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Aníbal Coronel, Fernando Huancas,
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Theoretical and numerical approaches of reaction term identification in a SIS reaction-diffusion system

Aníbal Coronel[a,*], Fernando Huancas[b], Mauricio Sepúlveda[c]

[a]*Departamento de Ciencias Básicas - Centro de Ciencias Exactas,Facultad de Ciencias, Universidad del Bío-Bío, Campus Fernando May, Andrés Bello 720, 3780000, Chillán, Chile*

[b]*Departamento de Matemática, Facultad de Ciencias Naturales, Matemáticas y del Medio Ambiente, Universidad Tecnológica Metropolitana, Las Palmeras No. 3360, 7800003, Ñuñoa-Santiago, Chile*

[c]*Centro de Investigación en Ingeniería Matemática (CI²MA) y Departamento de Ingeniería Matemática (DIM), Universidad de Concepción, Casilla 160-C, Concepción, Chile*

Abstract

We introduce the necessary conditions for existence and uniqueness of coefficients determination problem in a class of reaction-diffusion systems from a knowledge of an approximation of the state variables at the end of the processes. The system considered is a generalization of the susceptible-infectado-susceptible (SIS) model disease transmission under the assumption of diffusion. We introduce a formulation of the inverse problem as a constrained optimization problem for an appropriate cost functional. In the main results of the paper, we prove the existence of a minimizer for the cost functional, introduce a first order necessary optimality condition, deduce stability of the inverse problem unknowns with respect to the observations, and demonstrate the uniqueness up an additive constant of identification problem. In addition, we introduce a numerical approach of the inverse problem in the case of parameter identification problem and consider a numerical example.

Keywords: Inverse problem, parameter identification, SIS, reaction-diffusion systems
2000 MSC: 35R30, 49K20, 92D25, 92D30, 49N45

1. Introduction

The current literature well documented the mathematical modeling of epidemic spread [1, 2, 3, 4, 5, 6, 7]. Despite the advances, there are still aspects where mathematical analysis needs to be precise; an example of such a case is the problem of identifying coefficients from observations of state variables. In a broad sense, the approaches used to model the dynamics of epidemics are based on differential and difference equations, both deterministic and stochastic. One of the most used methodologies to formulate those mathematical models

*Corresponding author
Email addresses: `acoronel@ubiobio.cl` (Aníbal Coronel), `fhuancas@utem.cl` (Fernando Huancas), `mauricio@ing-mat.udec.cl` (Mauricio Sepúlveda)

is the compartmental approach, pioneered by Kermack-McKendrick [8]. In this context, the most basic model considers that the total population N is divided into two classes of individuals called susceptible and infected, denoted by S and I. Then, assuming that the compartment populations change by direct contact of infected individuals with susceptible ones or after having completed the infection period, the following mathematical model is deduced

$$\frac{dS}{dt} = -\beta SI + \gamma I, \quad \frac{dI}{dt} = \beta SI - \gamma I. \tag{1}$$

Here, βSI models the interaction of infected and susceptible individuals by applying the mass-action law, and γI models the recovery. If we additionally assume that the diffusion influences the dynamics of epidemics, we deduce that the model (1) is generalized to obtain the system

$$\frac{\partial S}{\partial t} - \Delta S = -\beta SI + \gamma I, \quad \frac{\partial I}{\partial t} - \Delta I = \beta SI - \gamma I. \tag{2}$$

We can extensively discuss the possible generalizations, which can be formulated by considering other variables affecting the dynamics spread. However, we focus on the analytical and numerical study of identifying reaction terms in (2) by assuming an observed profile for the infected population at finite time T.

An essential point in the mathematical modeling of epidemics is the selection of the function modeling the flow rate out of the susceptible class into the infectious class, well-known as horizontal incidence or infection force [9, 10]. Even though the most used incidence function in the mathematical epidemic articles is the mass-action-type function, other nonlinear functions have also been considered in the literature [11, 12, 13, 14], where the authors consider $f(S, I) = \beta S\sigma(S, I)$ with σ is defined by

$$\sigma(S,I) = \begin{cases} I, & & \text{(mass action)}, \\ \dfrac{I}{N}, & N > 0, & \text{(frequency dependent)}, \\ \dfrac{I}{S+I}, & & \text{(proportionate mixing)}, \\ (S)^{p-1}(I)^q, & 0 < p < 1,\ 0 < q < 1, & \text{(power law)}, \\ \dfrac{I}{c+S+I}, & c > 0 & \text{(asymptotic law)}. \end{cases} \tag{3}$$

For more information and discussion on other nonlinear models we refer to [12].

In this paper, we are interested in the determination of coefficients (β, γ) with a general function σ. Then, we propose a generalization of the functions given in (3), by considering the following properties of σ:

$$\sigma : \mathbb{R}_0^+ \times \mathbb{R}_0^+ \to \mathbb{R}_0^+ \text{ with } \mathbb{R}_0^+ = \mathbb{R}^+ \cup \{0\}, \text{ where } \mathbb{R}^+ = (0, \infty); \tag{4a}$$

$$\sigma(S, I) > 0 \text{ for } (S, I) \in \mathbb{R}^+ \times \mathbb{R}^+; \quad \sigma(S, 0) = 0 \text{ for } S \in \mathbb{R}^+; \tag{4b}$$

$$|\sigma(S, I)| \le c_1(S^r + I^r) + c_2 \text{ for } (S, I) \in \mathbb{R}^+ \times \mathbb{R}^+ \text{ and some } c_1, c_2 \ge 0 \text{ and } r > 0; \tag{4c}$$

$$\partial_1\sigma(S,I),\ \partial_2\sigma(S,I),\ \partial_{12}\sigma(S,I) > 0 \text{ for } (S,I) \in \mathbb{R}^+ \times \mathbb{R}^+; \tag{4d}$$
$$\partial_{11}\sigma(S,I) > 0,\ \partial_{22}\sigma(S,I) > 0 \text{ for } (S,I) \in \mathbb{R}^+ \times \mathbb{R}^+. \tag{4e}$$

Hence, in this paper, we study the determination of coefficients (β, γ) in a reaction-diffusion system of the following type

$$S_t - \Delta S = -\beta(x)S\sigma(S,I) + \gamma(x)I, \qquad \text{in } Q_T := \Omega \times [0,T], \tag{5}$$
$$I_t - \Delta I = \beta(x)S\sigma(S,I) - \gamma(x)I, \qquad \text{in } Q_T, \tag{6}$$
$$\nabla S \cdot \mathbf{n} = \nabla I \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma := \partial\Omega \times [0,T], \tag{7}$$
$$(S,I)(x,0) = (S_0, I_0)(x), \qquad \text{in } \Omega, \tag{8}$$

from knowledge of σ and an observed measurement for $(S,I)^t$ at $t = T$ given by the function $(S^{obs}, I^{obs})^t$ defined on $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$. This inverse problem is formulated more appropriately as follows

> Given the functions S_0, I_0, S^{obs}, and I^{obs} defined on Ω, and the function σ satisfying (4), find the functions β and γ defined on Ω, such that $(S,I)(\cdot,T)$, the solution of the initial boundary value problem l(5)-(8) at $t = T$, is as close as to the observation data (S^{obs}, I^{obs}). (9)

The notation $\partial\Omega$ is used for the boundary of Ω with outer unit normal vector field $\mathbf{n}$. We notice that, the problem (9) is introduced to validate the proposed mathematical models with experimental data or to solve well known model calibration problem.

We approach the analysis of (9) by considering both an analytical and a numerical perspectives. Firstly, in the case of our analytical study, we consider an equivalent reformulation of the inverse problem (9) as the constrained optimization problem

$$\inf_{(\beta,\gamma)\in U_{ad}(\Omega)} J(\beta,\gamma) \quad \text{subject to } (S_{(\beta,\gamma)}, I_{(\beta,\gamma)}) \text{ solution of (5)-(8)}, \tag{10}$$

where the cost functional and the admissible set are defined by

$$J(\beta,\gamma) := \frac{1}{2}\|(S_{(\beta,\gamma)}, I_{(\beta,\gamma)})(\cdot,T) - (S^{obs}, I^{obs})\|^2_{L^2(\Omega)^2} + \frac{\Gamma}{2}\|\nabla(\beta,\gamma)\|^2_{L^2(\Omega)^2}, \quad \Gamma > 0, \tag{11}$$
$$U_{ad}(\Omega) = \mathcal{A}(\Omega) \cap H^{[\![d/2]\!]+1}(\Omega)^2, \tag{12}$$
$$\mathcal{A}(\Omega) = \Big\{(\beta,\gamma) \in C^\alpha(\overline{\Omega})^2 \quad : \quad (\beta,\gamma)(x) \in]0,1[^2 \text{ on } \Omega \text{ and } \nabla(\beta,\gamma) \in L^2(\Omega)^2 \Big\}. \tag{13}$$

Here $H^m(\Omega)$ and $C^\alpha(\overline{\Omega})$ denote the standard Sobolev and Hölder spaces $W^{m,2}(\Omega)$ and $C^{0,\alpha}(\overline{\Omega})$, respectively. The first term of J is introduced to make mathematical precise sense of the term "as close as" in (9) and the second term is proposed to regularize the cost function with an appropriate selection of the regularization parameter Γ. Then by applying the applying the methodology of optimal control theory we get the following seven main results results: (i) the global classical solutions of (5)-(8), (ii) the existence of solutions of the optimization problem (10), (iii) the definition of an adjoint system, (iv) the definition of a first order necessary optimality condition for (10), (v) the stability of the direct problem solution with respect to the coefficients, (vi) the stability of the adjoint problem solution with respect to the coefficients and the observations, and (vii) the necessary condition for local uniqueness of (10). Second, in the case of our numerical study, we consider the adjoint based methodology with the discretize-then-differentiate strategy as is described in [15]. We begin discretizing the direct problem by an IMEX (implicit for the diffusion term and explicit for the advection) scheme and proving that the approximation is consistent with the biological model in the sense that it is positivity preserving and convergent. Then by considering the parameter identification, we introduce a discrete cost function, define a discrete adjoint state and calculate a discrete gradient. This exact gradient and BFGS method allows the develop the numerical examples for the parameter identification.

We remark that there are several works focused on the analytical approaches for optimal control problems for reaction-diffusion problems, for instance [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. Particularly, the study of the inverse problem (10), was initiated by Xiang and Liu in [26], where the authors develop a well detailed analysis of one-dimensional ($d = 1$) problem with σ give by the "proportionate mixing" given in (3). An extension to $d \geq 1$ was developed in [19], by introducing appropriate assumptions and functional framework such that the results of [26] are still valid in higher spatial dimensions. Some advances, in order to research the application of the methodology to similar systems and to define the consistent general assumptions are recently given in [18], where the authors consider σ give by the "power law" given in (3).

The paper is organized as follows. In Section 2, we present the assumptions, statement and results for our theoretical study. In Section 3, we present the results for the numerical analysis of the inverse problem. Meanwhile, in Section 4, we present a numerical example.

2. Analytical study of the inverse problem

We consider that the inverse problem (9) is equivalent to the optimization problem (10).

2.1. Assumptions on coefficients, initial-boundary conditions and the spatial domain

Throughout the paper, we consider the assumptions:

(A1) The set $\Omega \subset \mathbb{R}^d$ is an open bounded and convex set with smooth boundary of class C^∞.

(A2) The initial condition is considered with the regularity $(S_0, I_0) \in C^{2,\alpha}(\Omega)^2 \times L^\infty(\Omega)^2$ and such that $(S_0, I_0)(x) \in \mathbb{R}_0^+ \times \mathbb{R}_0^+$ and $(S_0 + I_0)(x) \in \mathbb{R}^+$ on Ω.

(A3) The function σ is assumed to be satisfy the properties given on (4).

(A4) The functions $(\beta, \gamma) \in U_{ad}(\Omega)$ with $U_{ad}(\Omega)$ defined in (12).

(A5) The observation function is assumed such that $(S^{obs}, I^{obs}) \in C^{2+\alpha,1+\alpha/2}(\Omega)^2$.

2.2. Well posedness of the direct problem (5)-(8)

Theorem 2.1. *Consider that $\Omega, (S_0, I_0), \sigma$ and (β, γ) satisfy the assumptions (A1)-(A4). Then, the initial boundary value problem* (5)-(8) *admits a unique positive classical solution $(S, I) \in C^{2+\alpha,1+\alpha/2}(Q_T)^2$ and $(S, I)(x, t)$ is bounded on $\overline{Q}_T$ for any $T > 0$.*

Proof. Let us consider that $\mathbf{f}_1(S, I) = -\beta(x)S\sigma(S, I)+\gamma(x)I$ and $\mathbf{f}_2(S, I) = \beta(x)S\sigma(S, I)-\gamma(x)I$. From (A3) (see (4b)) and (A4), we deduce that

$$\mathbf{f}_1(0, I) = -\beta(x)\ 0\ \sigma(0, I) + \gamma(x)I = \gamma(x)I \geq 0,$$
$$\mathbf{f}_2(S, 0) = \beta(x)S\sigma(S, 0) - \gamma(x)\ 0 = 0 \geq 0,$$

for all $(S, I) \in R^+ \times R^+$, i.e. $\mathbf{f}$ is quasi-positive or satisfies the condition (P) considered in [27]. Then, from (A2), (A3) and application of Lemma 1.1 in [27], we deduce the local existence and uniqueness of non-negative solutions for (5)-(8) on the interval $[0, T_*)$. Additionally, adding (5) and (6) and rearranging the initial and boundary conditions, we deduce the following initial-boundary value problem

$$(S + I)_t - \Delta(S + I) = 0, \quad \text{in } Q_T, \tag{14}$$
$$\nabla(S + I) \cdot \mathbf{n} = 0, \quad \text{on } \Gamma, \tag{15}$$
$$(S + I)(x, 0) = (S_0 + I_0)(x), \quad \text{in } \Omega, \tag{16}$$

An application of the maximum principle, implieas that $\|(S+I)(\cdot, t)\|_{L^\infty(\Omega)} \leq \|S_0+I_0\|_{L^\infty(\Omega)}$ for $t \in [0, T_*)$. Thus, we have the existence and uniqueness of non-negative and bounded solution for (5)-(8) on the interval $[0, T_*)$ and $(S, I)(x, t) \in [0, \|S_0+I_0\|_{L^\infty(\Omega)}]^2$ on $\Omega\times[0, T_*)$.

From (A3) (more precisely (4c)) and Lema 2.1 in [28] (see also Theorem 1 in [29]), we can prove that the local result implies a global ones, i.e. the global existence and uniqueness of non-negative classical solutions for (5)-(8). Now, the regularity $C^{2+\alpha,1+\alpha/2}(\overline{Q}_T)$ of the solution is due to the regularity of $\sigma, (\beta, \gamma)$ and (S_0, I_0) given on assumptions (A2)-(A4) and by follow by application of the standard arguments given for instance in [30, 31, 32]. □

2.3. Existence of solutions of the optimization problem (10)

Lemma 1. *Consider that $\Omega, (S_0, I_0), \sigma$ and (S^{obs}, I^{obs}) satisfy the assumptions (A1)-(A3) and (A5). Then, there exists at least one solution of the optimization problem*(10).

Proof. We proof the existence by the standard strategy of a minimizing sequence and use the appropriate compactness inclusions. We observe that $U_{ad}(\Omega) \neq \emptyset$ and also we have that $J(\beta, \gamma)$ is bounded for any $(\beta, \gamma) \in U_{ad}(\Omega)$. Then, we can define $\{(\beta_n, \gamma_n)\}_{n\in\mathbb{N}} \subset \mathcal{U} := U_{ad}(\Omega) \cap \mathcal{M}$ a minimizing sequence of J, with $\mathcal{M}$ a bounded closed set of $H^{[\![d/2]\!]+1}(\Omega)^2$. By the compact embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^\alpha(\Omega)$ for $\alpha \in]0, 1/2]$, we deduce that the minimizing sequence $\{(\beta_n, \gamma_n)\}$ is bounded in the strong topology of $C^\alpha(\overline{\Omega})^2$ for all $\alpha \in]0, 1/2]$, since there exists a positive constant C (independent of β_n, γ_n and n) such that

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

Notice that the right hand is bounded by the fact that $(\beta_n, \gamma_n) \in \mathcal{M} \subset H^{[\![d/2]\!]+1}(\Omega)^2$. Let us consider the notation (S_n, I_n) for the solution of the system (5)-(8) with (β_n, γ_n) instead of (β, γ). From the fact that $(\beta_n, \gamma_n) \in C^{\alpha}(\overline{\Omega})^2$ for all $\alpha \in]0, 1/2]$ and Theorem 2.1, we have that $(S_n, I_n) \in C^{2+\alpha, 1+\frac{\alpha}{2}}(\overline{Q}_T)^2$ and also $\{(S_n, I_n)\}_{n\in\mathbb{N}}$ is a bounded sequence in the strong topology of $C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T)^2$ for all $\alpha \in]0, 1/2]$. Thus, the boundedness of the minimizing sequence and the corresponding sequence $\{(S_n, I_n)\}_{n\in\mathbb{N}}$, implies that there exist

$$(\overline{\beta}, \overline{\gamma}) \in C^{1/2}(\Omega)^2 \cap U_{ad}(\Omega), \qquad (\overline{S}, \overline{I}) \in C^{2+\frac{1}{2},1+\frac{1}{4}}(\overline{Q}_T)^2,$$

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

$$(\beta_n, \gamma_n) \to (\overline{\beta}, \overline{\gamma}) \quad \text{uniformly on } C^{\alpha}(\Omega)^2, \tag{17}$$

$$(S_n, I_n) \to (\overline{S}, \overline{I}) \quad \text{uniformly on } \left[C^{\alpha,\frac{\alpha}{2}}(\overline{Q}_T) \cap C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T)\right]^2. \tag{18}$$

Moreover, we can deduce that $(\overline{S}, \overline{I})$ is the solution of the initial boundary value problem (5)-(8) 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

$$J(\overline{\beta}, \overline{\gamma}) \leq \lim_{n\to\infty} J(\beta_n, \gamma_n) = \inf_{(\beta,\gamma)\in U_{ad}(\Omega)} J(\beta, \gamma). \tag{19}$$

Then, $(\overline{\beta}, \overline{\gamma})$ is a solution of (10) and the prove of existence is concluded. □

2.4. Definition and some properties of the adjoint system for (5)-(8)

Theorem 2.2. *Consider that $\Omega, (S_0, I_0), (\beta, \gamma), \sigma$ and (S^{obs}, I^{obs}) satisfying the assumptions (A1)-(A5). Moreover, consider (p_1, p_2) the solution of the adjoint system to* (5)-(8) *defined by the following backward boundary value problem*

$$(p_1)_t + \Delta p_1 = -\overline{\beta}(x)\Big[\sigma(\overline{S}, \overline{I}) + \overline{S}\partial_1\sigma(\overline{S}, \overline{I})\Big](p_1 - p_2) \qquad \text{in } Q_T, \tag{20}$$

$$(p_2)_t + \Delta p_2 = \Big[-\overline{\beta}(x)\overline{S}\partial_2\sigma(\overline{S}, \overline{I}) + \overline{\gamma}(x)\Big](p_1 - p_2) \qquad \text{in } Q_T, \tag{21}$$

$$\nabla p_1 \cdot \mathbf{n} = \nabla p_2 \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma, \tag{22}$$

$$(p_1, p_2)(x, T) = (\overline{S}, \overline{I})(x, T) - (S^{obs}, I^{obs})(x), \qquad \text{in } \Omega, \tag{23}$$

where $(\overline{\beta}, \overline{\gamma})$ is a solution of (10) *and $(\overline{S}, \overline{I})$ is the solution of* (5)-(8) *with $(\overline{\beta}, \overline{\gamma})$ instead of (β, γ). Then, the solution of* (20)-(23) *satisfy the following estimates*

$$\|(p_1, p_2)(\cdot, t)\|^2_{L^2(\Omega)^2} \leq C, \qquad \|(p_1, p_2)(\cdot, t)\|^2_{H^1_0(\Omega)^2} \leq C, \tag{24}$$

$$\|\Delta(p_1, p_2)(\cdot, t)\|^2_{L^2(\Omega)^2} \leq C, \qquad \|(p_1, p_2)(\cdot, t)\|^2_{L^\infty(\Omega)^2} \leq C, \tag{25}$$

for $t \in [0, T]$, with C a generic positive constant.

Proof. We rewrite the end boundary backward problem (5)-(8) as the following initial boundary value problem

$$(q_1)_\tau - \Delta q_1 = \overline{\beta}(x)\Big[\sigma(S^*, I^*) + S^*\partial_1\sigma(S^*, I^*)\Big](q_1 - q_2) \qquad \text{in } Q_T, \tag{26}$$

$$(q_2)_\tau - \Delta q_2 = -\Big[-\overline{\beta}(x)S^*\partial_2\sigma(S^*, I^*) + \overline{\gamma}(x)\Big](q_1 - q_2) \qquad \text{in } Q_T, \tag{27}$$

$$\nabla q_1 \cdot \mathbf{n} = \nabla q_2 \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma, \tag{28}$$

$$(q_1, q_2)(x, 0) = (\overline{S}, \overline{I})(x, T) - (S^{obs}, I^{obs})(x), \qquad \text{in } \Omega, \tag{29}$$

by considering $\tau = T - t$ for $t \in [0, T]$, $(q_1, q_2)(\mathbf{x}, \tau) = (p_1, p_2)(\mathbf{x}, T - \tau)$, and $(S^*, I^*)(\mathbf{x}, \tau) = (\overline{S}, \overline{I})(\mathbf{x}, T - \tau)$. Multiplying (26) by q_1, (27) by q_2 and integrating by parts on Ω, we get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{d\tau}\|(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} + \|\nabla(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} \\
&\leq \int_\Omega \Big|\overline{\beta}(x)\Big[\sigma(S^*, I^*) + S^*\partial_1\sigma(S^*, I^*)\Big](q_1 - q_2)q_1 \\
&\qquad - \Big[-\overline{\beta}(x)S^*\partial_2\sigma(S^*, I^*) + \overline{\gamma}(x)\Big](q_1 - q_2)q_2\Big| dx.
\end{aligned} \tag{30}$$

By applying the fact that $(\beta, \gamma) \in U_{ad}(\Omega)$ and the assumption (A3), we deduce that there is a positive constant C such that

$$\frac{1}{2}\frac{d}{d\tau}\|(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} + \|\nabla(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} \leq C\|(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2}. \tag{31}$$

Then, a straightforward application of Gronwall inequality and the initial condition (29), implies the first estimate in (24). Moreover, from (31), we follow that

$$\|\nabla(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} \leq C\|(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2}.$$

Then from the first estimate in (24) and the definition of the norm of $H^1_0(\Omega)$ we deduce the second estimate in (24).

On the other hand, proceeding similar, multiplying (26) by Δq_1, (27) by Δq_2 and integrating on Ω, we deduce that there is a positive constant C such that

$$\begin{aligned}
&\frac{1}{2}\frac{d}{d\tau}\|(q_1, q_2)(\cdot, \tau)\|^2_{H^1_0(\Omega)^2} + \|\Delta(q_1, q_2)(\cdot, \tau)\|^2_{H^1_0(\Omega)^2} \\
&\leq C\left(\epsilon\|(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2} + \frac{1}{4\epsilon}\|\Delta(q_1, q_2)(\cdot, \tau)\|^2_{L^2(\Omega)^2}\right),
\end{aligned}$$

for any $\epsilon > 0$. Then, for $\epsilon > C/4$, by using the first estimate in (24) we deduce the first estimate in (25). Now, from (25), and the first estimate in (24), we have that the norm of (p_1, p_2) is bounded in the norm of $H^2(\Omega)^2$. Thus, by the standard embedding theorem of $H^2(\Omega)^2 \subset L^\infty(\Omega)^2$, we easily deduce the second estimate in (25).

□

2.5. First order optimality condition(5)-(8)

Theorem 2.3. *Consider that the assumptions and the notation of Theorem 2.2 are satisfied and also consider the symbol* $<,>$ *to the canonical inner product in* $L^2(\Omega)^2$*. Then, the inequality*

$$\iint_{Q_T} \Big[(\hat{\beta}-\overline{\beta})\overline{S}\sigma(\overline{S},\overline{I}) - (\hat{\gamma}-\overline{\gamma})\overline{I}\Big](p_1-p_2)dxdt \\ + \Gamma \Big\langle \nabla(\overline{\beta},\overline{\gamma}), \nabla\Big((\hat{\beta},\hat{\gamma})-(\overline{\beta},\overline{\gamma})\Big)\Big\rangle \geq 0, \tag{32}$$

is satisfied for any $(\hat{\beta},\hat{\gamma}) \in U_{ad}(\Omega)$.

Proof. Let us choose $(\hat{\beta},\hat{\gamma}) \in U_{ad}(\Omega)$, define $(\beta^\epsilon,\gamma^\epsilon) \in U_{ad}(\Omega)$ by the relation $(\beta^\epsilon,\gamma^\epsilon) = (1-\epsilon)(\overline{\beta},\overline{\gamma}) + \epsilon(\hat{\beta},\hat{\gamma})$, for $\epsilon \in [0,1]$, and consider (S^ϵ, I^ϵ) and $(\overline{S},\overline{I})$ solutions of (5)-(8) with $(\beta^\epsilon,\gamma^\epsilon)$ and $(\overline{\beta},\overline{\gamma})$ instead of (β,γ). Then, subtracting the systems for (S^ϵ, I^ϵ) and $(\overline{S},\overline{I})$, dividing by ϵ, defining $(z_1^\epsilon, z_2^\epsilon) := \epsilon^{-1}((S^\epsilon, I^\epsilon) - (\overline{S},\overline{I}))$, and using the fact that

$$\begin{aligned} h^\epsilon &:= -\frac{1}{\epsilon}\Big\{\beta^\epsilon(x)S^\epsilon\sigma(S^\epsilon,I^\epsilon) - \overline{\beta}(x)\overline{S}\sigma(\overline{S},\overline{I})\Big\} + \frac{1}{\epsilon}\Big\{\gamma^\epsilon(x)I^\epsilon - \overline{\beta}(x)\overline{I}\Big\} \\ &= -\beta^\epsilon(x)\left\{\left[\frac{S^\epsilon\sigma(S^\epsilon,I^\epsilon) - \overline{S}\sigma(\overline{S},I^\epsilon)}{S^\epsilon - \overline{S}}\right] z_1^\epsilon + \left[\frac{\overline{S}\sigma(\overline{S},I^\epsilon) - \overline{S}\sigma(\overline{S},\overline{I})}{I^\epsilon - \overline{I}}\right] z_2^\epsilon\right\} \\ &\quad - (\hat{\beta}-\overline{\beta})(x)\overline{S}\sigma(\overline{S},\overline{I}) + \gamma^\epsilon(x)z_2^\epsilon + (\hat{\beta}-\overline{\beta})(x)\overline{I}, \end{aligned}$$

we deduce the system

$$(z_1^\epsilon)_t - \Delta z_1^\epsilon = h^\epsilon, \quad \text{in } Q_T, \tag{33}$$
$$(z_2^\epsilon)_t - \Delta z_2^\epsilon = -h^\epsilon, \quad \text{in } Q_T, \tag{34}$$
$$\nabla z_1^\epsilon \cdot \mathbf{n} = \nabla z_2^\epsilon \cdot \mathbf{n} = 0, \quad \text{on } \Gamma, \tag{35}$$
$$(z_1^\epsilon, z_2^\epsilon)(x,0) = 0, \quad \text{in } \Omega. \tag{36}$$

Now, by considering (z_1,z_2) the limit of $(z_1^\epsilon, z_2^\epsilon)$ when $\epsilon \to 0$, and observing that h^ϵ converges to

$$\begin{aligned} h := -\overline{\beta}(x)\Big[\Big(\sigma(\overline{S},\overline{I}) + \overline{S}\partial_1\sigma(\overline{S},\overline{I})\Big)z_1 + \overline{S}\partial_2\sigma(\overline{S},\overline{I})\Big)z_2 \\ - (\hat{\beta}-\overline{\beta})(x)\overline{S}\sigma(\overline{S},\overline{I}) + \overline{\gamma}(x)z_2 + (\hat{\beta}-\overline{\beta})(x)\overline{I}. \end{aligned}$$

Then, taking the limit of (33)-(36) when $\epsilon \to 0$, we have that (z_1,z_2) satisfies the initial boundary value problem

$$(z_1)_t - \Delta z_1 = h, \quad \text{in } Q_T, \tag{37}$$
$$(z_2)_t - \Delta z_2 = -h, \quad \text{in } Q_T, \tag{38}$$
$$\nabla z_1 \cdot \mathbf{n} = \nabla z_2 \cdot \mathbf{n} = 0, \quad \text{on } \Gamma, \tag{39}$$
$$(z_1, z_2)(x,0) = (0,0), \quad \text{in } \Omega. \tag{40}$$

From the definition of (S^ϵ, I^ϵ) and using the hypothesis that $(\overline{S}, \overline{I})$ is an optimal solution of (10), we follow that

$$
\begin{aligned}
J_\epsilon := J(\beta^\epsilon, \gamma^\epsilon) &= \frac{1}{2}\|(S^\epsilon, I^\epsilon)(\cdot, T) - (S^{obs}, I^{obs})\|^2_{L^2(\Omega)^2} + \frac{\Gamma}{2}\|\nabla(\beta^\epsilon, \gamma^\epsilon)\|^2_{L^2(\Omega)^2}, \\
\frac{dJ_\epsilon}{d\epsilon}\Big|_{\epsilon=0} &= \left\langle (S^\epsilon, I^\epsilon)(\cdot, T) - (S^{obs}, I^{obs}), \frac{\partial}{\partial\epsilon}(S^\epsilon, I^\epsilon)(\cdot, T) \right\rangle\Big|_{\epsilon=0} \\
&\quad + \Gamma\left\langle \nabla(\overline{\beta}, \overline{\gamma}), \nabla\Big((\hat{\beta}, \hat{\gamma}) - (\overline{\beta}, \overline{\gamma})\Big)\right\rangle \\
&= \big\langle (\overline{S}, \overline{I})(\cdot, T) - (S^{obs}, I^{obs}), (z_1, z_2)(\cdot, T)\big\rangle \\
&\quad + \Gamma\left\langle \nabla(\overline{\beta}, \overline{\gamma}), \nabla\Big((\hat{\beta}, \hat{\gamma}) - (\overline{\beta}, \overline{\gamma})\Big)\right\rangle \geq 0,
\end{aligned} \tag{41}
$$

with (z_1, z_2) solution of (37)-(40). From (20)-(23) and (37)-(40), we observe that, we can rewrite the first term of (41) as follows

$$
\begin{aligned}
&\big\langle (\overline{S}, \overline{I})(\cdot, T) - (S^{obs}, I^{obs}), (z_1, z_2)(\cdot, T)\big\rangle = \langle (p_1, p_2)(\cdot, T), (z_1, z_2)(\cdot, T)\rangle \\
&\quad = \iint_{Q_T} \frac{\partial}{\partial t}\Big((p_1, p_2)\cdot(z_1, z_2)\Big)dxdt \\
&\quad = \iint_{Q_T} \Big\{(p_1, p_2)\cdot\Delta(p_1, p_2) - (z_1, z_2)\cdot\Delta(p_1, p_2) \\
&\qquad\qquad - \Big[(\hat{\beta} - \overline{\beta})\overline{S}\sigma(\overline{S}, \overline{I}) - (\hat{\gamma} - \overline{\gamma})\overline{I}\Big](p_1 - p_2)\Big\}dxdt.
\end{aligned}
$$

Hence, by using the fact that $\iint_{Q_T}\Big((p_1, p_2)\cdot\Delta(p_1, p_2) - (z_1, z_2)\cdot\Delta(p_1, p_2)\Big)dxdt = 0$ and the inequality (41), we conclude the proof of (32). □

2.6. Continuous dependence results

Theorem 2.4. *Consider that the assumptions of Theorems 2.1 and 2.2 are satisfied. Let us assume that the sets of functions* $\{(S, I), (p_1, p_2)\}$ *and* $\{(\hat{S}, \hat{I}), (\hat{p}_1, \hat{p}_2)\}$ *are solutions to the systems* (5)-(8) *and* (5)-(8) *with the data* $\{(\beta, \gamma), (S^{obs}, I^{obs})\}$ *and* $\{(\hat{\beta}, \hat{\gamma}), (\hat{S}^{obs}, \hat{I}^{obs})\}$*, respectively. Then, the estimates*

$$
\|((\hat{S}, \hat{I}) - (S, I))(\cdot, t)\|^2_{L^2(\Omega)^2} \leq C\|(\hat{\beta}, \hat{\gamma}) - (\beta, \gamma)\|^2_{L^2(\Omega)^2}, \tag{42}
$$

$$
\begin{aligned}
&\|((\hat{p}_1, \hat{p}_2) - (p_1, p_2))(\cdot, t)\|^2_{L^2(\Omega)^2} \\
&\quad \leq C\left(\|(\hat{\beta}, \hat{\gamma}) - (\beta, \gamma)\|^2_{L^2(\Omega)^2} + \|(\hat{S}^{obs}, \hat{I}^{obs}) - (S^{obs}, I^{obs})\|^2_{L^2(\Omega)^2}\right),
\end{aligned} \tag{43}
$$

holds for any $t \in [0, T]$ *and* C *a generic positive constant.*

Proof. For the sake of clarity of the presentation, we consider the notation $\delta\mathbf{x} = \hat{\mathbf{x}} - \mathbf{x}$ and $\delta g(\mathbf{x}) = g(\hat{\mathbf{x}}) - g(\mathbf{x})$. For instance $\delta(S, I) = (\hat{S}, \hat{I}) - (S, I)$, $\delta(\beta, \gamma) = (\hat{\beta}, \hat{\gamma}) - (\beta, \gamma)$, and $\delta\sigma(S, I) = \sigma(\hat{S}, \hat{I}) - \sigma(S, I)$. From the definition of (S, I) and $(\hat{S}, \hat{I})$ given by (5)-(8) and also the definition of (p_1, p_2) and $(\hat{p}_1, \hat{p}_2)$ satisfying (20)-(23), we deduce that $(\delta S, \delta I)$ and $(\delta p_1, \delta p_2)$ are solutions of the following systems

$$(\delta S)_t + \Delta(\delta S) = -\hat{\beta}(x)\hat{S}\sigma(\hat{S}, \hat{I}) + \hat{\gamma}(x)\hat{I} + \beta(x)S\sigma(S, I) - \gamma(x)I, \quad \text{in } Q_T, \tag{44}$$

$$(\delta I)_t + \Delta(\delta I) = \hat{\beta}(x)\hat{S}\sigma(\hat{S}, \hat{I}) - \hat{\gamma}(x)\hat{I} - \beta(x)S\sigma(S, I) + \gamma(x)I, \quad \text{in } Q_T, \tag{45}$$

$$\nabla\delta u_1 \cdot \mathbf{n} = \nabla\delta u_2 \cdot \mathbf{n} = 0, \quad \text{on } \Gamma, \tag{46}$$

$$(\delta S, \delta I)(x, 0) = 0, \quad \text{in } \Omega. \tag{47}$$

and

$$\begin{aligned}(\delta p_1)_t - \Delta(\delta p_1) &= -\hat{\beta}(x)\Big[\sigma(\hat{S}, \hat{I}) + \hat{S}\partial_1\sigma(\hat{S}, \hat{I})\Big](\hat{p}_1 - \hat{p}_2) \\ &\quad + \beta(x)\Big[\sigma(S, I) - S\partial_1\sigma(S, I)\Big](p_1 - p_2), \quad \text{in } Q_T,\end{aligned} \tag{48}$$

$$\begin{aligned}(\delta p_2)_t - \Delta(\delta p_2) &= \Big[- \hat{\beta}(x)\hat{S}\partial_2\sigma(\hat{S}, \hat{I}) + \hat{\gamma}(x)\Big](\hat{p}_1 - \hat{p}_2) \\ &\quad - \Big[- \beta(x)S\partial_2\sigma(S, I) + \gamma(x)\Big](p_1 - p_2), \quad \text{in } Q_T,\end{aligned} \tag{49}$$

$$\nabla\delta p_1 \cdot \mathbf{n} = \nabla\delta p_2 \cdot \mathbf{n} = 0, \quad \text{on } \Gamma, \tag{50}$$

$$(\delta p_1, \delta p_2)(x, T) = (\delta S, \delta I)(x, T) - (\delta S^{obs}, \delta I^{obs})(x), \quad \text{in } \Omega. \tag{51}$$

We observe that the right hand side of (44) can be rewritten as follows

$$\begin{aligned}RHS_{(44)} = &-\hat{\beta}(x)\left[\frac{\hat{S}\sigma(\hat{S}, \hat{I}) - S\sigma(S, \hat{I})}{\hat{S} - S}\right]\delta S - \beta(x)\left[\frac{S\sigma(S, \hat{I}) - S\sigma(S, I)}{\hat{I} - I}\right]\delta I \\ &- \delta\beta(x)S\sigma(S, \hat{I}) + \hat{\gamma}(x)\delta I + \delta\gamma(x)I,\end{aligned}$$

A similar expressions for the right hand side of (45), (48) and (49), in terms of δS, δI, δp_1, δp_2, $\delta\beta$ and $\delta\gamma$. Then, the proofs of (42) and (43) are reduced to get a priori estimations for the systems in (48)-(51).

We develop the proof of (42) as follows. Let us consider the system for $(\delta S, \delta I)$ in (44)-(47), by testing the equation in (44) by δS and (44) by δI, adding the results, we get the estimate

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|(\delta S, \delta I)(\cdot, t)\|^2_{L^2(\Omega)^2} &+ \|\nabla(\delta S, \delta I)(\cdot, t)\|^2_{L^2(\Omega)^2} \\ &\leq C\left(2\|(\delta S, \delta I)(\cdot, t)\|^2_{L^2(\Omega)^2} + \|(\delta\beta, \delta\gamma)\|^2_{L^2(\Omega)^2}\right).\end{aligned}$$

Then, by application of Gronwall inequality and the initial condition for $\delta(S, I)$ given in (47), we get

$$\|(\delta S, \delta I)(\cdot, t)\|^2_{L^2(\Omega)^2} \leq C\left(\|(\delta S, \delta I)(\cdot, 0)\|^2_{L^2(\Omega)^2} + \|(\delta\beta, \delta\gamma)\|^2_{L^2(\Omega)^2}\right) = C\|(\delta\beta, \delta\gamma)\|^2_{L^2(\Omega)^2},$$

for any $t \in]0, T]$, which implies (42).

The proof of (43) is developed as follows. Let us consider the system for $(\delta p_1, \delta p_2)$ in (48)-(51), by testing the equation in (48) by δp_1 and (48) by δp_2, we get the estimate

$$
\begin{aligned}
&-\frac{1}{2}\frac{d}{dt}\|(\delta p_1, \delta p_2)(\cdot,t)\|^2_{L^2(\Omega)^2} + \|\nabla(\delta(p_1,p_2))(\cdot,t)\|^2_{L^2(\Omega)^2} \\
&\leq C\Big(\|(\delta p_1, \delta p_2)(\cdot,t)\|^2_{L^2(\Omega)^2} + \|(\delta S, \delta I)(\cdot,t)\|^2_{L^2(\Omega)^2} + \mathbb{D}\mathbb{A}^\infty\|(\delta\beta,\delta\gamma)\|^2_{L^2(\Omega)^2}.
\end{aligned}
$$

Integrating on $[t,T]$ we get

$$
\|(\delta p_1, \delta p_2)(\cdot,t)\|^2_{L^2(\Omega)^2} \leq C\Big(\|(\delta p_1, \delta p_2)(\cdot,T)\|^2_{L^2(\Omega)^2} + \|(\delta\beta,\delta\gamma)\|^2_{L^2(\Omega)^2}\Big),
$$

which concludes the proof of (43) by using the end condition (51). □

2.7. A uniqueness result of the inverse problem

Theorem 2.5. *Let us consider* $\mathbf{c} \in \mathbb{R}^4_+$ *(fix) and* $\mathcal{U}_{\mathbf{c}}(\Omega) \subset U_{ad}(\Omega)$ *defined as follows*

$$
\mathcal{U}_{\mathbf{c}}(\Omega) = \Big\{(\beta,\gamma) \in U_{ad}(\Omega)\ :\ \|(\beta,\gamma)\|_{L^1(\Omega)^2} = \mathbf{c}\Big\}. \tag{52}
$$

Consider that $\Omega, (S_0, I_0), \sigma$ *and* (S^{obs}, I^{obs}) *satisfy the assumptions (A1)-(A3) and (A5). Then, there exists at least one solution of* (10) *and there exist* $\Theta \in \mathbb{R}^+$ *such that the solution of* (10) *is uniquely defined, up an additive constant, on* $\mathcal{U}_{\mathbf{c}}(\Omega)$ *for any regularization parameter* $\Gamma > \Theta$.

Proof. We observe that we can prove the existence by application of Lemma 1. Meanwhile, we prove the uniqueness by application of the stability result given on Theorem 2.4 and the necessary optimality condition of Theorem 2.3.

Let us consider $\{(S,I),(p_1,p_2)\}$ and $\{(\hat{S},\hat{I}),(p_1,\hat{}p_2)\}$ solutions of systems (5)-(8) and (5)-(8) with the coefficients and observations given by $\{(\beta,\gamma),(S,I)^{obs}\}$ and $\{(\hat{\beta},\hat{\gamma}),(\hat{S},\hat{I})^{obs}\}$, respectively. From Theorem 2.3 and the hypothesis that (β,γ) and $(\hat{\beta},\hat{\gamma})$ are solutions of (10), we have that the following inequalities

$$
\begin{aligned}
&\iint_{Q_T}\Big[(\overline{\overline{\beta}}-\beta)S\sigma(S,I) - (\overline{\overline{\gamma}}-\gamma)I\Big](p_1-p_2)dxdt \\
&\qquad\qquad + \Gamma\Big\langle \nabla(\beta,\gamma), \nabla\Big((\overline{\overline{\beta}},\overline{\overline{\gamma}}) - (\beta,\gamma)\Big)\Big\rangle \geq 0, \quad \forall(\overline{\overline{\beta}},\overline{\overline{\gamma}}) \in U_{ad}(\Omega),
\end{aligned} \tag{53}
$$

$$
\begin{aligned}
&\iint_{Q_T}\Big[(\underline{\underline{\beta}}-\hat{\beta})\hat{S}\sigma(\hat{S},\hat{I}) - (\underline{\underline{\gamma}}-\hat{\gamma})\hat{I}\Big](\hat{p}_1-\hat{p}_2)dxdt \\
&\qquad\qquad + \Gamma\Big\langle \nabla(\hat{\beta},\hat{\gamma}), \nabla\Big((\underline{\underline{\beta}},\underline{\underline{\gamma}}) - (\hat{\beta},\hat{\gamma})\Big)\Big\rangle \geq 0, \quad \forall(\underline{\underline{\beta}},\underline{\underline{\gamma}}) \in U_{ad}(\Omega),
\end{aligned} \tag{54}
$$

are satisfied, respectively. In particular, selecting $(\overline{\overline{\beta}},\overline{\overline{\gamma}}) = (\hat{\beta},\hat{\gamma})$ in (53) and $(\underline{\underline{\beta}},\underline{\underline{\gamma}}) = (\beta,\gamma)$ in (54), and adding both inequalities, we get

$$
\Gamma\|\nabla((\hat{\beta},\hat{\gamma}) - (\beta,\gamma))\|^2_{L^2(\Omega)^2}
$$

$$\leq \iint_{Q_T} \Big[(\hat{\beta}-\beta)S\sigma(S,I) - (\hat{\gamma}-\gamma)I\Big](p_1-p_2)$$
$$+ \Big[(\beta-\hat{\beta})\hat{S}\sigma(\hat{S},\hat{I}) - (\gamma-\hat{\gamma})\hat{I}\Big](\hat{p}_1-\hat{p}_2)dxdt$$
$$\leq C\Big[\|(\hat{\beta},\hat{\gamma})-(\beta,\gamma)\|_{L^2(\Omega)^2} + \|(\hat{p}_1,\hat{p}_2)-(p_1,p_2)\|_{L^2(\Omega)^2} + \|(\hat{S},\hat{I})-(S,I)\|_{L^2(\Omega)^2}\Big].$$

From assumption (A3), Theorem 2.1, Theorem 2.5, and Lemma 2.4 we deduce that

$$\Gamma\|\nabla((\hat{\beta},\hat{\gamma})-(\beta,\gamma))\|^2_{L^2(\Omega)^2} \leq C\Big(\|(\hat{\beta},\hat{\gamma})-(\beta,\gamma)\|_{L^2(\Omega)^2} + \|(\hat{S},\hat{I})^{obs}-(S,I)^{obs}\|_{L^2(\Omega)^2}\Big). \tag{55}$$

Now, considering that $(\hat{\beta},\hat{\gamma}),(\beta,\gamma) \in \mathcal{U}_{\mathbf{c}}(\Omega)$, by the generalized Poincaré inequality, we have that

$$\|(\hat{\beta},\hat{\gamma})-(\beta,\gamma)\|_{L^2(\Omega)^2} \leq C_{poi}\Big(\|\nabla((\hat{\beta},\hat{\gamma})-(\beta,\gamma))\|_{L^2(\Omega)^2} + \|(\hat{\beta},\hat{\gamma})-(\beta,\gamma)\|_{L^1(\Omega)^2}\Big) \tag{56}$$
$$\leq C_{poi}\|\nabla((\hat{\beta},\hat{\gamma})-(\beta,\gamma))\|_{L^2(\Omega)^2}.$$

Then, using the estimate (56) in (55), we have that

$$\Big(\Gamma - C_{poi}C\Big)\|\nabla((\hat{\beta},\hat{\gamma})-(\beta,\gamma))\|^2_{L^2(\Omega)^2} \leq C\|(\hat{S},\hat{I})^{obs}-(S,I)^{obs}\|_{L^2(\Omega)^2}.$$

Thus, selecting $\Theta = C_{poi}C$ we deduce the uniqueness up an additive constant. □

3. Numerical solution of the inverse problem

In this section, we introduce a numerical scheme to approximate the optimization problem (10). For clarity of the presentation, we restrict our presntation the one-dimensional case ($d=1$) and observe that it can be straightforward extended to higher dimensions on cartesian grids. Moreover, we consider that the reaction coefficients β and γ can be parametrized by the finite set of parameters denoted by $\mathbf{e} = (e_1,\ldots,e_k) \in \mathbb{R}^k$, i.e. $\beta(x) = \beta(x;\mathbf{e})$ and $\gamma(x) = \gamma(x;\mathbf{e})$. Our presentations of the IMEX method for discretization of the direct problem is based mainly in [33, 34, 35, 36, 37]. Concerning to the discretization of the inverse problem, we introduce a discrete adjoint state and calculate a discrete gradient, by adapting the discretization of the flux-diffusion identification in scalar strongly degenerate parabolic equations [38, 39].

Let us consider that $\Omega =]0,L[, \partial\Omega = \{0,L\}$ and $\Gamma_T = \{0,L\}\times[0,T]$. Concerning to the discretization of Q_T, we select $M,N \in \mathbb{N}$ such that the discretization of Ω is given by $x_k = k\Delta x$ for $k = 0,\ldots,M+1$ with $\Delta x = L/(M+1)$, and the discretization of $[0,T]$ is given by $t_n = n\Delta t$ for $n = 0,\ldots,N$ with $\Delta t = 1/N$. The approximation of a given function $G : \Omega\times\mathbb{R}_+ \to \mathbb{R}$ at (x_k,t_n) is denoted by G^n_k.

The approximation of the initial boundary value problem (5)-(6) we introduce the following IMEX method

$$\frac{S^{n+1}_k - S^n_k}{\Delta t} = \frac{1}{\Delta x^2}\Big[S^{n+1}_{k-1} - 2S^{n+1}_k + S^{n+1}_{k+1}\Big] - \beta(x_k)S^n_k\sigma(S^n_k,I^n_k) + \gamma(x_k)I^n_k, \tag{57}$$

$$\frac{I_k^{n+1} - I_k^n}{\Delta t} = \frac{1}{\Delta x^2}\Big[I_{k-1}^{n+1} - 2I_k^{n+1} + I_{k-1}^{n+1}\Big] + \beta(x_k)S_k^n\sigma(S_k^n, I_k^n) - \gamma(x_k)I_k^n, \tag{58}$$

$$\frac{S_1^n - S_0^n}{\Delta x} = \frac{S_{M+1}^n - S_M^n}{\Delta x} = \frac{I_1^n - I_0^n}{\Delta x} = \frac{I_{M+1}^n - I_M^n}{\Delta x} = 0, \tag{59}$$

$$S_k^0 = S_0(x_k), \quad I_k^0 = I_0(x_k). \tag{60}$$

In the case of (57) and (58) we have that $k = 1, \ldots, M$. In order to give a more compact presentation of (57)-(60) we set the notation

$$\mathbf{S}^n = (S_1^n, \ldots, S_M^n)^t, \quad \mathbf{I}^n = (I_1^n, \ldots, I_M^n)^t, \tag{61a}$$

$$\mathbf{U}^n = (S_1^n, \ldots, S_M^n, I_1^n, \ldots, I_M^n)^t = \begin{pmatrix} \mathbf{S}^n \\ \mathbf{I}^n \end{pmatrix} \tag{61b}$$

$$\mathbb{L} = \frac{\Delta t}{\Delta x^2} H \quad \text{with} \quad \mathbb{H} = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}_{M\times M} \tag{61c}$$

$$F_S(\mathbf{U}^n) = \begin{pmatrix} -\beta(x_1)S_1^n\sigma(S_1^n, I_1^n) + \gamma(x_1)I_1^n \\ \vdots \\ -\beta(x_M)S_M^n\sigma(S_M^n, I_M^n) + \gamma(x_M)I_M^n \end{pmatrix}, \tag{61d}$$

$$F_I(\mathbf{U}^n) = \begin{pmatrix} \beta(x_1)S_1^n\sigma(S_1^n, I_1^n) - \gamma(x_1)I_1^n \\ \vdots \\ \beta(x_M)S_M^n\sigma(S_M^n, I_M^n) - \gamma(x_M)I_M^n \end{pmatrix}, \tag{61e}$$

$$F(\mathbf{U}^n) = \begin{pmatrix} F_S(\mathbf{U}^n) \\ F_I(\mathbf{U}^n) \end{pmatrix}, \qquad \overline{\mathbb{L}} = \begin{pmatrix} \mathbb{I}_M + \mathbb{L} & \\ & \mathbb{I}_M + \mathbb{L} \end{pmatrix}, \tag{61f}$$

where $\mathbb{I}_M$ is the identity matrix of size M. We observe that (57)-(60) can be rewritten as follows

$$\mathbf{S}^{n+1} - \mathbf{S}^n = -\mathbb{L}\mathbf{S}^{n+1} + \Delta t F_S(\mathbf{U}^n), \quad \mathbf{I}^{n+1} - \mathbf{I}^n = -\mathbb{L}\mathbf{I}^{n+1} + \Delta t F_I(\mathbf{U}^n),$$

which is equivalently to

$$\overline{\mathbb{L}}\mathbf{U}^{n+1} = \mathbf{U}^{n+1} + \Delta t F(\mathbf{U}^n). \tag{62}$$

Hence, we have stated the IMEX scheme to approximate the direct problem.

For discretization of the inverse problem (10), we begin by considering the discret cost function J_Δ defined as follows

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

$$+\frac{\Gamma}{2}\frac{\Delta x}{2}\sum_{k=1}^{M}\Big(|\beta'(x_k)|^2+|\gamma'(x_k)|^2\Big). \tag{63}$$

Here β' and γ' denotes spatial derivatives, since we have assumed that $d=1$. Then, the solution of the inverse problem (10), is replaced by the following parameter identification problem

$$\inf_{\mathbf{e}\in\mathbb{R}^k}\mathcal{J}_\Delta(\mathbf{e}),\quad \mathcal{J}_\Delta(\mathbf{e})=J_\Delta(S_\Delta,I_\Delta), \tag{64}$$

$$\text{subject to } (S_\Delta,I_\Delta) \text{ solution of (57)-(60).} \tag{65}$$

Then, in order to calculate $\nabla_{\mathbf{e}}\mathcal{J}_\Delta(\mathbf{e})$ we introduce a discrete adjoint state for the IMEX scheme (57)-(60).

Testing (57) by $(p_1)_k^{n+1}$, we deduce $E_\Delta^S=0$ with E_Δ^S defined as follows

$$\begin{aligned}
E_\Delta^S &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\left\{S_k^{n+1}-S_k^n-\frac{\Delta t}{\Delta x^2}\Big(S_{k-1}^{n+1}-2S_k^{n+1}+S_{k+1}^{n+1}\Big)-\Delta t\ F_k(\mathbf{u}^n)\right\}(p_1)_k^{n+1},\\
&=\sum_{n=0}^{N-1}\sum_{k=1}^{M}S_k^n\left[(p_1)_k^n-(p_1)_k^{n+1}-\frac{\Delta t}{\Delta x^2}\Big((p_1)_{k-1}^n-2(p_1)_k^n+(p_1)_{k+1}^n\Big)\right]-\Delta t\ F_k(\mathbf{u}^n)(p_1)_k^{n+1}\\
&+\sum_{k=1}^{M}\left[S_k^N-\frac{\Delta t}{\Delta x^2}\Big(S_{k-1}^N-2S_k^N+S_{k+1}^N\Big)\right](p_1)_k^N-\left[S_k^0-\frac{\Delta t}{\Delta x^2}\Big(S_{k-1}^0-2S_k^0+S_{k+1}^0\Big)\right](p_1)_k^0\\
&-\frac{\Delta t}{\Delta x^2}\sum_{n=0}^{N-1}\Big[S_1^n(p_1)_2^n-S_M^n(p_1)_{M+1}^n+S_{M+1}^n(p_1)_M^n-S_1^n(p_1)_0^n\Big].
\end{aligned}$$

Similarly, by testing (58) by $(p_2)_k^{n+1}$, we deduce $E_\Delta^I=0$ with E_Δ^I defined as follows

$$\begin{aligned}
E_\Delta^I &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\left\{I_k^{n+1}-I_k^n-\frac{\Delta t}{\Delta x^2}\Big(I_{k-1}^{n+1}-2I_k^{n+1}+I_{k+1}^{n+1}\Big)-\Delta t\ F_{k+M}(\mathbf{u}^n)\right\}(p_2)_k^{n+1},\\
&=\sum_{n=0}^{N-1}\sum_{k=1}^{M}I_k^n\left[(p_2)_k^n-(p_2)_k^{n+1}-\frac{\Delta t}{\Delta x^2}\Big((p_2)_{k-1}^n-2(p_2)_k^n+(p_2)_{k+1}^n\Big)\right]-\Delta t\ F_{k+M}(\mathbf{u}^n)(p_2)_k^{n+1}\\
&+\sum_{k=1}^{M}\left[I_k^N-\frac{\Delta t}{\Delta x^2}\Big(I_{k-1}^N-2I_k^N+I_{k+1}^N\Big)\right](p_2)_k^N-\left[I_k^0-\frac{\Delta t}{\Delta x^2}\Big(I_{k-1}^0-2I_k^0+I_{k+1}^0\Big)\right](p_2)_k^0\\
&-\frac{\Delta t}{\Delta x^2}\sum_{n=0}^{N-1}\Big[I_1^n(p_2)_2^n-I_M^n(p_2)_{M+1}^n+I_{M+1}^n(p_2)_M^n-I_1^n(p_2)_0^n\Big].
\end{aligned}$$

Then, denoting by $\mathbf{p}_1^n=((p_1)_1^n,\ldots,(p_1)_M^n)^t$, $\mathbf{p}_2^n=((p_2)_1^n,\ldots,(p_2)_M^n)^t$, we define the Lagrangian $\mathcal{L}_\Delta$ for (64)-(65) by the following relation

$$\mathcal{L}_\Delta(\mathbf{u},\mathbf{p}_1^n,\mathbf{p}_2^n)=J_\Delta(\mathbf{u})-E_\Delta^S(\mathbf{u},\mathbf{p}_1^n)-E_\Delta^I(\mathbf{u},\mathbf{p}_2^n).$$

We notice that

$$\frac{d\mathcal{L}_\Delta}{d\mathbf{e}}(\mathbf{u},\mathbf{p}_1^n,\mathbf{p}_2^n)=\frac{\partial\mathcal{L}_\Delta}{\partial\mathbf{u}}(\mathbf{u},\mathbf{p}_1^n,\mathbf{p}_2^n)\frac{\partial u}{\partial\mathbf{e}}+\frac{\partial\mathcal{L}_\Delta}{\partial\mathbf{e}}(\mathbf{u},\mathbf{p}_1^n,\mathbf{p}_2^n).$$

We select $\mathbf{p}_1^n$ and $\mathbf{p}_2^n$ such that $\partial_{\mathbf{u}}\mathcal{L}_\Delta=0$, i.e.

$$\begin{aligned}\frac{(p_1)_k^n-(p_1)_k^{n+1}}{\Delta t}&=\frac{1}{\Delta x^2}\Big[(p_1)_{k-1}^n-2(p_1)_k^n+(p_1)_{k+1}^n\Big]\\&\quad-\beta(x_k)\Big[\sigma(S_k^n,S_k^n)+S_k^n\partial_1\sigma(S_k^n,S_k^n)\Big]\Big((p_1)_k^{n+1}-(p_2)_k^{n+1}\Big),\end{aligned}\tag{66}$$

$$\begin{aligned}\frac{(p_2)_k^n-(p_2)_k^{n+1}}{\Delta t}&=\frac{1}{\Delta x^2}\Big[(p_2)_{k-1}^n-2(p_2)_k^n+(p_2)_{k+1}^n\Big]\\&\quad+\Big[-\beta(x_k)S_k^n\partial_2\sigma(S_k^n,S_k^n)+\gamma(x_k)\Big]\Big((p_1)_k^{n+1}-(p_2)_k^{n+1}\Big),\end{aligned}\tag{67}$$

$$\frac{(p_1)_1^n-(p_1)_0^n}{\Delta x}=\frac{(p_1)_{M+1}^n-(p_1)_M^n}{\Delta x}=\frac{(p_2)_1^n-(p_2)_0^n}{\Delta x}=\frac{(p_2)_{M+1}^n-(p_2)_M^n}{\Delta x}=0,\tag{68}$$

$$(p_1)_k^N=S_k^N-S_k^{obs},\quad (p_2)_k^N=I_k^N-I_k^{obs}.\tag{69}$$

The scheme (66)-(69) is called the adjoint scheme. Hence, we have that

$$\begin{aligned}\nabla_{\mathbf{e}}\mathcal{J}_\Delta(\mathbf{e})&=\Delta t\sum_{n=0}^{N-1}\sum_{k=1}^{M}\Big[\nabla_{\mathbf{e}}\beta(x_1)S_k^n\sigma(S_k^n,I_k^n)-\nabla_{\mathbf{e}}\gamma(x_k)I_k^n\Big]\Big((p_1)_k^{n+1}-(p_2)_k^{n+1}\Big)\\&\quad+\frac{\Gamma}{2}\frac{\Delta x}{2}\sum_{k=1}^{M}\Big(|\nabla_{\mathbf{e}}\beta'(x_k)|^2+|\nabla_{\mathbf{e}}\gamma'(x_k)|^2\Big).\end{aligned}\tag{70}$$

defines the gradient which is used for numerical solution of parameter optimization problem.

4. A numerical example

In our example we consider that the initial condition $(S_0,I_0)(x)=(x,2-x)/2$. The vector of parameters to indentify are $\mathbf{e}=(e_1,e_2,e_3,e_4)$ and we consider that the coefficients are parameterized as follows $\beta(x)=e_1+e_2x$ and $\gamma(x)=e_3+e_4x$. The function σ considered is $\sigma(S,I)=I$, i.e. the corresponding to mass mass action (see (3)). We construct the observation profile at $T=0.6$ by considering a numerical simulation of the direct problem with $\mathbf{e}^{obs}=(0.00018,0.00001,0.144,0.0001)$, $M=200$ and $N=100000$ (i.e., $\Delta x=5E-3$ and $\Delta t=6E-6$). The state simulation on Q_T is shown on Figure 1(a),(b). We consider the initial guess $\mathbf{e}=(0.0001,0.00001,0.1,0.0011)$ and get that the identified parameters are $\mathbf{e}^\infty=(0.000017,0.000012,0.133,0.00015)$. The numerical identification is developed by considering $M=100$ and $N=1000$ or, equivalently, $\Delta x=1.0E-2$ and $\Delta t=5.\overline{9}E-4$. Moreover, we have considered the regularization parameter $\Gamma=0$. The comparison of the observed, identified and initial guess profiles are shown in Figure 1(c)–(f).

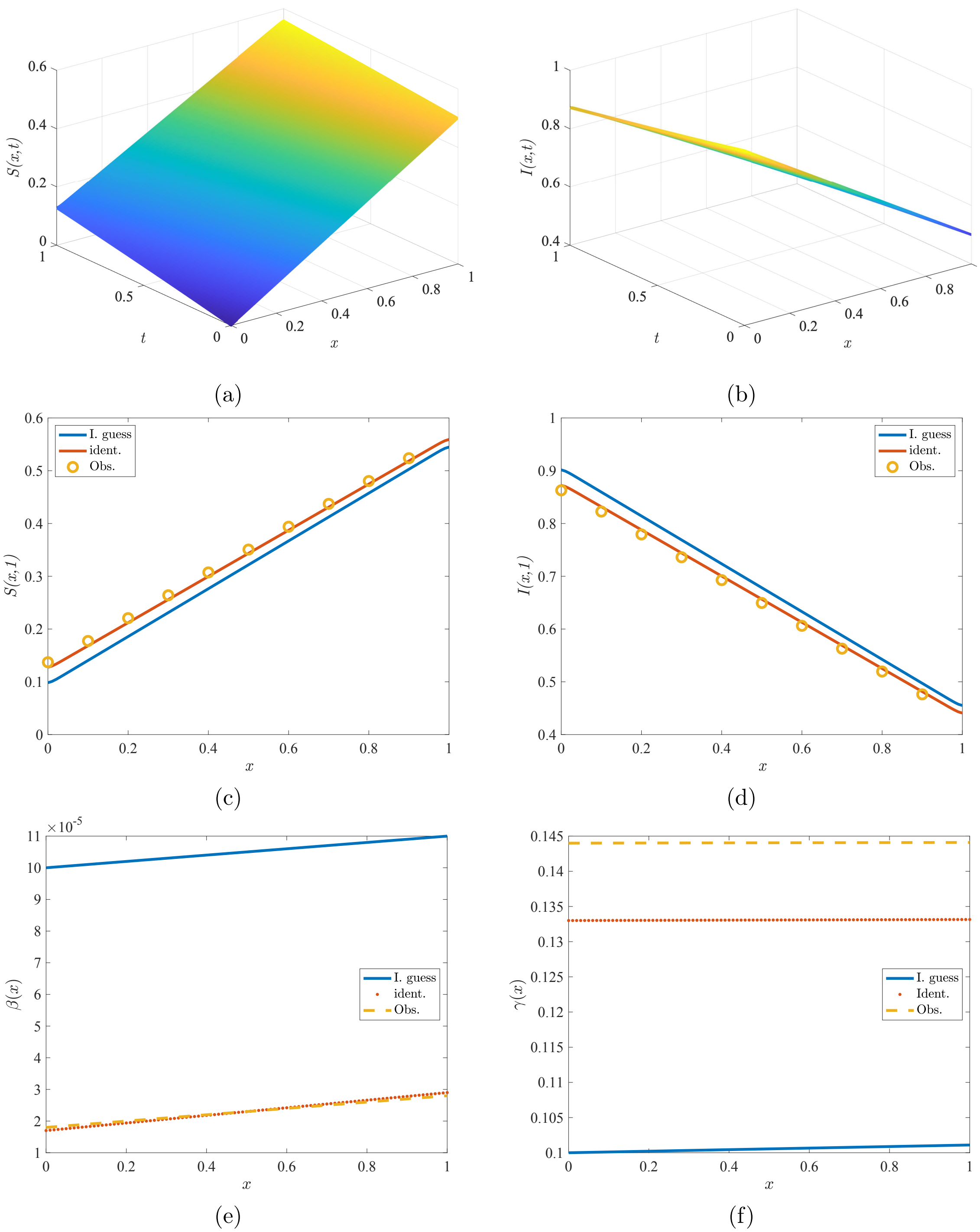

Figure 1: Results for numerical example. In (a) and (b) we show the numerical solution. In (c) and (d) we show the comparison of initial guess, observed and identified profiles at $T = 1$ for suceptibles and infective functions. In (e) and (f) we show the comparison of initial guess, observed, and identified function β and γ.

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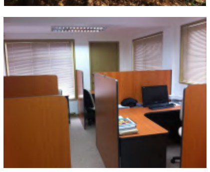

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