Predicting Invasive Species' Dynamics Using a Mechanistic-statistical Approach « Focus on *Xylella fastidiosa* »

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Plan

1. Framework
2. Data - *Xylella fastidiosa*(Xf)
3. Bayesian *model-averaging*
4. PDE-based Inference Approach
5. Prediction Approach
6. Results: Inference
7. Results: Prediction
8. Perspectives

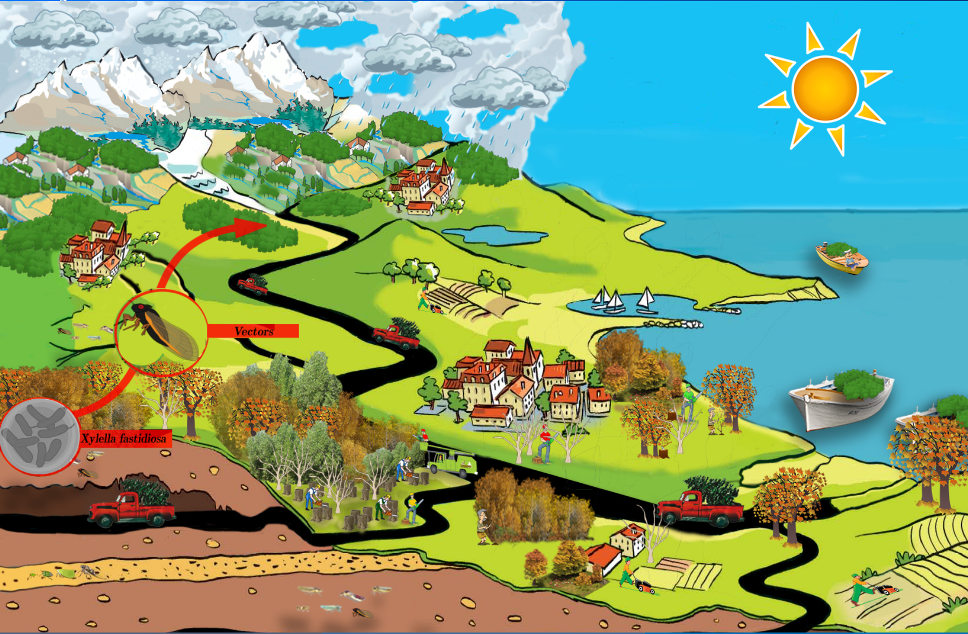
Plan

Framework - Biological Invasions

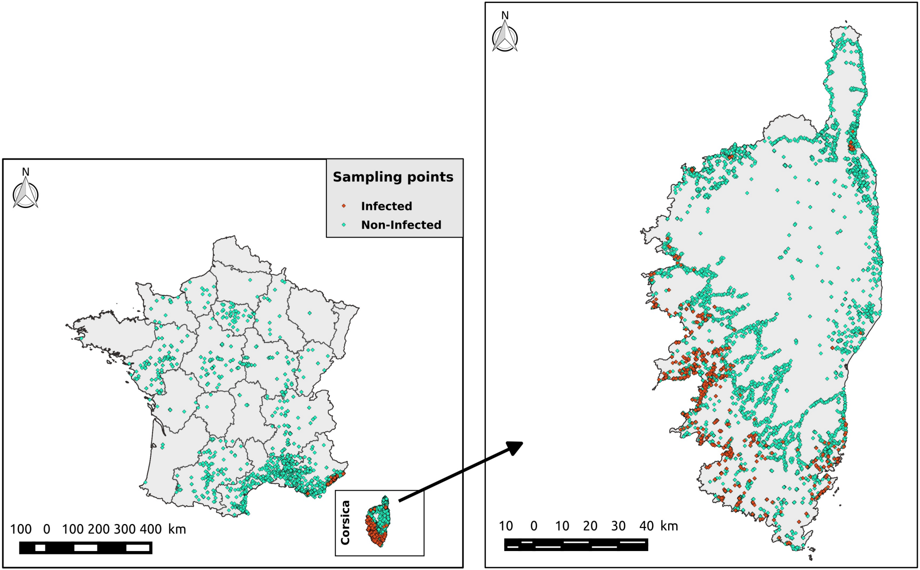
- Invasion of new territories by alien organisms a core topic in mathematical modeling.
  In particular:
  - Reconstructing the past dynamics of the alien organisms
  - Predicting their future spatial extents
- Stages of the biological invasion process:
  - Arrival
  - Establishment
  - Spread
  - Concentration

Plan

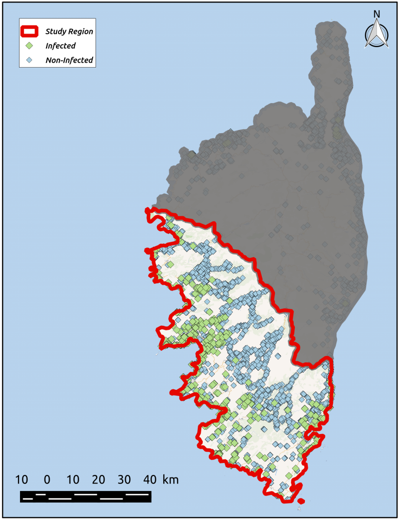
Xylella fastidiosa

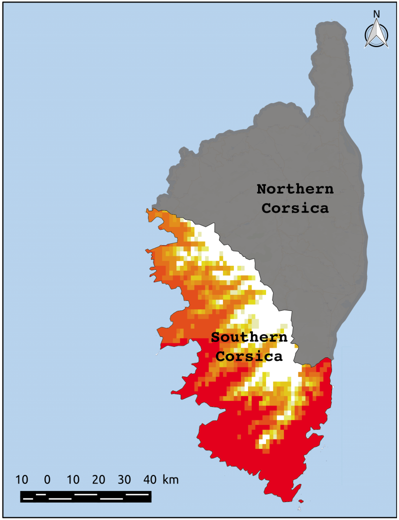


Epidemiosurveillance of data: Situation in France



Epidemiosurveillance data: Situation in South Corsica

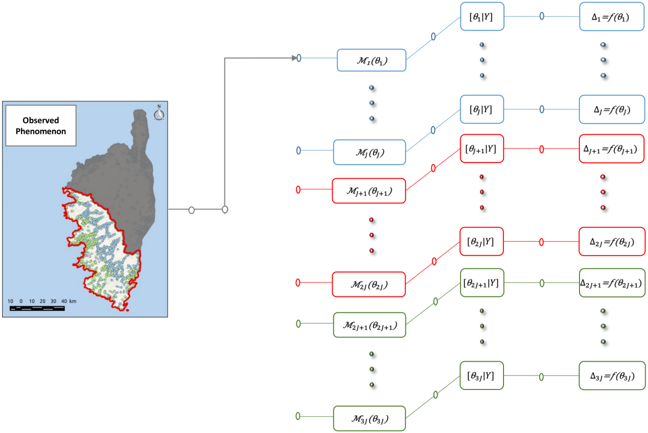




- ∼ **9000** plants sampled **since 2015** of which **900** have been diagnosed as **infected** (real-time PCR);
- For those ∼ 9000 plants, **geographic coordinates** and **sampling dates** are available;
- We also consider T, the average of the minimum daily temperature over January and February b/n 1995 and 2003 (Map of T with 1 km grid resolution on the right);

Plan

Strategy


Observed
Phenomenon
10 0 10 20 30 40 km
$\mathcal{M}_1(\theta_1)$
$\mathcal{M}_J(\theta_J)$
$\mathcal{M}_{J+1}(\theta_{J+1})$
$\mathcal{M}_{2J}(\theta_{2J})$
$\mathcal{M}_{2J+1}(\theta_{2J+1})$
$\mathcal{M}_{3J}(\theta_{3J})$
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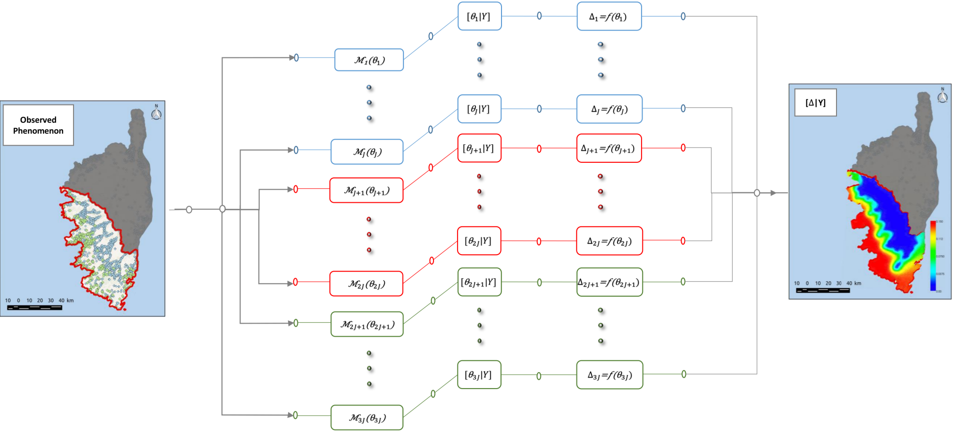
Strategy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Principles

The BMA posterior distribution of Δ is

$$[\Delta|Y] = \sum_{k=1}^{n} [\Delta|Y, \mathcal{M}_k] \times [\mathcal{M}_k|Y]$$

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- (blue) Posterior distribution of Δ given $\mathcal{M}_k$: Its empirical approximation is provided using the AMIS algorithm by the means of a weighted posterior sample of Θ;
- (red) Posterior Probability that $\mathcal{M}_k$ is the correct model;
- (green) Integrated likelihood of $\mathcal{M}_k$;

Principles

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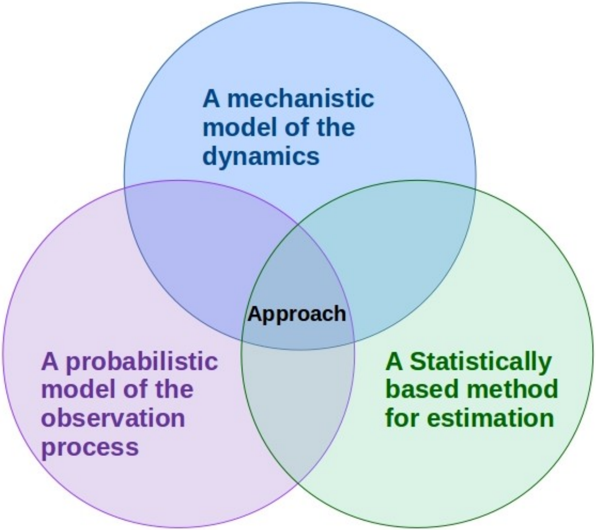
Posterior distribution of Δ given $\mathcal{M}_k$: Its empirical approximation is provided using the AMIS algorithm by the means of a weighted posterior sample of Θ;

Posterior Probability that $\mathcal{M}_k$ is the correct model;

Integrated likelihood of $\mathcal{M}_k$;

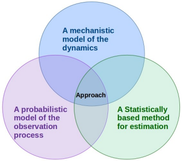
Plan

The Mechanistic-statistical Approach



Wikle 2003, Roques et *al.* 2011, Soubeyrand et Roques 2013

The Mechanistic-statistical Approach



Competing Process models

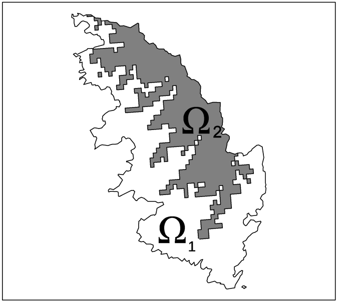
We assume that the dynamics of Xf is described by various models where $u(t, \mathbf{x})$ is the probability of a plant to be infected at time t in $\mathbf{x}$. The families of models considered are grounded on particular types of parabolic PDE.

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,\mathbf{x}) = \overbrace{D_j(\mathbf{x})}^{\text{Diffusion cœfficient}} \Delta u(t,\mathbf{x}) + \overbrace{f_i^j(u),}^{\text{Reproduction term}} & t \geq \tau_0,\ \mathbf{x} \in \Omega, \\ \nabla u(t,\mathbf{x}).n(\mathbf{x}) = 0, & t \geq \tau_0,\ \mathbf{x} \in \partial\Omega, \\ u(\tau_0, \mathbf{x}) = u_0(\mathbf{x}), & \mathbf{x} \in \Omega, \end{cases}$$

$$D_j(\mathbf{x}) = \sum_{k=1}^{2} D_k^j \mathbb{1}(\mathbf{x} \in \Omega_k^j), \ \ \forall j \leq J.$$

Competing Process models

Family i	Diffusion	$f_i^j(u), \forall j \leq J$
1	Homogeneous	$bu\left(1-\frac{u}{K}\right)\mathbb{1}(\mathbf{x}\in\Omega_1^j)-\alpha u\mathbb{1}(\mathbf{x}\in\Omega_2^j)$
2	Heterogeneous	$bu\left(1-\frac{u}{K}\right)\mathbb{1}(\mathbf{x}\in\Omega_1^j)-\alpha u\mathbb{1}(\mathbf{x}\in\Omega_2^j)$
3	Heterogeneous	$bu\left(1-\frac{u}{K}\right)$



- $\Omega_1^j = \Omega_1(T,\hat{T}_j) = \{\mathbf{x}\in\Omega : T(\mathbf{x}) > \hat{T}_j\}$
- $\Omega_2^j = \Omega_2(T,\hat{T}_j) = \{\mathbf{x}\in\Omega : T(\mathbf{x}) \leq \hat{T}_j\}$
- $\Omega = \Omega_1^j \bigcup \Omega_2^j$
- $\Omega_1^j \bigcap \Omega_2^j = \emptyset$

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3	Heterogeneous	$bu\left(1-\frac{u}{K}\right)$

- D : dispersal rate
- b : intrinsic growth rate of the pathogen infection
- $K \in (0,1]$: plateau for the probability of infection
- α : decrease rate of infection in Ω_2
- $\mathbb{1}(\mathbf{x}\in\Omega_k^j)$: characteristic function which is equal to 1 in Ω_k^j and 0 elsewhere.

Competing Process models

$$\begin{cases} \frac{\partial u}{\partial t} = D_j(\mathbf{x})\Delta u + f_i^j(u), & \text{in } \Omega \\ \nabla u.n = 0, & \text{on } \partial\Omega \\ u_0(\mathbf{x}) = u(\tau_0, \mathbf{x}), & \text{in } \Omega \end{cases}$$

For the initial conditions:

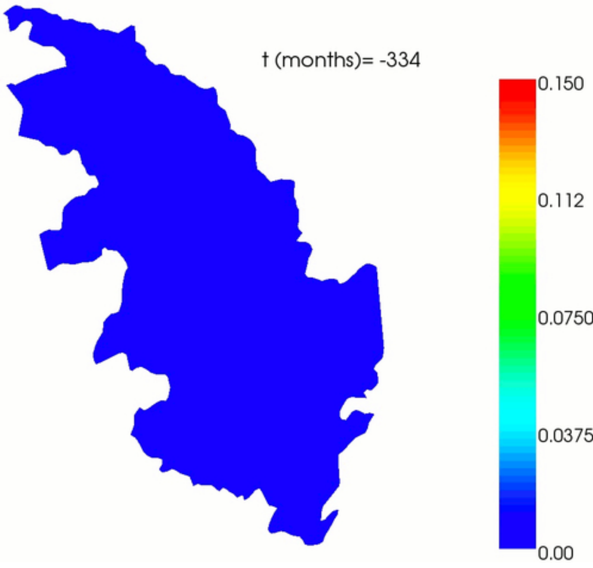
- The disease is introduced at time τ_0
- $\tilde{\mathbf{x}}_0 = (\tilde{x}_0, \tilde{y}_0)$ is the central point of the disease introduction
- The probability of infection at τ_0 in $\mathbf{x}$ satisfies:

$$u_0(\mathbf{x}) = p_0 \exp\left(-\frac{\|\mathbf{x} - \tilde{\mathbf{x}}_0\|^2}{2\sigma^2}\right)$$

where $\sigma^2 = \frac{r_0^2}{q}$ and q is the 0.95-quantile of the χ^2 distribution with 2 degrees of freedom. Then, at τ_0, 95% of the infected hosts are located in the ball $\mathcal{B}(\tilde{\mathbf{x}}_0, r_0)$. p_0, is the infection probability at $(\tau_0, \tilde{\mathbf{x}}_0)$.

Numerical Simulation

$$\begin{cases} \frac{\partial u}{\partial t} = D\Delta u + bu(1-\frac{u}{K})\mathcal{X}_{\Omega_1} - \alpha u \mathcal{X}_{\Omega_2}, & \text{in } \Omega \\ \nabla u.n = 0, & \text{on } \partial\Omega \\ u_0(\mathbf{x}) = u(\tau_0, \mathbf{x}), & \text{in } \Omega \end{cases}$$



Numerical solution with $D = 3.17 \times 10^5$, $b = 0.05$, $K = 0.15$, $\alpha = 0.26$, $\tilde{\mathbf{x}}_0 = (1176023, 6183750)$, $r_0 = 5000m$ $p_0 = 0.1$, $\tau_0 = -335$, $\hat{T} = 5.4^\circ$C.

Data model

Let $\mathcal{I}$ be a sample of size I that contains all the sampled hosts.

- t_i the sampling time of host i
- $\mathbf{x}_i$ its location
- Y_i its sanitary state observed at time t_i

Probabilistic Model of Observation

We assume that the measurements Y_i are, conditionally to u, independent random variables with Bernoulli distributions:

$$Y_i \sim \mathcal{B}in(1, u(t_i, \mathbf{x}_i)), \ \forall i \in \mathcal{I},$$

where u depends on the set of parameters Θ and on the model structure.

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Limitation

This data model is an extremely simplified version of the true observation process, a version that does not take into account per example the probability of false negatives, the dependency in the spatio-temporal process of collect $\{(t_i, \mathbf{x}_i, Y_i) : i \in \mathcal{I}\}$ and other proprieties of the observation process.

Bayes' rule

The posterior distribution of the unknown, hereafter dubbed Θ, is derived by Bayes' rule:

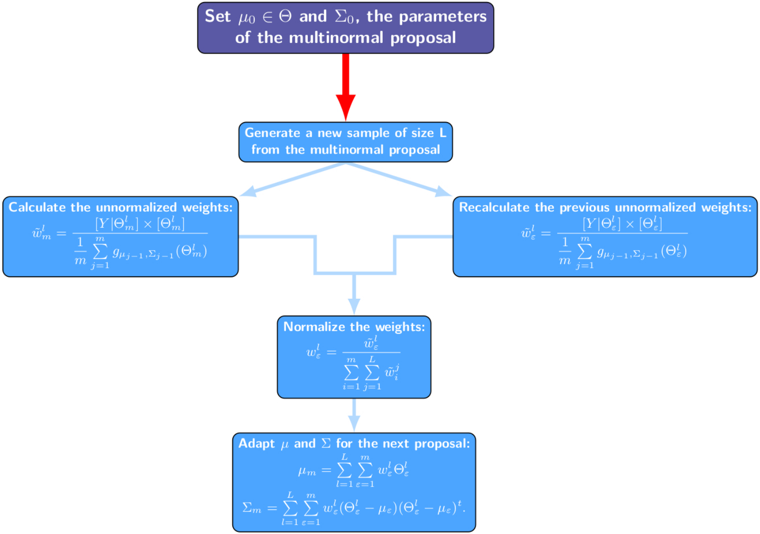
Likelihood

Prior

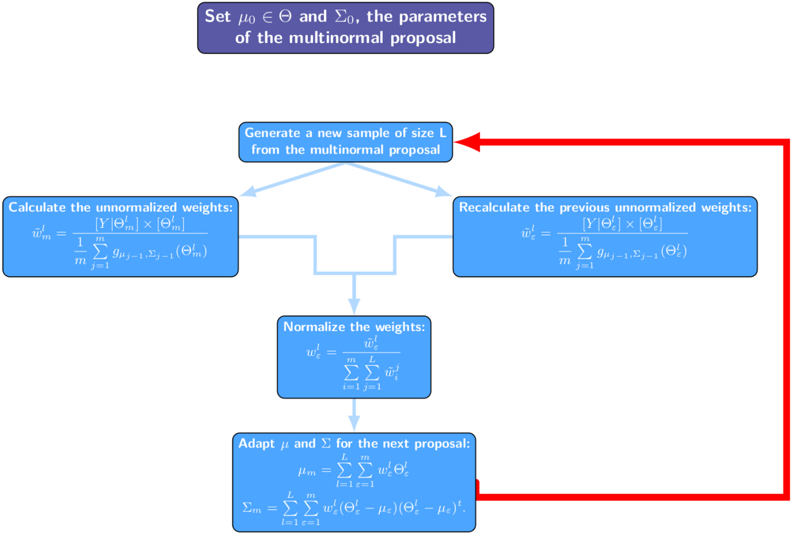
$$[\Theta|Y] = \frac{[Y|\Theta] \times [\Theta]}{[Y]}$$

Evidence

Bayesian Inference with AMIS



Bayesian Inference with AMIS



AMIS convergence

- The theoretical convergence of the AMIS has been proved (Cornuet et al., 2012; Jean-Marin et al. 2014) at a cost of slight modifications. After M iterations of the AMIS, for any integrable function h, the self normalized AMIS estimator of $\widehat{\mathbb{E}_\Pi(h(\Theta))} = \int h(\Theta)\Pi(\Theta)\sigma(dx)$ is as follows:

$$\widehat{\mathbb{E}_\Pi(h(\Theta))} = \frac{1}{\sum_{l=1}^{L}\sum_{m=1}^{M}\tilde{w}_m^l}\sum_{l=1}^{L}\sum_{m=1}^{M}\tilde{w}_m^l h(\Theta_m^l).$$

- When $M, L_1, \cdots, L_{M-1}$ are fixed, $\widehat{\mathbb{E}_\Pi(h(\Theta))} \xrightarrow[L_M\to\infty]{\mathbb{P}} \mathbb{E}_\Pi(h(\Theta))$.

Imposing compactness restrictions on the simulation space or upper bounds on the target density Π will allow for the estimator to remain unbiased and for its convergence to be established.

Why use AMIS?

1. AMIS can be easily parallelized;
2. Tuning parameters are automatically adapted across the algorithm iterations;
3. AMIS allows for an integral recycling of all past simulations;
4. AMIS is constructed sequentially and adaptevely;
5. AMIS provides a significant improvement in stability and effective sample size due to the introduction of a recycling procedure (Cornuet et *al.*, 2012);

Plan

BMA: Principles

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Approximating the Integrated Likelihood

Criteria	Harmonic Mean Estimators(HME)
HME_1	$\left\{ \sum_{s=1}^{S} \frac{1}{[Y\|\Theta^{(s)}, \mathcal{M}_k] \times [\Theta^{(s)}\|\mathcal{M}_k]} w^{(s)} \right\}^{-1}$
HME_2	$\left\{ \sum_{s=1}^{S} \frac{g(\Theta^{(s)})}{[Y\|\Theta^{(s)}, \mathcal{M}_k] \times [\Theta^{(s)}\|\mathcal{M}_k]} w^{(s)} \right\}^{-1}$

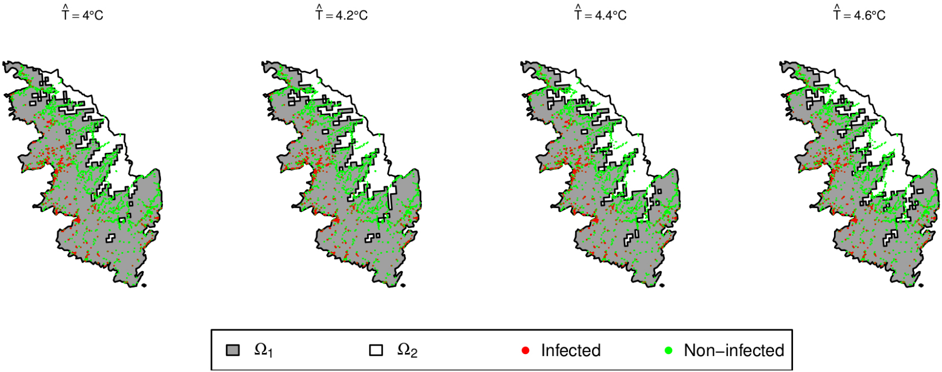
- $\{\Theta^{(s)}, w^{(s)}\}_{s=1}^{S}$ a weighted sample of size S drawn from the posterior distribution of Θ
- $f(.)$ is an importance p_k-dimensional probability density and natural choices to match the posterior would be multivariate normal with mean and covariance from the $\Theta^{(s)}$.
- HME_1 is consistent when $S \to \infty$ but it is indeed unstable
- HME_2 is unbiased, consistent and satisfies a Gaussian central limit theorem if

$$\int \frac{g(\Theta_k)}{[Y|\Theta_k, \mathcal{M}_k] \times [\Theta_k|\mathcal{M}_k]} d\Theta_k < \infty$$

Criteria	Other Estimators of $[\mathcal{M}_k \vert Y]$
WAIC_1	$\dfrac{exp(-\frac{1}{2}\text{dWAIC}_1^k)}{\sum_{j=1}^n exp(-\frac{1}{2}d\text{WAIC}_1^j)}$
WAIC_2	$\dfrac{exp(-\frac{1}{2}\text{dWAIC}_2^k)}{\sum_{j=1}^n exp(-\frac{1}{2}d\text{WAIC}_2^j)}$
DIC_1	$\dfrac{exp(-\frac{1}{2}\text{dDIC}_1^k)}{\sum_{j=1}^n exp(-\frac{1}{2}d\text{WAIC}_1^j)}$
DIC_2	$\dfrac{exp(-\frac{1}{2}\text{dDIC}_2^k)}{\sum_{j=1}^n exp(-\frac{1}{2}\text{dDIC}_2^j)}$
IC_1	$\dfrac{exp(-\frac{1}{2}\text{dIC}^k)}{\sum_{j=1}^n exp(-\frac{1}{2}d\text{IC}^j)}$
BIC_1	$\dfrac{exp(-\frac{1}{2}\text{dBIC}^k)}{\sum_{j=1}^n exp(-\frac{1}{2}d\text{BIC}^j)}$

Plan

Application to One Model Structure: Selection of $\hat{T}$



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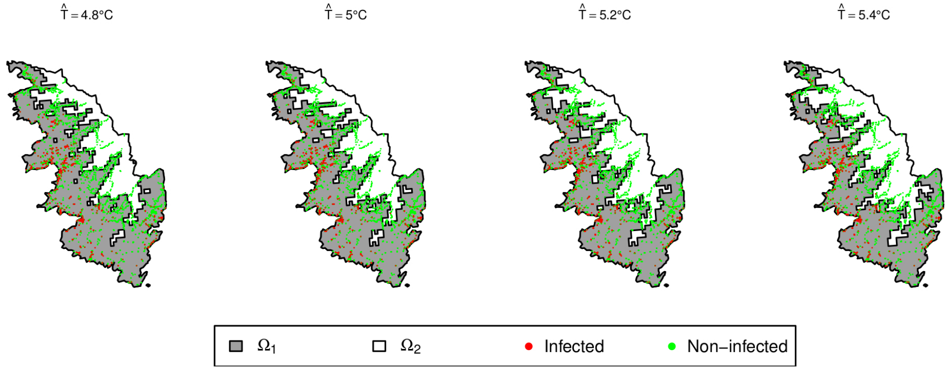

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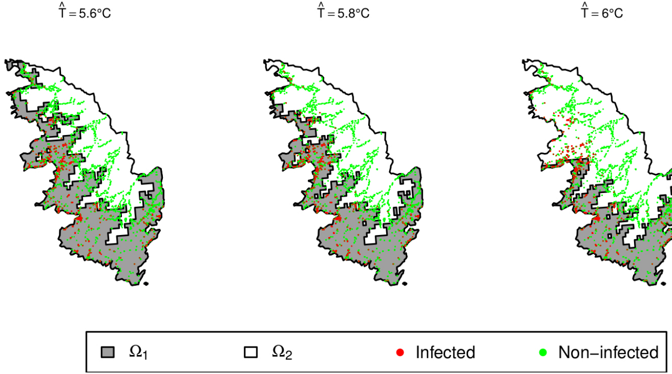

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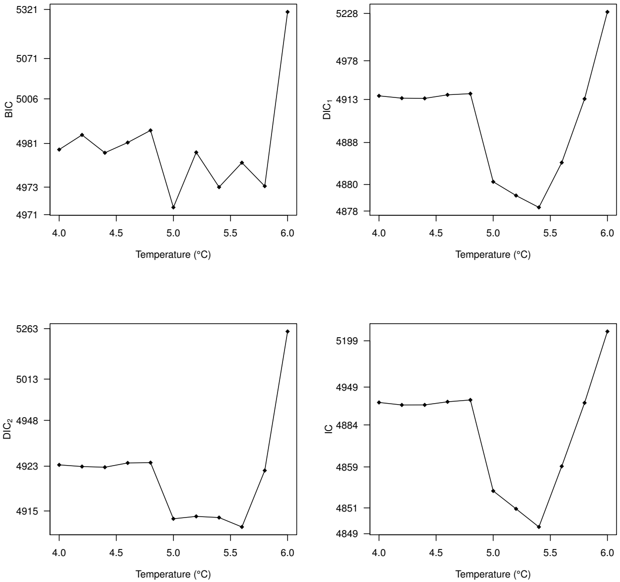


Application to One Model: Inference of the *posterior* distribution of Θ

Let $\Theta = [D; b; K; \alpha; \tau_0; \tilde{\mathbf{x}}_0]$, r_0, p_0 are fixed and $\hat{T} = 5.4\,^\circ$ C is selected.

The prior distribution is uniform and vague over the parameter space.

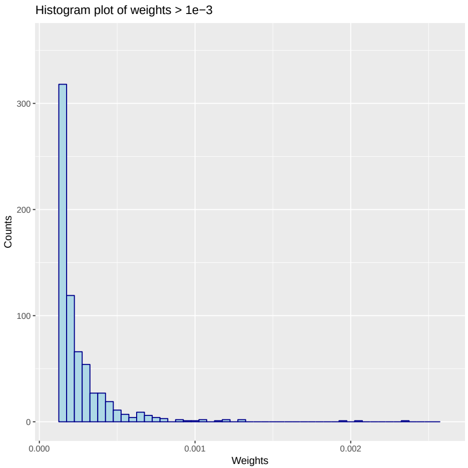
And, the introduction points are only generated in Ω_1

Initialization: We used,

$$\mu = \begin{bmatrix} 10^5 \\ 0.1 \\ 0.1 \\ 2 \\ 1191369 \\ 6076691 \\ -335 \end{bmatrix} \in \Theta \text{ and } \Sigma = \begin{bmatrix} 10^{10} & & & & & & \\ & 0.01 & & & & & \\ & & 0.01 & & (0) & & \\ & & & 1 & & & \\ & (0) & & & 10^8 & & \\ & & & & & 10^8 & \\ & & & & & & 2500 \end{bmatrix}$$

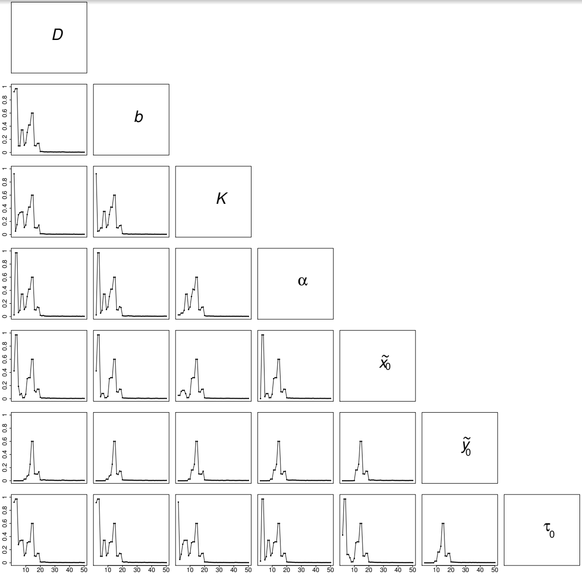
for the initial parameters of the multi-normal proposal

Importance Weights



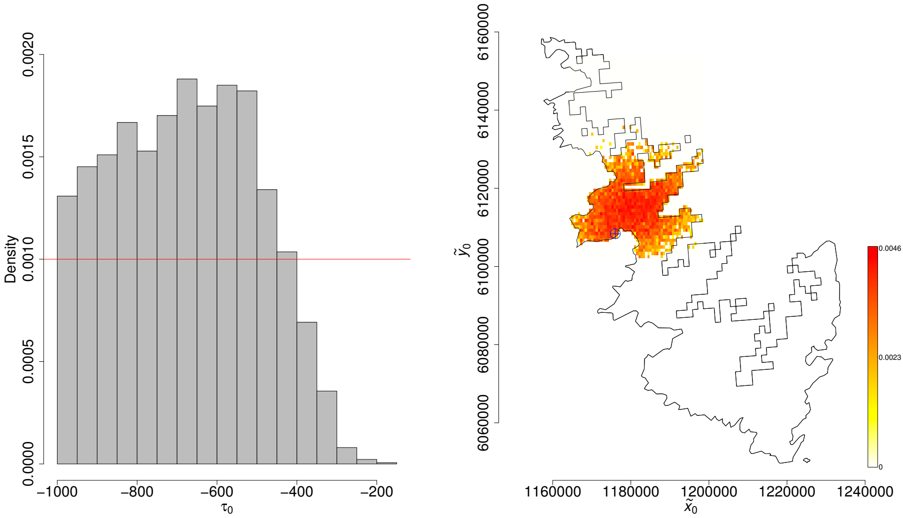
0.0026080735
0.0023748224
0.0020296469
0.0019714157
0.0013218297
0.0012909493
0.0012142132
0.0012120195
0.0011568165
0.0010675652
0.0010555070
0.0009843055
0.0009736781
0.0009130111
0.0008805903
0.0008244563
0.0008042306
0.0007916683
0.0007484289
0.0007388762

Stabilization of the AMIS algorithm



Variation in the deviation measure between the assessments of the posterior distribution at iteration $m-1$ and $m > 1$ of the AMIS algorithm.

Marginal and 2D Posterior distributions



Posterior distributions of the introduction time τ_0 (histogram) and the introduction point $\tilde{\mathbf{x}}_0$ (color palette). The prior for τ_0 was uniform over $[-1000, 0]$ (red line). The value of $\tilde{\mathbf{x}}_0$ having the largest weight in AMIS is indicated by a blue dot. The prior for $\tilde{\mathbf{x}}_0$ was uniform over the space delimited by the contours.

Marginal and 2D Posterior distributions

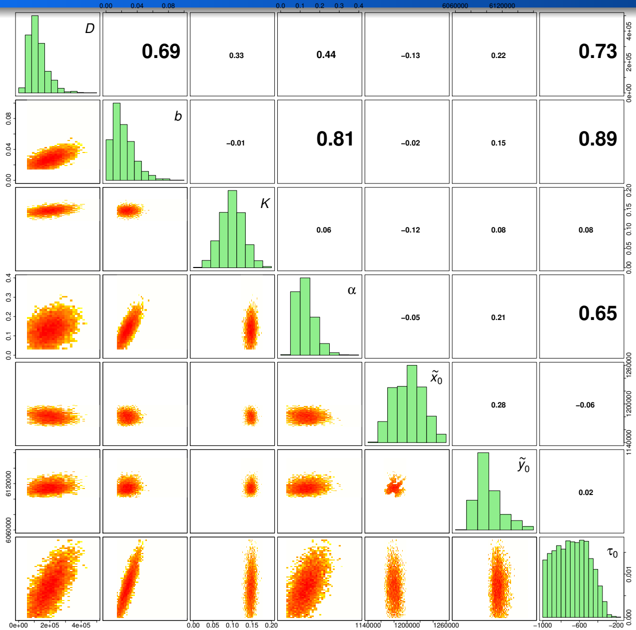


Table: Posterior medians, means and standard deviations of parameters of the reaction-diffusion-absorption equation.

Parameter	Unit	Median	Mean	Standard deviation
D	$\mathrm{m}^2\cdot$ month^{-1}	1.8×10^5	2.0×10^5	0.7×10^5
b	month^{-1}	0.026	0.027	0.008
K	probability	0.147	0.148	0.007
α	month^{-1}	0.12	0.13	0.05
τ_0	month	-680	-681	179

Goodness-of-fit

The Brier Score is computed as follows:

$$\text{BS} = \frac{1}{I}\sum_{i=1}^{I}\left(Y_i^{\text{obs}} - u(t_i, \mathbf{x}_i)\right)^2.$$

- I the number of sampled hosts
- Y_i^{obs} observed sanitary status
- $u(t_i, \mathbf{x_i})$ the solution of the model given Θ

	Median	Mean	CI(95%)
BS	0.0828	0.0828	[0.0827; 0.0829]

Goodness-of-fit

The probabilistic predictions provided by the model can also be compared to simple but data-informed predictions via the Brier skill score:

$$\mathsf{BSS} = 1 - \frac{\mathsf{BS}}{\mathsf{BS}_{\mathsf{ref}}}; \mathsf{BS}_{\mathsf{ref}} = (1/I)\sum_{i=1}^{I}(Y_i^{\mathsf{obs}} - \bar{Y}^{\mathsf{obs}})^2.$$

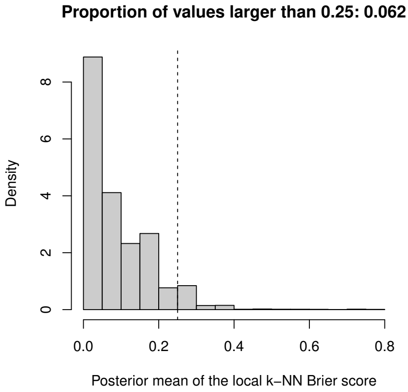
- $\mathsf{BS}_{\mathsf{ref}}$ is the Brier score for a reference forecast (here the climatology)
- $\bar{Y}^{\mathsf{obs}}$ mean of $\{Y_i^{\mathsf{obs}} : i = 1, \ldots, I\}$

	Median	Mean	CI(95%)
BSS	0.031	0.031	$[0.029, 0.032]$

Goodness-of-fit

The local Brier Score (LBS) based on the k-NN satisfies:

$$\text{LBS}_k(i) = \frac{1}{k+1} \sum_{i' \in i \cup \mathcal{V}_k(i)} \left(Y_{i'} - u(t_{i'}, \mathbf{x}_{i'})\right)^2; \; i = 1, \cdots, I.$$



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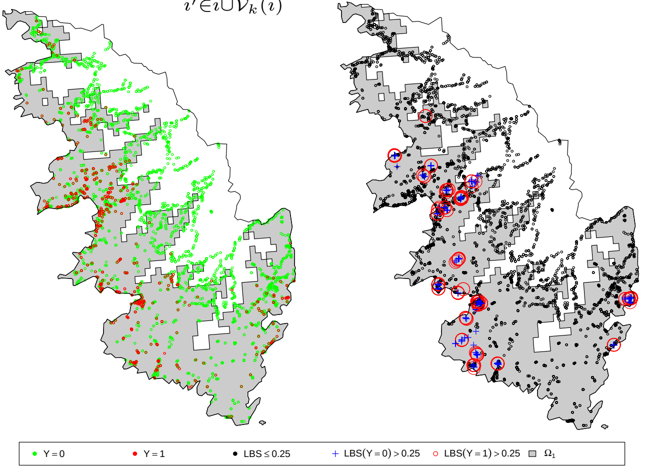
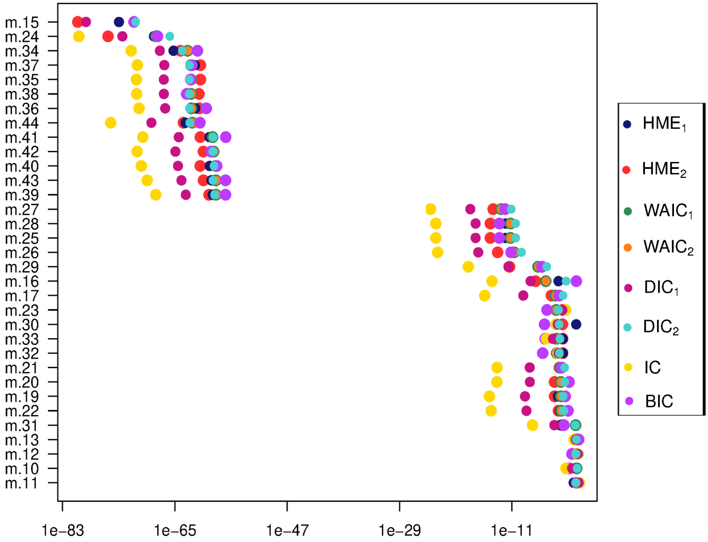


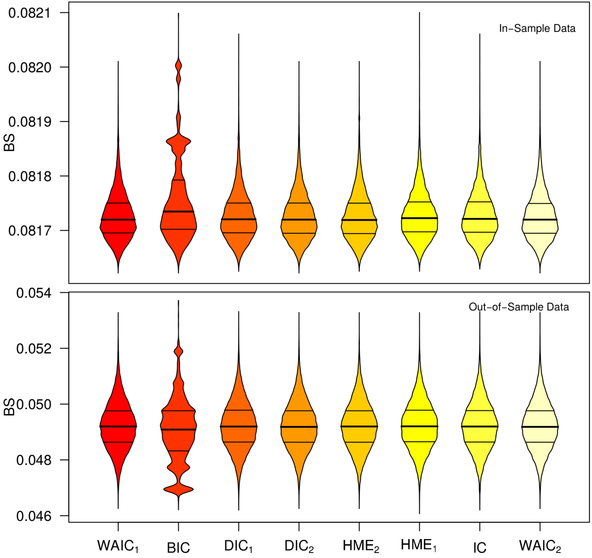
Plan

Posterior model probability



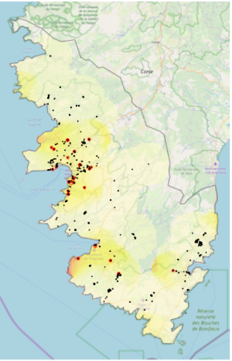
Posterior model probability values approximated using all the alternative methods

Brier Score


0.0821
0.0820
0.0819
0.0818
0.0817
BS
In−Sample Data
0.054
0.052
0.050
0.048
0.046
BS
Out−of−Sample Data
WAIC1
BIC
DIC1
DIC2
HME2
HME1
IC
WAIC2

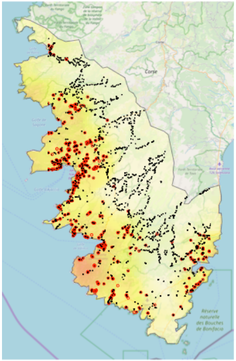
In & out-of-sample Predictions

Estimated proportions of positive results



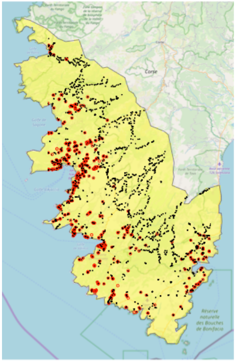
bw: 10 km -- Range of values: [0 , 0.495]

Estimated proportions of positive results



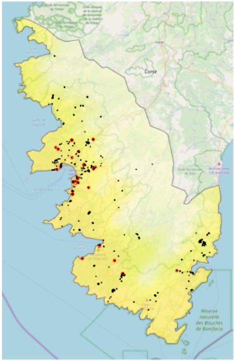
bw: 10 km -- Range of values: [0 , 0.352]

Climatology



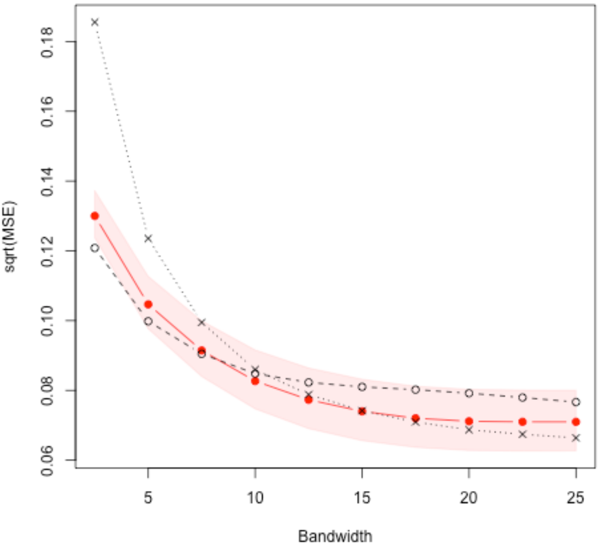
bw: 10 km -- Range of values: [0.098 , 0.098]

averageU



bw: 10 km -- Range of values: [0 , 0.147]

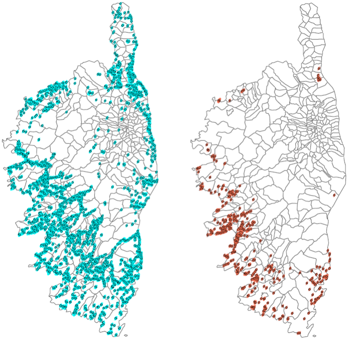
Root-mean-square error (RMSE)



Plan

Conclusion and Discussion

- Design control and surveillance based on model predictions
- Incorporate into those models the possibility of multiple introductions of Xf $((\mathbf{x}_0^1, \tau_0^1), \cdots, (\mathbf{x}_0^N, \tau_0^N))$ and then enlarge the study domain to entire Corsica
- Use additional covariates for defining the sub-domains
- Infer $\hat{T}$ jointly with the other parameters



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THANK YOU

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