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

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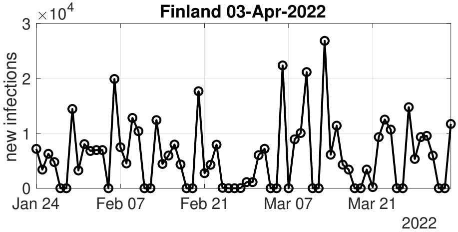
Daily counts of new infection cases



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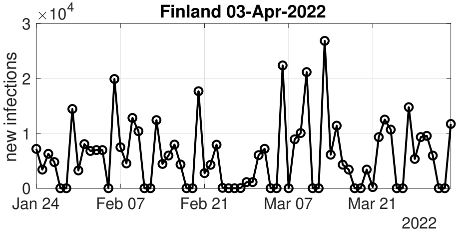

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Design of adapted sanitary measures and impact evaluation requires:

→ efficient monitoring tools *epidemiological model,*

→ robustness to low quality of the data *handle outlier values,*

→ reliable confidence levels *credibility intervals.*

Main challenges of epidemic surveillance

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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,

$$\mathbb{P}(Z_t|Z_{t-1}, Z_{t-2}, \ldots) = \text{Poisson}\left(p_t(\boldsymbol{\theta})\right), \quad p_t(\boldsymbol{\theta}) = R_t \sum_{u=1}^{\tau_\phi} \Phi_u Z_{t-u} + O_t$$

- Φ: serial interval function, i.e., infection delay distribution
- $\mathbf{R} = (R_1, \cdots, R_T)$ reproduction numbers at day $t = 1, \ldots, T$
- $\mathbf{O} = (O_1, \cdots, O_T)$ errors at day $t = 1, \ldots, T$

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Probability distribution of unknown parameters

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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)

Two quantities of interest:

- reproduction number $\mathbf{R} = (\mathsf{R}_1, \ldots, \mathsf{R}_T)$
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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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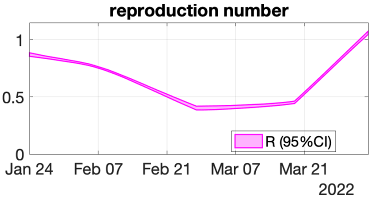

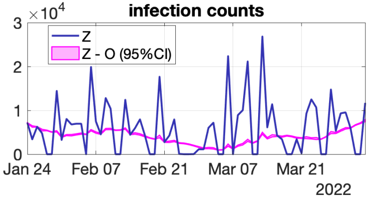

$\mathsf{R}_T \in [1.05, 1.08] \quad \Longrightarrow \quad \mathsf{R}_T \geq 1$ with probability at least 0.95

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,
- $\mathrm{A} \in \mathbb{R}^{d \times d}$ invertible linear operator.

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

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else $\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^{n+\frac{1}{2}}$ with probability depending on $\boldsymbol{\theta}^{n+\frac{1}{2}}$ and $\boldsymbol{\theta}^n$,

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

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

$\Longrightarrow$ move toward regions of high probability

Monte Carlo Samplers

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

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

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

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.

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

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

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

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

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

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

If $\mathrm{A} \in \mathbb{R}^{c\times d}$ with $c \leq d$ is **full rank**, consider invertible extension $\overline{\mathrm{A}} \in \mathbb{R}^{d\times d}$.

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Dual methods: $\boldsymbol{\theta}^{n+\frac{1}{2}} = \mathrm{A}^{-1}\tilde{\mu}(\tilde{\boldsymbol{\theta}}^{n}) + \sqrt{2\gamma}\xi^{n+1}, \quad \xi^{n+1} \sim \mathcal{N}_d(0, \mathrm{A}^{-1}\mathrm{A}^{-\top})$

Proximal Langevin Monte Carlo

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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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`*dual` : $\overline{\mathsf{D}}_1 = \begin{pmatrix} -1 & 0\dots0 \\ 0 & \\ \vdots & \mathsf{D}_1 \\ 0 & \end{pmatrix} \Longrightarrow$ invertible extension of D_1.

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Data $N = 2.10^3$, $d = 20$
X: independent Rademacher r.v., rows normalized to 1.

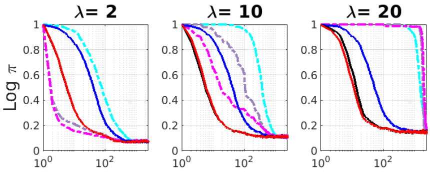
Convergence indicator:

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

high probability regions

Comparaison of the MCMC samplers

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



– gain to use 1st 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

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

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

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MCMC dual samplers:
[RWdual] random walk in the dual space
[Mdual] Moreau drift in the dual space
[PGdual] proximal-gradient type drift in the dual space

$$\mathbf{R}^{n+\frac{1}{2}} = \begin{cases} \mathbf{R}^n \\ \overline{\mathsf{D}}_2^{-1}\tilde{\mu}_{\mathsf{R}}^{\mathtt{M}}(\tilde{\boldsymbol{\theta}}^n) \\ \overline{\mathsf{D}}_2^{-1}\tilde{\mu}_{\mathsf{R}}^{\mathtt{PG}}(\tilde{\boldsymbol{\theta}}^n) \end{cases} + \sqrt{2\gamma_{\mathsf{R}}}\xi_{\mathsf{R}}^{n+1}; \quad \mathbf{O}^{n+\frac{1}{2}} = \begin{cases} \mathbf{O}^n \\ \tilde{\mu}_{\mathsf{O}}^{\mathtt{M}}(\tilde{\boldsymbol{\theta}}^n) \\ \tilde{\mu}_{\mathsf{O}}^{\mathtt{PG}}(\tilde{\boldsymbol{\theta}}^n) \end{cases} + \sqrt{2\gamma_{\mathsf{O}}}\xi_{\mathsf{O}}^{n+1}.$$

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Gaussian perturbation:

- $\xi_{\mathsf{R}}^{n+1} \sim \mathcal{N}(0, \overline{\mathsf{D}}_2^{-1}\overline{\mathsf{D}}_2^{-\top})$,
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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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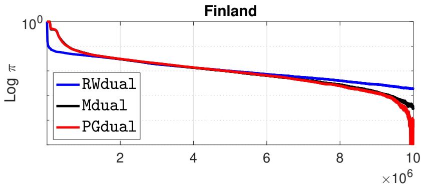
Convergence of the Markov chains



Take home messages:

- MCMC samplers for composite distributions with constrained support

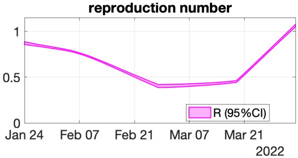
$$\pi(\boldsymbol{\theta}) \propto \exp\left(-f(\boldsymbol{\theta}) - g(\mathrm{A}\boldsymbol{\theta})\right) \mathbb{1}_{\mathcal{D}}(\boldsymbol{\theta})$$

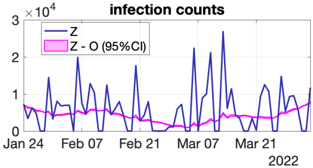
- Comparison on a toy example: faster convergence when
  - taking into account 1^{st} order information on π
  - using adequate covariance in the Gaussian proposal

- CI estimates of R_t and $\mathrm{Z}^{(D)}$ published daily for 200+ countries

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

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





Ongoing work:

- Generation of realistic synthetic data to assess estimation performance.

Research directions:

- New epidemiological models for low quality data, possibly graph data;
- Automated and data-driven selection of hyperparameters $\gamma_{\mathrm{R/O}}$, $\lambda_{\mathrm{R/O}}$

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Two-year postdoc position
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