual}(\mathbf{R}^{(k)}, \mathbf{O}^{(k)}; \underline{\lambda}^{(k)})$

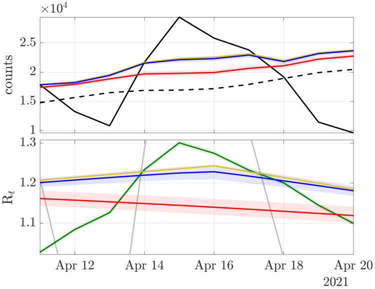
 # Sample $\underline{\lambda}$ *at fixed* $\mathbf{R}^{(k+1)}, \mathbf{O}^{(k+1)}$

$\lambda_\mathsf{R}^{(k+1)} \sim \Gamma(T + \alpha_\mathsf{R}, \|\mathbf{D}_2 \mathbf{R}^{(k+1)} + \delta\| + \beta_\mathsf{R})$

$\lambda_\mathsf{O}^{(k+1)} \sim \Gamma(T + \alpha_\mathsf{O}, \|\mathbf{O}^{(k+1)}\| + \beta_\mathsf{O})$

Germany, from February 21, 2021 to May 1, 2021





$\mathbf{R}^{\mathsf{MLE}}$: Maximum Likelihood Estimate

$\mathbf{R}^{\mathsf{EpiEstim}}$ and 95% CIs

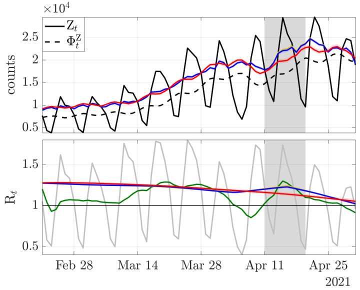
$\mathbf{R}^{\mathsf{MAP}}$ and $\mathbf{Z}-\mathbf{O}^{\mathsf{MAP}}$

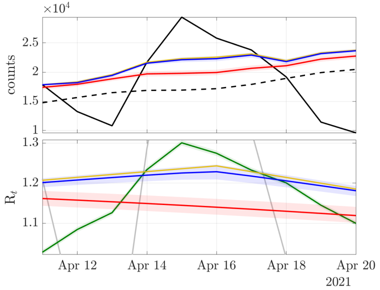
$\widehat{\mathbf{R}}^{\mathsf{Mean\,(PG)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\mathsf{Mean\,(PG)}}$ and 95% CIs

$\widehat{\mathbf{R}}^{\mathsf{Mean\,(H)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\mathsf{Mean\,(H)}}$ and 95% CIs

Hierarchical Bayesian Model for COVID-19 propagation

Germany, from February 21, 2021 to May 1, 2021





$\mathbf{R}^{\text{MLE}}$: Maximum Likelihood Estimate

$\mathbf{R}^{\text{EpiEstim}}$ and 95% CIs

$\mathbf{R}^{\text{MAP}}$ and $\mathbf{Z}-\mathbf{O}^{\text{MAP}}$

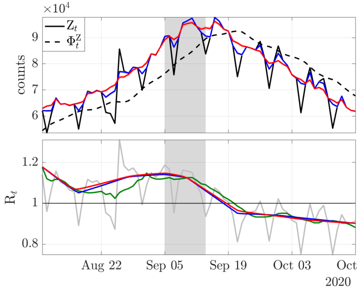
$\widehat{\mathbf{R}}^{\text{Mean (PG)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\text{Mean (PG)}}$ and 95% CIs

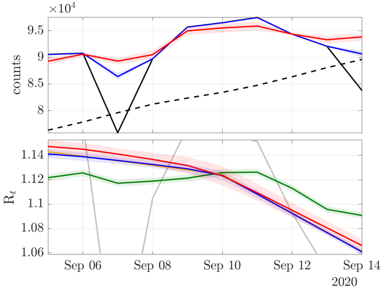
$\widehat{\mathbf{R}}^{\text{Mean (H)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\text{Mean (H)}}$ and 95% CIs

Area covered by the Credibility Intervals

	EpiEstim	PGdual	Hierarchical
India	0.42	0.40 ± 0.01	0.58 ± 0.01
Germany	1.09	1.56 ± 0.02	2.13 ± 0.01
France	0.36	0.46 ± 0.01	1.35 ± 0.07
South Korea	0.82	0.79 ± 0.03	0.89 ± 0.01

India, from August 9, 2020 to October 17, 2020





$\mathbf{R}^{\mathrm{MLE}}$: Maximum Likelihood Estimate

$\mathbf{R}^{\mathrm{EpiEstim}}$ and 95% CIs

$\mathbf{R}^{\mathrm{MAP}}$ and $\mathbf{Z} - \mathbf{O}^{\mathrm{MAP}}$

$\widehat{\mathbf{R}}^{\mathrm{Mean\,(PG)}}$, $\mathbf{Z} - \widehat{\mathbf{O}}^{\mathrm{Mean\,(PG)}}$ and 95% CIs

$\widehat{\mathbf{R}}^{\mathrm{Mean\,(H)}}$, $\mathbf{Z} - \widehat{\mathbf{O}}^{\mathrm{Mean\,(H)}}$ and 95% CIs

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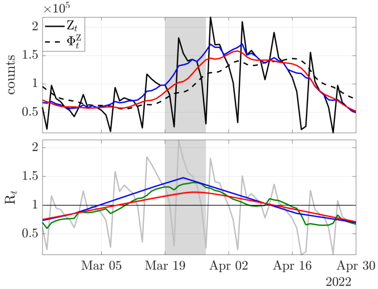
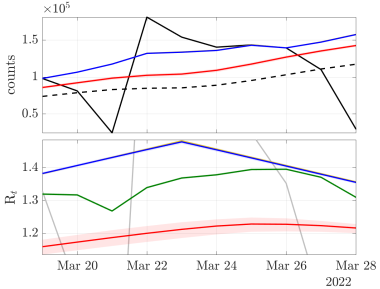
France, from February 20, 2022 to April 20, 2022





$\mathbf{R}^{\mathrm{MLE}}$: Maximum Likelihood Estimate

$\mathbf{R}^{\mathrm{EpiEstim}}$ and 95% CIs

$\mathbf{R}^{\mathrm{MAP}}$ and $\mathbf{Z} - \mathbf{O}^{\mathrm{MAP}}$

$\widehat{\mathbf{R}}^{\mathrm{Mean\,(PG)}}$, $\mathbf{Z} - \widehat{\mathbf{O}}^{\mathrm{Mean\,(PG)}}$ and 95% CIs

$\widehat{\mathbf{R}}^{\mathrm{Mean\,(H)}}$, $\mathbf{Z} - \widehat{\mathbf{O}}^{\mathrm{Mean\,(H)}}$ and 95% CIs

Area covered by the Credibility Intervals

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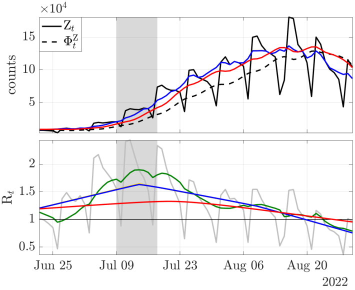
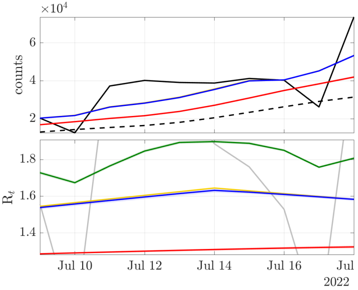
South Korea	0.82	0.79 ± 0.03	0.89 ± 0.01

South Korea, from June 22, 2022 to August 30, 2022





$\mathbf{R}^{\mathrm{MLE}}$: Maximum Likelihood Estimate
$\mathbf{R}^{\mathrm{EpiEstim}}$ and 95% CIs
$\mathbf{R}^{\mathrm{MAP}}$ and $\mathbf{Z}-\mathbf{O}^{\mathrm{MAP}}$

$\widehat{\mathbf{R}}^{\mathrm{Mean\,(PG)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\mathrm{Mean\,(PG)}}$ and 95% CIs
$\widehat{\mathbf{R}}^{\mathrm{Mean\,(H)}}$, $\mathbf{Z}-\widehat{\mathbf{O}}^{\mathrm{Mean\,(H)}}$ and 95% CIs

Area covered by the Credibility Intervals

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