The optimal control approach to analyze some inverse problems for reaction-diffusion systems arising from epidemiology

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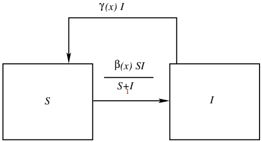
Overview

1. SIS model results
2. Indirectly transmitted diseases
3. Tumor growth models
4. Numerical solution

SIS MODEL RESULTS

SIS model: direct problem and inverse problem



Direct problem: Given $\{\beta, \gamma, S_0, I_0\}$ find $\{S, I\}$ such that

$$
\begin{aligned}
S_t - \Delta S &= -\beta(\mathbf{x})\frac{SI}{S+I} + \gamma(\mathbf{x})I, && (\mathbf{x}, t) \in Q_T := \Omega \times [0, T],\\
I_t - \Delta I &= \beta(\mathbf{x})\frac{SI}{S+I} - \gamma(\mathbf{x})I, && (\mathbf{x}, t) \in Q_T,\\
\nabla S \cdot \mathbf{n} &= \nabla I \cdot \mathbf{n} = 0, && (\mathbf{x}, t) \in \Gamma := \partial\Omega \times [0, T],\\
S(\mathbf{x}, 0) &= S_0(\mathbf{x}), \quad I(\mathbf{x}, 0) = I_0(\mathbf{x}), && \mathbf{x} \in \Omega,
\end{aligned}
$$

Inverse problem: Given $\{S_0, I_0, S^{obs}(\cdot, T), I^{obs}(\cdot, T)\}$ find $\{\beta, \gamma\}$ such that $\{S_{\beta,\gamma}, I_{\beta,\gamma}\}$ is the solution of a SIS model satisfying $S_{\beta,\gamma}(\cdot, T) \equiv S^{obs}(\cdot, T)$ and $I_{\beta,\gamma}(\cdot, T) \equiv I^{obs}(\cdot, T)$.

Inverse problem results

- The inverse problem for onedimensional and restrictive condition for the stability result of a SIS model.
  Xiang & Liu (2015)
- The extension to the multidimensional case with a more general assumption for the stability result.
  Coronel, Huancas & Sepúlveda (2019)
- The extension to the multidimensional case with the infection force of the type $S^n I^n$ instead of $SI/(S+I)$.
  Coronel, Friz, Hess & Zegarra (2019)
- The extension to the model of indirectly transmitted diseases model.
  Coronel, Huancas & Sepúlveda (2019)
- The identification of diffusion when the diffusion is space dependent function.
  A. Coronel, F. Huancas, I. Hess & A. Tello (2024)
- Identification of reaction in a reaction-diffusion system for tumor growth.
  PhD thesis of I. Hess . . . stay in Seville with collaboration of F. Guillén-Gonzaáles

SIS model

The direct problem is reduced to: Given S_0, I_0, β, γ find S, I such that

$$
\begin{aligned}
\frac{\partial S}{\partial t} - \Delta S &= -\beta(\mathbf{x})\frac{SI}{S+I} + \gamma(\mathbf{x})I, && (\mathbf{x}, t) \in Q_T := \Omega \times [0, T],\\
\frac{\partial I}{\partial t} - \Delta I &= \beta(\mathbf{x})\frac{SI}{S+I} - \gamma(\mathbf{x})I, && (\mathbf{x}, t) \in Q_T,\\
\nabla S \cdot \mathbf{n} &= \nabla I \cdot \mathbf{n} = 0, && (\mathbf{x}, t) \in \Gamma := \partial\Omega \times [0, T],\\
S(\mathbf{x}, 0) &= S_0(\mathbf{x}), \quad I(\mathbf{x}, 0) = I_0(\mathbf{x}), && \mathbf{x} \in \Omega.
\end{aligned}
$$

The Inverse Problem is defined as follows: Given $T > 0$ and the set of functions $\{S_0, I_0, S^{obs}, I^{obs}\}$ defined on Ω, find the functions β and γ such that $(S, I)(\mathbf{x}, T) = (S^{obs}, I^{obs})(\mathbf{x})$ for $\mathbf{x} \in \Omega$ with (S, I) the solution of the forward problem.

The inverse problem may be recasting as the optimization problem

$$
\inf J(\beta, \gamma) \quad \text{subject to } (\beta, \gamma) \in U_{ad}(\Omega) \text{ and } (S, I) \text{ solution of SIS model,}
$$

where J and $U_{ad}(\Omega)$ are appropriately defined.

SIS model

We consider the admissible set $U_{ad}(\Omega)$ and the functional $J : U_{ad}(\Omega) \to \mathbb{R}$ defined as follows

$$U_{ad}(\Omega) = \mathcal{A}(\Omega) \cap \left[H^{[\![d/2]\!]+1}(\Omega) \times H^{[\![d/2]\!]+1}(\Omega) \right],$$

$$J(\beta,\gamma) := \frac{1}{2} \left[\|S(\cdot,T) - S^{obs}\|^2_{L^2(\Omega)} + \|I(\cdot,T) - I^{obs}\|^2_{L^2(\Omega)} \right] + \frac{\Gamma}{2} \left[\|\nabla\beta\|^2_{L^2(\Omega)} + \|\nabla\gamma\|^2_{L^2(\Omega)} \right],$$

with $[\![\cdot]\!]$ the integer part function, $\Gamma \in \mathbb{R}^+$ an appropriate regularization parameter and

$$\mathcal{A}(\Omega) = \Big\{ (\beta,\gamma) \in C^{\alpha}(\overline{\Omega}) \times C^{\alpha}(\overline{\Omega}) \;:\; \mathrm{Ran}(\beta) \subseteq [\underline{b}, \overline{b}] \subset]0,1[, \\ \mathrm{Ran}(\gamma) \subseteq [\underline{r}, \overline{r}] \subset]0,1[, \quad \nabla\beta,\ \nabla\gamma \in L^2(\Omega) \Big\},$$

where $\mathrm{Ran}(f)$ denotes the range of a function f. We note that $U_{ad}(\Omega) = \mathcal{A}(\Omega)$ when $d = 1$ and coincides with the admissible set considered by Xiang & Liu (2015).

SIS model

We consider the following set of assumptions:

(SIS0) The open bounded and convex set Ω is such that $\partial\Omega$ is C^1.

(SIS1) The initial conditions S_0 and I_0 are belong to $C^{2,\alpha}(\overline{\Omega})$ and satisfy the inequalities

$$S_0(\mathbf{x}) \geq 0, \quad I_0(\mathbf{x}) \geq 0, \quad \int_\Omega I_0(\mathbf{x})d\mathbf{x} > 0, \quad S_0(\mathbf{x}) + I_0(\mathbf{x}) \geq \phi_0 > 0,$$

on Ω, for some positive constant ϕ_0;

(SIS2) The observation functions S^{obs} and I^{obs} are belong to $L^2(\Omega)$.

We consider that the adjoint system to SIS model is given by

$$\begin{aligned}
&\frac{\partial P}{\partial t} + \Delta P = \overline{\beta}(\mathbf{x})\frac{\overline{I}^2}{(\overline{S}+\overline{I})^2}(P-Q), && (\mathbf{x},t) \in Q_T := \Omega \times [0,T],\\
&\frac{\partial Q}{\partial t} + \Delta Q = \left(\overline{\beta}(\mathbf{x})\frac{\overline{S}^2}{(\overline{S}+\overline{I})^2} - \overline{\gamma}(\mathbf{x})\right)(P-Q), && (\mathbf{x},t) \in Q_T,\\
&\nabla P\cdot\mathbf{n} = \nabla Q\cdot\mathbf{n} = 0, && (\mathbf{x},t) \in \Gamma := \partial\Omega \times [0,T],\\
&P(\mathbf{x},T) = \overline{S}(\mathbf{x},T) - S^{obs}(\mathbf{x}), \quad Q(\mathbf{x},T) = \overline{I}(\mathbf{x},T) - I^{obs}(\mathbf{x}), && \mathbf{x} \in \Omega,
\end{aligned}$$

where $(\overline{\beta},\overline{\gamma}) \in U_{ad}$ and $(\overline{S},\overline{I})$ is the corresponding solution of SIS model with $(\overline{\beta},\overline{\gamma})$ instead of (β,γ).

SIS model: Direct problem

Theorem

Consider that the hypotheses (SIS0)-(SIS2) are satisfied. If $(\beta, \alpha) \in C^{\alpha}(\overline{\Omega}) \times C^{\alpha}(\overline{\Omega})$, the initial boundary value problem SIS admits a unique positive classical solution (S, I), such that S and I are belong to $C^{2+\alpha, 1+\alpha/2}(\overline{Q}_T)$ and also S and I are bounded on $\overline{Q}_T$, for any given $T \in \mathbb{R}^+$.

The existence and the uniqueness can be developed by the Shauder's theory for parabolic equations. Meanwhile, the positive behavior of the solution is a consequence of the maximum principle.

SIS model

Theorem

Consider that the following hypotheses (SIS0)-(SIS3) are satisfied. Then,
(i) There exists at least one solution of optimization problem (IP).
(ii) Let us consider $(\overline{\beta},\overline{\gamma})$ *is the solution of IP and* $(\overline{S},\overline{I})$ *the corresponding solutions of SIS with* $(\overline{\beta},\overline{\gamma})$ *instead of* (β,γ)*. Then,* (P,Q) *is bounded in* $L^{\infty}(0,t;H^2(\Omega))$ *for almost all time t in* $]0,T]$*. In particular* (P,Q) *is bounded in* $L^{\infty}(0,t;L^{\infty}(\Omega))$ *for almost all time t in* $]0,T]$*.*
(iii) Let us consider $\overline{S},\overline{I},\overline{\beta},\overline{\gamma}$*, P and Q as is given in (ii). Then, the following inequality*

$$\int_{Q_T}\left[(\hat{\beta}-\overline{\beta})\frac{\overline{S}\,\overline{I}}{\overline{S}+\overline{I}}-(\hat{\gamma}-\overline{\gamma})\overline{I}\right](P-Q)+\Gamma\Big[\int_{\Omega}\nabla\overline{\beta}\cdot\nabla(\hat{\beta}-\overline{\beta})+\nabla\overline{\gamma}\cdot\nabla(\hat{\gamma}-\overline{\gamma})\Big]\geq 0,$$

is satisfied for all $(\hat{\beta},\hat{\gamma})\in U_{ad}(\Omega)$*.*
(iv) The mapping $(\beta,\gamma)\mapsto(S,I)$ *is continuous from* $U_{ad}(\Omega)\subset[L^2(\Omega)]^2$ *to* $L^{\infty}(0,t;L^2(\Omega))$ *for almost all time t in* $]0,T]$*.*
(v) The mapping $(\beta,\gamma,S^{obs},I^{obs})\mapsto(P,Q)$ *is continuous from* $U_{ad}(\Omega)\times L^2(\Omega)\times L^2(\Omega)\subset[L^2(\Omega)]^4$ *to* $L^{\infty}(0,t;L^2(\Omega))$ *for almost all time t in* $]0,T]$*.*
(vi) Given $\mathbf{c}=(c_1,c_2)\in\mathbb{R}^2_+$ *(fix) define* $\mathcal{U}_{\mathbf{c}}(\Omega)=\left\{(\beta,\gamma)\in U_{ad}(\Omega)\,:\,\int_{\Omega}(\beta,\gamma)d\mathbf{x}=\mathbf{c}\right\}$*.*
Then, there exist $\overline{\Gamma}\in\mathbb{R}^+$ *such that the solution of IP is uniquely defined, up an additive constant, on* $\mathcal{U}_{\mathbf{c}}(\Omega)$ *in the* $L^2(\Omega)$ *sense for any regularization parameter* $\Gamma>\overline{\Gamma}$*.*

(i) Existence 1/2

We note that $U_{ad}(\Omega) \neq \emptyset$ and $J(\beta, \gamma)$ is bounded for any $(\beta, \gamma) \in U_{ad}(\Omega)$. The fact that $U_{ad}(\Omega) \neq \emptyset$ follows for instance by considering the pair of functions $(\beta, \gamma)(\mathbf{x}) = (\underline{b} + \overline{b}, \underline{r} + \overline{r})/2$, which is belong to $U_{ad}(\Omega)$. The boundedness of J is deduced by the following three facts: the bounded behavior of S and T on $\overline{Q}_T$ as consequence of part (i), the hypothesis (SIS2) and the fact that $\nabla\beta,\ \nabla\gamma \in L^2(\Omega)$ by the definition of $U_{ad}(\Omega)$. Then, we can consider that $\{(\beta_n, \gamma_n)\} \subset \mathcal{U}$ is a minimizing sequence of J.

On the other hand, we claim the compact embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^{\alpha}(\Omega)$ for $\alpha \in]0, 1/2]$. Indeed, it can be deduced using two results. First, we have the Sobolev embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^{\theta}(\Omega)$ with $\theta = 1/2$ for d odd and $\theta \in]0, 1[$ for d even. Then, for all d we have the continuous embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^{1/2}(\Omega)$. Second, we have the compact embedding $C^{1/2}(\Omega) \subset C^{\alpha}(\Omega)$ for all $\alpha \in]0, 1/2]$. Hence our claim follows from the chain of embeddings $H^{[\![d/2]\!]+1}(\Omega) \subset C^{1/2}(\Omega) \subset C^{\alpha}(\Omega)$ for all $\alpha \in]0, 1/2]$.

The compact embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^{\alpha}(\Omega)$ for $\alpha \in]0, 1/2]$, implies that the minimizing sequence $\{(\beta_n, \gamma_n)\}$ is bounded in the strong topology of $C^{\alpha}(\overline{\Omega}) \times C^{\alpha}(\overline{\Omega})$ for all $\alpha \in]0, 1/2]$, since there exists a positive constant C (independent of β, γ and n) such that

$$\|\beta_n\|_{C^{\alpha}(\overline{\Omega})} + \|\gamma_n\|_{C^{\alpha}(\overline{\Omega})} \leq C\Big(\|\beta_n\|_{H^{[\![d/2]\!]+1}(\Omega)} + \|\gamma_n\|_{H^{[\![d/2]\!]+1}(\Omega)}\Big), \quad \forall \alpha \in]0, 1/2].$$

Now, we note that the right hand is bounded by the fact that $\beta_n, \gamma_n \in H^{[\![d/2]\!]+1}(\Omega)$ (the definition of $U_{ad}(\Omega)$).

(i) Existence 2/2

Let us denote by (S_n, I_n) the solution of the SIS model corresponding to (β_n, γ_n). Then, by considering the fact that $\{(\beta_n, \gamma_n)\}$ is belong to $C^\alpha(\overline{\Omega}) \times C^\alpha(\overline{\Omega})$ for all $\alpha \in]0, 1/2]$, by (i), we have that S_n and I_n are belong to the Hölder space $C^{2+\alpha, 1+\frac{\alpha}{2}}(\overline{Q}_T)$ and also $\{(S_n, I_n)\}$ is a bounded sequence in the strong topology of $C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T) \times C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T)$ for all $\alpha \in]0, 1/2]$.

The boundedness of the minimizing sequence and the corresponding sequence $\{(S_n, I_n)\}$, implies that there exist

$$(\overline{\beta}, \overline{\gamma}) \in \left[C^{1/2}(\Omega) \times C^{1/2}(\Omega)\right] \cap U_{ad}(\Omega), \qquad (\overline{S}, \overline{T}) \in C^{2+\frac{1}{2},1+\frac{1}{4}}(\overline{Q}_T) \times C^{2+\frac{1}{2},1+\frac{1}{4}}(\overline{Q}_T),$$

and the subsequences again labeled by $\{(\beta_n, \gamma_n)\}$ and $\{(S_n, I_n)\}$ such that

$$\beta_n \to \overline{\beta}, \quad \gamma_n \to \overline{\gamma} \quad \text{uniformly on } C^\alpha(\Omega),$$
$$S_n \to \overline{S}, \quad I_n \to \overline{I} \quad \text{uniformly on } C^{\alpha,\frac{\alpha}{2}}(\overline{Q}_T) \cap C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T).$$

Moreover, we can deduce that $(\overline{S}, \overline{I})$ is the solution of the SIS model corresponding to the coefficients $(\overline{\beta}, \overline{\gamma})$.

Hence, by Lebesgue's dominated convergence theorem, the weak lower-semicontinuity of L^2 norm, and the definition of the minimizing sequence, we have that

$$J(\overline{\beta}, \overline{\gamma}) \le \lim_{n\to\infty} J(\beta_n, \gamma_n) = \inf_{(\beta,\gamma)\in U_{ad}(\Omega)} J(\beta, \gamma).$$

Then, $(\overline{\beta}, \overline{\gamma})$ is a solution of of optimization problem.

(ii) Boundedness of (P, Q) 1/3

The proof of that AP is the adjoint system for SIS we can follow by the standard arguments in optimal control theory. Now, in order to get the $L^\infty(0, t; H^2(\Omega))$ estimates, let us consider an arbitrary $t \in]0, T]$ and we claim that

$$
\begin{aligned}
&\|P(\cdot,t)\|^2_{L^2(\Omega)} + \|Q(\cdot,t)\|^2_{L^2(\Omega)} \le C,\\
&\|\nabla P(\cdot,t)\|_{L^2(\Omega)} + \|\nabla Q(\cdot,t)\|_{L^2(\Omega)} \le C,\\
&\|\Delta P(\cdot,t)\|_{L^2(\Omega)} + \|\Delta Q(\cdot,t)\|_{L^2(\Omega)} \le C,\\
&\|P(\cdot,t)\|_{L^\infty(\Omega)} \le C, \quad \|Q(\cdot,t)\|_{L^\infty(\Omega)} \le C,
\end{aligned}
$$

for a some positive generic constants C. We can prove the claims by standard estimates for an initial value problem equivalent to AP. Indeed, in order to transform in an initial boundary problem we introduce the change of variable $\tau = T - t$ for $t \in [0, T]$. Moreover, consider the notation $w_1(\cdot,\tau) = P(\cdot, T-\tau)$, $w_2(\cdot,\tau) = Q(\cdot, T-\tau)$, $S^*(\cdot,\tau) = \bar{S}(\cdot, T-\tau)$, and $I^*(\cdot,\tau) = \bar{I}(\cdot, T-\tau)$. Then, the adjoint system AP is equivalent to the system

$$
\begin{aligned}
&(w_1)_\tau - \Delta w_1 = \bar{\beta}(\mathbf{x}) \left(\frac{I^*}{S^* + I^*} \right)^2 (w_1 - w_2), && \text{in } Q_T,\\
&(w_2)_\tau - \Delta w_2 = \bar{\beta}(\mathbf{x}) \left(\frac{S^*}{S^* + I^*} \right)^2 (w_1 - w_2) - \bar{\gamma}(\mathbf{x})(w_1 - w_2), && \text{in } Q_T,\\
&\nabla w_1 \cdot \mathbf{n} = \nabla w_2 \cdot \mathbf{n} = 0, && \text{on } \Gamma,\\
&w_1(\mathbf{x},0) = \bar{S}(\mathbf{x},T) - S^{obs}(\mathbf{x}), \quad w_2(\mathbf{x},0) = \bar{I}(\mathbf{x},T) - I^{obs}(\mathbf{x}), && \text{in } \Omega.
\end{aligned}
$$

Now, we proceed to get the corresponding estimates for AP*.

(ii) Boundedness of (P, Q) 2/3

In order the L^2 and H_0^1 estimates, we test the first equation by w_1 and the second equation by w_2, and sum the results to get that

$$\frac{1}{2}\frac{d}{d\tau}\left(\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right) + \|\nabla w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|\nabla w_2(\cdot,\tau)\|^2_{L^2(\Omega)}$$

$$\leq \int_\Omega |\bar{\beta}(\mathbf{x})| \left(\frac{I^*}{S^* + I^*}\right)^2 |w_1^2 - w_1 w_2| \, d\mathbf{x} + \int_\Omega \left(|\bar{\beta}(\mathbf{x})| \left(\frac{S^*}{S^* + I^*}\right)^2 + |\bar{\gamma}(\mathbf{x})| \right) |w_1 w_2 - w_2^2| \, d$$

$$\leq \left(\bar{b} + \bar{r}\right) \left[\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right].$$

Then, from the Gronwall inequality, we obtain

$$\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)} \leq \exp\left(2(\bar{b} + \bar{r})T\right) \left(\|w_1(\cdot,0)\|^2_{L^2(\Omega)} + \|w_2(\cdot,0)\|^2_{L^2(\Omega)}\right),$$

which implies the L^2 estimate. . . .

$$\|\nabla w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|\nabla w_2(\cdot,\tau)\|^2_{L^2(\Omega)} \leq (\bar{b} + \bar{r}) \exp\left(2(\bar{b} + \bar{r})T\right) \left(\|w_1(\cdot,0)\|^2_{L^2(\Omega)} + \|w_2(\cdot,0)\|^2_{L^2}\right.$$

and we can follow the H_0^1 estimate.

(ii) Boundedness of (P, Q) 3/3

Using the fact that

$$\int_\Omega (w_i)_\tau \Delta w_i \, d\mathbf{x} = -\int_\Omega \nabla[(w_i)_\tau] \cdot \nabla w_i \, d\mathbf{x} + \int_{\partial\Omega} (w_i)_\tau \nabla(w_i) \cdot \mathbf{n} \, dS = -\frac{1}{2}\frac{d}{d\tau}\|w_i(\cdot,\tau)\|^2_{L_2(\Omega)},$$

for $i = 1, 2$. We note that, multiplying the first equation by Δw_1, multiplying the second equation by Δw_2, integrating on Ω, and adding the results, we deduce that

$$\frac{1}{2}\frac{d}{d\tau}\left(\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right) + \|\Delta w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|\Delta w_2(\cdot,\tau)\|^2_{L^2(\Omega)}$$
$$\leq (\overline{b} + \overline{r})\left[2\epsilon\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + 2\epsilon\|w_2(\cdot,\tau)\|^2_{L^2(\Omega)} + \frac{1}{2\epsilon}\|\Delta w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \frac{1}{2\epsilon}\|\Delta w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right]$$

for any $\epsilon > 0$. Then, we have that

$$\frac{1}{2}\frac{d}{d\tau}\left(\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right) + \left(1 - \frac{(\overline{b} + \overline{r})}{2\epsilon}\right)\left(\|\Delta w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|\Delta w_2(\cdot,\tau)\|^2_{L^2}\right.$$
$$\leq 2\epsilon(\overline{b} + \overline{r})\left[\|w_1(\cdot,\tau)\|^2_{L^2(\Omega)} + \|w_2(\cdot,\tau)\|^2_{L^2(\Omega)}\right].$$

Now, by selecting $\epsilon > (\overline{b}+\overline{r})/2$ and using the estimate L^2 estimate we get the inequality for $\Delta P, \Delta Q$.
The norm of $P(\cdot, t)$ and $Q(\cdot, t)$ are bounded in the norm of $H^2(\Omega)$ for any $t \in]0, T]$. Thus, by the standard embedding theorem of $H^2(\Omega) \subset L^\infty(\Omega)$, we easily deduce that $P(\cdot, t)$ and $Q(\cdot, t)$ are bounded in $L^\infty(\Omega)$.

(iii) Necesary Optimality condition 1/2

Let us consider an arbitrary pair $(\hat{\beta}, \hat{\gamma}) \in U_{ad}$ and introduce the notation

$$\begin{aligned}(\beta^\varepsilon, \gamma^\varepsilon) &= (1-\varepsilon)(\bar{\beta}, \bar{\gamma}) + \varepsilon(\hat{\beta}, \hat{\gamma}) \in U_{ad}, \\ J_\varepsilon &= J(\beta^\varepsilon, \gamma^\varepsilon) = \frac{1}{2}\int_\Omega \left(\left| S^\varepsilon(\mathbf{x}, t) - S^{obs}(\mathbf{x}) \right|^2 + \left| I^\varepsilon(\mathbf{x}, t) - I^{obs}(\mathbf{x}) \right|^2 \right) d\mathbf{x} \\ &\quad + \frac{\delta}{2}\int_\Omega \left(|\nabla\beta^\varepsilon(\mathbf{x})|^2 + |\nabla\gamma^\varepsilon(\mathbf{x})|^2 \right) d\mathbf{x},\end{aligned}$$

where $(S^\varepsilon, I^\varepsilon)$ is the solution of SIS with $(\beta^\varepsilon, \gamma^\varepsilon)$ instead of (β, γ). Now, using the hypothesis that $(\bar{\beta}, \bar{\gamma})$ is an optimal solution of IP and taking the Fréchet derivative of J_ε, we have that

$$\begin{aligned}\left.\frac{dJ_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} &= \int_\Omega \left(\left| S^\varepsilon(\mathbf{x}, t) - S^{obs}(\mathbf{x}) \right| \left.\frac{\partial S^\varepsilon}{\partial\varepsilon}\right|_{\varepsilon=0} + \left| I^\varepsilon(\mathbf{x}, t) - I^{obs}(\mathbf{x}) \right| \left.\frac{\partial I^\varepsilon}{\partial\varepsilon}\right|_{\varepsilon=0} \right) d\mathbf{x} \\ &\quad + \delta\int_\Omega \left[\nabla\bar{\beta}\nabla\left(\hat{\beta} - \bar{\beta}\right) + \nabla\bar{\gamma}\nabla\left(\hat{\gamma} - \bar{\gamma}\right) \right] d\mathbf{x} \geq 0,\end{aligned}$$

where $\partial_\varepsilon S^\varepsilon$ and $\partial_\varepsilon I^\varepsilon$ for $\varepsilon = 0$ are calculated by analyzing the sensitivities of solutions for SIS with respect to perturbations of (β, γ).

(iii) Necesary Optimality condition 2/2

Let us consider

$$(z_1^\varepsilon, z_2^\varepsilon) = \frac{1}{\varepsilon}\left(S^\varepsilon - \bar{S}, I^\varepsilon - \bar{I}\right),$$

$$\mathbb{F}_u = \frac{1}{S^\varepsilon - \bar{S}}\left[\frac{S^\varepsilon}{S^\varepsilon + I} - \frac{S}{S+I}\right] \quad \mathbb{F}_v = \frac{1}{I^\varepsilon - \bar{I}}\left[\frac{I^\varepsilon}{S + I^\varepsilon} - \frac{I}{S+I}\right]$$

we deduce the following system

$$\begin{aligned}
(z_1^\varepsilon)_t - \Delta z_1^\varepsilon &= -\beta^\varepsilon(\mathbf{x})\mathbb{F}_u I^\varepsilon z_1^\varepsilon - \beta^\varepsilon(\mathbf{x})(\bar{S})^m \mathbb{F}_v z_2^\varepsilon \\
&\quad - (\hat{\beta} - \bar{\beta})(\bar{S})^m(\bar{I})^n + \gamma^\varepsilon(\mathbf{x}) z_2^\varepsilon + (\hat{\gamma} - \bar{\gamma})\bar{I}, && \text{in } Q_T, \\
(z_2^\varepsilon)_t - \Delta z_2^\varepsilon &= \beta^\varepsilon(\mathbf{x})\mathbb{F}_u I^\varepsilon z_1^\varepsilon + \beta^\varepsilon(\mathbf{x})(\bar{S})^m \mathbb{F}_v z_2^\varepsilon \\
&\quad + (\hat{\beta} - \bar{\beta})(\bar{S})^m(\bar{I})^n - \gamma^\varepsilon(\mathbf{x}) z_2^\varepsilon - (\hat{\gamma} - \bar{\gamma})\bar{I}, && \text{in } Q_T, \\
\nabla z_1^\varepsilon \cdot \mathbf{n} &= \nabla z_2^\varepsilon \cdot \mathbf{n} = 0, && \text{on } \Gamma, \\
z_1^\varepsilon(\mathbf{x}, 0) &= z_2^\varepsilon(\mathbf{x}, 0) = 0, && \text{in } \Omega.
\end{aligned}$$

Then, denoting by (z_1, z_2) the limit of $(z_1^\varepsilon, z_2^\varepsilon)$ when $\varepsilon \to 0 \ldots$

(iv) continous dependence DP 1/2

Lemma

Consider that the following hypotheses (SIS0)-(SIS3) are satisfied. Let us consider that (S, I) and $(\tilde{S}, \tilde{I})$ are the corresponding solutions of SIS model with coefficients $(\beta, \gamma) \in U_{ad}(\Omega)$ and $(\tilde{\beta}, \tilde{\gamma}) \in U_{ad}(\Omega)$, respectively. Then, there exist the positive constant C such that the inequality

$$\|(\hat{S} - S)(\cdot, t)\|^2_{L^2(\Omega)} + \|(\hat{I} - I)(\cdot, t)\|^2_{L^2(\Omega)} \leq C\Big(\|\hat{\beta} - \beta\|^2_{L^2(\Omega)} + \|\hat{\gamma} - \gamma\|^2_{L^2(\Omega)}\Big),$$

holds for any $t \in [0, T]$.

(iv) continous dependence DP 2/2

Now, by notational convenience we consider $\delta S, \delta I, \delta\beta$ and $\delta\gamma$ defined as follows

$$\delta S = \hat{S} - S, \quad \delta I = \hat{I} - I, \quad \delta\beta = \hat{\beta} - \beta, \quad \delta\gamma = \hat{\gamma} - \gamma.$$

Then, from the system SIS for (S, I) and $(\hat{S}, \hat{S})$ we have that $(\delta S, \delta I)$ satisfy the initial boundary value problem

$$\begin{aligned}
(\delta S)_t - \Delta(\delta S) &= -\hat{\beta}(\mathbf{x})\left(\frac{\hat{S}}{\hat{S}+\hat{I}} - \frac{S}{S+I}\right) - \delta\beta(\mathbf{x})\left(\frac{\hat{S}}{\hat{S}+\hat{I}}\right) + \hat{\gamma}(\mathbf{x})\delta I + \gamma(\mathbf{x})I, && \text{in } \in Q_T,\\
(\delta I)_t - \Delta(\delta I) &= \hat{\beta}(\mathbf{x})\left(\frac{\hat{S}}{\hat{S}+\hat{I}} - \frac{S}{S+I}\right) + \delta\beta(\mathbf{x})\left(\frac{\hat{S}}{\hat{S}+\hat{I}}\right) - \hat{\gamma}(\mathbf{x})\delta I - \gamma(\mathbf{x})I, && \text{in } \in Q_T,\\
\nabla(\delta S)\cdot\mathbf{n} &= \nabla(\delta I)\cdot\mathbf{n} = 0, && \text{on } \in \Gamma,\\
(\delta S)(\mathbf{x},0) &= (\delta I)(\mathbf{x},0) = 0, && \text{in } \Omega.
\end{aligned}$$

(v) continous dependence AP 1/2

Lemma

Consider that the following hypotheses (SIS0)-(SIS3) are satisfied. Let us consider that (S, I) and $(\tilde{S}, \tilde{I})$ are the corresponding solutions of SIS model with coefficients $(\beta, \gamma) \in U_{ad}(\Omega)$ and $(\tilde{\beta}, \tilde{\gamma}) \in U_{ad}(\Omega)$, respectively. Moreover consider that (P, Q) and $(\tilde{P}, \tilde{Q})$ are the solutions of the adjoint problems for (S, I) and $(\tilde{S}, \tilde{I})$ with (S^{obs}, I^{obs}) and $(\tilde{S}^{obs}, \tilde{I}^{obs})$ as observations, respectively. Then, there exist the positive constant C such that the inequality

$$\begin{aligned} \|(\hat{P} - P)(\cdot, t)\|^2_{L^2(\Omega)} + \|(\hat{Q} - Q)(\cdot, t)\|^2_{L^2(\Omega)} \\ \leq \tilde{C}_1 \left(\|\hat{\beta} - \beta\|^2_{L^2(\Omega)} + \|\hat{\gamma} - \gamma\|^2_{L^2(\Omega)} \right) \\ + \tilde{C}_2 \left(\|\hat{S}^{obs} - S^{obs}\|^2_{L^2(\Omega)} + \|\hat{I}^{obs} - I^{obs}\|^2_{L^2(\Omega)} \right) \end{aligned}$$

holds for any $t \in [0, T]$.

(v) continous dependence AP 2/2

We consider that $\delta P = \hat{P} - P$ and $\delta Q = \hat{Q} - Q$ which satisfy the system

$$
\begin{aligned}
(\delta P)_t + \Delta(\delta P) &= \hat{\beta}(\mathbf{x}) \left(\frac{\hat{I}}{\hat{S} + \hat{I}} \right)^2 (\hat{P} - \hat{Q}) - \beta(\mathbf{x}) \left(\frac{I}{S + I} \right)^2 (P - Q), && \text{in } Q_T, \\
(\delta Q)_t + \Delta(\delta Q) &= \left(\hat{\beta}(\mathbf{x}) \left(\frac{\hat{S}}{\hat{S} + \hat{I}} \right)^2 - \hat{\gamma}(\mathbf{x}) \right) (\hat{P} - \hat{Q}) \\
&\quad - \left(\beta(\mathbf{x}) \left(\frac{S}{S + I} \right)^2 - \gamma(\mathbf{x}) \right) (P - Q), && \text{in } Q_T, \\
\nabla(\delta P) \cdot \mathbf{n} &= \nabla(\delta Q) \cdot \mathbf{n} = 0, && \text{on } \Gamma, \\
(\delta P)(\mathbf{x}, T) &= \delta S(\mathbf{x}, T) - \left(\hat{S}^{obs}(\mathbf{x}) - S^{obs}(\mathbf{x}) \right), && \text{in } \Omega, \\
(\delta Q)(\mathbf{x}, T) &= \delta I(\mathbf{x}, T) - \left(\hat{I}^{obs}(\mathbf{x}) - I^{obs}(\mathbf{x}) \right), && \text{in } \Omega.
\end{aligned}
$$

Lemma

Consider that the following hypotheses (SIS0)-(SIS3) are satisfied. Let us consider that (S, I) and $(\tilde{S}, \tilde{I})$ are the corresponding solutions of SIS model with coefficients $(\beta, \gamma) \in U_{ad}(\Omega)$ and $(\tilde{\beta}, \tilde{\gamma}) \in U_{ad}(\Omega)$, respectively. Moreover consider that (P, Q) and $(\tilde{P}, \tilde{Q})$ are the solutions of the adjoint problems for (S, I) and $(\tilde{S}, \tilde{I})$ with (S^{obs}, I^{obs}) and $(\tilde{S}^{obs}, \tilde{I}^{obs})$ as observations, respectively. If $\int_\Omega (\beta, \gamma) dx = \int_\Omega (\tilde{\beta}, \tilde{\gamma}) dx$, the estimate

$$\|\tilde{\beta} - \beta\|^2_{L^2(\Omega)} + \|\tilde{\gamma} - \gamma\|^2_{L^2(\Omega)} \leq \Psi \left[\|\tilde{S}^{obs} - S^{obs}\|^2_{L^2(\Omega)} + \|\tilde{I}^{obs} - I^{obs}\|^2_{L^2(\Omega)} \right],$$

is valid for some constant $\Psi > 0$.

Xiang& Liu (2015). Let us consider the notation of item (v). If there exists $x_0 \in \Omega$ such that $(\beta, \gamma)(x_0) = (\tilde{\beta}, \tilde{\gamma})(x_0)$ the estimate

$$\max_{\mathbf{x} \in \Omega} |(\tilde{\beta} - \beta)(\mathbf{x})|^2 + \max_{\mathbf{x} \in \Omega} |(\tilde{\gamma} - \gamma)(\mathbf{x})|^2 \leq \Psi \left[\|\tilde{S}^{obs} - S^{obs}\|^2_{L^2(\Omega)} + \|\tilde{I}^{obs} - I^{obs}\|^2_{L^2(\Omega)} \right],$$

is valid.

(vi) Stability IP 2/4

Xiang & Liu uses the following result:

Lemma

For $\rho \in C[0,1]$ *we have* $\max_{x\in[0,1]} |\rho(x)| \leq |\rho(x_0)| + \|\nabla\rho\|_{L^2(\Omega)}$

We use a generalized Poincaré inequality

$$\|\rho\|_{L^p(\Omega)} \leq C(\|\rho\|_{L^1(\Omega)} + \|\nabla\rho\|_{L^p(\Omega)}) \qquad \forall \rho \in W^{1,p}(\Omega).$$

(vi) Stability IP

Using the fact that (β, γ) and $(\tilde{\beta}, \tilde{\gamma})$ are solutions of IP we have

$$\int_{Q_T} \left[(\hat{\beta} - \beta) \frac{SI}{S+I} - (\hat{\gamma} - \gamma) I \right] (P - Q) d\mathbf{x} dt$$
$$+ \Gamma \left[\int_\Omega \nabla \beta \cdot \nabla (\hat{\beta} - \beta) d\mathbf{x} + \int_\Omega \nabla \gamma \cdot \nabla (\hat{\gamma} - \gamma) d\mathbf{x} \right] \geq 0, \quad \forall (\hat{\beta}, \hat{\gamma}) \in U_{ad}(\Omega),$$
$$\int_{Q_T} \left[(\hat{\beta} - \tilde{\beta}) \frac{\tilde{S}\ \tilde{I}}{\tilde{S} + \tilde{I}} - (\hat{\gamma} - \tilde{\gamma}) \tilde{I} \right] (\tilde{P} - \tilde{Q}) d\mathbf{x} dt$$
$$+ \Gamma \left[\int_\Omega \nabla \tilde{\beta} \cdot \nabla (\hat{\beta} - \tilde{\beta}) d\mathbf{x} + \int_\Omega \nabla \tilde{\gamma} \cdot \nabla (\hat{\gamma} - \tilde{\gamma}) d\mathbf{x} \right] \geq 0, \quad \forall (\hat{\beta}, \hat{\gamma}) \in U_{ad}(\Omega),$$

Then, selecting $(\hat{\beta}, \hat{\gamma}) = (\overline{\beta}, \overline{\gamma})$ in the first inequality and $(\hat{\beta}, \hat{\gamma}) = (\beta, \gamma)$ in the second inequality, rearranging some terms and applying the Cauchyy-Schwarz we deduce that

$$\Gamma \left[\|\nabla (\tilde{\beta} - \beta)\|^2_{L^2(\Omega)} + \|\nabla (\tilde{\gamma} - \gamma)\|^2_{L^2(\Omega)} \right]$$
$$\leq \int_{Q_T} |\tilde{\beta} - \beta| \left| \frac{\tilde{S}\ \tilde{I}}{\tilde{S} + \tilde{I}} (\tilde{P} - \tilde{Q}) - \frac{SI}{S+I} (P - Q) \right| d\mathbf{x} dt + \int_{Q_T} |\tilde{\gamma} - \gamma| \left| \tilde{I} (\tilde{P} - \tilde{Q}) - I(P - Q) \right| \mathbf{x} dt$$

(vi) Stability IP 4/4

$$\Gamma\left[\|\nabla(\tilde\beta-\beta)\|^2_{L^2(\Omega)}+\|\nabla(\tilde\gamma-\gamma)\|^2_{L^2(\Omega)}\right]$$
$$\leq \Theta_1\left[\|\tilde\beta-\beta\|^2_{L^2(\Omega)}+\|\tilde\gamma-\gamma\|^2_{L^2(\Omega)}\right]+\Theta_2\left[\|\tilde S-S\|^2_{L^\infty(0,T;L^2(\Omega))}+\|\tilde I-I\|^2_{L^\infty(0,T;L^2(\Omega))}\right]$$
$$+\Theta_3\left[\|\tilde P-P\|^2_{L^\infty(0,T;L^2(\Omega))}+\|\tilde Q-Q\|^2_{L^\infty(0,T;L^2(\Omega))}\right]$$
$$\leq\left[\Theta_1+\Theta_2+\Theta_3\right]\left[\|\tilde\beta-\beta\|^2_{L^2(\Omega)}+\|\tilde\gamma-\gamma\|^2_{L^2(\Omega)}\right]+\Theta_3\left[\|\tilde S^{obs}-S\|^2_{L^2(\Omega)}+\|\tilde I^{obs}-I\|^2_{L^2(\Omega)}\right]$$

Now, considering that $(\hat\beta,\hat\gamma),(\beta,\gamma)\in\mathcal{U}_{\mathbf{c}}(\Omega)$, by the generalized Poincaré inequality, we have that there exist a positive constant C_{poi} such that

$$\|\hat\beta-\beta\|^2_{L^2(\Omega)}+\|\hat\gamma-\gamma\|^2_{L^2(\Omega)}$$
$$\leq C_{poi}\left(\|\nabla(\hat\beta-\beta)\|^2_{L^2(\Omega)}+\|\nabla(\hat\gamma-\gamma)\|^2_{L^2(\Omega)}+\|\hat\beta-\beta\|^2_{L^1(\Omega)}+\|\hat\gamma-\gamma\|^2_{L^1(\Omega)}\right)$$
$$=C_{poi}\left(\|\nabla(\hat\beta-\beta)\|^2_{L^2(\Omega)}+\|\nabla(\hat\gamma-\gamma)\|^2_{L^2(\Omega)}\right).$$

Thus

$$\left(\Gamma-\overline{\Gamma}\right)\left[\|\nabla(\hat\beta-\beta)\|^2_{L^2(\Omega)}+\|\nabla(\hat\gamma-\gamma)\|^2_{L^2(\Omega)}\right]\leq\Upsilon_2\left[\|\hat S^{obs}-S^{obs}\|^2_{L^2(\Omega)}+\|\hat I^{obs}-I^{obs}\|^2_{L^2(\Omega)}\right]$$

which implies the desired uniqueness for $\overline{\Gamma}=(\Theta_1+\Theta_2+\Theta_3)C_{poi}$.

MODELLING ASSUMPTIONS

Modelling Assumptions 1/3

The mathematical model for invasion and persistence of parasites through spatially distributed host populations assumes that [6]:

(A0) There are two independent host populations H_1 and H_2 which are spatially distributed over non-coincident spatial domains Ω_1 and Ω_2 of $\subset \mathbb{R}^d$ $(d = 1, 2, 3)$; i.e. $\Omega_1 \cap \Omega_2 \neq \emptyset$ and $\Omega_1 \cap \Omega_2 \neq \Omega_i$, $i = 1, 2$; respectively. Here non-coincident The region Ω_1 is a reservoir where live a parasite which, in most of the cases of interest, is benign on the population H_1 and lethal on the population H_2.

(A1) Each host population is subdivided into three subclasses: susceptible individuals who are capable to be infected, infective individuals who have contracted the disease and are capable to transmitting it, and recovered individuals. The notation φ, ψ and χ is used to represent the population densities of the subclasses of susceptible, infective and recovered individuals from the total population $H_1 = \varphi + \psi + \chi$, while u, v, and w is used to represent the population densities of the susceptible, infective and recovered subclasses of the total population $H_2 = u + v + w$.

Modelling assumptions 2/3

(A2) The susceptible individuals in the host population H_1 can contract the disease from cross contacts with infected hosts from H_1 or with the environment.

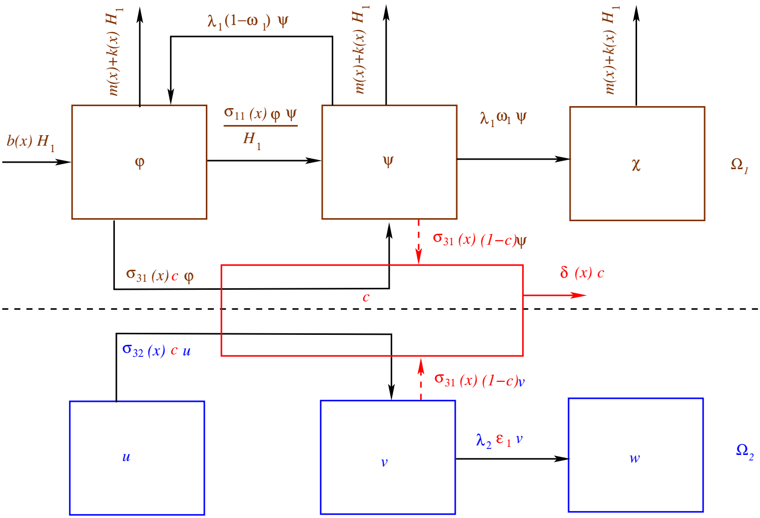
(A3) The susceptible individuals in the host population H_2 are infected by contact with the environment but there is neither cross infection from infected hosts from H_2 nor crisscross infection with H_1.

(A4) There is a contaminant on the habitat or environment. The proportion of contaminant is represented by c.

Modelling assumptions 3/3

(A5) There is spatial heterogeneity into the coefficients.

- The population H_1 follow a logistic dynamic with a space dependent birth-rate $b(x)$, which is identical in each subclass, offspring being susceptible at birth because the disease is assumed to be benign in H_1.
- The spatially density dependent mortality rate $m(x)+k(x)H_1$ is considered allowing a spatially variable carrying capacity.
- Any demographic effect, besides a disease-induced mortality, on the population H_2 is ignored.
- $1/\lambda_i$ is the duration of the infective stage in population H_i, $i = 1, 2$.
- A fixed proportion $w_1 \in [0, 1]$ of infective individuals from H_1 become permanently immune, a proportion $1 - w_1 \in [0, 1]$ reentering to the susceptible class.
- The disease can be lethal in the second host population with a fixed survival rate $\varepsilon_1 \in [0, 1]$.



$m(x)+k(x)\ H_1$
$\lambda_1(1-\omega_1)\ \psi$
$m(x)+k(x)\ H_1$
$m(x)+k(x)\ H_1$
$b(x)\ H_1$
φ
$\frac{\sigma_{11}(x)\ \varphi\ \psi}{H_1}$
ψ
$\lambda_1\omega_1\ \psi$
χ
Ω_1
$\sigma_{31}(x)\ (1-c)\psi$
$\sigma_{31}(x)\ c\ \varphi$
$\delta\ (x)\ c$
c
$\sigma_{32}(x)\ c\ u$
$\sigma_{31}(x)\ (1-c)v$
$\lambda_2\ \varepsilon_1\ v$
u
v
w
Ω_2

Modelling: governing equations

$$\left.\begin{aligned}
&\partial_t\varphi - \mathrm{div}(d_{11}(x)\nabla\varphi) \\
&\quad = -\sigma_{11}(x)\frac{\varphi\psi}{H_1} - \sigma_{31}(x)c\varphi + (1-w_1)\lambda_1\psi \\
&\qquad + b(x)H_1 - (m(x)+k(x)H_1)\varphi, \\
&\partial_t\psi - \mathrm{div}(d_{12}(x)\nabla\psi) \\
&\quad = \sigma_{11}(x)\frac{\varphi\psi}{H_1} + \sigma_{31}(x)c\varphi - \lambda_1\psi \\
&\qquad -(m(x)+k(x)H_1)\psi, \\
&\partial_t\chi - \mathrm{div}(d_{13}(x)\nabla\chi) \\
&\quad = w_1\lambda_1\psi - (m(x)+k(x)H_1)\chi,
\end{aligned}\right\}\text{in } Q_{1,T} = \Omega_1\times]0,T[,$$

$$\left.\begin{aligned}
&\partial_t u - \mathrm{div}(d_{21}(x)\nabla u) = -\sigma_{32}(x)cu, \\
&\partial_t v - \mathrm{div}(d_{22}(x)\nabla v) = \sigma_{32}(x)cu - \lambda_2 v, \\
&\partial_t w - \mathrm{div}(d_{23}(x)\nabla w) = \varepsilon_1\lambda_2 v,
\end{aligned}\right\}\text{in } Q_{2,T} = \Omega_2\times]0,T[,$$

$$\partial_t c = \sigma_{13}(x)(1-c)\tilde{\psi} + \sigma_{23}(x)(1-c)\tilde{v} - \delta(x)c, \qquad \text{in } Q_T = (\Omega_1\cup\Omega_2)\times]0,$$

Modelling: initial and boundary conditions

We consider no-flux boundary conditions

$$d_{11}(x)\frac{\partial\varphi}{\partial\eta_1} = d_{12}(x)\frac{\partial\psi}{\partial\eta_1} = d_{13}(x)\frac{\partial\chi}{\partial\eta_1} = 0, \quad \text{on } \Gamma_{1,T} = \partial\Omega_1 \times]0, T[,$$
$$d_{21}(x)\frac{\partial u}{\partial\eta_2} = d_{22}(x)\frac{\partial v}{\partial\eta_2} = d_{23}(x)\frac{\partial w}{\partial\eta_2} = 0, \quad \text{on } \Gamma_{2,T} = \partial\Omega_2 \times]0, T[,$$

where η_i are the unit normal vector to $\partial\Omega_i$ and the initial conditions are

$$\varphi(x,0) = \varphi_0(x), \quad \psi(x,0) = \psi_0(x), \quad \chi(x,0) = \chi_0(x), \qquad \text{in } Q_{1,T},$$
$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x), \quad w(x,0) = w_0(x), \qquad \text{in } Q_{2,T},$$
$$c(x,0) = c_0(x), \quad \text{in } Q_T.$$

Moreover, we assume that $c_0(x) \in [0,1]$ for $x \in \Omega_1 \cup \Omega_2$.

DEFINITIONS OF DIRECT AND INVERSE PROBLEMS

Direct Problem

Notation:

$$
\begin{aligned}
\mathbf{h}_1 &= (\varphi, \psi, \chi) & \boldsymbol{\sigma}_1 &= (\sigma_{11}, \sigma_{31}, b, m, k) & \mathbb{D}_1 &= \operatorname{diag}(d_{11}, d_{12}, d_{13}) \\
\mathbf{h}_2 &= (u, v, w) & \boldsymbol{\sigma}_2 &= (\sigma_{32}, b, m, k) & \mathbb{D}_2 &= \operatorname{diag}(d_{21}, d_{22}, d_{23}) \\
& & \boldsymbol{\sigma}_3 &= (\sigma_{13}, \sigma_{23}, \delta) & &
\end{aligned}
$$

$$\boxed{\mathbf{h} = (\mathbf{h}_1, \mathbf{h}_2, c)} \quad \boxed{\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)}$$

Definition

The direct problem is defined as follows: Given $\boldsymbol{\sigma}, \mathbb{D}_i$ and the initial conditions find $\mathbf{h}$ the solution of the following IBVP

$$
\begin{aligned}
\partial_t \mathbf{h}_1 - \operatorname{div}(\mathbb{D}_1(x)\nabla \mathbf{h}_1) &= F(\mathbf{h}_1, c; \boldsymbol{\sigma}_1(x)) && \text{in } Q_{1,T}, \\
\partial_t \mathbf{h}_2 - \operatorname{div}(\mathbb{D}_2(x)\nabla \mathbf{h}_2) &= G(\mathbf{h}_2, c; \boldsymbol{\sigma}_2(x)) && \text{in } Q_{2,T}, \\
\partial_t c &= K(\mathbf{h}_1, \mathbf{h}_2, c; \boldsymbol{\sigma}_3(x)) && \text{in } Q_T, \\
\mathbb{D}_i(x)\frac{\partial \mathbf{h}_i}{\partial \eta_i} &= 0 && \text{on } \Gamma_{i,T}, \\
& \text{initial conditions}
\end{aligned}
$$

Inverse Problem

Definition

The direct problem is defined as follows: Given $\boldsymbol{\sigma}, \mathbb{D}_i$ and the initial conditions find $\mathbf{h}$ the solution of the following IBVP

$$
\begin{aligned}
\partial_t \mathbf{h}_1 - \mathrm{div}(\mathbb{D}_1(x)\nabla \mathbf{h}_1) &= F(\mathbf{h}_1, c; \boldsymbol{\sigma}_1(x)) && \text{in } Q_{1,T},\\
\partial_t \mathbf{h}_2 - \mathrm{div}(\mathbb{D}_2(x)\nabla \mathbf{h}_2) &= G(\mathbf{h}_2, c; \boldsymbol{\sigma}_2(x)) && \text{in } Q_{2,T},\\
\partial_t c &= K(\mathbf{h}_1, \mathbf{h}_2, c; \boldsymbol{\sigma}_3(x)) && \text{in } Q_T,\\
\mathbb{D}_i(x)\frac{\partial \mathbf{h}_i}{\partial \eta_i} &= 0 && \text{on } \Gamma_{i,T},\\
&\text{initial conditions}
\end{aligned}
$$

Definition

The inverse problem is defined as follows: Given $\mathbb{D}_i$, initial conditions and some experimental data at time T given by $\mathbf{h}^{obs}(\cdot, T)$, find the coefficients $\boldsymbol{\sigma}$ such that the solution $\mathbf{h}(\cdot, T)$ of the IBVP for $\boldsymbol{\sigma}$ is “very close” to $\mathbf{h}^{obs}(\cdot, T)$.

WELL POSEDNESS OF DIRECT PROBLEM

Notation

In order to simplify the presentation of our results and proofs we consider the following notation

$$\begin{aligned}
\mathcal{L}^p &= \mathbf{L}^p(\Omega_1) \times \mathbf{L}^p(\Omega_2) \times L^p(\Omega_1 \cup \Omega_2), \\
\mathbb{L}^p &= \Big[\mathbf{L}^p(\Omega_1)\Big]^5 \times \mathbf{L}^p(\Omega_2) \times \mathbf{L}^p(\Omega_1 \cup \Omega_2), \\
\mathcal{C}^\alpha &= \Big[C^{0,\alpha}(\overline{\Omega}_1)\Big]^5 \times C^{0,\alpha}(\overline{\Omega}_2) \times \Big[C^{2,\alpha}\Big(\overline{\Omega_1 \cup \Omega_2} \backslash \mathcal{D}\Big)\Big]^2 \times C^{2,\alpha}(\overline{\Omega_1 \cup \Omega_2}),
\end{aligned}$$

with $\mathcal{D} = (\partial\Omega_1 \cap \overline{\Omega}_2) \cup (\partial\Omega_2 \cap \overline{\Omega}_1)$; and analogously to $\mathcal{L}^p$ we consider the notation for the functional spaces $\mathcal{W}^{m,p}$ and $\mathcal{H}^m$.

Hypothesis

(H0) The sets Ω_1 and Ω_2 are open bounded convex sets of $\mathbb{R}^d$ such that $\partial\Omega_i$ are of $C^{3,\alpha}$ regularity.

(H1) The functions modelling the initial conditions are non-negative and satisfying the following regularity conditions: $\varphi_0, \psi_0, \chi_0$ are continuous on $\overline{\Omega_1}$; u_0, v_0, w_0 are continuous on $\overline{\Omega_2}$; and c_0 is continuous on $\overline{\Omega_1 \cup \Omega_2} \backslash \mathcal{D}$. Moreover, we assume that $c_0(x) \in [0,1]$ on $\Omega_1 \cup \Omega_2$.

(H2) The diffusion coefficients $d_{i,j}$ for $(i,j) \in \{1,2\} \times \{1,2,3\}$ are positive functions, bounded from below on Ω_i and belong $C^{2,\alpha}(\overline{\Omega_i}) \cap L^\infty(\Omega_i)$.

(H3) The coefficients are componentwise strictly positive on their domains of definition, i.e. $\sigma_{11}, \sigma_{31}, b, m$, and k are strictly positive on $\overline{\Omega}_1$; σ_{32} is strictly positive on $\overline{\Omega}_2$; δ is strictly positive on $\overline{\Omega_1 \cup \Omega_2}$; σ_{13} is strictly positive on $\overline{\Omega}_1$ and identically 0 outside of $\overline{\Omega}_1$; σ_{23} is strictly positive on $\overline{\Omega}_2$ and identically 0 outside of $\overline{\Omega}_2$. Moreover, $\boldsymbol{\theta} \in \mathcal{C}^\alpha$ and the birth and mortality rates are such that $b(x) - m(x)$ is strictly positive for all $x \in \Omega_1$.

Well posedness of the direct problem

Theorem (Fitzgibbon, Langlais & Morgan, 2007)

If the requirements listed above in (H0)-(H3) are met, then the direct problem has a unique, classical, global nonnegative solution $\varphi, \psi, \chi, u, v, w$*, and* c*, which is componentwise non-negative;* φ, ψ, *and* χ *are uniformly bounded on* $Q_1 = \Omega_1 \times]0, \infty[$, u, v, *and* w, *are uniformly bounded on* $Q_2 = \Omega_2 \times]0, \infty[$, *and* c *is uniformly bounded on* $Q = (\Omega_1 \cup \Omega_2) \times]0, \infty[$*; and* $c(x, t) \in [0, 1]$ *on* Q*.*

The proof is divided in four big parts: the local existence is followed by Banach fixed point argument; the componentwise non-negativity is deduced by application of the weak maximum principle for scalar parabolic equations; the global well posedness is a consequence of L_∞ estimates of solution components; and the global existence is proved by using the results for discontinuous coefficients and uniform estimates using cut-off functions.

INVERSE PROBLEM RESULTS

Inverse problem

We reformulate the inverse problem as an optimization problem. Let us consider the following cost functional

$$J(\mathbf{h},\boldsymbol{\sigma}) = \frac{1}{2}\left\|(\mathbf{h}_1,\mathbf{h}_2,c)(\cdot,T) - (\mathbf{h}_1^{obs},\mathbf{h}_2^{obs},c^{obs})\right\|_{\mathcal{L}^2}^2 + \frac{\Gamma}{2}\|\nabla\boldsymbol{\theta}\|_{\mathbb{L}^2}^2, \quad \Gamma > 0,$$

where $\mathbf{h}_1^{obs} = (\phi^{obs},\psi^{obs},\chi^{obs})$, $\mathbf{h}_2^{obs} = (u^{obs},v^{obs},w^{obs})$. Thus the inverse problem is formalized as the following optimization problem

$$\text{Find } \overline{\boldsymbol{\theta}} \in U_{ad} \ : \ J(\overline{\boldsymbol{\theta}}) = \inf_{\boldsymbol{\theta}\in U_{ad}} J(\boldsymbol{\theta}) \quad \text{subject to } (\mathbf{h}_1,\mathbf{h}_2,c) \text{ is solution of direct problem.}$$

where $U_{ad} := U_{ad}(\Omega_1,\Omega_2)$ is the admissible set

$$\begin{aligned} U_{ad}(\Omega) &= \mathcal{A}(\Omega_1,\Omega_2)\cap\mathcal{H}^{[\![d/2]\!]+1} \\ \mathcal{A}(\Omega_1,\Omega_2) &= \left\{\boldsymbol{\theta} := (\boldsymbol{\theta}_1,\boldsymbol{\theta}_2,\boldsymbol{\theta}_3)\in\mathcal{C}^\alpha \ : \quad \mathrm{Ran}(\boldsymbol{\theta}) \subseteq \prod_{i=1}^{9}[\underline{r}_i,\overline{r}_i] \subset \mathbb{R}_+^9, \quad \nabla\boldsymbol{\theta}\in\mathbb{L}^2\right\} \end{aligned}$$

Results

The main results are the following:

(a) the existence of solutions for the inverse problem,

(b) a well defined adjoint state,

(c) the introduction of first order optimality condition,

(d) the stability of a direct problem solution with respect to the coefficients of the reaction term,

(e) the stability of the adjoint problem solution with respect to the coefficients of the reaction term and the observations,

(f) the uniqueness of the identification problem.

(a) the existence of solutions for the inverse problem

Theorem

Let us consider that (H0)-(H3) and the following hypothesis

(H4) The observation function $(\mathbf{h}_1^{obs}, \mathbf{h}_2^{obs}, c^{obs})$ *belongs* $\mathcal{L}^2$,

are valid. Moreover consider the on $\mathcal{U} := \mathcal{A}(\Omega_1, \Omega_2) \cap \mathcal{M}$ *with* $\mathcal{M}$ *a bounded closed set of* $\mathcal{H}^{[\![d/2]\!]+1}$ *containing the constant functions. Then, there exists at least one solution of optimization problem on* $\mathcal{U}$.

(b) Adjoint state 1/2

We introduce the adjoint state

$$
\begin{aligned}
\partial_t \mathbf{p}_i + \mathrm{div}(\mathbb{D}_i(x)\nabla \mathbf{p}_i) &= \mathbf{q}_i(x, \mathbf{p}_i, s; \overline{\mathbf{h}}_i, \overline{c}, \overline{\boldsymbol{\theta}}_i(x)), \qquad \text{in } Q_{i,T}, \quad i = 1, 2, \\
\partial_t s &= \varsigma(x, \mathbf{p}_1, \mathbf{p}_2, s; \overline{c}, \overline{\boldsymbol{\theta}}_3(x)), \quad \text{in } Q_T, \\
(\mathbb{D}_i(x)\nabla \mathbf{h}_i) \cdot \boldsymbol{\eta}_i &= 0, \quad \text{on } \Gamma_{i,T}, \quad i = 1, 2, \\
\mathbf{p}_i(x, T) &= \overline{\mathbf{h}}_i(x, T) - \mathbf{h}_i^{obs}(x), \quad \text{in } \Omega_i, \quad i = 1, 2, \\
s(x, T) &= \overline{c}(x, T) - c^{obs}(x), \quad \text{in } \Omega_1 \cup \Omega_2,
\end{aligned}
$$

where the functions $\mathbf{q}_i$ and ς are defined as follows

$$
\begin{aligned}
q_{11} = {} & \left[\overline{\sigma}_{11}(x)\frac{\overline{\psi}(\overline{\varphi} + \overline{\psi})}{(H_1)^2} + \overline{\sigma}_{31}(x)\overline{c}\right](p_{12} - p_{11}) + \Big(\overline{b}(x) - \overline{m}(x)\Big)p_{11} \\
& -\overline{k}(x)\Big(2\overline{\varphi}p_{11} + \overline{\psi}p_{12} + \overline{\chi}p_{13}\Big), \\
q_{12} = {} & \overline{\sigma}_{11}(x)\frac{\overline{\varphi}(\overline{\varphi} + \overline{\chi})}{(H_1)^2}(p_{12} - p_{11}) + (1 - \omega_1\lambda_1 + \overline{b}(x))p_{11} - \overline{m}(x)p_{12} + \omega_1\lambda_1(p_{13} - p_{12} \\
& -\overline{k}(x)\Big(\overline{\varphi}p_{11} + 2\overline{\psi}p_{12} + \overline{\chi}p_{13}\Big) + \overline{\sigma}_{13}(x)(1 - \overline{c})s, \\
q_{13} = {} & -\overline{\sigma}_{11}(x)\frac{\overline{\varphi}\overline{\psi}}{(H_1)^2}(p_{12} - p_{11}) - \overline{b}(x)p_{11} - \overline{k}(x)\Big(\overline{\varphi}p_{11} + \overline{\psi}p_{12} + 2\overline{\chi}p_{13}\Big), \\
q_{21} = {} & \overline{\sigma}_{32}(x)\overline{c}(p_{22} - p_{21}), \qquad q_{22} = \varepsilon\lambda_2(p_{23} - p_{22}) + \overline{\sigma}_{23}(x)(1 - \overline{c})s, \qquad q_{23} = 0, \\
\varsigma = {} & \overline{\sigma}_{31}(x)\tilde{\overline{\psi}}(\tilde{p}_{12} - \tilde{p}_{11}) + \overline{\sigma}_{32}(x)\tilde{\overline{v}}(\tilde{p}_{22} - \tilde{p}_{21}) - (\overline{\sigma}_{13}(x)\tilde{\overline{\psi}} + \overline{\sigma}_{23}(x)\tilde{\overline{v}} + \overline{\delta}(x))s.
\end{aligned}
$$

(b) Adjoint state 2/2

Theorem

Assume that the hypothesis (H0)-(H4) are satisfied, consider that $\overline{\theta}$ is the solution of optimization problem and $(\overline{\mathbf{h}}_1, \overline{\mathbf{h}}_2, \overline{c})$ is the corresponding solution of direct problem with $\overline{\theta}$ instead of θ. Then, the adjoint system is given by the system defined previously. Moreover, the pair $(\mathbf{p}_1, \mathbf{p}_2)$ is bounded in $L^\infty(0, t; [H^2(\Omega_1)]^3 \times [H^2(\Omega_2)]^3)$ for almost all time t in $]0, T]$ and the solution of the adjoint system is bounded in $L^\infty(0, t; \mathcal{L}^\infty)$ for almost all time t in $]0, T]$.

(c) first order optimality condition

Theorem

Assume that the hypothesis (H0)-(H4) are satisfied and consider the notation $\overline{\theta}, (\overline{\mathbf{h}}_1, \overline{\mathbf{h}}_2, \overline{c})$ and $(\mathbf{p}_1, \mathbf{p}_2, s)$ as is given in Theorem for adjoint state. Then, the following inequality

$$
\begin{aligned}
&\int\!\!\int_{Q_{1,T}} \Big\{ \Big[(\hat{\sigma}_{11} - \overline{\sigma}_{11}) \frac{\overline{\varphi}\,\overline{\psi}}{\overline{H}_1} + (\hat{\sigma}_{31} - \overline{\sigma}_{31}) \Big] (p_{11} - p_{12}) + bH_1 p_{11} - (m + kH_1)\overline{\mathbf{h}}_1 \cdot \overline{\mathbf{p}}_1 \Big\} d \\
&+ \int\!\!\int_{Q_{2,T}} (\hat{\sigma}_{32} - \overline{\sigma}_{32})(p_{21} - p_{22})dxdt \\
&+ \int\!\!\int_{Q_T} \Big\{ \Big(\hat{\sigma}_{13} - \overline{\sigma}_{13} \Big)(1 - \overline{c})\tilde{\overline{\varphi}} s + \Big(\widehat{\sigma_{23}} - \overline{\sigma_{23}} \Big)(1 - \overline{c})\tilde{v} \\
&\qquad - (\hat{\delta} - \overline{\delta})\overline{c} \Big\} sdxdt + \Gamma \int_{\Omega_1} \nabla\overline{\theta}_1 \cdot \nabla(\hat{\theta}_1 - \overline{\theta}_1)dx + \Gamma \int_{\Omega_2} \nabla\overline{\theta}_2 \cdot \nabla(\hat{\theta}_2 - \overline{\theta}_2)dx \\
&+ \Gamma \int_{\Omega_1 \cup \Omega_2} \nabla\overline{\theta}_3 \cdot \nabla(\hat{\theta}_3 - \overline{\theta}_3)dx \Big] \geq 0, \quad \forall \hat{\theta} \in U_{ad},
\end{aligned}
$$

is satisfied.

(d)-(e) stability of a direct and adjoint problem solutions . . .

Theorem

Assume that the hypothesis (H0)-(H4) are valid. Then, considering the norm induced topologies of $\mathbb{L}^2$, $L^\infty(0,t;\mathcal{L}^2)$, *and* $\mathbb{L}^2 \times \mathcal{L}^2$ *we have that the assertions*

(i) *The mapping* $\theta \mapsto (\mathbf{h}_1, \mathbf{h}_2, c)$ *is continuous from* $U_{ad} \subset \mathbb{L}^2$ *to* $L^\infty(0,t;\mathcal{L}^2)$ *for almost all time* t *in* $]0,T]$.

(ii) *The mapping* $(\theta, \mathbf{h}_1^{obs}, \mathbf{h}_2^{obs}, c^{obs}) \mapsto (\mathbf{p}_1, \mathbf{p}_2, s)$ *is continuous from* $U_{ad} \times \mathcal{L}^2 \subset \mathbb{L}^2 \times \mathcal{L}^2$ *to* $L^\infty(0,t;\mathcal{L}^2)$ *for almost all time* t *in* $]0,T]$.

are satisfied.

(f) the uniqueness of the identification problem ...

Theorem

Let us define the set

$$\mathcal{U}_{\mathbf{c}} = \left\{ \theta \in \mathcal{U} \;:\; \int_{\Omega} \theta(x)dx = \mathbf{c}, \quad \mathbf{c} = (c_1, \ldots, c_9) \in \mathbb{R}^9_+ \right\}$$

with $\mathcal{U}$ the set defined on Theorem for existence of solutions. Then, for each $\mathbf{c}$*, the solution of optimization problem is uniquely defined, up to an additive constant, on $\mathcal{U}_{\mathbf{c}}$ in the $\mathbb{L}^2$ sense for any large enough regularization parameter* Γ*.*

MATHEMATICAL MODEL FOR TUMOR GROWTH

Direct problem: Mathematical model

The cancerous cells invasion taking place in a bounded domain $\Omega \subset \mathbb{R}^d$, $(d = 1, 2, 3)$ with smooth boundary $\partial\Omega$ can be modelled by the reaction-diffusion system:

$$\begin{aligned}
u_t - d_1\Delta u &= \alpha_1 g_1(u)u - (\beta_1 v + \gamma_1 w)u && \text{in } Q_T,\\
v_t - d_2\Delta v &= \alpha_2 g_2(v)v - (\beta_2 u + \gamma_2 w)v && \text{in } Q_T,\\
w_t - d_3\Delta w &= -\alpha_3 w + U && \text{in } Q_T,\\
u(x,0) = u_0(x),\ v(x,0) &= v_0(x),\ \ w(x,0) = w_0(x) && \text{in } \Omega,\\
\frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} &= \frac{\partial w}{\partial \mathbf{n}} = 0 && \text{on } \Gamma_T.
\end{aligned}$$

where $u(x,t)$ is the tumor cells density, $v(x,t)$ the normal cells density and $w(x,t)$ is the drug concentration.

- $Q_T := \Omega \times (0,T)$ and $\Gamma_T := \partial\Omega \times (0,T)$.
- $\alpha_1(x), \alpha_2(x)$ growth rates;
- $\alpha_3(x)$ reabsorption rate for the drug;
- $\beta_1(x), \beta_2(x)$ death rates by competition;
- $\gamma_1(x), \gamma_2(x)$ death rates by treatment;
- $U(x,t) \geq 0$ drug injected;
- $d_1, d_2, d_3 > 0$ are the diffusivity;
- $\mathbf{n}$ is the unit normal.

Parameter calibration problem

We consider the direct problem

$$
\begin{aligned}
&\partial_t u_1 - d_1 \Delta u_1 = \Big(\theta_1 g_1(u_1) - (\theta_4 u_2 + \theta_6 u_3)\Big) u_1, && \text{in } Q_T := \Omega \times (0, T),\\
&\partial_t u_2 - d_2 \Delta u_2 = \Big(\theta_2 g_2(u_2) - (\theta_5 u_1 + \theta_7 u_3)\Big) u_2, && \text{in } Q_T,\\
&\partial_t u_3 - d_3 \Delta u_3 = -\theta_3 u_3 + U, && \text{in } Q_T,\\
&(u_1, u_2, u_3)(x, 0) = (u_{1,0}, u_{2,0}, u_{3,0})(x), && \text{in } \Omega,\\
&\nabla u_1 \cdot \mathbf{n} = \nabla u_2 \cdot \mathbf{n} = \nabla u_3 \cdot \mathbf{n} = 0, && \text{on } \Gamma_T := \partial\Omega \times (0, T).
\end{aligned}
$$

Inverse problem is defined as follows:

> Given $\mathbf{u}^{obs}$ and $\mathbf{u}_0$ defined on Ω, find the set of real functions defining the components of $\boldsymbol{\theta}$ defined on Ω, such that the solution $\mathbf{u}$ of the direct problem satisfy the final time condition $\mathbf{u}(x, T) = \mathbf{u}^{obs}(x)$ for $x \in \Omega$.

Optimal control problem

Defining $J, \mathcal{J}$ and the admissible set $S_{ad}(\Omega)$ as follows

$$J(\mathbf{u}) = \frac{1}{2}\left\|\mathbf{u}(\cdot, T) - \mathbf{u}^{obs}\right\|^2_{[L^2(\Omega)]^3}, \qquad \mathcal{J}(\boldsymbol{\theta}) = J(\mathbf{u}_{\boldsymbol{\theta}}) + \frac{\Gamma}{2}\|\boldsymbol{\theta}\|^2_{[L^2(\Omega)]^7},$$

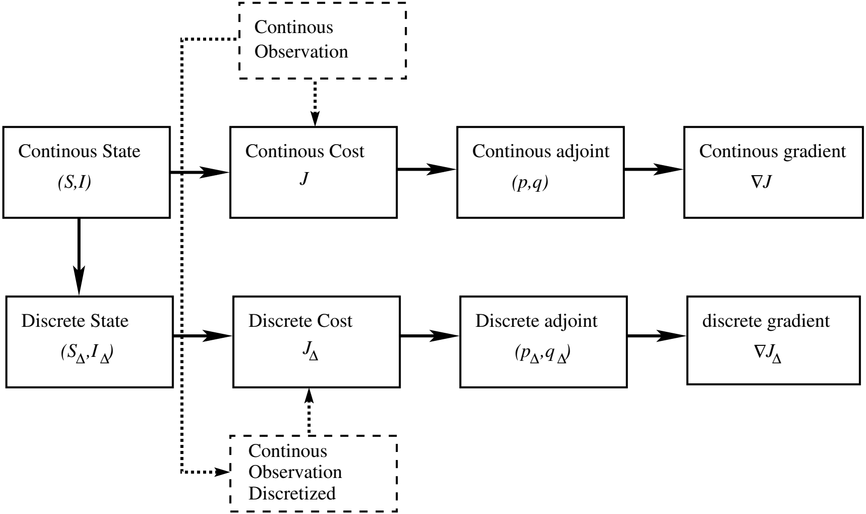
$$S_{ad}(\Omega) = \left\{\boldsymbol{\theta} \in [L^2(\Omega)]^7 \ : \ \boldsymbol{\theta}(x) \in \prod_{k=1}^{7} [0, \theta_k^{\max}] \quad \text{a.e. } x \in \Omega\right\},$$

we recast the parameter identification problem as the following optimization problem:

$$\left.\begin{array}{l} \text{Given } \mathbf{u}^{obs} \text{ and } \mathbf{u}_0, \text{ find } \overline{\boldsymbol{\theta}} \text{ such that:} \\ \mathcal{J}(\overline{\boldsymbol{\theta}}) := \min\limits_{\boldsymbol{\theta} \in S_{ad}(\Omega)} \mathcal{J}(\boldsymbol{\theta}) \text{ subject to } \mathbf{u}_{\boldsymbol{\theta}} \text{ solution of direct problem.} \end{array}\right\}$$

NUMERICAL SOLUTION

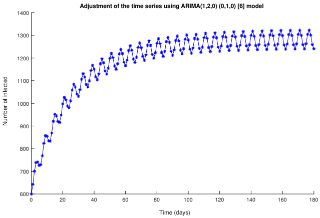
METHODOLOGY


Continous Observation
Continous State
(S,I)
Continous Cost
J
Continous adjoint
(p,q)
Continous gradient
∇J
Discrete State
(S_Δ, I_Δ)
Discrete Cost
J_Δ
Discrete adjoint
(p_Δ, q_Δ)
discrete gradient
∇J_Δ
Continous Observation Discretized

ODE MODELS

ODE model

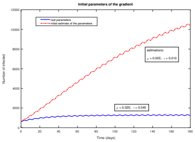
$$
\left.\begin{aligned}
\frac{d}{dt}S(t) &= \Lambda - \mu\, S(t) - \frac{\beta(t)S(t)\, I(t)}{1 + kI(t)},\\
\frac{d}{dt}I(t) &= \frac{\beta(t)S(t)\, I(t)}{1 + kI(t)} - (\mu + \gamma)\, I(t) - m.
\end{aligned}\right\}
$$

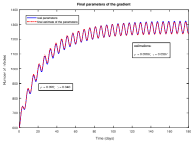


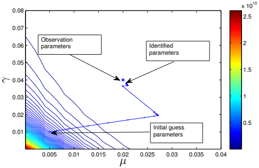
$$
\left.\begin{aligned}
\frac{d}{dt}S(t) &= 400 - 0.02\, S(t) - \frac{3\,[0.2 + \sin(\pi t/3)]\, S(t)\, I(t)}{10000 + 100\, I(t)},\\
\frac{d}{dt}I(t) &= \frac{3\,[0.2 + \sin(\pi t/3)]\, S(t)\, I(t)}{10000 + 100\, I(t)} - (0.02 + 0.04)\, I(t) - 10,\\
S(0) &= 14000, \quad I(0) = 600.
\end{aligned}\right\}
$$

ODE Inverse

$$\text{Minimize } J(\mu,\gamma) = \delta \left\| I_{\mu,\gamma} - I^{obs} \right\|^2_{L_2(0,T)} := \delta \int_0^T (I_{\mu,\gamma} - I^{obs})^2(\tau)d\tau$$







	μ	γ
observation parameters	0.0200	0.0400
initial guess parameters	0.0005	0.0100
identified parameters	0.0206	0.0387

F. Novoa-Muñoz, S. Espinoza, A, Coronel, I. Hess (2019)

DIFUSION IDENTIFICATION

Finite volume approximation of direct problem

$$
\begin{aligned}
\frac{S_k^{n+1} - S_k^n}{\Delta t} &= \frac{1}{\Delta x^2}\left[d_1(x_k) S_{k+1}^{n+1} - \Big(d_1(x_k) + d_1(x_{k-1})\Big) S_k^{n+1} + d_1(x_{k-1}) S_{k-1}^{n+1}\right] \\
&\quad - \beta(x_k) S_k^{n+1} I_k^n + \gamma(x_k) I_k^{n+1} \\
\frac{I_k^{n+1} - I_k^n}{\Delta t} &= \frac{1}{\Delta x^2}\left[d_2(x_k) I_{k+1}^{n+1} - \Big(d_2(x_k) + d_2(x_{k-1})\Big) I_k^{n+1} + d_2(x_{k-1}) I_{k-1}^{n+1}\right] \\
&\quad + \beta(x_k) S_k^{n+1} I_k^n - \gamma(x_k) I_k^{n+1} \\
\frac{S_1^n - S_0^n}{\Delta x} &= \frac{S_{M+1}^n - S_M^n}{\Delta x} = 0, \quad \frac{I_1^n - I_0^n}{\Delta x} = \frac{I_{M+1}^n - I_M^n}{\Delta x} = 0, \\
S_k^0 &= S_0(x_k), \quad I_k^0 = I_0(x_k).
\end{aligned}
$$

$$
\begin{pmatrix} I_M + L_S + \Delta t \beta D I^n & -\Delta t \gamma \\ -\Delta t \beta D I^n & I_M + L_I + \Delta t \gamma \end{pmatrix} \begin{pmatrix} S^{n+1} \\ I^{n+1} \end{pmatrix} = \begin{pmatrix} S^n \\ I^n \end{pmatrix}
$$

Numerical scheme 1D: Liu & Yang (2022) ...has several properties: preserves the biological meaning (such as positivity) and is unconditionally convergent.

Inverse problem

$$\begin{aligned}
&\partial_t S - \mathrm{diver}(d_1(x)\nabla S) = -\beta(x)SI + \gamma(x)I, && \text{in } Q_T,\\
&\partial_t I - \mathrm{diver}(d_2(x)\nabla I) = \beta(x)SI - \gamma(x)I, && \text{in } Q_T,\\
&\nabla S\cdot\mathbf{n} = \nabla I\cdot\mathbf{n} = 0, && \text{in } \Gamma_T,\\
&(S,I)(x,0) = (S_0,I_0)(x), && \text{on } \Omega,
\end{aligned}$$

Parameter identification problem: The diffusion coefficients d_1 and d_2 depend of a finite number of parameters denoted by $\mathbf{e} = (e_1, \dots, e_n)$ which is explicitly denoted by $d_i(x) = d_i(x;\mathbf{e})$ for $i = 1, 2$.

$$\inf_{\mathbf{e}\in\mathbb{R}^n} \mathcal{J}_\Delta(\mathbf{e}), \quad \mathcal{J}_\Delta(\mathbf{e}) = J_\Delta(S_\Delta, I_\Delta),$$

subject to (S_Δ, I_Δ) solution of numerical scheme for direct problem,

$$J_\Delta(S_\Delta, I_\Delta) := \frac{\Delta x}{2}\sum_{k=1}^{M}(S_k^N - S_k^{obs})^2 + \frac{\Delta x}{2}\sum_{k=1}^{M}(I_k^N - I_k^{obs})^2.$$

Adjoint scheme and discrete gradient

$$\frac{P_k^n - P_k^{n+1}}{\Delta t} = \frac{1}{\Delta x^2}\Big[d_1(x_{k-1})P_{k-1}^n - \Big(d_1(x_k) + d_1(x_{k-1})\Big)P_k^n + d_1(x_k)S_{k+1}^{n+1}\Big]$$
$$- \beta(x_k)(P_k^n - Q_k^n)$$

$$\frac{Q_k^n - Q_k^{n+1}}{\Delta t} = \frac{1}{\Delta x^2}\Big[d_2(x_{k-1})Q_{k+1}^{n+1} - \Big(d_2(x_k) + d_2(x_{k-1})\Big)I_k^{n+1} + d_2(x_k)Q_{k+1}^{n+1}\Big]$$
$$+ \Big(\beta(x_k)S_k^n - \gamma(x_k)\Big)(Q_k^n - P_k^n)$$

$$\frac{P_1^n - P_0^n}{\Delta x} = \frac{P_{M+1}^n - P_M^n}{\Delta x} = 0, \quad \frac{Q_1^n - Q_0^n}{\Delta x} = \frac{Q_{M+1}^n - Q_M^n}{\Delta x} = 0,$$
$$P_k^N = |S_k^N - S_k^{obs}|, \quad Q_k^N = |I_k^N - I_k^{obs}|.$$

$$\nabla_{\mathbf{e}}\mathcal{J}_\Delta(\mathbf{e})$$
$$= -\frac{\Delta t}{\Delta x}\sum_{n=0}^{N}\sum_{k=1}^{M}\Big[\nabla_{\mathbf{e}}d_1(x_k)S_{k+1}^n - \Big(\nabla_{\mathbf{e}}d_1(x_k) + \nabla_{\mathbf{e}}d_1(x_{k-1})\Big)S_k^n + \nabla_{\mathbf{e}}d_1(x_{k-1})S_{k-1}^n\Big]P_k^n$$
$$+ \Big[\nabla_{\mathbf{e}}d_2(x_k)I_{k+1}^n - \Big(\nabla_{\mathbf{e}}d_2(x_k) + \nabla_{\mathbf{e}}d_2(x_{k-1})\Big)I_k^n + \nabla_{\mathbf{e}}d_2(x_{k-1})I_{k-1}^n\Big]Q_k^n$$
$$+ \Gamma\sum_{k=0}^{M+1}\Big[d_1(x_k)\nabla_{\mathbf{e}}d_1(x_k) + d_2(x_k)\nabla_{\mathbf{e}}d_2(x_k)\Big].$$

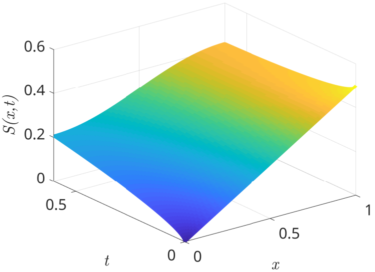
Example 1: Identification of a constant diffusion

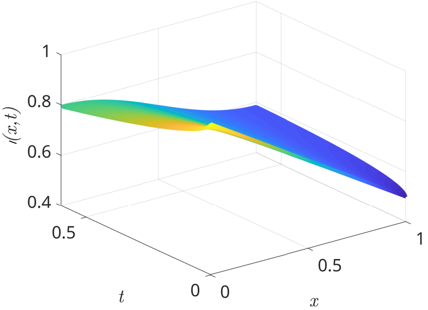
We consider

$$\beta(x) = 0.000284535, \quad \gamma(x) = 0.144, \quad (S_0, I_0)(x) = \frac{1}{2}(x, 2-x),$$

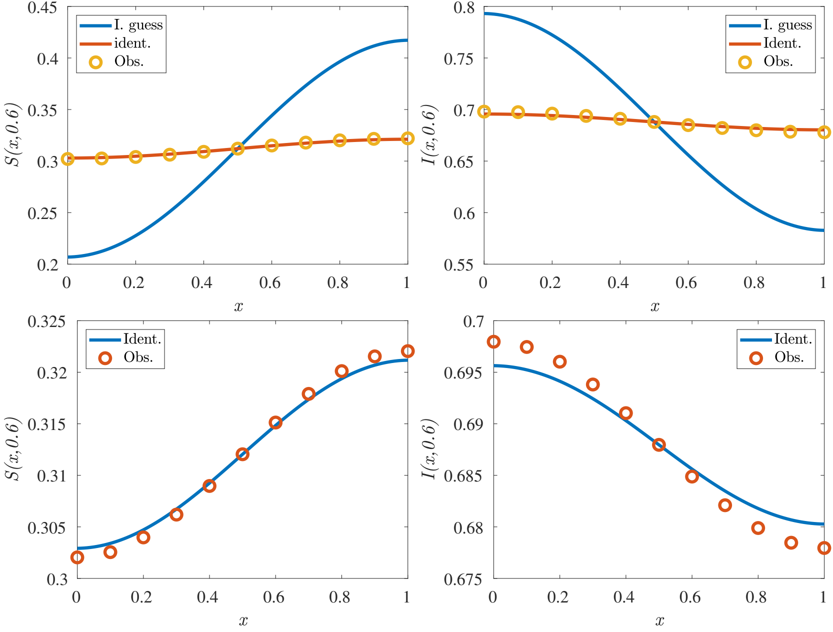
$$\color{red}{\mathbf{e} = (e_1, e_2), \quad d_1(x;\mathbf{e}) = e_1, \quad d_2(x;\mathbf{e}) = e_2}.$$

We construct the observation profile at $T = 0.6$ by considering a numerical simulation of the direct problem with $\mathbf{e}^{obs} = (0.5, 0.5)$, $M = 200$ and $N = 100000$ (i.e., $\Delta x = 5E-3$ and $\Delta x = 6E-6$).





Example 1: inital guess $\mathbf{e} = (0.1, 0.1)$, $\mathbf{e}^{\infty} = (0.52294, 0.55149)$, $\mathbf{e}^{obs} = (0.5, 0.5)$



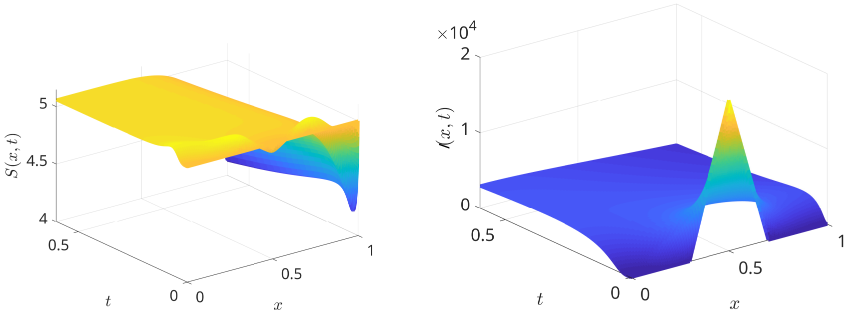
Example 2: Identification of a quadratic diffusion function

We consider $\beta(x) = 0.000284535$, $\gamma(x) = 0.144$, and

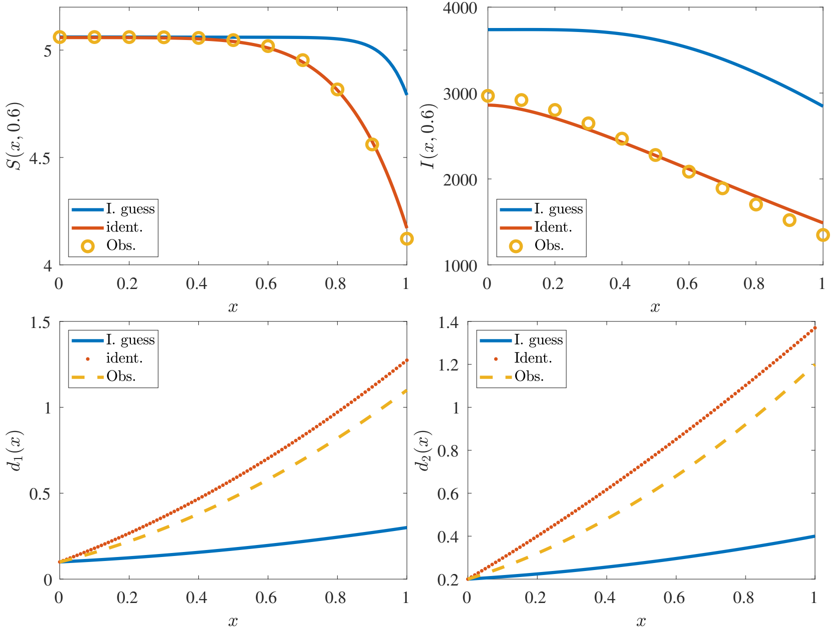
$$I_0(x) = \begin{cases} 0, & x \leq 0.3, \\ 100000x - 30000, & 0.3 < x \leq 0.5, \\ -100000x + 70000, & 0.5 < x \leq 0.7, \\ 0, & \text{otherwise.} \end{cases}$$

$$d_1(x; \mathbf{e}) = 0.1 + e_1 x + e_2 x^2, \quad d_2(x; \mathbf{e}) = 0.2 + e_3 x + e_4 x^2.$$

We construct the observation profile at $T = 0.6$ by considering a numerical simulation of the direct problem with $\mathbf{e}^{obs} = (0.5, 0.5, 0.5, 0.5)$, $M = 200$ and $N = 100000$ (i.e., $\Delta x = 5E-3$ and $\Delta x = 6E-6$).



Example 2: $\mathbf{e}^0 = 0.1 \ldots \mathbf{e}^\infty = (0.75143, 0.42256, 0.95842, 0.21146)$, $\mathbf{e}^{obs} = 0.5 \ldots$



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Congratulations, Kisko G-G & Manolo G-B,
on your 60th Birthday!