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Identification of a power-like reaction term in a reaction-diffusion SIS model

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Abstract

In this paper, we introduce the necessary conditions for the reaction term determination in a class of reaction-diffusion systems, based on knowledge of an approximation of the state variables at the end of the processes. The system considered is a generalization of the susceptible-infected-susceptible (SIS) model of disease transmission, assuming spatial displacement of individuals. We consider that the reaction term is defined by a power incidence function, and the coefficients are space-time-dependent functions modeling the disease and recovery rates. We introduce a formulation of the inverse problem as a constrained optimization problem for an appropriate cost functional. The main results of the paper are the existence of a minimizer for the cost functional; the definition of a first-order necessary optimality condition; the proofs of stability of the state and adjoint equations with respect to the coefficients, the power of the incidence, and the observations; and the introduction of a biological consistent numerical approximation of the optimal control problem. Moreover, we present some numerical examples of the parameter identification problem.

Keywords: power incidence function, inverse problem, parameter identification, SIS, reaction-diffusion systems

MSC Classification: 35R30 49K20 92D25 92D30 49N45

1 Introduction

The reaction-diffusion models have recently attracted significant interest for modeling disease transmission across different biological populations, as they often better capture many aspects of the processes as is documented in the recent survey articles [31, 42] (see also the books [4, 5, 8, 11, 15, 53, 66]). This is especially true when we consider the spatial movement of populations and, consequently, the diffusion of the disease and the interactions of individuals occur in the spatial domain. In the broader sense, accounting for the spatial dependence of the model variables is a better improvement than the standard compartmental models based on ordinary differential equations when a law for diffusion modelling is applied. The typical assumption is that the spatial diffusion of individuals satisfies Fick's law. However, generalizing disease models from ordinary differential equations to partial differential equations involves subtle details. For instance, the model of individual interactions is not always directly evident from measurements; the formulation of the boundary conditions, the well-posedness of the model, and the numerical approximation are also involved. Particularly, we emphasize that it is necessary to identify an appropriate model of the interaction based on disease observations.

In a pioneering work, Kermack and McKendrick introduced a model of epidemiological dynamics [48]. Initially the authors have considered that a population of N individuals is divided into three classes or compartments: susceptible, infected, and recovered; assumed that the size of the populations of each compartment changes by direct contact of infected individuals with susceptible ones or after having completed the infection period; and suppose that there is immunity after the infection period, formulate the ordinary differential equation system known as the susceptible–infected–recovered (SIR) system. Subsequently, they have modified their original proposal to consider the case of infection propagation under the assumption of immunity, obtaining the SIS mathematical model: $s = -\beta si + \gamma i$ and $i' = \beta si - \gamma i$, with $s = s(t)$ and $i = i(t)$ the populations of susceptible and infected compartments in a time t, respectively. Here, βsi models the interaction of infected and susceptible individuals by applying the mass-action law, and γi models the recovery. The coefficients β and γ are called the transmission and recovery rates, respectively. Afterwards, an extensive list of generalizations of the assumptions to get SIS have been introduced, which can be grouped into five types: nonlinear mechanisms more general than mass action [12, 29, 30, 33, 35, 45, 76]; the inclusion of spatial displacement of individuals by introducing the concept of diffusion [3, 6, 14, 26, 27, 46, 49, 50, 54, 68, 71]; the consideration of variable coefficients [3, 56, 57]; the inclusion of other type of compartments like asymptomatic, hospitalized, and quarantined individuals [68, 71]; and the spread of the epidemics attending to multi-populations [9, 34, 56, 57, 74, 75]. Particularly, in the present work we are interested in a nonlinear mechanisms identification in SIS reaction-diffusion system.

The influence spatial of displacement of the individuals have considered in a first time in the works [3, 47, 67], where the authors justified and introduced generalized models based on partial differential equations that incorporate diffusion. Moreover, from the works of Capasso and Serio [12] and Anderson and May [5], several proposals to improve the mass-action incidence mechanism model have been made [25, 37, 39, 51, 65]. We recall that the authors of [12] find that the mass-action law is imprecise and consequently is open to refinement due to their lack of precision when it is applied to model the saturated infection force for a large-scale epidemic, and in [5] it was introduced an explicit criticism of modeling with the mass-action law. More recently, [37] introduced a discussion of other factors that determine the desease dynamics not considered by the mass action, and [51] showed that classical mass action does not adequately capture the dynamics of COVID-19. Hence, in the presenet work, we are interested in the case of a particular generalization of the mass-action law interaction modeled by a power-law of the form $\beta s^q i^p$ where p and q are positive constants, which, for the first time, was introduced in [59] for ordinary differential equations models (see also [38, 40, 41, 58, 59, 62]) and recently analyzed in [69, 70, 72] in the context of reaction-diffusion systems.

In this article we consider that the disease transmission is modeled by the following reaction-diffusion system:

$$S_t - d_S \Delta S = -\beta(x,t) S^q I^p + \gamma(x,t) I, \qquad \text{in } Q_T := \Omega \times [0,T], \tag{1}$$
$$I_t - d_I \Delta I = \beta(x,t) S^q I^p - \gamma(x,t) I, \qquad \text{in } Q_T, \tag{2}$$
$$\nabla S \cdot \mathbf{n} = \nabla I \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma := \partial\Omega \times [0,T], \tag{3}$$
$$(S,I)(x,0) = (S_0, I_0)(x), \qquad \text{in } \Omega, \tag{4}$$

where the habitat $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$ is an open and bounded domain with boundary $\partial\Omega$ and outer unit normal vector field $\mathbf{n}$; the unknowns $S = S(x,t)$ and $I = I(x,t)$ are the density of susceptible and infected individuals at the position x and time t, respectively; p and q are positive constants; $\beta(x,t)$ and $\gamma(x,t)$ are the disease transmission and recovery rates, respectively; $S_0(x)$ and $I_0(x)$ are the initial conditions; and d_S and d_I are positive constants modeling the motility of susceptible and infected individuals, respectively. The Neumann boundary condition (3) means that there is no flux of individuals across the boundary of the habitat during the epidemic event. We observe that the power incidence is reduced to the mass-action incidence mechanism when $p = q = 1$, which have been researched by several authors, see for instance [24, 28, 55, 77, 79]. Additionally, we notice that the total population size in the mathematical model (1)–(4) is constant, since adding the equations (1) and (2), integrating over Ω, applying the Green's formula, and using the boundary conditions (3), we deduce that

$$\frac{d}{dt}\int_\Omega (S+I)(x,t)dx = \int_\Omega \Big(d_S \Delta S + d_I \Delta I \Big) dx = \int_{\partial\Omega} \Big(d_S \nabla S \cdot \mathbf{n} dS + d_I \nabla S \cdot \mathbf{n} dS \Big) = 0,$$

or equivalently $\int_\Omega (S+I)(x,t)dx = \int_\Omega (S_0 + I_0)(x,t)dx$ for any $t > 0$. The well-posedness of strong solutions of (1)–(4) is troublesome because, specifically for the case $p, q \in (0,1)$, since the standard methodologies lack of direct applicability, for instance, the reaction term is not Lipschitz. Recently, [72] introduced the framework and extensively established the analysis of the well-posedness and the asymptotic behavior of strong solutions to (1)–(4). Particularly, the authors of [72] consider that p, q are positive constants, β, γ are positive Hölder continuous functions, and the initial conditions are positive continuous functions (see Theorem 1 for details).

The aim of this paper is to analyze the identification of the reaction coefficients and the exponents of the power-law from measurements of susceptible and infected populations at some fixed time. To provide a more precise formulation of the inverse problem, we begin by defining appropriate notation and a formal framework. In the context of the previous notation the identification problem is defined as follows: Given a observation of the susceptible and infected populations at time $T > 0$, denoted by S^{obs} and I^{obs} defined from Ω to $\mathbb{R}^+$, determine β, γ, p and q such that $(S, I)(\cdot, T)$, the solution of (1)–(4), is "as close as" to (S^{obs}, I^{obs}). This identification problem can be recast as an optimal control problem as follows. Let us beginning by considering the cost function J, the reduced cost function $\mathcal{J}$, and the admisible set U_{ad} defined as follows:

$$J(S,I) = \frac{1}{2}\left\|(S,I)(\cdot,T) - (S^{obs}, I^{obs})\right\|^2_{L^2(\Omega)^2} + \frac{\Gamma}{2}\int_0^T \|\nabla(\beta,\gamma)(\cdot,t)\|^2_{L^2(\Omega)^2}\,dt, \tag{5}$$

$$\mathcal{J}(\beta,\gamma,p,q) = J(S_{(\beta,\gamma,p,q)}, I_{(\beta,\gamma,p,q)}), \tag{6}$$

$$\begin{aligned} U_{ad} = \Big\{ &(\beta,\gamma,p,q) \in C^{\alpha,\alpha/2}(Q_T)^2 \times [0,\infty)^2 \ : \ \nabla\beta, \nabla\gamma \in L^2(Q_T), \\ &(\beta,\gamma)(x,t) \in [\underline{\beta},\overline{\beta}] \times [\underline{\gamma},\overline{\gamma}] \subset \mathbb{R}^2_+ \text{ on } Q_T \Big\} \cap (H^{[\![d/2]\!]+1}(\Omega)^2 \times \mathbb{R}^2_+), \end{aligned} \tag{7}$$

where $\Gamma \geq 0$ is a positive constant. The notations $C^{\alpha,\alpha/2}(Q_T)$, $C(\overline{\Omega})$, $L^2(\Omega)$ and $H^{[\![d/2]\!]+1}(\Omega)$ are the standard notation for Hölder, continuous, Lebesgue, and Sobolev space of functions, respectively [1, 32]; and $(S_{(\beta,\gamma,p,q)}, I_{(\beta,\gamma,p,q)})$ denotes the solution of the reaction-diffusion system of (1)–(4) for β, γ, p, and q. Hence, the identification problem is formulated as the optimal control problem:

$$\left.\begin{array}{l} \text{Find } (\overline{\beta},\overline{\gamma},\overline{p},\overline{q}) \in U_{ad} \text{ such that} \\ \mathcal{J}(\overline{\beta},\overline{\gamma},\overline{p},\overline{q}) = \displaystyle\inf_{(\beta,\gamma,p,q)\in U_{ad}} \mathcal{J}(\beta,\gamma,p,q), \\ \text{subject to } (S_{(\beta,\gamma,p,q)}, I_{(\beta,\gamma,p,q)}) \text{ solution of (1)–(4).} \end{array}\right\} \tag{8}$$

The particular case of the optimal control problem (8) with p, q fixed and β and γ independents of t is analized in [19]. Moreover, various studies have explored analytical approaches for other optimal control in reaction-diffusion systems [7, 13, 17–23, 78, 80]. Regarding the identification of reaction coefficients, Xiang and Liu [80] initially analyzed the one-dimensional case ($d = 1$) by assuming the incidence function $SI/(S+I)$ rather than mass-action kinetics. This was later extended to $d \geq 1$ in [17].

The main contributions of the paper are the following: the existence of solutions of the optimal control problem (8); the definition of an adjoint system; the introduction of a first order optimality condition; the continuous dependence of the state equation solutions with respect to the coefficients and the power exponentes; and the continuous dependence of the adjoint equation solutions with respect to the coefficients, the power exponentes, and the observation functions. In a broad sense, the existence of solutions of the optimal control problem is developed considering the minimization sequences methodology, the first order result is deduced by introducing the sensitivity equation, the continuos dependence results are proved by application of the energy estimates, and the introduction of a consistent numerical approximation of the control problem by the discretize-then-optimize methodology. In addition we present some numerical simulations for the particular case of the optimal control problem known as the parameter identification problem, where we consider that the coefficients are parameterized by a finite number of parameters.

2 Analytical results of the optimal control problem

2.1 Assumptions and well-posedness of state equations

The analysis of well-posedness of the initial boundary problem (1)–(4) is historically related to the contributions of Alikakos [2] and Masuda [64]. In [2] the author analyze the case of $\beta = 1$, $\gamma = 0$, $p \in [1, (n+1)/n)$ and $q = 1$ and in [64] the author generalize the result of [2] to the case $p > 0$. Subsequently, [44, 52, 73] obtains results for similar results of global existence of classical solutions with the reaction terms given by $-S^q I^p + \lambda S^{\overline{q}} I^{\overline{p}}$ and $S^q I^p - S^{\overline{q}} I^{\overline{p}}$ with $p, q, \overline{p}, \overline{q} \in [1, \infty)$ and $\lambda \in [0, 1]$. The analysis of the case $p, q, \overline{p}, \overline{q} \in (0, 1)$ is more delicate, since, the products $S^q I^p$ and $S^{\overline{q}} I^{\overline{p}}$ are not Lipschitz, and the existing theories of the dynamical systems cannot be applied directly, we refer to the extensively discussion developed in [33, 44]. Afterwards, and recently, in [72] the authors have obtained the global existence of classical solutions when $p, q, \overline{p}, \overline{q} \in [0, \infty)$. Moreover the authors of [72] have analized (1)–(4) by assuming that $(\beta, \gamma, p, p) \in U_{ad}$ and the initial conditions are positive continuous functions.

In this paper we adapte the assumptions introduced in [72] and define the following hypothesis

(H0) The open bounded convex set Ω is such that $\partial\Omega$ is C^1.
(H1) The functions constants p and q are positive, and the functions β and γ are positive and bounded Hölder functions, i.e.

$$p, q \in [0, \infty), \beta, \gamma \in C^{\alpha, \alpha/2}(Q_T), \quad (\beta, \gamma)(x, t) \in [\underline{\beta}, \overline{\beta}] \times [\underline{\gamma}, \overline{\gamma}] \subset \mathbb{R}^2_+,$$

where $\underline{\beta}$, $\overline{\beta}$, $\underline{\gamma}$, and $\overline{\gamma}$ are some strictly positive constants.
(H2) The initial conditions S_0 and I_0 belong to $C(\overline{\Omega})$ with $S_0(x) \geq 0$ and $I_0(x) \geq 0$ on $\overline{\Omega}$ and satisfying the relations: $I_0(x) > 0$ on an open subset of $\overline{\Omega}$, $S_0(x) > 0$ on $\overline{\Omega}$ for $q \in (0, 1)$, and $I_0(x) > 0$ on $\overline{\Omega}$ for $p \in (0, 1)$.
(H3) The observation functions S^{obs} and I^{obs} are belong to $C(\overline{\Omega})$.

The biological interpretation of the hypotheses is discussed in [72] and the the role in the mathemathical analysis is the following: (H0) is necessary to get the appropriate compactness used to prove the existence of solutions for the inverse problem; (H1)-(H2) are necessary to get the well-posedness and strictly positive behavior of the solution for the direct problem; and (H3) is necessary to get the stability result and existence of strong solutions of the adjoint problem.

Theorem 1 *[72, theorem 2.3] Assume that the hypothesis (H0)-(H2) are satisfied. Then, the initial boundary value problem for a reaction-diffusion system (1)–(4) admits a unique positive classical solution (S, I), such that S and I are belong to $C^{2+\alpha,1+\alpha/2}(\overline{Q}_T)$. Furthermore, the relations*

$$\|S(\cdot,t)\|_{L^\infty(\Omega)}, \|I(\cdot,t)\|_{L^\infty(\Omega)} \leq C, \quad \forall t \geq 0, \tag{9}$$

$$\limsup_{t\to\infty} \|S(\cdot,t)\|_{L^\infty(\Omega)}, \limsup_{t\to\infty} \|I(\cdot,t)\|_{L^\infty(\Omega)} \leq C, \tag{10}$$

are satisfied for all $t \geq 0$, for some a positive generic constants C, depending only on the initial data.

2.2 Existence of solutions of the optimal control problem.

Theorem 2 *Assume that the assumptions (H0)-(H3) are satisfied. Then, there exists at least one solution of (8).*

Proof The proof is based on the standard technique of minimizing sequence. We begin, by observing that $(\beta(x,t), \gamma(x,t), p, q) = (\underline{\beta} + \overline{\beta}, \underline{\gamma} + \overline{\gamma}, 2, 2)/2$ is an admissible control, implying that the admissible sete U_{ad} is not empty. Moreover, by Theorem 1 we deduce that $\mathcal{J}$ is bounded, and we can consider that $\{(\beta_n, \gamma_n, p_n, q_n)\} \subset \mathcal{M} \subset U_{ad}(\Omega)$ is a minimizing sequence of $\mathcal{J}$ with $\mathcal{M}$ a bounded and closed set. From Theorem 6[32, pp. 270] and Theorem 1.3.1[1, pp. 11] we deduce the compact embedding $H^{[\![d/2]\!]+1}(\Omega) \subset C^\alpha(\Omega)$ for $\alpha \in]0, 1/2]$ for Ω bounded and convex (see [17] for details). It implies that $\{(\beta_n, \gamma_n)(\cdot, t)\}$ is bounded in the strong topology of $C^\alpha(\overline{\Omega})^2$ for all $\alpha \in]0, 1/2]$, equivalently, there exists a positive constant C (independent of β, γ and n) such that

$$\|\beta_n(\cdot,t)\|_{C^\alpha(\overline{\Omega})} + \|\gamma_n(\cdot,t)\|_{C^\alpha(\overline{\Omega})} \leq C\Big(\|\beta_n(\cdot,t)\|_{H^{[\![d/2]\!]+1}(\Omega)} + \|\gamma_n(\cdot,t)\|_{H^{[\![d/2]\!]+1}(\Omega)}\Big),$$

for all $\alpha \in]0, 1/2]$ and $t \geq 0$. Notice that the right hand is bounded by the definition of $\mathcal{M}$. Let S_n and I_n the corresponding solution of (1)-(4) with $(\beta_n, \gamma_n, p_n, q_n)$ instead of (β, γ, p, q). Moreover, by Theorem 1, we follow that $\{(S_n, I_n)\}$ is a bounded sequence in the strong topology of $C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T)^2$ for all $\alpha \in]0, 1/2]$. Then, the boundedness of the minimizing sequence and the corresponding sequence $\{(S_n, I_n)\}$, implies that there exist

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

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

$$\beta_n \to \overline{\beta}, \quad \gamma_n \to \overline{\gamma} \quad \text{uniformly on } C^{\alpha,\alpha/2}(\overline{Q}_T), \quad (p_n, q_n) \to (\overline{p}, \overline{q}), \tag{11}$$

$$S_n \to \overline{S}, \quad I_n \to \overline{I} \quad \text{uniformly on } C^{\alpha,\frac{\alpha}{2}}(\overline{Q}_T) \cap C^{2+\alpha,1+\frac{\alpha}{2}}(\overline{Q}_T). \tag{12}$$

Moreover, we can deduce that $(\overline{S}, \overline{I})$ is the solution of the initial boundary value problem of (1)-(4) corresponding to the coefficients $(\overline{\beta}, \overline{\gamma}, \overline{p}, \overline{q})$. Hence, by Lebesgue's dominated convergence theorem, the weak lower-semicontinuity of the L^2 norm, and the definition of the minimizing sequence, we have that

$$\mathcal{J}(\overline{\beta}, \overline{\gamma}, \overline{p}, \overline{q}) \leq \lim_{n\to\infty} \mathcal{J}(\beta_n, \gamma_n, p_n, q_n) = \inf_{(\beta,\gamma,p,q)\in U_{ad}} \mathcal{J}(\beta, \gamma, p, q). \tag{13}$$

Then, $(\overline{\beta}, \overline{\gamma}, \overline{p}, \overline{q})$ is a solution of (8). □

2.3 Continuous adjoint state.

Let us define (w_1, w_2) as the solution of the following backward boundary value problem

$$(w_1)_t + d_S \Delta w_1 = q\bar{\beta}(x,t)\bar{S}^{q-1}\bar{I}^p(w_1 - w_2), \qquad \text{in } Q_T, \tag{14}$$
$$(w_2)_t + d_I \Delta w_2 = (p\bar{\beta}(x,t)\bar{S}^q\bar{I}^{p-1} - \bar{\gamma}(x,t))(w_1 - w_2), \qquad \text{in } Q_T, \tag{15}$$
$$\nabla w_1 \cdot \mathbf{n} = \nabla w_2 \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma, \tag{16}$$
$$(w_1, w_2)(x,T) = \Big(\bar{S}(x,T) - S^{obs}(x), \bar{I}(x,T) - I^{obs}(x)\Big), \qquad \text{in } \Omega, \tag{17}$$

where $(\bar{\beta}, \bar{\gamma}, \bar{p}, \bar{q}) \in U_{ad}$ is a solution of the optimal control problem (8) and $(\bar{S}, \bar{I})$ is the corresponding solution of (1)-(4) with $(\bar{\beta}, \bar{\gamma}, \bar{p}, \bar{q})$ instead of (β, γ, p, q).

Theorem 3 *Assume that the assumptions (H0)-(H3) are satisfied. Then, The adjoint system to (1)-(4) is given by the system (14)-(17). Moreover, the solution (14)-(17) is bounded in $L^\infty(0,t;H^2(\Omega))$ for almost all time t in $]0,T]$. In particular the solution (14)-(17) is bounded in $L^\infty(0,t;L^\infty(\Omega))$ for almost all time t in $]0,T]$.*

Proof The proof of the fact that (14)-(17) is the adjoint system of (1)-(4) can be developed by the standard arguments of optimal control theory, see for instance [36]. Now, in order to get the other properties of the result we apply the standard energy estimates methodology. For $L^\infty(0,t;H^2(\Omega))$ estimates, we set $t \in]0,T]$ and claim that

$$\|(w_1, w_2)(\cdot,t)\|^2_{L^2(\Omega)^2} \le C, \qquad \|(\nabla w_1, \nabla w_2)(\cdot,t)\|_{L^2(\Omega)^2} \le C, \tag{18}$$
$$\|(\Delta w_1, \Delta w_2)(\cdot,t)\|_{L^2(\Omega)^2} \le C, \qquad \|w_1(\cdot,t)\|_{L^\infty(\Omega)} \le C, \qquad \|w_2(\cdot,t)\|_{L^\infty(\Omega)} \le C, \tag{19}$$

for a positive generic constant C. The rest of the proof is dedicated to prove the claims (18)-(19). We begin by defining the change of variable $\tau = T - t$ for $t \in [0,T]$. Moreover, consider the notation $w_1^*(\cdot,\tau) = w_1(\cdot, T-\tau)$, $w_2^*(\cdot,\tau) = w_2(\cdot,T-\tau)$, $S^*(\cdot,\tau) = \bar{S}(\cdot,T-\tau)$, and $I^*(\cdot,\tau) = \bar{I}(\cdot,T-\tau)$. Then, the adjoint system (14)-(17) is equivalent to the system

$$(w_1^*)_t - d_S\Delta w_1^* = -q\bar{\beta}(x,T-t)S^{*q-1}I^{*p}(w_1^* - w_2^*), \qquad \text{in } Q_T, \tag{20}$$
$$(w_2)_t - d_I\Delta w_2 = -(p\bar{\beta}(x,T-t)S^{*q}I^{*p-1} - \bar{\gamma}(x,t-T))(w_1^* - w_2^*), \qquad \text{in } Q_T, \tag{21}$$
$$\nabla w_1^* \cdot \mathbf{n} = \nabla w_2^* \cdot \mathbf{n} = 0, \qquad \text{on } \Gamma, \tag{22}$$
$$(w_1, w_2)(x,0) = \Big(\bar{S}(x,T) - S^{obs}(x), \bar{I}(x,T) - I^{obs}(x)\Big), \qquad \text{in } \Omega, \tag{23}$$

Now, we proceed to get the estimates.

To prove (18), we proceed as follows. We multiply (20) by w_1^* and (21) by w_2^*, integrate on Ω and use the Green formula, add the resulting equalities, apply the Cauchy inequality, rearranging some terms, and applying the Theorem 1, we can deduce the following estimate

$$\frac{1}{2}\frac{d}{d\tau}\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} + \|(\nabla w_1^*, \nabla w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \le C\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \tag{24}$$

Then, by the Gronwall inequality, we obtain

$$\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \le e^{2CT}\|(w_1^*, w_2^*)(\cdot,0)\|^2_{L^2(\Omega)^2}, \tag{25}$$

which implies the first estimation in (18). Moreover, from (24) and (25), we have that

$$\|(\nabla w_1^*, \nabla w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \le C\, e^{2CT}\, \|(w_1^*, w_2^*)(\cdot,0)\|^2_{L^2(\Omega)^2}$$

and by the definition of the norm of $H_0^1(\Omega)$ we deduce the second estimate in (18).

On the other hand, using the fact that

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

for $i = 1, 2$. We note that, multiplying (20) by Δw_1, multiplying (21) by Δw_2, integrating on Ω, and adding the results, we deduce that

$$\begin{aligned}&\frac{1}{2}\frac{d}{d\tau}\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{H_0^1(\Omega)^2} + \|(\Delta w_1^*, \Delta w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2}\\ &\quad\le C\Big[\epsilon\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} + \frac{1}{4\epsilon}\|(\Delta w_1^*, \Delta w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2}\Big],\end{aligned}$$

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

$$\frac{1}{2}\frac{d}{d\tau}\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{H_0^1(\Omega)^2} + \frac{4\epsilon - C}{4\epsilon}\|(\Delta w_1^*, \Delta w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \le \epsilon C\|(w_1^*, w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2}.$$

Now, by selecting $\epsilon > C/4$ and using the estimate (25) we get

$$\|(\Delta w_1^*, \Delta w_2^*)(\cdot,\tau)\|^2_{L^2(\Omega)^2} \le \frac{4\epsilon^2 C}{4\epsilon - C} e^{2CT}\|(w_1^*, w_2^*)(\cdot,0)\|^2_{L^2(\Omega)^2},$$

which implies the first inequality in (19). From the previous estimates, we notice that the norms of w_1 and w_2 are bounded in the norm of $H^2(\Omega)$. Thus, by the standard embedding theorem of $H^2(\Omega) \subset L^\infty(\Omega)$, we easily deduce the last two estimates in (19) and conclude the proof of the theorem. □

2.4 First order optimality condition

Theorem 4 *Assume that the assumptions (H0)-(H3) are satisfied and consider that $(\bar{S}, \bar{I})$ $(\bar{w}_1, \bar{w}_2)$ are the solutions of the state and adjoint systems for the optimal control solution $(\bar{\beta}, \bar{\gamma}, \bar{p}, \bar{q})$. Then, the following inequality*

$$\begin{aligned}&\int_{Q_T}\Big\{-\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\Big[\ln(\bar{S})(\hat{q}-\bar{q}) + \ln(\bar{I})(\hat{p}-\bar{p})\Big]\\ &\qquad + \Big[(\hat{\beta}(x,t)-\bar{\beta}(x,t))\bar{S}^{\bar{q}}\bar{I}^{\bar{p}} - (\hat{\gamma}(x,t)-\bar{\gamma}(x,t))\bar{I}\Big](w_2 - w_1)\Big\}dxdt\\ &\quad + \Gamma\int_{Q_T}\Big[\nabla\overline{\beta}\cdot\nabla(\hat{\beta}-\overline{\beta}) + \nabla\overline{\gamma}\cdot\nabla(\hat{\gamma}-\overline{\gamma})\Big]dxdt \ge 0, \quad \forall(\hat{\beta},\hat{\gamma}) \in U_{ad}(\Omega),\end{aligned} \tag{26}$$

is satisfied.

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

$$(\beta^\varepsilon, \gamma^\varepsilon, p^\varepsilon, q^\varepsilon) = (1-\varepsilon)(\bar{\beta}, \bar{\gamma}, \bar{p}, \bar{q}) + \varepsilon(\hat{\beta}, \hat{\gamma}, \hat{p}, \hat{q}) \in U_{ad}, \quad \varepsilon \in (0,1),$$

$$\mathcal{J}_\varepsilon = \frac{1}{2}\|(S^\varepsilon, I^\varepsilon)(\cdot,T) - (S^{obs}, I^{obs})\|^2_{L^2(\Omega)^2} + \frac{\Gamma}{2}\int_0^T \|(\nabla\beta^\varepsilon, \nabla\gamma^\varepsilon)(\cdot,t)\|^2_{L^2(Q_T)^2}dt,$$

where $(S^\varepsilon, I^\varepsilon)$ is the solution of (1)-(4) with $(\beta^\varepsilon, \gamma^\varepsilon, p^\varepsilon, q^\varepsilon)$ instead of (β, γ, p, q) and $\mathcal{J}_\varepsilon = J(\beta^\varepsilon, \gamma^\varepsilon, p^\varepsilon, q^\varepsilon)$. Now, using the hypothesis that $(\bar{\beta}, \bar{\gamma}, \bar{p}, \bar{q})$ is an optimal solution of (8) and taking the Fréchet derivative of J_ε, we have that

$$\frac{d\mathcal{J}_\varepsilon}{d\varepsilon}\Big|_{\varepsilon=0} = \int_\Omega\left(\Big|S^\varepsilon(x,T) - S^{obs}(x)\Big|\frac{\partial S^\varepsilon}{\partial\varepsilon}\Big|_{\varepsilon=0} + \Big|I^\varepsilon(x,T) - I^{obs}(x)\Big|\frac{\partial I^\varepsilon}{\partial\varepsilon}\Big|_{\varepsilon=0}\right)dx$$

$$+\Gamma\int_{Q_T}\left[\nabla\bar{\beta}\nabla\left(\hat{\beta}-\bar{\beta}\right)+\nabla\bar{\gamma}\nabla\left(\hat{\gamma}-\bar{\gamma}\right)\right]dxdt\geq 0, \tag{27}$$

where $\partial_\varepsilon S^\varepsilon$ and $\partial_\varepsilon I^\varepsilon$ for $\varepsilon=0$ are calculated by analyzing the sensitivities of solutions for (1)-(4) with respect to perturbations of (β,γ,p,q).

From the definition of $(S^\varepsilon, I^\varepsilon)$ and $(\bar{S},\bar{I})$ we have that

$$(S^\varepsilon)_t - d_S\Delta S^\varepsilon = -\beta^\varepsilon(x,t)(S^\varepsilon)^{q^\varepsilon}(I^\varepsilon)^{p^\varepsilon}+\gamma^\varepsilon(x,t)I^\varepsilon, \quad \text{in } Q_T, \tag{28}$$

$$(I^\varepsilon)_t - d_I\Delta I^\varepsilon = \beta^\varepsilon(x,t)(S^\varepsilon)^{q^\varepsilon}(I^\varepsilon)^{p^\varepsilon}-\gamma^\varepsilon(x,t)I^\varepsilon, \quad \text{in } Q_T, \tag{29}$$

$$\nabla S^\varepsilon\cdot\mathbf{n}=\nabla I^\varepsilon\cdot\mathbf{n}=0, \quad \text{on } \Gamma, \tag{30}$$

$$(S^\varepsilon, I^\varepsilon)(x,0)=(S_0,I_0)(\mathbf{x}), \quad \text{in } \Omega, \tag{31}$$

and

$$(\bar{S})_t - d_S\Delta\bar{S} = -\bar{\beta}(x,t)(\bar{S})^{\bar{p}}(\bar{I})^{\bar{q}}+\bar{\gamma}(x,t)\bar{I}, \quad \text{in } Q_T, \tag{32}$$

$$(\bar{I})_t - d_I\Delta\bar{I} = \bar{\beta}(x,t)(\bar{S})^{\bar{p}}(\bar{I})^{\bar{q}}-\bar{\gamma}(x,t)\bar{I}, \quad \text{in } Q_T, \tag{33}$$

$$\nabla\bar{S}\cdot\mathbf{n}=\nabla\bar{I}\cdot\mathbf{n}=0, \quad \text{on } \Gamma, \tag{34}$$

$$(\bar{S},\bar{I})(x,0)=(S_0,I_0)(x), \quad \text{in } \Omega. \tag{35}$$

Let us consider the notation $(z_1^\varepsilon, z_2^\varepsilon)=\varepsilon^{-1}\left(S^\varepsilon-\bar{S}, I^\varepsilon-\bar{I}\right)$ and observe that

$$\begin{aligned}
G^\varepsilon &= -\frac{1}{\varepsilon}\Big[\beta^\varepsilon(x,t)(S^\varepsilon)^{q^\varepsilon}(I^\varepsilon)^{p^\varepsilon}-\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\Big]+\frac{1}{\varepsilon}\Big[\gamma^\varepsilon(x,t)I^\varepsilon-\bar{\gamma}(x,t)\bar{I}\Big]\\
&= -\beta^\varepsilon(x,t)\frac{\Big[(S^\varepsilon)^{q^\varepsilon}-(\bar{S})^{q^\varepsilon}\Big]}{S^\varepsilon-\bar{S}}(I^\varepsilon)^{p^\varepsilon}z_1^\varepsilon-\beta^\varepsilon(x,t)(\bar{S})^{q^\varepsilon}\frac{\Big[(I^\varepsilon)^{p^\varepsilon}-(\bar{I})^{p^\varepsilon}\Big]}{I^\varepsilon-\bar{I}}z_2^\varepsilon\\
&\quad -\beta^\varepsilon(x,t)\frac{\Big[(\bar{S})^{q^\varepsilon}-(\bar{S})^{q^\varepsilon}\Big]}{q^\varepsilon-\bar{q}}(\bar{I})^{p^\varepsilon}(\hat{q}-\bar{q})-\beta^\varepsilon(x,t)(\bar{S})^{q^\varepsilon}\frac{\Big[(\bar{I})^{p^\varepsilon}-(\bar{I})^{p^\varepsilon}\Big]}{p^\varepsilon-\bar{p}}(\hat{p}-\bar{p})\\
&\quad -(\hat{\beta}(x,t)-\bar{\beta}(x,t))(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}+\gamma^\varepsilon(x,t)z_2^\varepsilon+(\hat{\gamma}(x,t)-\bar{\gamma}(x,t))\bar{I},
\end{aligned}$$

Then, subtracting the system (32)-(35) from (28)-(31), and dividing by ε, we deduce the following system

$$(z_1^\varepsilon)_t - d_S\Delta z_1^\varepsilon = G^\varepsilon, \quad \text{in } Q_T, \tag{36}$$

$$(z_2^\varepsilon)_t - d_I\Delta z_2^\varepsilon = -G^\varepsilon, \quad \text{in } Q_T, \tag{37}$$

$$\nabla z_1^\varepsilon\cdot\mathbf{n}=\nabla z_2^\varepsilon\cdot\mathbf{n}=0, \quad \text{on } \Gamma, \tag{38}$$

$$(z_1^\varepsilon, z_2^\varepsilon)(x,0)=0, \quad \text{in } \Omega. \tag{39}$$

Denoting by (z_1,z_2) the limit of $(z_1^\varepsilon, z_2^\varepsilon)$ when $\varepsilon\to 0$, from (36)-(39), we deduce that

$$(z_1)_t - d_S\Delta z_1 = G, \quad \text{in } Q_T, \tag{40}$$

$$(z_2)_t - d_I\Delta z_2 = -G, \quad \text{in } Q_T, \tag{41}$$

$$\nabla z_1\cdot\mathbf{n}=\nabla z_2\cdot\mathbf{n}=0, \quad \text{on } \Gamma, \tag{42}$$

$$(z_1,z_2)(x,0)=0, \quad \text{in } \Omega, \tag{43}$$

where

$$\begin{aligned}
G &= -\bar{q}\bar{\beta}(x,t)(\bar{S})^{\bar{q}-1}(\bar{I})^{\bar{p}}z_1-\Big[\bar{p}\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}-1}-\bar{\gamma}(x,t)\Big]z_2-\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\ln(\bar{S})(\hat{q}-\bar{q})\\
&\quad -\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\ln(\bar{I})(\hat{p}-\bar{p})-(\hat{\beta}(x,t)-\bar{\beta}(x,t))(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}+(\hat{\gamma}(x,t)-\bar{\gamma}(x,t))\bar{I}.
\end{aligned}$$

Thus, in (27) we have that

$$\frac{dJ_\varepsilon}{d\varepsilon}\Big|_{\varepsilon=0}=\int_\Omega\left(\left|S^\varepsilon(x,T)-S^{obs}\right|z_1(x,T)+\left|I^\varepsilon(x,T)-I^{obs}\right|z_2(x,T)\right)dx$$

$$+\Gamma\int_{Q_T}\left[\nabla\bar{\beta}\nabla\left(\hat{\beta}-\bar{\beta}\right)+\nabla\bar{\gamma}\nabla\left(\hat{\gamma}-\bar{\gamma}\right)\right]dxdt\geq 0, \tag{44}$$

where (z_1, z_2) is the solution of (40)-(43).

On the other hand, from (14)-(17) and (40)-(41), we deduce that

$$\begin{aligned}\frac{\partial}{\partial t}(w_1z_1+w_2z_2) &= w_1\Delta z_1+w_2\Delta z_2-z_1\Delta w_1-z_2\Delta w_2\\ &-\bar{\beta}(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\Big[\ln(\bar{S})(\hat{q}-\bar{q})+\ln(\bar{I})(\hat{p}-\bar{p})\Big]+\Big[(\hat{\beta}-\bar{\beta})\bar{S}^{\bar{q}}\bar{I}^{\bar{p}}-(\hat{\gamma}-\bar{\gamma})\bar{I}\Big](w_2-w_1).\end{aligned}$$

Then, we deduce the following identity

$$\begin{aligned}&\int_\Omega\Big(\Big|\bar{S}(x,T)-S^{obs}(x)\Big|z_1(x,T)+\Big|\bar{I}(x,T)-I^{obs}(x)\Big|z_2(x,T)\Big)dx\\ &=\int_\Omega\Big(w_1(x,T)z_1(x,T)+w_2(x,T)z_2(x,T)\Big)dx=\int_{Q_T}\frac{\partial}{\partial t}(w_1z_1+w_2z_2)dxdt\\ &=\int_{Q_T}\Big\{-\bar{\beta}(x,t)(\bar{S})^{\bar{q}}(\bar{I})^{\bar{p}}\Big[\ln(\bar{S})(\hat{q}-\bar{q})+\ln(\bar{I})(\hat{p}-\bar{p})\Big]\\ &\qquad+\Big[(\hat{\beta}(x,t)-\bar{\beta}(x,t))\bar{S}^{\bar{q}}\bar{I}^{\bar{p}}-(\hat{\gamma}(x,t)-\bar{\gamma}(x,t))\bar{I}\Big](w_2-w_1)\Big\}dxdt\end{aligned} \tag{45}$$

Hence, we can conclude the proof of (26) by replacing (45) in the first term of (44). □

2.5 Continuos dependence results

Theorem 5 *Assume that the assumptions (H0)-(H3) are satisfied. The mapping* $(\beta,\gamma,p,q)\mapsto(S,I)$ *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* $]0,T]$.

Proof Let us consider the set of functions $\{S,I\}$ and $\{\hat{S},\hat{I}\}$ as solutions to the direct problem (1)-(4) and with data $\{\beta,\gamma,p,q\}$ and $\{\hat{\beta},\hat{\gamma},\hat{p},\hat{q}\}$, respectively. Then, we can prove that there exist the positive constant C such that the inequality

$$\|(\hat{S}-S,\hat{I}-I)(\cdot,t)\|^2_{L^2(\Omega)^2}\leq C\Big[\|(\hat{\beta}-\beta,\hat{\gamma}-\gamma)(\cdot,t)\|^2_{L^2(\Omega)^2}+|\hat{p}-p|+|\hat{q}-q|\Big] \tag{46}$$

holds for any $t\in[0,T]$. We begin by considering the notation δZ defined by $\delta Z=\hat{Z}-Z$. Then, from an algebraic manipulation of the corresponding systems for for (S,I) and $(\hat{S},\hat{S})$ we deduce that $(\delta S,\delta I)$ satisfy the initial boundary value problem

$$(\delta S)_t-d_S\Delta(\delta S)=\delta F, \quad \text{in } Q_T, \tag{47}$$

$$(\delta I)_t-d_I\Delta(\delta I)=-\delta F, \quad \text{in } Q_T, \tag{48}$$

$$\nabla(\delta S)\cdot\mathbf{n}=\nabla(\delta I)\cdot\mathbf{n}=0, \quad \text{on } \Gamma, \tag{49}$$

$$(\delta S,\delta I)(x,0)=0, \quad \text{in } \Omega, \tag{50}$$

where

$$\begin{aligned}\delta F &= -\hat{\beta}(x,t)(\hat{S}^{\hat{q}}-S^{\hat{q}})\hat{I}^{\hat{p}}-\hat{\beta}(x,t)\hat{S}^{\hat{q}}(\hat{I}^{\hat{p}}-I^{\hat{p}})-\delta\beta(x,t)S^{\hat{q}}I^{\hat{p}}-\beta(x,t)(S^{\hat{q}}-S^q)I^{\hat{p}}\\ &-\beta(x,t)S^q(\hat{I}^{\hat{p}}-I^p)+\gamma(x,t)\delta I+\delta\gamma(x,t)\hat{I}\\ &=-\hat{q}\hat{\beta}(x,t)\left[\int_S^{\hat{S}}u^{\hat{q}-1}du\right]\hat{I}^{\hat{p}}-\hat{p}\hat{\beta}(x,t)\hat{S}^{\hat{q}}\left[\int_I^{\hat{I}}u^{\hat{p}-1}du\right]-\delta\beta(x,t)S^{\hat{q}}I^{\hat{p}}\end{aligned}$$

$$- \beta(x,t)\ln(S)\left[\int_q^{\hat{q}} S^u du\right] I^{\hat{p}} - \beta(x,t)S^q\ln(I)\left[\int_p^{\hat{p}} I^u du\right] + \gamma(x,t)\delta I + \delta\gamma(x,t)\hat{I}.$$

To prove (46), we test the equations (47) and (48) by δS and δI, respectively. Then, adding the results, integrating on Ω, applying the Cauchy-Schwarz inequality, and Theorem 1, we get

$$\frac{1}{2}\frac{d}{dt}\|(\delta S,\delta I)(\cdot,t)\|^2_{L^2(\Omega)^2} + d_S\|\nabla(\delta S)(\cdot,t)\|^2_{L^2(\Omega)} + d_I\|\nabla(\delta I)(\cdot,t)\|^2_{L^2(\Omega)}$$
$$\leq C\Big[\|(\delta S,\delta I)(\cdot,t)\|^2_{L^2(\Omega)^2} + \|(\hat{\beta}-\beta,\hat{\gamma}-\gamma)(\cdot,t)\|^2_{L^2(\Omega)^2} + |\hat{p}-p| + |\hat{q}-q|\Big] \tag{51}$$

Then, using the Gronwall inequality and (50), we deduce (46). □

Theorem 6 *Assume that the assumptions (H0)-(H3) are satisfied. The mapping* $(\beta,\gamma,p,q,S^{obs},I^{obs}) \mapsto (w_1,w_2)$ *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* $]0,T]$.

Proof By similar arguments to the proof of the item (iv) we prove that the inequality

$$\|(\hat{w}_1-w_1,\hat{w}_2-w_2)(\cdot,t)\|^2_{L^2(\Omega)^2}$$
$$\leq C\Big(\|(\hat{\beta}-\beta,\hat{\gamma}-\gamma)(\cdot,t)\|^2_{L^2(\Omega)} + |\hat{p}-p| + |\hat{q}-q| + \|(\hat{S}^{obs}-S^{obs},\hat{I}^{obs}-I^{obs})\|^2_{L^2(\Omega)^2}\Big),$$

holds for any $t\in[0,T]$, which implies the result of the item. □

2.6 Comments on the uniqueness of the control problem

It is well known, broadly speaking, the inverse problem suffers from ill-posedness regarding uniqueness. A precise case of non–uniqueness for constant endemic equilibria. To be more precise we consider (1)–(4) with positive and constant coefficients β and γ. It is well known that the total population $N=\int_\Omega (S_0+I_0)(x)dx$ is conserved. In the classical mass action incidence function model ($p=q=1$), the system admits the disease-free equilibrium $(N,0)$ and, whenever $R_0 := \beta N/\gamma > 1$, the endemic equilibrium

$$(S_*,I_*) = \left(\frac{N}{R_0},\, N\Big(1-\frac{1}{R_0}\Big)\right),$$

Observing that the Laplacian vanishes for constant functions, the pair $(S,I)(x,t) = (S_*,I_*)$ is a stationary solution of the power-incidence model if and only if

$$\beta S_*^q I_*^p = \gamma I_*, \text{ or equivalently } \gamma = \beta S_*^q I_*^{p-1}.$$

Hence, once the endemic equilibrium (S_*,I_*) is fixed, the above relation represents only one scalar constraint for the four parameters (β,γ,p,q). Consequently, there exist infinitely many parameter sets producing the same constant endemic equilibrium. For instance, fixing $p=1$, any choice of $\beta>0$ and $q>0$ together with $\gamma=\beta S_*^q$ generates the same stationary solution $(S,I)(x,t)=(S_*,I_*)$. This simple observation shows that, when only constant endemic states are observed, the inverse problem of identifying the parameters (β,γ,p,q) cannot be uniquely solvable.

Although the inverse problem is generally ill-posed in terms of uniqueness, it is possible to establish conditions for local uniqueness, as demonstrated in [17, 19, 80]. These studies strategically employ the necessary optimality conditions and continuous dependence results to derive uniqueness within specific subsets of the admissible set. However, in the present case, it is not possible to establish conditions that extend such estimates, nor specifically to prove that an inequality of the form

$$\|(\hat{\beta}-\beta,\hat{\gamma}-\gamma)(\cdot,t)\|^2_{L^2(\Omega)^2}+|\hat{p}-p|+|\hat{q}-q|\leq C\|(\hat{S}-S,\hat{I}-I)(\cdot,t)\|^2_{L^2(\Omega)^2} \tag{52}$$

for any $t>0$ and some $C>0$ depending on the regularization parameter Γ.

3 Numerical approximation of the optimal control problem

In this section, we develop a numerical approximation of the optimal control problem (8). We focus on the one-dimensional spatial case and the parameter identification problem or, equivalently, we consider that $\Omega\subset\mathbb{R}$ and the reaction coefficients β and γ are parametrized by the finite set of parameters $\mathbf{e}=(e_1,\ldots,e_k)\in\mathbb{R}^k$, i.e. $\beta(x,t)=\beta(x,t;\mathbf{e})$ and $\gamma(x,t)=\gamma(x,t;\mathbf{e})$. In a broad sense, we consider a finte difference discretization on the state equation based mainly in [43, 60, 61, 63, 81]; and concerning to the discretization of control problem, we define a discrete adjoint state and discrete gradient, by adapting the results given [10, 16].

3.1 Discretization of the state equations

In order to discretize (1)-(4) we define a finite difference scheme. We consider that $\Omega=]0,L[$, $\partial\Omega=\{0,L\}$ and $\Gamma_T=\{0,L\}\times[0,T]$. We define the discretization of Q_T by selecting $M,N\in\mathbb{N}$ such that the partition 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_k^n. Hence, the approximation of the initial boundary value problem (1)-(4) is given by

$$\frac{S_k^{n+1}-S_k^n}{\Delta t}=\frac{d_S}{\Delta x^2}\Big[S_{k-1}^{n+1}-2S_k^{n+1}+S_{k+1}^{n+1}\Big]-R_{\text{lin}}, \tag{53}$$

$$\frac{I_k^{n+1}-I_k^n}{\Delta t}=\frac{d_I}{\Delta x^2}\Big[I_{k-1}^{n+1}-2I_k^{n+1}+I_{k-1}^{n+1}\Big]+R_{\text{lin}}, \tag{54}$$

$$\frac{S_1^n-S_0^n}{\Delta x}=\frac{S_{M+1}^n-S_M^n}{\Delta x}=\frac{I_1^n-I_0^n}{\Delta x}=\frac{I_{M+1}^n-I_M^n}{\Delta x}=0, \tag{55}$$

$$S_k^0=S_0(x_k),\quad I_k^0=I_0(x_k), \tag{56}$$

where $k=1,\ldots,M$ and the function R_{lin} in a linearization of the reation term and is defined by the relations (53) and (54) is defined as follows

$$R_{\text{lin}}=\Big[q\beta_k^{n+1}(S_k^n)^{q-1}(I_k^n)^p\Big]S_k^{n+1}+\Big[p\beta_k^{n+1}(S_k^n)^q(I_k^n)^{p-1}+\gamma_k^{n+1}\Big]I_k^{n+1}$$

$$-(p+q-1)\beta_k^{n+1}(S_k^n)^q(I_k^n)^p - \gamma_k^{n+1} I_k^n \tag{57}$$

The approximation (57) is introduced to avoid the solution of nonlinear systems as is considered in the case of the implicit method.

In order to give a more compact presentation of (53)-(56) we consider the notation

$$\mathbf{S}^n = (S_1^n, \ldots, S_M^n)^t, \quad \mathbf{I}^n = (I_1^n, \ldots, I_M^n)^t, \quad \mathbf{U}^n = \begin{pmatrix} \mathbf{S}^n \\ \mathbf{I}^n \end{pmatrix}, \tag{58a}$$

$$\mathbb{L}_S = \frac{d_S \Delta t}{\Delta x^2}\mathbb{H}, \ \mathbb{L}_I = \frac{d_I \Delta t}{\Delta x^2}\mathbb{H}, \quad \text{with} \quad \mathbb{H} = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}_{M\times M} \tag{58b}$$

$$\mathbf{G}^n = \Big(\beta_1^n(S_1^n)^q(I_1^n)^p - \gamma_1^n I_1^n, \ldots, \beta_M^n(S_M^n)^q(I_1^n)^p - \gamma_M^n I_M^n\Big)^t \tag{58c}$$

$$\mathbb{G}_S^n = \Delta t\,\frac{\partial \mathbf{G}^n}{\partial \mathbf{S}^n}, \quad \mathbb{G}_I^n = \Delta t\,\frac{\partial \mathbf{G}^n}{\partial \mathbf{I}^n}, \qquad \mathbf{F}^n = \begin{pmatrix} \mathbb{G}_S^n \mathbf{S}^n + \mathbb{G}_I^n \mathbf{I}^n - \Delta t\,\mathbf{G}^n \\ -\mathbb{G}_S^n \mathbf{S}^n - \mathbb{G}_I^n \mathbf{I}^n + \Delta t\,\mathbf{G}^n \end{pmatrix}, \tag{58d}$$

$$\mathbb{L}^n = \begin{pmatrix} \mathbb{I}_M + \mathbb{L}_S + \mathbb{G}_S^n & \mathbb{G}_I^n \\ -\mathbb{G}_S^n & \mathbb{I}_M + \mathbb{L}_I - \mathbb{G}_I^n \end{pmatrix}, \tag{58e}$$

where $\mathbb{I}_M$ is the identity matrix of size M. We observe that (53)-(56) can be rewritten as follows

$$\begin{aligned} \Big(\mathbb{I}_M + \mathbb{L}_S + \mathbb{G}_S\Big)\mathbf{S}^{n+1} + \mathbb{G}_I \mathbf{I}^{n+1} &= \mathbf{S}^n + \mathbb{G}_S \mathbf{S}^n + \mathbb{G}_I \mathbf{I}^n - \Delta t\,\mathbf{G}^n \\ -\mathbb{G}_S \mathbf{S}^{n+1} + \Big(\mathbb{I}_M + \mathbb{L}_I - \mathbb{G}_I\Big)\mathbf{I}^{n+1} &= \mathbf{S}^n - \mathbb{G}_S \mathbf{S}^n - \mathbb{G}_I \mathbf{I}^n + \Delta t\,\mathbf{G}^n \end{aligned}$$

which is equivalently to

$$\mathbb{L}^n \mathbf{U}^{n+1} = \mathbf{U}^n + \mathbf{F}^n. \tag{59}$$

Hence, we have stated the finite difference scheme (53)-(56) is equivalent to (59).

We notice that the numerical solutions obtained with the numerical scheme (53)-(56) preserve the key biological properties, such as positivity, boundedness, and the invariance of the total population. These features are crucial for both the biological consistency of the simulation and the subsequent numerical analysis of the epidemic model. More precisely, by applying the argumentes given in Theorem 2.6 [60] we can proof the following result.

Theorem 7 *Assume that the hypothesis (H0)-(H2) are satisfied. Then, there exists a unique solution* (S^n, I^n) *of the numerical scheme* (53)-(56). *Moreover, the solutions remain positive and bounded for arbitrary positive stepsizes* Δt *and* Δx *and the scheme is unconditionally convergent.*

3.2 Discret adjoint scheme and discrete gradient

For discretization of the optimal control problem, we begin by considering the discrete cost function J_Δ and the reduced cost functions $\mathcal{J}_\Delta$ defined as follows

$$J_\Delta(S_\Delta, I_\Delta) = \frac{\Delta x}{2}\sum_{k=1}^{M}\Big[(S_k^N - S_k^{obs})^2 + (I_k^N - I_k^{obs})^2\Big] + \frac{\Gamma \Delta x \Delta t}{2}\sum_{k=1}^{N}\sum_{k=1}^{M}\Big[|\partial_x \beta_k^n|^2 + |\partial_x \gamma_k^n|^2\Big], \quad (60)$$

$$\mathcal{J}_\Delta(\mathbf{e}, p.q) = J_\Delta(S_\Delta(\mathbf{e}, p.q), I_\Delta(\mathbf{e}, p.q)). \quad (61)$$

Then, the solution of the inverse problem (8), is replaced by the following parameter identification problem

$$\left.\begin{array}{l} \text{Find } (\overline{\mathbf{e}}, \overline{p}, \overline{q}) \in U_\Delta \text{ such that} \\ \mathcal{J}_\Delta(\overline{\mathbf{e}}, \overline{p}, \overline{q}) = \inf\limits_{(\mathbf{e},p,q)\in U_\Delta} \mathcal{J}_\Delta(\mathbf{e}, p, q) \\ \text{subject to } (S_\Delta, I_\Delta) \text{ solution of (53)-(56),} \end{array}\right\} \quad (62)$$

where $U_\Delta \subset \mathbb{R}^k \times (0,\infty)^2$ is a set such that $(\beta(x,t,\mathbf{e}), \gamma(x,t,\mathbf{e}), p, q) \in U_{ad}$.

In order to calculate the discrete gradient we introduce a discrete adjoint state for the finite differece scheme (53)-(56). Testing (53) by ${w_1}_k^{n+1}$, we deduce $E_\Delta^S = 0$ with E_Δ^S defined as follows

$$\begin{aligned} E_\Delta^S &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\Big\{S_k^{n+1} - S_k^n - \frac{d_S\Delta t}{\Delta x^2}\Big(S_{k-1}^{n+1} - 2S_k^{n+1} + S_{k+1}^{n+1}\Big) - \Delta t\, R_{\text{lin}}\Big\}(w_1)_k^{n+1}, \\ &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\Big\{S_k^n\Big[(w_1)_k^n - (w_1)_k^{n+1} - \frac{d_S\Delta t}{\Delta x^2}\Big((w_1)_{k-1}^n - 2(w_1)_k^n + (w_1)_{k+1}^n\Big)\Big] \\ &\qquad - \Delta t\, R_{\text{lin}}(w_1)_k^{n+1}\Big\} + \sum_{k=1}^{M}\Big[S_k^n - \frac{d_S\Delta t}{\Delta x^2}\Big(S_{k-1}^n - 2S_k^n + S_{k+1}^n\Big)\Big](w_1)_k^n\Big|_{n=0}^{N} \\ &- \frac{d_S\Delta t}{\Delta x^2}\sum_{n=0}^{N-1}\Big[S_1^n(w_1)_2^n - S_M^n(w_1)_{M+1}^n + S_{M+1}^n(w_1)_M^n - S_1^n(w_1)_0^n\Big]. \end{aligned}$$

Similarly, by testing (54) by $(p_2)_k^{n+1}$, we deduce $E_\Delta^I = 0$ with E_Δ^I defined as follows

$$\begin{aligned} E_\Delta^I &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\Big\{I_k^{n+1} - I_k^n - \frac{d_I\Delta t}{\Delta x^2}\Big(I_{k-1}^{n+1} - 2I_k^{n+1} + I_{k+1}^{n+1}\Big) + \Delta t\, R_{\text{lin}}\Big\}(w_2)_k^{n+1}, \\ &= \sum_{n=0}^{N-1}\sum_{k=1}^{M}\Big\{I_k^n\Big[(w_2)_k^n - (w_2)_k^{n+1} - \frac{d_I\Delta t}{\Delta x^2}\Big((w_2)_{k-1}^n - 2(w_2)_k^n + (w_2)_{k+1}^n\Big)\Big] \end{aligned}$$

$$+\Delta t\, R_{\text{lin}}(w_2)_k^{n+1}\Big\} + \sum_{k=1}^{M}\Big[I_k^n - \frac{d_I \Delta t}{\Delta x^2}\Big(I_{k-1}^n - 2I_k^n + I_{k+1}^n\Big)\Big](w_2)_k^n\Big|_{n=0}^{N}$$

$$-\frac{d_I \Delta t}{\Delta x^2}\sum_{n=0}^{N-1}\Big[I_1^n(w_2)_2^n - I_M^n(w_2)_{M+1}^n + I_{M+1}^n(w_2)_M^n - I_1^n(w_2)_0^n\Big].$$

Then, denoting by $\mathbf{w}_1^n = ((w_1)_1^n, \ldots, (w_1)_M^n)^t$, $\mathbf{w}_2^n = ((w_2)_1^n, \ldots, (w_2)_M^n)^t$, and $\mathbf{W}^n = (\mathbf{w}_1^n, \mathbf{w}_2^n)^t$, we define the Lagrangian $\mathcal{L}_\Delta = \mathcal{L}_\Delta\Big(S_\Delta, I_\Delta, (w_1)_\Delta, (w_2)_\Delta\Big)$ for (62) by the following relation

$$\mathcal{L}_\Delta = \mathcal{J}_\Delta(\mathbf{e}, p, q) - E_\Delta^S\Big(S_\Delta, I_\Delta, (w_1)_\Delta\Big) - E_\Delta^I\Big(S_\Delta, I_\Delta, (w_2)_\Delta\Big).$$

We notice that $\nabla_{(\mathbf{e},p,q)}\mathcal{L}_\Delta = \partial_{S_\Delta}\mathcal{L}_\Delta \partial_{(\mathbf{e},p,q)} S_\Delta + \partial_{I_\Delta}\mathcal{L}_\Delta \partial_{(\mathbf{e},p,q)} I_\Delta + \partial_{(\mathbf{e},p,q)}\mathcal{L}_\Delta$. Then, we select $\mathbf{w}_1^n$ and $\mathbf{w}_2^n$ such that $\partial_{S_\Delta}\mathcal{L}_\Delta = \partial_{I_\Delta}\mathcal{L}_\Delta = 0$, i.e.

$$\frac{(w_1)_k^n - (w_1)_k^{n+1}}{\Delta t} = \frac{d_S}{\Delta x^2}\Big[(w_1)_{k-1}^n - 2(w_1)_k^n + (w_1)_{k+1}^n\Big] - \partial_{S_k^n} R_{\text{lin}}\Big((w_1)_k^{n+1} - (w_2)_k^{n+1}\Big), \tag{63}$$

$$\frac{(w_2)_k^n - (w_2)_k^{n+1}}{\Delta t} = \frac{d_I}{\Delta x^2}\Big[(w_2)_{k-1}^n - 2(w_2)_k^n + (w_2)_{k+1}^n\Big] - \partial_{I_k^n} R_{\text{lin}}\Big((w_1)_k^{n+1} - (w_2)_k^{n+1}\Big), \tag{64}$$

$$\frac{(w_1)_{k+1}^n - (w_1)_k^n}{\Delta x} = \frac{(w_2)_{k+1}^n - (w_2)_k^n}{\Delta x} = 0, \quad k = 0, M, \tag{65}$$

$$(w_1)_k^N = S_k^N - S_k^{obs}, \quad (w_2)_k^N = I_k^N - I_k^{obs}. \tag{66}$$

The scheme (63)-(66) is called the adjoint scheme. Hence, we have that

$$\nabla_{(\mathbf{e},p,q)}\mathcal{J}_\Delta(\mathbf{e}, p, q) = \Delta t \sum_{n=0}^{N-1}\sum_{k=1}^{M} \nabla_{(\mathbf{e},p,q)} R_{\text{lin}}\Big((w_1)_k^{n+1} - (w_2)_k^{n+1}\Big) + \frac{\Gamma \Delta x \Delta t}{2}\sum_{n=1}^{N}\sum_{k=1}^{M}\Big(|\nabla_{\mathbf{e}}\partial_x \beta_k^n|^2 + |\nabla_{\mathbf{e}}\partial_x \gamma_k^n|^2\Big). \tag{67}$$

defines the discrete gradient.

4 Numerical examples

In this section we develop three numerical examples focused on the the identification of the powers of the incidence function (Example 1), the identification of the reaction coefficients (Example 1) and the simultaneous identification of the reaction coefficients and the incidence function (Example 3). For the solution of the optimization problem we have considered used the function `fminunc` of Matlab. The synthetic observations are obtained by considering that $(\Delta t, \Delta x) = (1e-3, 5e-4)$, the identification is developed with $(\Delta t, \Delta x) = (1e-2, 5e-3)$ and in all examples $\Gamma = 0$.

4.1 Example 1: Identification of the incidence function

In this example we consider the identification of the powers in the incidence function, i.e. $\mathbf{e} = (p, q)$, by assuming that $\Omega = [0,1]$, $T = 1$, $d_S = 0.001$, $d_I = 0.003$, $\beta = 0.01$ and $\gamma = 0.006$. We construct a synthetic observation by considering the initial conditions given by

$$S_0(x) = 5, \qquad I_0(x) = \begin{cases} 0.001 & x \in [0, 0.3) \cup (0.7, 1], \\ 9.995x - 2.9975 & x \in [0.3, 0.5], \\ -9.995x + 6.9975 & x \in (0.5, 0.7], \end{cases}$$

and the powers of the incidence function $p = q = 1$. The simulation with $\mathbf{e}^{obs} = (1,1)$ is presented in Figures 1-(a)-(b). We develop the identification by considering the initial guess $\mathbf{e} = (2,2)$ and get that the identified parameters are $\mathbf{e}^{\infty} = (0.8926, 1.0046)$. The numerical identification results showing the comparison of the observed, identified and initial guess profiles are shown in Figures 1-(c)-(d).

In Figure 2 we show the behavior of the cost function. We observe that the cost function remains relatively invariant near $\mathbf{e}^{obs}$, resulting in a plateau that hinders the optimization progress. However, in spite slow descent behavior, we get develop the convergence to the numerical optimal value of the parameters as is shown in Figure 2-(d).

4.2 Example 2: Identification of the reaction coefficients

In this example we consider the identification of the reaction coefficients β and γ, by assuming that $\Omega = [0,1]$, $T = 1$, $d_S = 0.003$, $d_I = 0.002$, and $p = q = 1$. We consider that β and γ are of the following form

$$\beta(x,t) = \beta_0 \left[1 + \alpha_0 \exp\left(\frac{-k_0 (x - x_m)^2}{2\sigma_m^2} \right) \right] \left[1 - \frac{\alpha_1}{1 + \exp(-k_1 (t - t_c))} \right], \tag{68}$$

$$\gamma(x) = \gamma_{\max} + (\gamma_{\max} - \gamma_{\min}) \exp\left(\frac{-k_2 (x - x_h)^2}{2\sigma_h^2} \right). \tag{69}$$

The second and third factors of the function β models the increased probability of contagion near hotspots, such as supermarkets or airports, and the influence of lockdowns or quarantines in reducing contact, respectively. The parameter β_0 is the natural disease transmission constant; α_0 is the urban intensity, x_m and σ_m are the center and the radius of the hotspots, respectively; α_1 is the effectiveness of the health policy measure; and t_c is the time from which the confinement or isolation policy comes into effect or is implemented. The function γ models the recovery rate in a health center located at x_h with radius σ_h. The parameters $\gamma_{\min}$ and $\gamma_{\max}$ are the slow and fast recovery rates. Moreover k_1, k_2, and k_3, are some appropriate constants. For definition

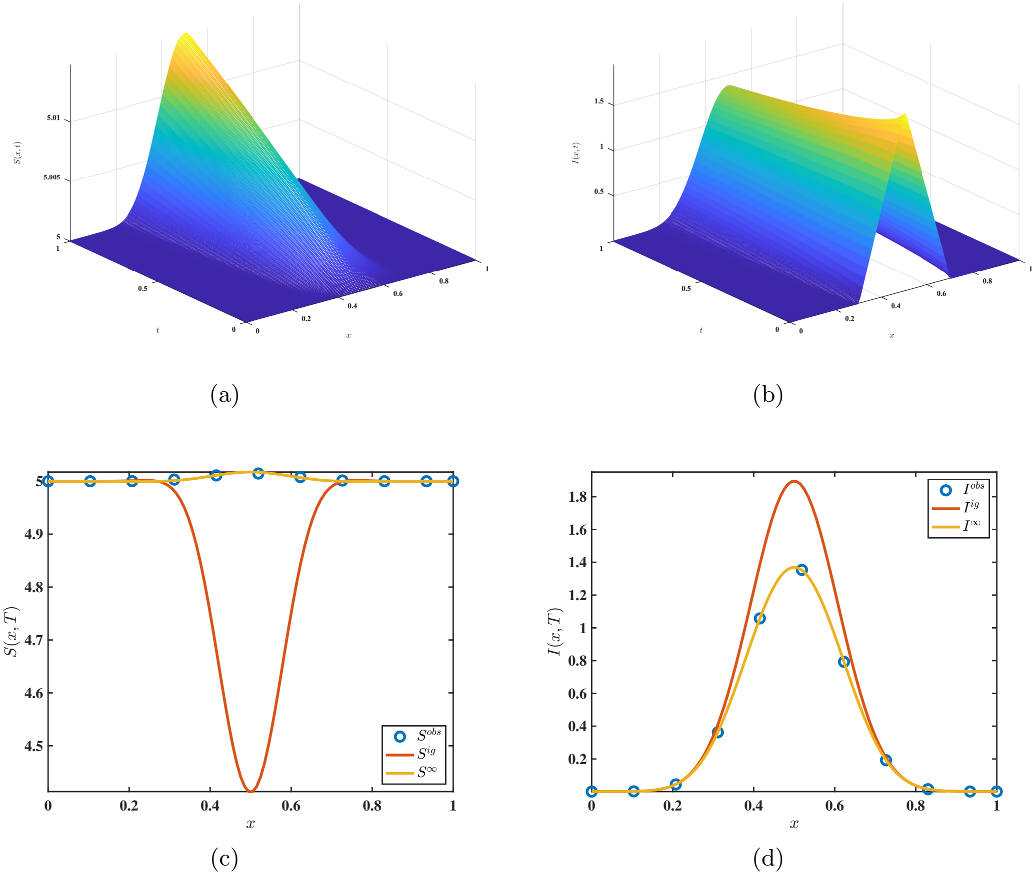


Fig. 1: Results of identification for Example1. (a) and (b) simulation results for $p = q = 1$, i.e. for mass action law, used to produce the synthetic observation data. (c) and (d) comparison of observed, initial guess, and identified profiles for susceptible and infected populations.

of the identification problem, we consider that the functions β and γ are parametrized by the vector $\mathbf{e} = (\beta_0, \alpha_0, k_0, \alpha_1, k_1, \gamma_{\min}, \gamma_{\max}, k_2)$ and the other parameters are fixed with the following values $x_m = 0.25$, $\sigma_m = 0.1$, $t_c = 0.5$, $x_h = 0.75$, and $\sigma_h = 0.1$.

We construct a synthetic observation by considering the incidence function with $p = q = 1$, the initial conditions

$$S_0(x) = -0.1562(10x + 1)(10x - 11), \tag{70}$$

$$I_0(x) = \begin{cases} 0.001 & x \in [0, 0.1) \cup (0.5, 1], \\ 9.995x - 0.9985 & x \in [0.1, 0.3], \\ -9.995x + 4.9985 & x \in (0.3, 0.5], \end{cases} \tag{71}$$

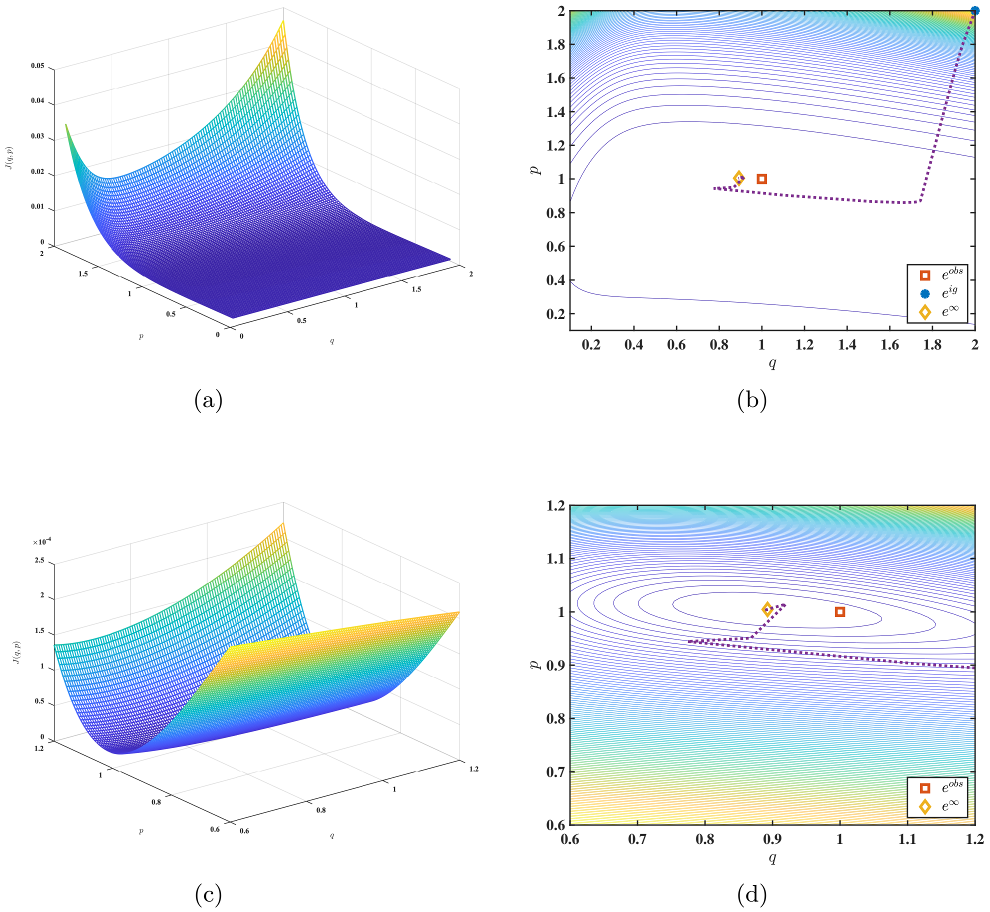


Fig. 2: Cost function for Example1. (a) the cost function for $p, q \in [0.1, 2]$. (b) contour levels of cost function for cost function in (a) with path of descent convergence. (c) and (d) are a zoom of (a) and (b), respectively, by considering that $p, q \in [0.6, 1.2]$

and the value of the parameters for β and γ are given by the values in $\mathbf{e}^{obs}$ given in Table 1. The simulation with $\mathbf{e}^{obs}$ is presented in Figures 3-(a) and (b). We develop the identification with the initial guess $\mathbf{e}^{ig}$ and obtain the identified parameters $\mathbf{e}^{\infty}$, booth are given in Table 1. A comparison of the observed, initial guess, and identified profiles is given in Figures 3-(a) and (b). Moreover, in Figure 4 we show a comparison of the observed, initial guess, and identified coefficients β and γ.

Table 1: Numerical values of the parameters for coefficients $\beta(x,t)$ and $\gamma(x)$ define in (68)-(69). Moreover, we consider $x_m = 0.25$, $\sigma_m = 0.1$, $t_c = 0.5$, $x_h = 0.75$, and $\sigma_h = 0.1$.

Parámetro	β_0	α_0	k_0	α_1	k_1	$\gamma_{\min}$	$\gamma_{\max}$	k_2
$\mathbf{e}^{obs}$	0.2000	1.5000	1.0000	0.7000	75.0000	0.0500	0.3000	1.0000
$\mathbf{e}^{ig}$	0.7000	1.0000	2.0000	0.5000	100.0000	0.0800	0.8000	2.0000
$\mathbf{e}^{\infty}$	0.3165	1.9463	0.9891	0.5746	99.9392	0.3429	0.5975	1.2640

4.3 Example 3: Identification of the reaction coefficients and the powers of the incidence function

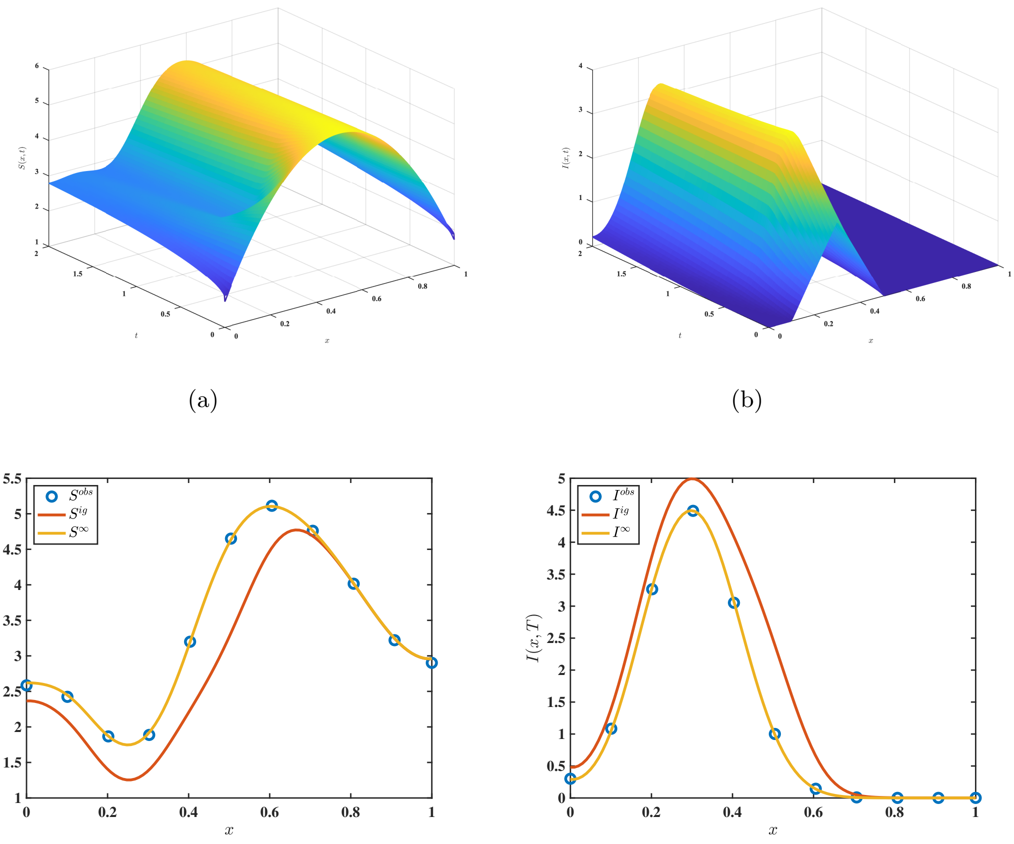
In this example we consider the identification of the reaction coefficients β and γ of the parametric form given in Example 2 (see (68) (69)) and assume that $\Omega = [0,1]$, $T = 1$, $d_S = 0.003$, $d_I = 0.002$. Moreover, we consider that the synthetic observation is those constructed in Example 2, i.e. by considering the incidence function with $p = q = 1$, the initial conditions given in (70)-(71), and the value of the parameters for β and γ given $\mathbf{e}^{obs}$ given in Table 2. We notice that, the simulation with $\mathbf{e}^{obs}$ is presented in Figures 3-(a) and (b), since corresponds to the same value of the parameters given for Example 2. In Table 2 we report the values of the identification parameters $\mathbf{e}^{\infty}$ by assuming the initial guess $\mathbf{e}^{ig}$. A comparison of the observed, initial guess, and identified profiles is given in Figures 5-(a) and (b). Moreover, in Figure 6 and Figure 7 we show a comparison of the observed, initial guess, and identified coefficients (β,γ) and the incidence function.

Table 2: Numerical values of the parameters for coefficients $\beta(x,t)$, $\gamma(x)$ given in (68)-(69) and the powers of the incidence function. Moreover, we consider $x_m = 0.25$, $\sigma_m = 0.1$, $t_c = 0.5$, $x_h = 0.75$, and $\sigma_h = 0.1$.

Parámetro	β_0	α_0	k_0	α_1	k_1	$\gamma_{\min}$	$\gamma_{\max}$	k_2	p	q
$\mathbf{e}^{obs}$	0.2000	1.5000	1.0000	0.7000	75.0000	0.0500	0.3000	1.0000	1.0000	1.0000
$\mathbf{e}^{ig}$	0.7000	1.0000	2.0000	0.5000	100.0000	0.0800	0.8000	2.0000	2.0000	2.0000
$\mathbf{e}^{\infty}$	0.3165	1.9463	0.9891	0.5746	99.9392	0.3429	0.5975	1.2640	1.0384	0.9211

5 Conclusion

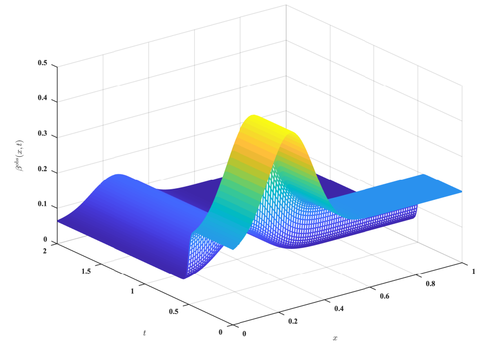
This paper presents a theoretical and numerical framework for reaction identification in a reaction-diffusion system arising from epidemiology. The identification problem is formulated as an optimal control problem, where state equations is defined by an initial boundary valued problem for a reaction–diffusion system modelling the susceptible and infected populations living a bounded habitat. The matrix diffusion is considered



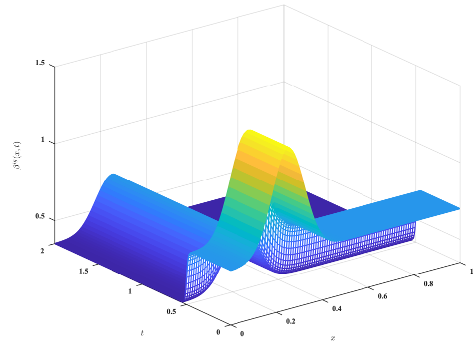
(a) (b) (c) (d)

Fig. 3: Results of identification for Example 2. (a) and (b) simulation results for $p = q = 1$, i.e. for mass action law, and the parameters $\mathbf{e}^{obs}$ in Table 1. (c) and (d) comparison of observed, initial guess, and identified profiles for susceptible and infected populations obtained with paremeters $\mathbf{e}^{obs}$, $\mathbf{e}^{ig}$, and$\mathbf{e}^{\infty}$, respectively, see Table 1.

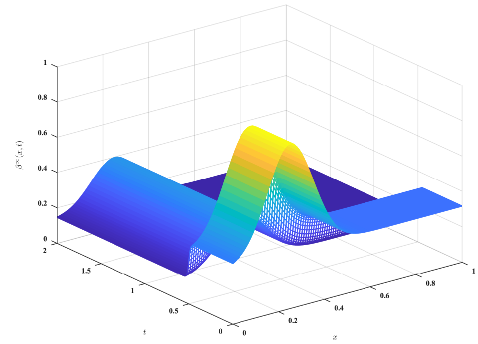
as a constant diagonal matrix. The reaction is defined by two coefficients, modeling the disease transmission and recovery rates, and the incidence function, modeling the interaction of susceptible and infected populations. These coefficients are space-time dependent functions and the incidence is a power function. Within the context of Hölder regularity, the state equations are well posed in the sense of positive strong solutions, by assuming that the coefficients are positive and bounded, the powers are positive, and the initial condition are positive. Concerning to the optimal control problem: the existence of solutions is proved; an adjoint system and a first order condition for optimality solutions are stablished and proved; and a continuos dependence of the state and adjoint equations with respect to the reaction coefficients, the



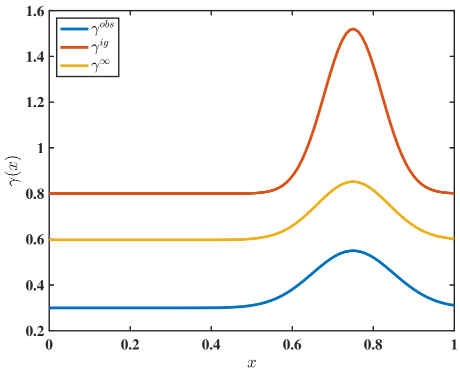
(a)



(b)



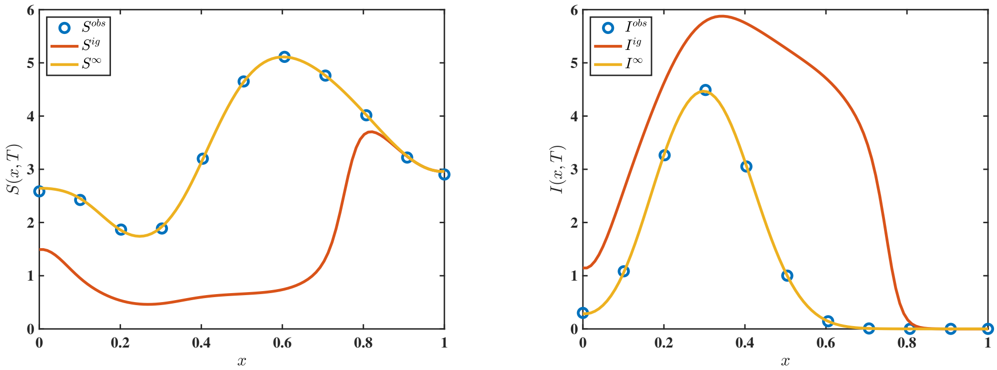
(c)



(d)

Fig. 4: Coefficients $\beta(x,t)$ and $\gamma(x)$ for Example 2. (a), (b) and (c) are the observed, initial guess, and identified coefficient β with parameters, respectively. (c) is comparison of observed, initial guess, and identified coefficient γ. The numerical values $\mathbf{e}^{obs}$, $\mathbf{e}^{ig}$, and$\mathbf{e}^{\infty}$ are given in Table 1

incidence powers, and the observation functions are introduced. Additionally a numerical approximation based on the IMEX and discretize-then-optimize methodologies is introduced and used to simulate the parameter identification problem in three examples. Hence, this work present a progres for the mathematical framework for reaction identification in reaction-diffusion systems arising from epidemiology and provides and make some advances for the numerical solution which needs some refinements in order to get the applications to experimental data.



(a) (b)

Fig. 5: Results of identification for Example 3. (a) and (b) show a comparison of observed, initial guess, and identified profiles for susceptible and infected populations obtained with paremeters $\mathbf{e}^{obs}$, $\mathbf{e}^{ig}$, and$\mathbf{e}^{\infty}$, respectively, see Table 2.

Declarations

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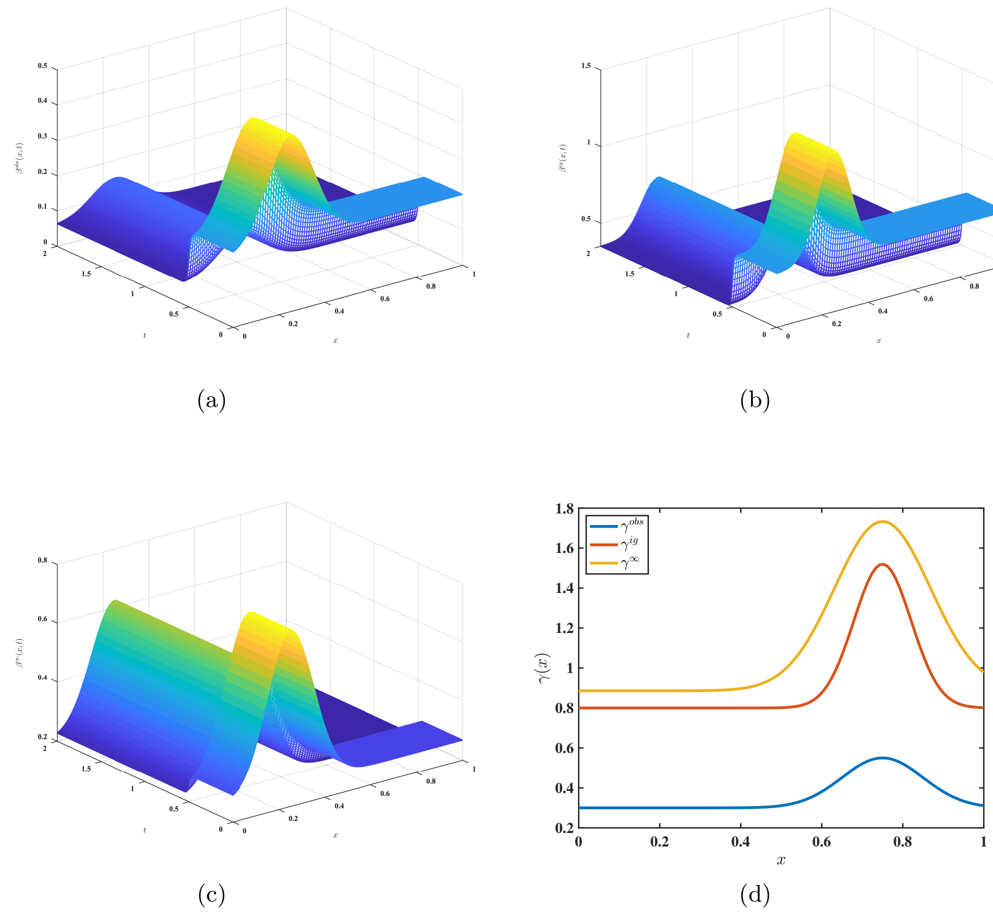

Fig. 6: Coefficients $\beta(x,t)$ and $\gamma(x)$ for Example 2. (a), (b) and (c) are the observed, initial guess, and identified coefficient β with parameters, respectively. (c) is comparison of observed, initial guess, and identified coefficient γ. The numerical values $\mathbf{e}^{obs}$, $\mathbf{e}^{ig}$, and$\mathbf{e}^{\infty}$ are given in Table 1

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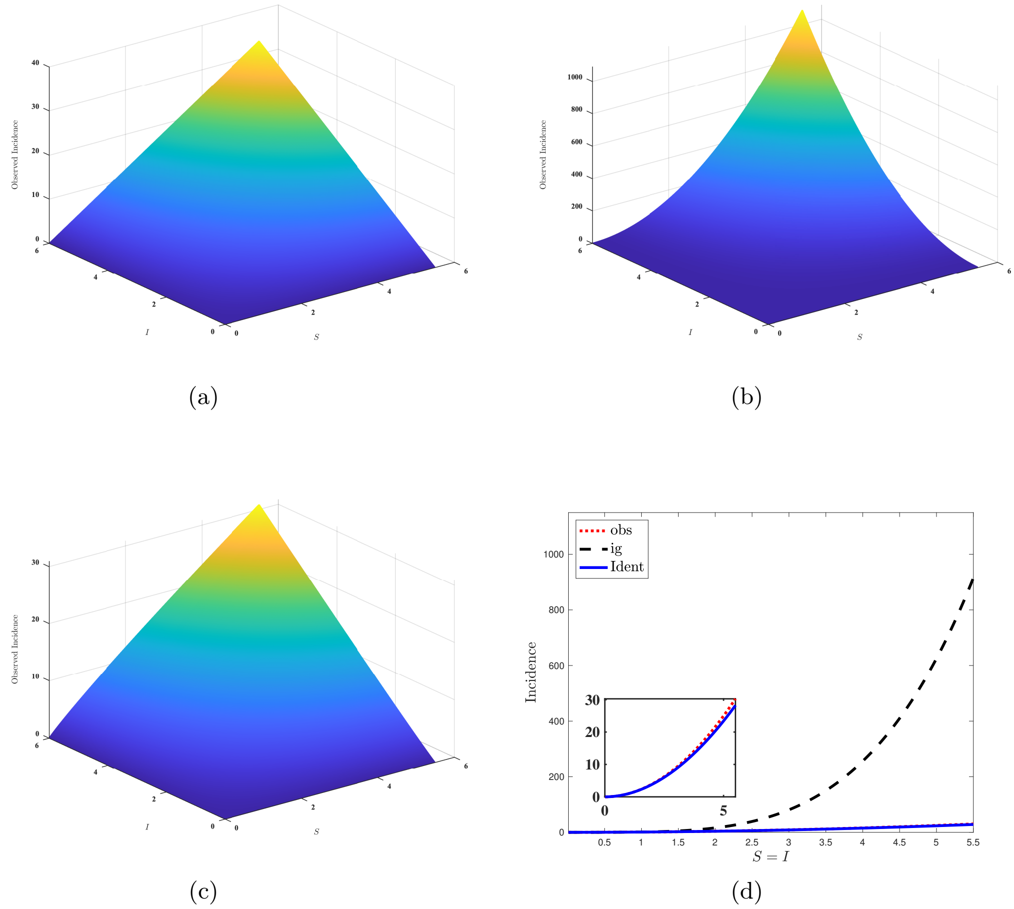

Fig. 7: Power incidence function for Example 3 for $(S, I) \in [0.1, 5.5] \times [0.1, 6]$. (a) Observed incidence function SI. (b) Initial guess incidence function $S^2 I^2$. (c) Identified incidence function $S^{0.9211} I^{1.0384}$. (c) Comparison of observed, initial guess, and identified incidence functions $S = I \in [0.1, 5.5]$. The numerical values $\mathbf{e}^{obs}$, $\mathbf{e}^{ig}$, and$\mathbf{e}^{\infty}$ are given in Table 2.

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