Proximal-Langevin samplers for nonsmooth composite posteriors: Application to the estimation of Covid19 reproduction number

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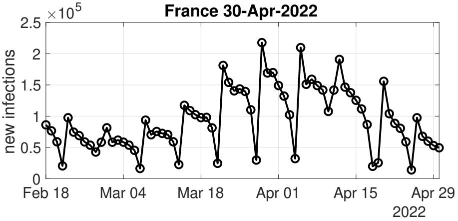
‡ Partly funded by *Fondation Simone et Cino Del Duca, Institut de France*

Daily counts of new infection cases



data collected
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Main challenges of epidemic surveillance

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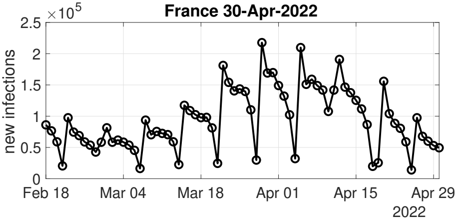

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$\longrightarrow$ efficient monitoring tools — *epidemiological model,*

$\longrightarrow$ robustness to low quality of the data — *handle outlier values,*

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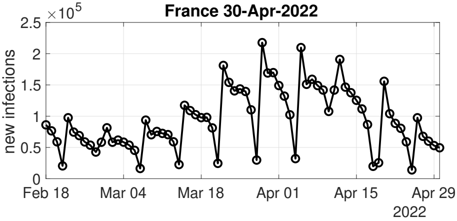

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Key indicator: reproduction number R_0 (Liu et al., 2018, *PNAS*)

"averaged number of secondary cases generated by a typical contagious individual"

$\Longrightarrow$ relaxed into an **effective time-varying reproduction number** R_t at day t

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

Propagation model of Covid19

Z_t: number of new infections at day t,

$$\mathbb{P}(\mathsf{Z}_t|\mathsf{Z}_{t-1},\mathsf{Z}_{t-2},\ldots) = \text{Poisson}\left(\mathsf{p}_t(\boldsymbol{\theta})\right), \quad \mathsf{p}_t(\boldsymbol{\theta}) = \mathsf{R}_t \sum_{u=1}^{\tau_\phi} \Phi_u \mathsf{Z}_{t-u} + \mathsf{O}_t$$

- Φ: serial interval function, i.e., infection delay distribution
- $\mathbf{R} = (\mathsf{R}_1, \cdots, \mathsf{R}_T)$ reproduction numbers at day $t = 1, \ldots, T$
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- $g(A\boldsymbol{\theta}) = \lambda_R \|D_2 \mathbf{R}\|_1 + \lambda_O \|\mathbf{O}\|_1, \qquad D_2 \in \mathbb{R}^{(T-2)\times T}$: discrete Laplacian matrix

(Artigas et al., 2022, EUSIPCO; Fort et al., 2023, IEEE Trans Sig Process)

Pandemic monitoring

Two quantities of interest:

- reproduction number $\mathbf{R} = (\mathrm{R}_1, \ldots, \mathrm{R}_T)$
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Level of confidence required to support high impact sanitary decisions:

$\Longrightarrow$ estimate **credibility intervals at level 95%** under the statistical model

$$\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O}) \sim \pi, \quad \text{with} \quad \pi(\boldsymbol{\theta}) \propto \exp\left(-f(\boldsymbol{\theta}) - g(\mathrm{A}\boldsymbol{\theta})\right) \mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$$

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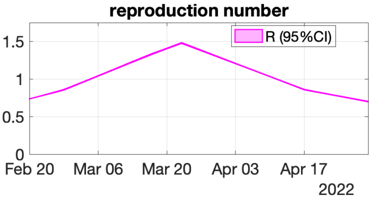

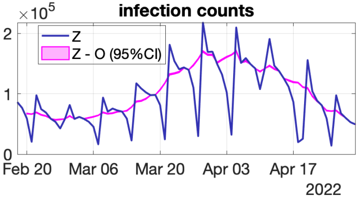

$R_T \in [0.70, 0.71] \quad \Longrightarrow \quad R_T < 1$ with probability at least 0.95

Credibility interval estimation of

$\boldsymbol{\theta} \equiv$ sample from a distribution[†] of the form:

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- $\boldsymbol{\theta} \in \mathbb{R}^d$ vector of parameters,
- f differentiable,
- $\mathcal{D} \subset \mathbb{R}^d$ admissible domain,
- g convex, non-smooth,
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Markov Chain Monte Carlo method

1) generate a Markov chain $\{\boldsymbol{\theta}^n, n \in \mathbb{N}\}$ such that

- $\boldsymbol{\theta}^{n+1}$ depends only on $\boldsymbol{\theta}^n$,
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2) compute credibility interval estimates from samples $\{\boldsymbol{\theta}^n, n \geq N\}$ for $N \gg 1$.

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Hastings-Metropolis type algorithm $\mathsf{C} \in \mathbb{R}^{d \times d}$ symmetric positive definite; $\gamma > 0$

1) Gaussian proposal: $\boldsymbol{\theta}^{n+\frac{1}{2}} = \mu(\boldsymbol{\theta}^n) + \sqrt{2\gamma}\xi^{n+1}, \quad \xi^{n+1} \sim \mathcal{N}_d(0, \mathsf{C});$

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Case of smooth π: Tempered Langevin dynamics (Roberts & Tweedie, 1996, *Bernoulli*)

$$\mu(\boldsymbol{\theta}) = \boldsymbol{\theta} + \gamma\sqrt{\mathsf{C}}\,\nabla \ln \pi(\boldsymbol{\theta})$$

$\Longrightarrow$ move toward regions of high probability

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Case of non-smooth π: proximal Langevin $\quad \pi \propto \exp\left(-f - g(\mathrm{A}\cdot)\right)\mathbb{1}_{\mathcal{D}}$

- f differentiable with gradient ∇f,
- g non-smooth, convex,

  with closed-form proximal operator $\mathrm{prox}_{\rho g} = (\mathrm{I} + \rho\partial g)^{-1}$, $\rho > 0$.

Purpose: compare different proximal design of the drift μ.

Purpose: drift term $\mu(\boldsymbol{\theta})$ adapted to $\pi \propto \exp\left(-f - g(\mathsf{A}\cdot)\right)\mathbb{1}_{\mathcal{D}}$, g non-smooth.

$$\operatorname{prox}_{\gamma g(\mathsf{A}\cdot)}(\boldsymbol{\theta}) = \underset{\boldsymbol{\varphi}\in\mathbb{R}^d}{\operatorname{argmin}} \left(\frac{1}{2}\|\boldsymbol{\theta} - \boldsymbol{\varphi}\|_2^2 + \gamma g(\mathsf{A}\boldsymbol{\varphi})\right)$$

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- Moreau drift: *smooth approximation of g by its Moreau envelop*

$$\mu^{\mathtt{M}}(\boldsymbol{\theta}) = \boldsymbol{\theta} - \gamma \nabla f(\boldsymbol{\theta}) - \frac{\gamma}{\rho} \mathsf{A}^\top (\mathsf{I} - \operatorname{prox}_{\rho g}) \mathsf{A}\boldsymbol{\theta}, \quad \rho = \gamma$$

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- PGdec drift: if $\mathsf{A}\mathsf{A}^\top = \nu \mathsf{I}$, with $\nu > 0 \Longrightarrow$ closed-form expression of $\operatorname{prox}_{\gamma g(\mathsf{A}\cdot)}$

$$\mu^{\mathtt{PGdec}}(\boldsymbol{\theta}) = \operatorname{prox}_{\gamma g(\mathsf{A}\cdot)} \left(\boldsymbol{\theta} - \gamma \nabla f(\boldsymbol{\theta}) \right)$$

extended to $g(\mathsf{A}\cdot) = \sum_{i=1}^{I} g_i(\mathsf{A}_i\cdot)$, with $\mathsf{A}_i\mathsf{A}_i^\top = \nu_i \mathsf{I}$, $\nu_i > 0$

(Fort et al., 2023, IEEE Trans Sig Process)

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- Random Walk drift: $\mu^{\mathtt{RM}}(\boldsymbol{\theta}) = \boldsymbol{\theta}$

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$\mathrm{A} \in \mathbb{R}^{d \times d}$ **invertible**

dual drift term $\tilde{\mu}(\tilde{\boldsymbol{\theta}})$, $\tilde{\boldsymbol{\theta}} = \mathrm{A}\boldsymbol{\theta}$, adapted to $\tilde{\pi} \propto \exp\left(-f(\mathrm{A}^{-1}\cdot) - g\right)\mathbb{1}_{\mathcal{D}}(\mathrm{A}^{-1}\cdot)$

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(Artigas, 2022, *EUSIPCO*; Fort et al., 2023, IEEE Trans Sig Process)

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- Dual Random Walk drift: $\tilde{\mu}^{\mathrm{RM}}(\tilde{\boldsymbol{\theta}}) = \tilde{\boldsymbol{\theta}}$

Toy example: MCMC for penalized logistic regression

Model
- $\mathsf{X} \in \mathbb{R}^{N \times d}$: covariates matrix,
- $\boldsymbol{\theta}^* \in \mathbb{R}^d$: piecewise constant regression vector,
- $\mathsf{Y} \in \{0, 1\}^N$: binary response vector

$$\mathsf{Y}_j \sim \text{Bernoulli}\left((1 + \exp(-(\mathsf{X}\boldsymbol{\theta}^*)_j))^{-1} \right), \quad \text{independent.}$$

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Data $\quad N = 2.10^3$, $d = 20$

X: independent Rademacher r.v., rows normalized to 1.

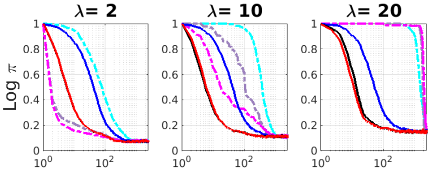
Convergence indicator:

$$\text{Log}\,\pi = \frac{\ln \pi_t(\boldsymbol{\theta}^n) - \ln \pi_t^*}{\ln \pi_t(\boldsymbol{\theta}^1) - \ln \pi_t^*}, \qquad \ln \pi_t^* = \max_{\boldsymbol{\theta} \in \mathbb{R}} \ln \pi_t(\boldsymbol{\theta})$$

high probability regions

Comparaison of the MCMC samplers

primal *dashed lines*	dual *solid lines*
`RW`	`RWdual`
`M`	`Mdual`
`PGdec`	`PGdual`



- gain to use 1^{st} order information vs. `RW`;
- primal samplers: the fastest at small λ;
- dual samplers: the fastest for medium to large λ, good for small λ.

$\Longrightarrow$ `Mdual` and `PGdual` fast convergence; robust to the choice of λ

Covid19 propagation model: $\boldsymbol{\theta} = (\mathbf{R}, \mathbf{O})$ of probability distribution

$$\pi(\boldsymbol{\theta}) \propto \exp\left(-\sum_{t=1}^{T}\left(-\mathsf{Z}_t \ln \mathsf{p}_t(\boldsymbol{\theta}) + \mathsf{p}_t(\boldsymbol{\theta})\right) - \lambda_{\mathsf{R}}\|\mathsf{D}_2\mathbf{R}\|_1 - \lambda_{\mathsf{O}}\|\mathbf{O}\|_1\right)\mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$$

$$\mathsf{D}_2 \in \mathbb{R}^{(T-2)\times T} \ \textbf{full rank} \quad \Longrightarrow \quad \overline{\mathsf{D}}_2 \in \mathbb{R}^{T\times T} \ \textbf{invertible} \text{ extension}$$

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MCMC dual samplers: [`RWdual`] random walk in the dual space
[`Mdual`] Moreau drift in the dual space
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$$\mathbf{R}^{n+\frac{1}{2}} = \begin{cases} \mathbf{R}^n \\ \overline{\mathsf{D}}_2^{-1}\tilde{\mu}_{\mathsf{R}}^{\mathtt{M}}(\tilde{\boldsymbol{\theta}}^n) \\ \overline{\mathsf{D}}_2^{-1}\tilde{\mu}_{\mathsf{R}}^{\mathtt{PG}}(\tilde{\boldsymbol{\theta}}^n) \end{cases} + \sqrt{2\gamma_{\mathsf{R}}}\xi_{\mathsf{R}}^{n+1}; \quad \mathbf{O}^{n+\frac{1}{2}} = \begin{cases} \mathbf{O}^n \\ \tilde{\mu}_{\mathsf{O}}^{\mathtt{M}}(\tilde{\boldsymbol{\theta}}^n) \\ \tilde{\mu}_{\mathsf{O}}^{\mathtt{PG}}(\tilde{\boldsymbol{\theta}}^n) \end{cases} + \sqrt{2\gamma_{\mathsf{O}}}\xi_{\mathsf{O}}^{n+1}.$$

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Hyperparameters:

- $(\lambda_{\mathsf{R}}, \lambda_{\mathsf{O}}) = (3.5\,\sigma_{\mathbf{Z}}\sqrt{6}/4, 0.05)$,
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- γ adjusted to reach 25% acceptance rate.

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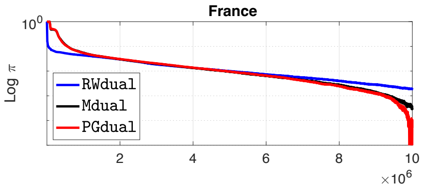
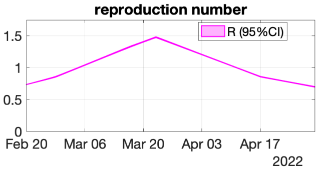
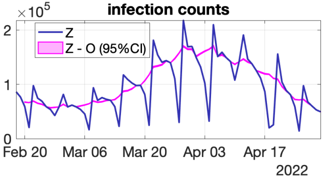
Convergence of the Markov chains



Credibility intervals of regularized reproduction number and corrected counts





CI estimates of R_t and $Z_t^{(D)}$ published daily for 200+ countries during $\sim$2 years

`https://perso.ens-lyon.fr/patrice.abry/`

`https://perso.math.univ-toulouse.fr/gfort/project/opsimore-2/`

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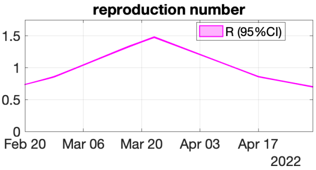
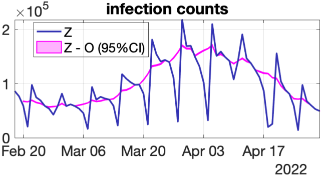


$\lambda_{\mathsf{R}} = 3.5 \times \mathrm{std}(\mathbf{Z})$



$\lambda_{\mathsf{O}} = 0.05$

$$\pi(\boldsymbol{\theta}) \propto \exp\left(-\sum_{t=1}^{T}\left(-\mathsf{Z}_t \ln \mathsf{p}_t(\boldsymbol{\theta}) + \mathsf{p}_t(\boldsymbol{\theta})\right) - \lambda_{\mathsf{R}}\|\mathsf{D}_2\mathbf{R}\|_1 - \lambda_{\mathsf{O}}\|\mathbf{O}\|_1\right)\mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta});$$

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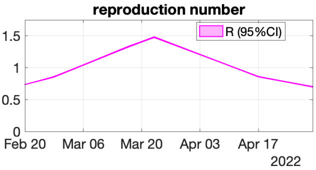

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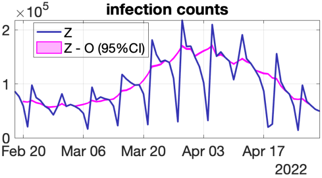

$\lambda_{\mathsf{O}} = 0.05$

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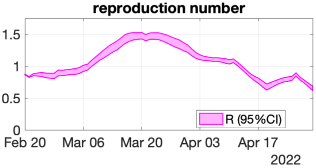

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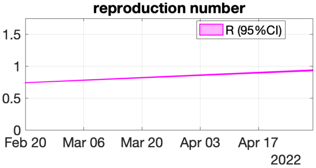
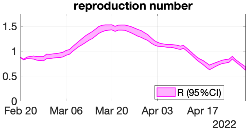
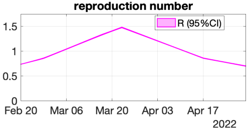


$\lambda_{\mathsf{R}} = 500 \times \mathrm{std}(\mathbf{Z})$

Expert choice: somehow arbitrary, subjective and costly



$\lambda_R = 0.5 \times \mathrm{std}(\mathbf{Z})$



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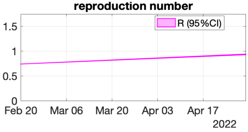
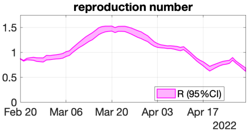


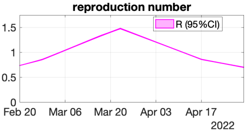
$\lambda_R = 500 \times \mathrm{std}(\mathbf{Z})$

Extension: a Hierarchical Bayesian epidemiological model

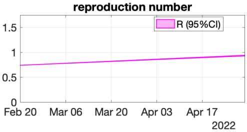
Expert choice: somehow arbitrary, subjective and costly



$\lambda_{\mathrm{R}} = 0.5 \times \mathrm{std}(\mathbf{Z})$



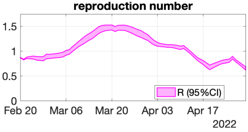
$\lambda_{\mathrm{R}} = 3.5 \times \mathrm{std}(\mathbf{Z})$



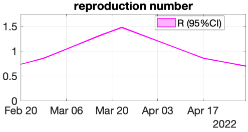
$\lambda_{\mathrm{R}} = 500 \times \mathrm{std}(\mathbf{Z})$

$$\ln \pi(\boldsymbol{\theta}|\boldsymbol{\lambda}) = \sum_{t=1}^{T} \left(\mathrm{Z}_t \ln \mathrm{p}_t(\boldsymbol{\theta}) - \mathrm{p}_t(\boldsymbol{\theta})\right) - \lambda_{\mathrm{R}} \|\mathrm{D}_2 \mathbf{R}\|_1 - \lambda_{\mathrm{O}} \|\mathbf{O}\|_1 + T \ln \lambda_{\mathrm{R}} + T \ln \lambda_{\mathrm{O}} + \mathrm{C}$$

Expert choice: somehow arbitrary, subjective and costly



$\lambda_R = 0.5 \times \mathrm{std}(\mathbf{Z})$



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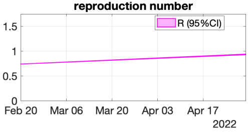

$\lambda_R = 500 \times \mathrm{std}(\mathbf{Z})$

$$\ln \pi(\boldsymbol{\theta}|\boldsymbol{\lambda}) = \sum_{t=1}^{T} (Z_t \ln p_t(\boldsymbol{\theta}) - p_t(\boldsymbol{\theta})) - \lambda_R \|D_2 \mathbf{R}\|_1 - \lambda_O \|\mathbf{O}\|_1 + T \ln \lambda_R + T \ln \lambda_O + C$$

Purpose: account for uncertainty in the choice of the priors $\boldsymbol{\lambda} := (\lambda_R, \lambda_O)$

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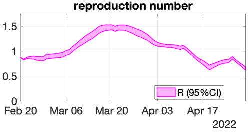

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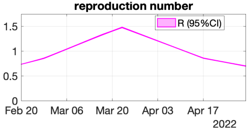

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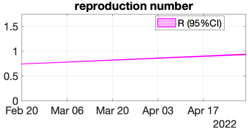

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$\Longrightarrow$ Conjugate Gamma hyperpriors: $\lambda_R \sim \Gamma(\alpha_R, \beta_R)$, $\lambda_O \sim \Gamma(\alpha_O, \beta_O)$

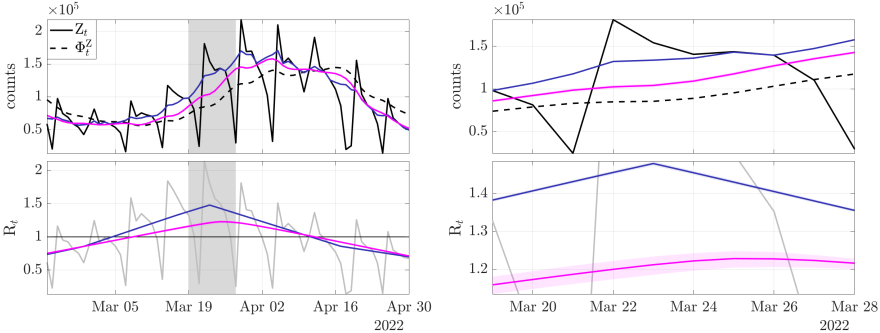
$$\lambda_R \mid \mathbf{R}, \mathbf{O} \sim \Gamma(T + \alpha_R, \|D_2 \mathbf{R}\|_1 + \beta_R), \quad \lambda_O \mid \mathbf{R}, \mathbf{O} \sim \Gamma(T + \alpha_O, \|\mathbf{O}\|_1 + \beta_O)$$

closed-form expression with direct sampling: Gibbs sampler alternating `PGdual` and Γ

Extension: a Hierarchical Bayesian epidemiological model

Principle: explore jointly the distribution of $(\mathbf{R}, \mathbf{O}, \lambda_\mathsf{R}, \lambda_\mathsf{O})$

$\Longrightarrow$ let $\boldsymbol{\lambda}$ adapt to data by varying around $(3.5 \times \mathrm{std}(\mathbf{Z}), 0.05)$



Area covered by the credibility intervals of **R**:

- `PGdual` targeting $\pi(\boldsymbol{\theta}|\boldsymbol{\lambda})$ by sampling $(\mathbf{R}, \mathbf{O})$: 0.46 ± 0.01
- `Gibbs` targeting $\pi(\boldsymbol{\theta}, \boldsymbol{\lambda})$ by sampling $(\mathbf{R}, \mathbf{O}, \lambda_\mathsf{R}, \lambda_\mathsf{O})$: 1.35 ± 0.07

Hierarchical distribution $\pi(\boldsymbol{\theta}, \boldsymbol{\lambda})$: more flexible, captures better intrinsic data variability

Conclusion and perspectives

Take home messages:

- Proximal Langevin based MCMC sampler for

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

  π composite distributions with constrained support

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Ongoing work:

- Online estimation scheme to process new counts on the fly
- New epidemiological models for low quality data: π not log-concave
- Monitoring different territories: spatiotemporal dynamics through graph inference