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Research article

Optimal control problem and reaction identification term for carrier-borne epidemic spread with a general infection force and diffusion

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Abstract: In this paper, we simultaneously study reaction identification and the optimal control problem for a reaction-diffusion system modeling carrier-borne epidemics with a general transmission function and vaccination. The state equations are given by a susceptible-infected-recovered reaction-diffusion system with zero-flux boundary conditions and initial conditions. The reaction is modeled by three terms: a general transmission function modeling the force of the infection or the effective contact between susceptible and infected individuals, a linear function for transition between susceptible and infected individuals, and a function for control of vaccination of susceptible individuals. The cost function consists of two parts: two terms related to parameter identification, comprising a regularized least squares cost function, and five terms related to the control of the population through vaccination. The optimal control problem is analyzed by applying the Dubovitskii and Milyutin formalism. In the main results, we deduce the well-posedness of the state equation, the existence of the optimal control problem, the existence of solutions of the adjoint state, and a first-order optimality condition. We develop a numerical approximation for the optimal control problem by employing an IMEX method to approximate the state equations. In this approach, the coefficients of the reaction terms and the control functions depend on a finite set of parameters. We provide two numerical examples to demonstrate the agreement of our numerical solution with the measurement observations.

Keywords: optimal control; parameter identification; SIR with diffusion; carrier-borne epidemic; first-order optimality condition

1. Introducction

1.1. Scope

In recent years, optimal control theory has been utilized as a crucial mathematical tool for making decisions in complex physical, biological, chemical, geometrical, and even economic situations [1,2]. In a broad sense, the optimal control problems achieve a goal by adjusting a function to a system solution, where the system can be, for instance, an ordinary differential equation, a partial differential equation, or an integral differential equation [3]. Historically, the theory of control has been applied to engineering and business, for instance, to calculate the optimal interplanetary trajectories for rockets and industrial inventories with part numbers running into the hundreds of thousands. The applications, methodologies, and even the concepts associated with control theory underwent an evolution that is well-detailed in the survey [4].

Another important aspect of optimal control theory is its foundation in key principles of optimization theory. For instance, in biology, optimizing the available resources among the competing requirements of a particular health problem is equivalent to solving an optimal control problem. More precisely, the problems of controlling the spread of epidemics and competing systems were studied using analogies with the industrial applications of optimal control, changing the language appropriately [5]. Particularly, a pioneering contribution to epidemic disease control is the work developed by Sanders [6], where the author obtained some results for a single population governed by a logistic equation. Afterward, an improvement was developed by Wickwire [7]. Currently, there is a long list of works focused mainly on the minimization of the infected population by implementing some vaccination strategies. For instance, we refer to [7–14], and this list of optimal control problems in vaccination applications is not exhaustive. We remark that in those works, the governing equations are ordinary differential equation systems. More recently the analysis of control problems has been extended in [15–23] to the case where the state equations modeling the spread of the dynamics are reaction-diffusion systems.

On the other hand, in the mathematical modeling of disease propagation through compartmental models, a particular immunization model was proposed by Wickwire [24]. The assumptions of the model introduced in [24] are contextualized for specific epidemics, such as typhoid fever, tuberculosis, and amoebic dysentery. In those diseases, the spread is at least partly caused by carriers who, although they show no explicit symptoms, can transmit the disease to the susceptible population. To be more precise, the author considers a closed population consisting of N individuals, which is partitioned into three subpopulations: susceptibles, infected, and recovered, with populations $s(t)$, $I(t)$, and $r(t)$, for $t \geq 0$, respectively. It is also assumed that a proportion $p \in [0, 1]$ of infected individuals (the carriers) show no explicit or at least noticeable symptoms, although they have the contingency to transmit the disease, and, when detected, they are immediately removed. Additionally, susceptibles are immunized, and at time t we have that $u(t)$ individuals are transferred from the susceptible class to the removed class. Then, we incorporate $u(t)$ as a control function, which we assume to be piecewise continuous and to take values in the interval $[0, 1]$. Then, the state equations are given by the ordinary differential equations system

$$s'(t) = -\beta s(t)i(t) - u(t), \tag{1.1}$$

$$i'(t) = \beta p s(t)i(t) - \gamma i(t), \tag{1.2}$$

$$r'(t) = \beta(1 - p)s(t)i(t) + \gamma i(t) + u(t), \tag{1.3}$$

$$s(0) = s_0,\ i(0) = i_0,\ r(0) = r_0, \tag{1.4}$$

where $\beta, \gamma \in (0, 1)$ are the constant rates, $(s_0, i_0, r_0) \in [0, N)^3$, and the cost function is given by

$$\int_0^{\infty} \Big(c_1 i(\tau) + c_2\beta(1-p)s(\tau)i(\tau) + ku(\tau)\Big)d\tau, \tag{1.5}$$

where c_1, c_2, and k are some appropriate positive constants. Note that $s_0(t)+i_0(t)+r_0(t) = s_0+i_0+r_0 = N$, which can be deduced by adding Eqs (1.1)–(1.3). We observe that the first term of the cost function in (1.5) is associated with the minimizing of the infective population, the second term is related to the detection of carriers and the isolation as soon as they are detected, and the third term is the optimal control. Roughly speaking, the main results in [24] are the characterization of the controls of (1.1)–(1.5) as bang-bang controllers providing an explicit formula for the switching curve.

1.2. Vaccination control and parameter identification problems

At the beginning of the 21st century, Behncke [8] introduced a generalized model and vaccination control for carrier-borne epidemics. The generalization of [8] is related to the infection force used in the modeling of the interaction between susceptible and infected populations. In the case of (1.1)–(1.4), the interaction is modeled by the mass-action law $\beta s(t)i(t)$. Utilizing standard interaction functions considered in the literature (see for instance [25]) like $\beta xy/(x+y)$ and $xy^p/(1+\alpha y^q)$, Behncke [8] introduced the following set $\mathcal{B}_{ad}$ for the interaction force:

$$\begin{aligned}\mathcal{B}_{ad} = \Big\{f : \mathbb{R}^2 \to [0,\infty)^2 \ : \quad & f(s,i) = 0 \text{ for } (s,i) \in \mathbb{R}^2 - [0,\infty)^2;\\ & f(0,i) = f(s,0) = 0 \text{ and } f(s,i) > 0 \text{ for } (s,i) \in (0,\infty)^2;\\ & \partial_{ss} f(s,i), \partial_{ii} f(s,i) \le 0 \text{ for } (s,i) \in [0,\infty)^2;\\ & \text{and } \partial_s f(s,i), \partial_i f(s,i), \partial_{si} f(s,i) > 0 \text{ for } (s,i) \in [0,\infty)^2\Big\}.\end{aligned} \tag{1.6}$$

Related to the efficiency or effectiveness of vaccination, consider the set

$$\mathcal{G}_{ad} = \Big\{g : [0,N] \to [0,\infty) \ : \ g'(s) \ge 0 \text{ and } g'(0) > 0\Big\}. \tag{1.7}$$

Let $a > 0$ be a base vaccine efficacy or efficiency independent of the proportion of susceptible individuals. We note that the set $\mathcal{G}_{ad}$ models the situation where vaccination is dynamic, and we have at least two basic scenarios: $g(s) = a + s$ represents the case where the efficacy or efficiency of the vaccine increases with the number of susceptible individuals in the population, and $g(s) = as + s^2$ represents the case where there is a rate of vaccine efficacy proportional to the susceptible population together with a herd immunity effect. Behncke [8] studied the following optimal control problem: Find the function u satisfying the system

$$s'(t) = f(s(t), i(t)) - u(t)g(s(t)), \tag{1.8}$$

$$i'(t) = pf(s(t), i(t)) - \gamma i(t), \tag{1.9}$$

$$s(0) = s_0,\ i(0) = i_0, \tag{1.10}$$

where $f \in \mathcal{B}_{ad}$, $g \in \mathcal{G}_{ad}$, and the cost function is given by

$$\int_0^T \Big(i(\tau) + c(s(t))g(s(t))u(\tau) + du(\tau)\Big)d\tau + ai(T), \tag{1.11}$$

with $c : [0, N] \to [0, \infty)$ such that $c'(s) \leq 0$, $T > 0$, $d \geq 0$ and $a \in [0, \gamma^{-1}]$. The author assumes that $u(t) \in [0, u_0]$, and proves that the solution of (1.8)–(1.11) is of bang-bang type.

On the other hand, the optimal control theory has recently been applied to solve the inverse problem arising from coefficient identification in reaction-diffusion mathematical models from epidemiology [26–30]. In [26], the authors considered the reaction-diffusion system

$$\begin{aligned}
&\partial_t S - \Delta S = -\beta(x)\frac{SI}{S+I} + \gamma(x)I, && \text{in} \quad Q_T = (0,T)\times\Omega,\\
&\partial_t I - \Delta I = \beta(x)\frac{SI}{S+I} - \gamma(x)I, && \text{in} \quad Q_T,\\
&\nabla S \cdot \eta = \nabla I \cdot \eta = 0, && \text{on} \quad \Sigma_T = (0,T)\times\partial\Omega,\\
&(S,I)(x,0) = (S_0, I_0)(x), && \text{in} \quad \Omega,
\end{aligned}$$

where $\Omega \subset \mathbb{R}^d$, $d \geq 1$, is a bounded set with smooth boundary $\partial\Omega$; η is the outward unit normal to $\partial\Omega$; $S(x,t)$ and $I(x,t)$ denote the density of the sub-classes of susceptible and infected populations at position x and time t, respectively; $T > 0$ denotes the time under which the dynamics are studied; and S_0 and I_0 are the initial distributions of susceptible and infected populations, respectively. The boundary condition models the fact that there is no population flux across the boundary, and both populations (susceptible and infected individuals) reside in a self-contained, isolated environment. Then, assuming that the additional measurements for susceptible and infected densities at T are given by $S^d(x)$ and $I^d(x)$, respectively, they analyze the problem of finding the functions β and γ such that

$$(\beta,\gamma) \in \left\{(f_1, f_2) : \Omega \to [0,\infty)^2 \ : \ (f_1, f_2)(x) \in (0,1)^2 \text{ for } x \in \Omega \text{ and } \nabla(f_1, f_2) \in L^2(\Omega)\right\}$$

considering the cost function

$$\frac{1}{2}\left\|(S,I)(\cdot,T) - (S^d, I^d)(\cdot)\right\|^2_{L^2(\Omega)} + \frac{N}{2}\left\|\nabla(\beta,\gamma)\right\|^2_{L^2(\Omega)}, \quad N > 0.$$

The results on existence and local uniqueness, in the context of smooth solutions, given in [26] is reduced to the case $d = 1$ and extended to $d > 1$ in [27]. Moreover, it is generalized to more general mathematical models in [28–31].

1.3. Simultaneous parameter identification and optimal control problems

In this article, we investigate the simultaneous study of parameter identification and the optimal control problem for a reaction-diffusion system modeling carrier-borne epidemics with a general transmission function and vaccination. More precisely, we consider that the population satisfies the assumptions introduced in [24].

Additionally, we assume that each population moves spatially toward the negative of the gradient of its respective population density, which is modeled by a diffusion term with a diagonal diffusion matrix. Thus, the state equations are given by

$$\partial_t S - \Delta S = -\beta(x) f(S,I) - u(t)g(S), \quad \text{in} \quad Q_T, \tag{1.12}$$

$$\partial_t I - \Delta I = p\beta(x) f(S,I) - \gamma(x)I, \quad \text{in} \quad Q_T, \tag{1.13}$$

$$\partial_t R - \Delta R = (1-p)\beta(x) f(S,I) + \gamma(x)I + u(t)g(S), \quad \text{in} \quad Q_T, \tag{1.14}$$

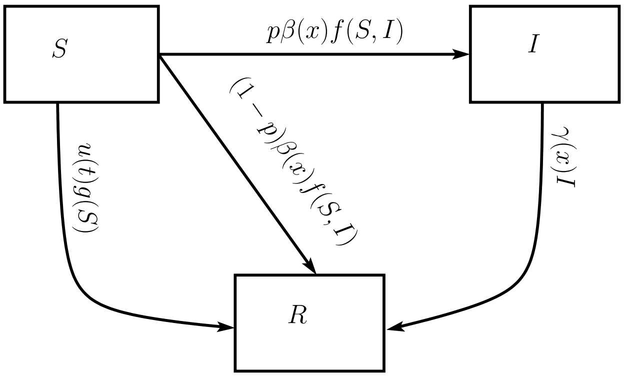


Figure 1. Compartmental representation of the system (1.12)–(1.16).

$$\nabla S\cdot\eta=\nabla I\cdot\eta=\nabla R\cdot\eta=0, \qquad \text{on} \quad \Sigma_T, \tag{1.15}$$

$$(S,I,R)(0,x)=(S_0,I_0,R_0)(x), \qquad \text{in} \quad \Omega, \tag{1.16}$$

where $R(x,t)$ denotes the density of the recovered population (see Figure 1). Here, the function u denotes the vaccination effort, g the efficiency or effectiveness of the vaccination program, β denotes the contagion rate, γ the recovery of the infected rate, and the initial conditions S_0, I_0, and R_0 are functions from Ω to $\mathbb{R}_0^+$. We assume that $p\in[0,1]$ is a given constant representing the proportion of carriers or infected individuals who exhibit no explicit symptoms but are still capable of transmitting the disease, and we assume that once these individuals are identified, they are promptly isolated or removed from the population.

Let us consider that we have measurements of the state variables at T given by $S^d(x), I^d(x)$, and $R^d(x)$. The cost function is defined as

$$\begin{aligned} J(S,I,R,\beta,\gamma,u)=&\frac{k_1}{2}\left\|(S,I,R)(\cdot,T)-(S^d,I^d,R^d)(\cdot)\right\|^2_{L^2(\Omega)}+\frac{k_2}{2}\left\|\nabla(\beta,\gamma)\right\|^2_{L^2(\Omega)}+k_3\iint_{Q_T}I(x,t)dxdt\\ &+k_4\iint_{Q_T}c(S(x,t))u(t)g(S(x,t))dxdt+k_5\iint_{Q_T}(1-p)\beta(x)f((S,I)(x,t))dxdt\\ &+k_6\int_0^T u(t)dt+k_7\int_\Omega I(x,T)dx, \end{aligned}\tag{1.17}$$

where k_i are some appropriate constants, and the function c is a monotonically decreasing and positive function ($c'(S)\le 0$ and $c(S)\ge 0$). Hence, we refer to the optimal control problem as the following optimization problem:

$$\left.\begin{array}{l} \text{Find the functions } \beta,\gamma,u \text{ minimizing the cost function } \mathcal{J} \text{ from } C(\Omega)^2\times L^2(0,T)\\ \text{to } \mathbb{R} \text{ defined by } \mathcal{J}(\beta,\gamma,u)=J(S,I,R,\beta,\gamma,u) \text{ with } J \text{ given on (1.17), and subject}\\ \text{to } (S,I,R,\beta,\gamma,u) \text{ satisfying the system (1.12)–(1.16).} \end{array}\right\}\tag{1.18}$$

Notice that the optimal control problem is a combination of the coefficient identification and optimal control problems. For similar optimal control problems on reaction-diffusion we refer to [32, 33].

In (1.17), the function c models the cost of vaccination as a function dependent on the susceptibles, and consequently the assumption that $c'(S)\le 0$, means that the vaccination at higher densities may be cheaper and easier. The first two terms of J are related to the inverse problem of coefficient identification problem, and the other terms consider the care of the infected, vaccination, and economic loss. Additionally, we observe the following facts: the third term represents the cost of infection during the time of disease propagation, the fourth term is related to the cost of vaccination, the fifth term models the cost of the interaction of susceptible and infected interaction, the sixth term represents the cost of implementing campaigns to support the vaccination effort, and the seventh term represents an additional cost resulting from the remaining infected population at the end of the process. It is worth noting that our choice of the linear form for the third term in the cost function (1.17), is motivated by its ability to provide greater control over the infected population without excessively amplifying the values of $I(x,t)$. This choice also contributes to improved numerical performance. In particular, this strategy is well-suited when the primary objective is to minimize the total spread of the infection rather than to smooth out local fluctuations [34, 35].

1.4. Methodology and main results of the paper

In this paper, we analyze (1.18) by applying the Dubovitskii and Milyutin formalism [31, 36–39]. Then, in order to reformulate in the context of the standard Dubovitskii and Milyutin notation, we introduce the following spaces

$$E = W^{1,2}(0,T;L^2(\Omega))^3 \times L^2(\Omega)^2 \times L^2(0,T), \quad \tilde{E} = L^2(0,T;H^2(\Omega))^3 \times L^\infty(0,T;H^1(\Omega))^3,$$

where the notation corresponds to Lebesgue and Sobolev spaces, see [40, 41] for details. Hence, the problem (1.18) can be rewritten as the optimization problem

$$\left.\begin{array}{l} \text{Minimize } J(S,I,R,\beta,\gamma,u) \text{ subject to } (S,I,R,\beta,\gamma,u) \in \mathcal{D} \\ \text{with } \mathcal{D} = \Big\{(S,I,R,\beta,\gamma,u) \in E : M(S,I,R,\beta,\gamma,u) = 0\Big\}, \end{array}\right\} \tag{1.19}$$

where $J : E \to \mathbb{R}$ is defined by (1.17), and the operator $M : E \to \tilde{E}$ is defined by

$$M(S,I,R,\beta,\gamma,u) = (\psi_1,\psi_2,\psi_3,\psi_4,\psi_5,\psi_6) \tag{1.20}$$

if only if

$$\partial_t S - \Delta S + \beta(x) f(S,I) + u(t) g(S) = \psi_1, \quad \text{in } Q_T, \tag{1.21}$$

$$\partial_t I - \Delta I - p\beta(x) f(S,I) + \gamma(x) I = \psi_2, \quad \text{in } Q_T, \tag{1.22}$$

$$\partial_t R - \Delta R - (1-p)\beta(x) f(S,I) - \gamma(x) I - u(t) g(S) = \psi_3, \quad \text{in } Q_T, \tag{1.23}$$

$$\nabla S \cdot \eta = \nabla I \cdot \eta = \nabla R \cdot \eta = 0, \quad \text{on } \Sigma_T, \tag{1.24}$$

$$(S,I,R)(0,x) - (S_0,I_0,R_0)(x) = (\psi_4,\psi_5,\psi_6), \quad \text{in } \Omega. \tag{1.25}$$

We observe that the system (1.12)–(1.16) is a particular case of the system (1.21)–(1.25) when $\psi_i = 0$, for $i = 1, \cdots, 6$.

The main results of this paper are the following: the existence and uniqueness of a positive solution of the initial-boundary value problem (1.12)–(1.16), the existence of solutions for the optimization problem (1.19), the differentiability properties of the operators M and J and the characterization of the descent and tangent, the existence of solutions for the adjoint system for (1.12)–(1.16), and the introduction of a first-order optimal condition. A summary of the methodology and results is schematically presented in Figure 2.

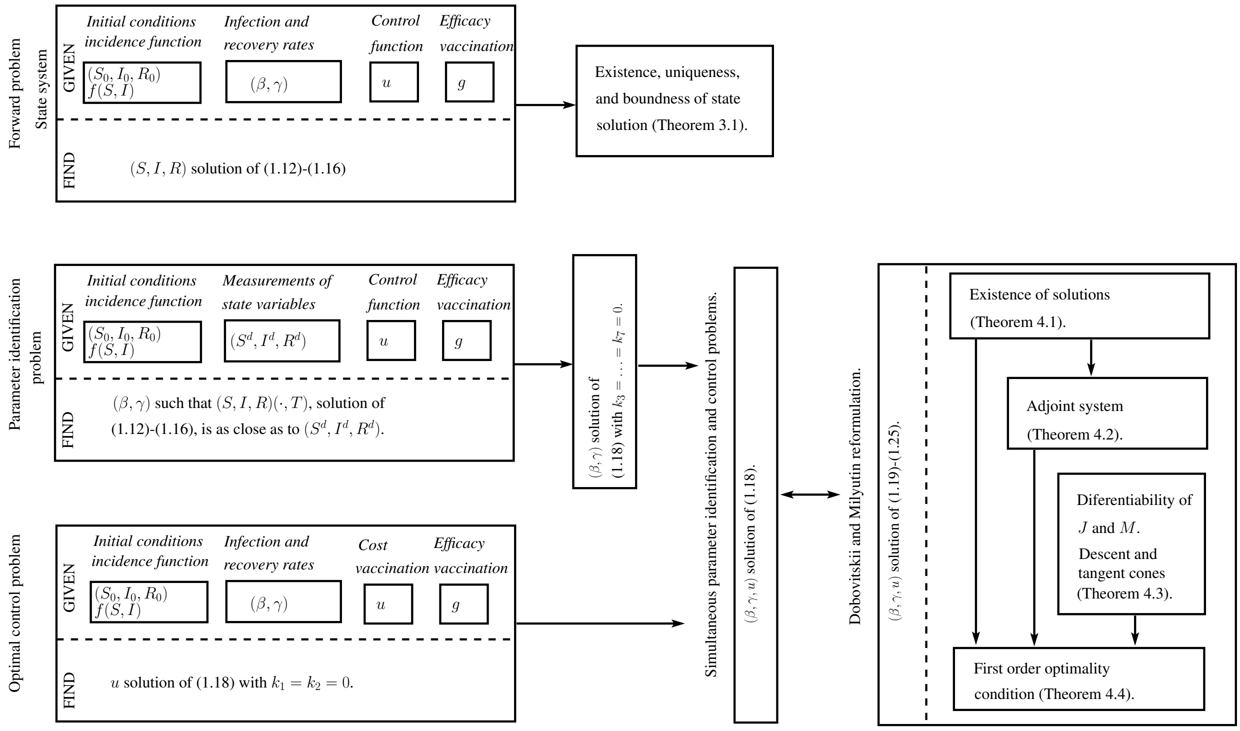


Figure 2. Flow chart diagram summarizing the methodology and results obtained in the paper.

1.5. A short review of related work

The literature on mathematical modeling in epidemiology is extensive, making it challenging to summarize all contributions in a brief survey. However, a comprehensive recent review was developed in [42]. One of the most influential approaches to mathematical modeling is based on the compartmental model methodology introduced in the pioneering work of Kermack and McKendrick [43]. They proposed and studied a deterministic SIR epidemic model by dividing the population into three compartments: susceptible, infected, and recovered. This methodology relies on certain assumptions that lead to a mathematical model governed by a system of ordinary differential equations. For a more extensive discussion, we refer to [44]. The generalization of the original compartmental models has been expanded to study various types of diseases affecting human, animal, and plant populations [45–48]. These different variants and extensions are associated with the incidence function, which models the interactions between susceptible and infected populations. Additionally, they explore the complex dynamics of specific diseases by incorporating several compartments and generalizing the models to include diffusion or partial differential equations. Therefore, our key improvements are focused on the following aspects:

- *General incidence function.* Observing the system (1.1)–(1.4), we have that the interaction of susceptible and infected is modeled by βsi, which is a bilinear function. It is reported that this kind of behavior is valid for small values of infected population and is unrealistic for large values [49]. Several extensions have been proposed in the literature, distinguishing at least two perspectives. First, we recall that the vast majority consider the interaction between susceptible, infected, and recovered populations as rates and assume them to be constant [32, 45–48, 50]. However, in recent years, some authors have argued that these interactions are dependent on some phenomena, such

as the seasonality, spatial heterogeneity, and the periodicity [51–54]. Second, there are proposals to generalize the nonlinear interaction, and in this sense Behncke [8] proposed a class of functions $\mathcal{B}_{ad}$ defined in (1.6), which at least generalizes the existing particular cases. We remark that the proposal of [8] is given in the context of ordinary differential equations and with constant infected and recovered rates. Hence, in this paper we extend the result of [8] to the case of partial differential equations models and with space dependent infected and recovered rates.
- *Simultaneous optimal control and model calibration problems.* In most studies, optimal control problems, such as those related to vaccination, are analyzed separately from model calibration issues. Moreover, we remark that there is research on the biological control of epidemics where the rates are typically assumed to be constant [55]. To calibrate the reaction terms in epidemic models that incorporate reaction-diffusion processes, these problems are complex and challenging to study because they involve solving an inverse problem [26, 32, 33]. Our contribution aims to generalize previous approaches to address these two issues, optimal control, and model calibration, simultianously. Specifically, in relation to the control problem identified, our proposal modifies the approach suggested by Behncke [8] by incorporating the geographical location of the population over which a disease spreads. We also consider that the infection rate is a function that depends on geographical location. We include a control parameter for vaccination efforts, where the effectiveness or efficacy of vaccination is contingent on the number of vaccinated susceptible individuals. Regarding the parameter identification problem, our proposal diverges from existing literature concerning the cost function. In this study, we introduce a cost function that not only facilitates the identification of the reaction coefficients, but also performs traditional optimal control over the state variables. Specifically, our approach optimizes not only the state variables but also accounts for the costs associated with vaccination and the economic impacts resulting from the disease.

Additionally, the contributions of the paper present a small progress in the numerical approximation of the inverse and model calibration problems.

1.6. Paper outline

The paper is organized as follows. In Section 2, we introduce the assumptions and relevant results for Dubovitskii-Milyutin formalism. In Section 3, we analyze the system (1.12)–(1.16). In Section 4, we present the results for the optimal control problem (1.19). In Section 5, we develop a numerical approximation of the optimal control problem and give two numerical examples. Finally, in Section 6, we present some conclusions and future work.

2. Preliminaries

In this section, we precisely state the assumptions and present some previous results of semigroup theory and Dubovitskii-Milyutin formalism.

2.1. Assumptions

Henceforth, we consider the following assumptions on the spatial domain, the coefficients of the state equation, and the observed functions:

(H1) The set $\Omega \subset \mathbb{R}^d$ for $d = 1, 2, 3$ is an open and bounded set of C^1 class.

(H2) The initial condition (S_0, I_0, R_0) belongs to the set $\mathcal{U}_0$ defined as

$$\mathcal{U}_0 = \Big\{(S, I, R) \in H^2(\Omega)^3 : \nabla S \cdot \eta = \nabla I \cdot \eta = \nabla R \cdot \eta = 0 \quad \text{on} \quad \partial\Omega\Big\}$$

and also the functions $S_0 \geq 0$, $I_0 \geq 0$, and $R_0 \geq 0$ on Ω.

(H3) The functions f and g are locally Lipschitz such that $(f, g) \in \mathcal{B}_{ad} \times \mathcal{G}_{ad}$, where $\mathcal{B}_{ad}$ and $\mathcal{G}_{ad}$ are the set functions defined in (1.6) and (1.7). Moreover, we assume $p \in [0, 1]$ is a fixed constant.

(H4) The functions $\beta, \gamma : \Omega \to \mathbb{R}$ and $u : [0, T] \to \mathbb{R}$ belong to admissible set $\mathcal{U}_{ad} = \mathcal{U} \times Z$ with $\mathcal{U}$ and Z defined as follows:

$$\begin{aligned} \mathcal{U} = \Big\{(\beta, \gamma) \in C(\Omega)^2 \quad &: \quad (\beta, \gamma)(x) \in [\beta_\star, \beta^\star] \times [\gamma_\star, \gamma^\star] \subset]0, 1[^2 \quad \text{on} \quad \Omega \\ &\text{and} \quad \|\nabla(\beta, \gamma)\|^2_{L^2(\Omega)} \quad \text{bounded}\Big\}, \\ Z = \Big\{h \in L^2(0, T) \quad &: \quad 0 \leq h(t) \leq 1, \quad t \in [0, T]\Big\}. \end{aligned}$$

(H5) The observed functions are such that $(S^d, I^d, R^d) \in L^2(\Omega)^3$.

2.2. A semigroup result

Theorem 2.1. *([56], Proposition 1.2, p. 175) Let X be a Banach space, $A : D(A) \subseteq X \to X$ be the infinitesimal generator of a C_0-semigroup of contractions on X, and $f : [0, T] \times X \to X$ a function which is measurable in t and Lipschitz in $x \in X$ uniformly with respect to $t \in [0, T]$. If $y_0 \in X$, then the initial value problem*

$$y'(t) = Ay(t) + f(t, y(t)), \in [0, T], \tag{2.1}$$

$$y(0) = y_0, \tag{2.2}$$

has a unique mild solution $y \in C([0, T]; X)$. Moreover, if X is a Hilbert space, A is self-adjoint and dissipative on X, and $y_0 \in D(A)$, the mild solution is a strong solution such that $y \in W^{1,2}(0, T; X)$.

2.3. Differential calculus on Banach Spaces. Dubovitskii-Milyutin formalism terminology and notation

To introduce the results of the differential calculus on Banach Spaces, we recall some aspects detailed in [57]. More precisely, we present the definitions of Fréchet Gâteaux differentiability.

Definition 2.1. *[57, Definition A.15, p. 453] Let X and Y be Banach spaces, and $U \subset X$ be a (non-empty) open subset of X. An operator $F : U \to Y$ is called* Fréchet differentiable *(briefly F-differentiable) at $x_0 \in U$ if there exists an operator $L(x_0) \in \mathcal{L}(X, Y)$ such that if $h \in X$ and $x_0 + h \in U$,*

$$F(x_0 + h) - F(x_0) = L(x_0)h + R(h, x_0)$$

with $R(h, x_0) = o(\|h\|_X)$, that is, $\|R(h, x_0)\|_Y / \|h\|_X$ converges to 0 when h goes to 0. $L(x_0)$ is called the Fréchet derivative *(or differential) of F at x_0, and we write $L(x_0) = F'(x_0)$.*

Definition 2.2. *[57, Definition A.17, p. 453] Let X and Y be Banach spaces, and $U \subset X$ be an open subset of X. An operator $F : U \subset X \to Y$ is called* Gâteaux differentiable *(briefly G-differentiable) at*

$x_0 \in U$ if there exists an operator $A(x_0) \in \mathcal{L}(X,Y)$ such that, for any $h \in X$ and any $t \in \mathbb{R}$ such that $x_0 + th \in U$,

$$\lim_{t\to 0} \frac{F(x_0+th) - F(x_0)}{t} = A(x_0)h.$$

$A(x_0)$ is called the Gâteaux derivative *(or differential) of F at x_0, and we write $A(x_0) = F'_G(x_0)$.*

On the other hand, the terminology and results related to the Dubovistskii and Milyutin formalism are presented below; for more details consult [58, 59]. Initially, we consider the generic optimization problem

$$\left.\begin{array}{r} \min \quad J(x), \quad \text{subject to:} \quad x \in Q = \bigcap_{i=1}^{n+1} Q_i, \\ \overset{\circ}{Q}_i \neq \emptyset, \quad i = 1,\ldots,n, \quad \text{(inequality constraints)} \\ Q_{n+1} = \{x \in X : M(x) = 0\}, \quad \text{(equality constraints)} \end{array}\right\} \tag{2.3}$$

where $J : X \to \mathbb{R}$ is a functional and M is a operator, with X and Y Banach spaces. The notation $\overset{\circ}{Q}_i$ is utilized for the interior of Q_i.

In the works of Dubovitskii and Milyutin [36, 37], the necessary conditions for local optimality at a point $x_0 \in X$ are derived through the separation of the conical approximations of the constraint sets $Q_i, i = 1,\ldots,k+1$, and the set $\{x \in X : J(x) < J(x_0)\}$. In these studies, the authors introduce the concepts of cones (of feasible direction, tangent, and descent, presented subsequently), which are non-empty and convex. Then, almost in a broad sense, they establish that x_0 is a local minimum of problem (2.3) if and only if there does not exist a common direction to all the conical approximations. The results of Dubovitskii and Milyutin demonstrate that this geometric property of local optimality of the point x_0 can be equivalently expressed in terms of the linear forms of the corresponding dual (or polar) cones. Then, to give the Dubovitskii and Milyutin theorem, we begin by presenting some terminology and notation in the following definitions.

Definition 2.3. *The vector $h \in X$ is said to be a descent direction of the functional $J : X \to \mathbb{R}$ at $x_0 \in X$ if there is a neighborhood V of h and $\alpha = \alpha(J, x_0, h) > 0$ such that the inequality $J(x_0 + \varepsilon\bar{h}) \leq J(x_0) - \varepsilon\alpha$ is satisfied for all $\varepsilon \in (0, \varepsilon_0)$ for any $\bar{h} \in V$. Additionally, we say that the functional J is regular decreasing at $x_0 \in X$ if the set of descent directions at x_0 is a convex set.*

Definition 2.4. *Let $h \in X$ and Q_i with $\overset{\circ}{Q}_i \neq \emptyset$ be the set defining the i-th inequality constraint. The vector h is said to be a feasible direction at $x_0 \in X$ if $x_0 + \varepsilon\bar{h} \in Q_i$ for all $\varepsilon \in (0, \varepsilon_0)$, and for any $\bar{h} \in V$, V a neighborhood of h. Additionally, the inequality constraint set Q_i is called regular at $x_0 \in X$ if the set of all feasible directions on Q_i at x_0 is a convex set.*

Definition 2.5. *Let $h \in X$ and Q_i with $\overset{\circ}{Q}_i = \emptyset$ be the set defining the i-th equality constraint. The vector h is said to be a tangent direction at $x_0 \in X$ if for each $\varepsilon \in (0, \varepsilon_0)$ there is $x(\varepsilon) \in Q_i$ such that $x(\varepsilon) = x_0 + \varepsilon h + r(\varepsilon) \in X$ for some neighborhood V of 0, $r(\varepsilon)^{-1} \in V$ for any $\varepsilon > 0$ small enough, or equivalently $\|r(\varepsilon)\| = o(\varepsilon)$. Additionally, if the set of all possible tangent directions is a vectorial subspace, it is said to be a tangent space, and also the equality constraint Q_i is called regular at x_0 if the set of all possible tangent directions for Q_i at x_0 define a convex set.*

Definition 2.6. *A set $K \subset X$, with X a real Banach space, is said to be a cone with vertex at zero if $\lambda x \in K$ for all $\lambda > 0$ and $x \in K$. Moreover, we call the dual cone for K to the set denoted by K^* and defined as follows $K^* = \{\varphi \in X^* : \varphi(x) \geq 0, \forall x \in K\}$.*

Proposition 2.2. *The descent, feasible, and tangent directions generate cones with vertex at zero. Moreover, the cones generated by descent and feasible directions are open sets.*

Theorem 2.3. *[58, Theorem 6.1, p. 40] (Dubovitskii-Milyutin Theorem) Consider the optimization problem* (2.3). *Assume that J has a local minimum at $x_0 \in Q = \bigcap_{i=1}^{n+1} Q_i$, J is regularly decreasing at x_0, with descent directions cone K_0, $Q_i, i = 1, \cdots, n$, are regular at x_0, with feasible directions cone K_i, and Q_{n+1} is regular at x_0, with tangent directions cone K_{n+1}. Then, there exist $n+1$ continuous linear functionals $G_i \in K_i^*$, not all identically zero, such that*

$$\sum_{i=1}^{n+1} G_i = 0.$$

Theorem 2.4. *[60, Theorem 4.21, p. 98] (Lyusternik Theorem) Let X and Y be a real Banach spaces with norms $\|\cdot\|_X$ and $\|\cdot\|_Y$, respectively, $g : X \to Y$ a given mapping, and let some $\overline{x} \in S := \{x \in X : g(x) = 0\}$. If g satisfies the assumptions that g is Fréchet differentiable on a neighborhood of $\bar{x}$, $g'(\cdot)$ is continuous at $\bar{x}$, and $g'(\bar{x})$ is a surjective map, then $\{x \in X : g'(\bar{x})(x) = 0\} \subset K_t(S, \bar{x})$.*

3. Existence of the solution of the state equation system

In this section we analyze the existence and uniqueness of solutions for the system (1.12)–(1.16). Hence we have the following result for (1.12)–(1.16).

Theorem 3.1. *Consider that the assumptions (H1)–(H4) are satisfied. Then, there is at most one strictly positive global strong solution of the system* (1.12)–(1.16) *belonging to $W^{1,2}(0, T; L^2(\Omega))^3$ such that*

$$(S, I, R) \in \left[L^2(0, T; H^2(\Omega))^3 \cap L^\infty(0, T; H^1(\Omega))^3\right], \tag{3.1}$$

$$\left\|\frac{\partial S}{\partial t}\right\|_{L^2(Q_T)} + \|S\|_{L^2(0,T;H^2(\Omega))} + \|S(t, \cdot)\|_{H^1(\Omega)} + \|S\|_{L^\infty(Q_T)} \leq K, \tag{3.2}$$

$$\left\|\frac{\partial I}{\partial t}\right\|_{L^2(Q_T)} + \|I\|_{L^2(0,T;H^2(\Omega))} + \|I(t, \cdot)\|_{H^1(\Omega)} + \|I\|_{L^\infty(Q_T)} \leq K, \tag{3.3}$$

$$\left\|\frac{\partial R}{\partial t}\right\|_{L^2(Q_T)} + \|R\|_{L^2(0,T;H^2(\Omega))} + \|R(t, \cdot)\|_{H^1(\Omega)} + \|R\|_{L^\infty(Q_T)} \leq K, \tag{3.4}$$

for a.e. $t \in [0, T]$ and for some generic positive constant K depending only on $\|\nabla(S_0, I_0, R_0)\|_{L^2(\Omega)}$, $\|(S_0, I_0, R_0)\|_{L^2(\Omega)}$, $\|(S_0, I_0, R_0)\|_{L^\infty(\Omega)}$, $\|f\|_{Lip}$, $\|g\|_{Lip}$, $\beta_\star, \beta^\star$, $\gamma_\star$, and $\gamma^\star$.

Proof. Our proof is based on the application of the theory of evolution equations in Banach spaces, or, to be precise, we use Theorem 2.1. We begin by considering the notation

$$\left.\begin{array}{l} X = L^2(\Omega)^3; \quad D(A) = \mathcal{U}_0; \quad \mathbf{y} = (S, I, R)^\top; \\ A : D(A) \subset X \to X \text{ such that } A\mathbf{y} = (\Delta S, \Delta I, \Delta R)^\top, \\ \mathbf{F} : [0, T] \times X \to X \text{ such that} \\ \mathbf{F}(t, \mathbf{y}(t)) = \Big(-\beta(x) f(y_1(t), y_2(t)) - u(t) g(y_1(t)), \quad p\beta(x) f(y_1(t), y_2(t)) - \gamma(x) y_2(t), \\ \qquad\qquad (1-p)\beta(x) f(y_1(t), y_2(t)) + \gamma(x) y_2(t) + u(t) g(y_1(t))\Big)^\top, \\ \text{and } \mathbf{y}_0 = (S_0, I_0, R_0)^\top. \end{array}\right\} \tag{3.5}$$

Here, "$\top$" indicates the transpose of a vector. Then, system (1.13)–(1.16) is equivalent to the following Cauchy problem:

$$\mathbf{y}'(t) = A\mathbf{y}(t) + \mathbf{F}(t, \mathbf{y}(t)), \quad \mathbf{y}(0) = \mathbf{y}_0. \tag{3.6}$$

We observe that X is a Hilbert space and the operator A is self-adjoint, semi-definite positive, and dissipative on X and $\mathbf{y}_0 \in D(A)$ (see [56] for details). Then, A satisfies the assumption of Theorem 2.1. However, we notice that the function $\mathbf{F}$ does not satisfy the Lipschitz condition required by Theorem 2.1, then we can not apply Theorem 2.1. Hence, the proof is developed by applying similar ideas to those used in [31, 33] to prove the existence of the solutions. The methodology consists of three steps which are described below.

Step (i). *Proof of existence and uniqueness of a local positive bounded solution.* We begin by defining a truncated problem. Let us consider $N > 0$ a fixed large number and the function $\mathbf{F}_N : [0, T] \times X \to X$ defined by

$$\mathbf{F}_N(t, \mathbf{y}(t)) = \begin{cases} \mathbf{F}(t, \mathbf{y}(t)), & \mathbf{y}(t) \in [-N, N]^3, \\ \mathbf{F}(t, P(\mathbf{y}(t))), & \mathbf{y}(t) \in \mathbb{R}^3 - [N, \infty]^3, \end{cases} \tag{3.7}$$

where P from $\mathbb{R}^3$ to $\mathrm{Ima}(P) = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \ : \ 0 \le |x_i \le N, i = 1, 2, 3\}$ is defined as follows:

$$P(x_1, x_2, x_3) = \Big(\xi_N(x_1), \xi_N(x_2), \xi_N(x_3)\Big) \quad \text{with} \quad \xi_N(a) = \min(\max(a, -N), N).$$

Notice that in practice, the truncation in (3.7) means that $\mathbf{y}_j(t)$ is replaced by $-N$ when $\mathbf{y}_j(t) < -N$, $\mathbf{y}_j(t)$ is preserved when $\mathbf{y}_j(t) \in [-N, N]$, and $\mathbf{y}_j(t)$ is replaced by N when $\mathbf{y}_j(t) > N$. Then, the Cauchy problem

$$\mathbf{y}_N'(t) = A\mathbf{y}_N(t) + \mathbf{F}_N(t, \mathbf{y}_N(t)), \quad \mathbf{y}_N(0) = \mathbf{y}_0 \tag{3.8}$$

is called the truancated Cauchy problem in the sense that it is a truncation of (3.6).

The existence of solutions for (3.8) is a consequence of Theorem 2.1 since we observe that assumption (H3) implies that the function $\mathbf{F}_N$ satisfies the Lipschitz hypothesis required by Theorem 2.1. For instance, one of the main estimates in the Lipschitz proof of $\mathbf{F}_N$ is the following:

$$\begin{aligned} \Big|\beta(x) f(\hat{a}, \hat{b}) - \beta(x) f(\bar{a}, \bar{b})\Big| &\le \beta^\star \Big\{\Big|f(\hat{a}, \hat{b}) - f(\bar{a}, 0)\Big| + \Big|f(0, \hat{b}) - f(\bar{a}, \bar{b})\Big|\Big\} \\ &\le \beta^\star \max\left\{\frac{|f(\hat{a}, \hat{b}) - f(\bar{a}, 0)|}{|\hat{a} - \bar{a}|} + \frac{|f(0, \hat{b}) - f(\bar{a}, \bar{b})|}{|\hat{b} - \bar{b}|}\right\}\Big(|\hat{a} - \bar{a}| + |\hat{b} - \bar{b}|\Big), \end{aligned}$$

which implies the Lipschitz hypothesis by the local Lipschitz assumption on f. Then, we can deduce that the Cauchy problem (3.8) has a unique strong solution $\mathbf{y}_N \in W^{1,2}(0,T;X)^3$ with $\mathbf{y}_N \in \left[L^2(0,T;H^2(\Omega))^3 \cap L^\infty(0,T;H^1(\Omega))^3\right]$.

In order to prove the boundedness of $\mathbf{y}_N$, we consider the uncoupled Cauchy problems

$$\mathbf{y}^{\pm\prime}_N(t) = A\mathbf{y}_N^{\pm} + \mathbf{F}_N(t,\mathbf{y}_N(t)) \pm \mathbf{M}, \quad \mathbf{y}_N^{\pm}(0) = \mathbf{y}_0 \pm \tilde{\mathbf{y}}_0, \tag{3.9}$$

where $\tilde{\mathbf{y}}_0 = \left(\|S_0\|_{L^\infty(\Omega)}, \|I_0\|_{L^\infty(\Omega)}, \|R_0\|_{L^\infty(\Omega)}\right)$, $\mathbf{M} = \left(\overline{M}, \overline{M}, \overline{M}\right)$ with $\overline{M} = \max\left\{\|\mathbf{F}\|_{L^\infty(\mathbb{R}^3)}, \left\|\mathbf{y}_0\right\|_{L^\infty(Q_T)}\right\}$, and we develop some estimates. We notice that the following two facts: the strong solution of (3.9) satisfies

$$\mathbf{y}_N^{\pm}(t) = e^{At}(\mathbf{y}_0 \pm \hat{\mathbf{y}}_0) + \int_0^t \left[e^{A(t-s)}\left(\mathbf{F}_N(s,\mathbf{y}_N(s)) \pm \mathbf{M}\right)\right] ds; \tag{3.10}$$

and the components of $\mathbf{y}_0 - \hat{\mathbf{y}}_0$ and $\mathbf{F}_N(s,\mathbf{y}_N(s)) - \mathbf{M}$ are negative for all $t \geq 0$ as a consequence of the definition of $\mathbf{M}$ and $\tilde{\mathbf{y}}_0$. We notice that e^{At} is positive since A is a self-adjoint and semi-definite positive operator [61, Theorem 1.7, p. 79]. From (3.10), we deduce that each component of $\mathbf{y}_N^-(t)$ is negative for all $t \geq 0$. Similarly, we deduce that the components of $\mathbf{y}_N^+(t)$ are positive for all $t \geq 0$, since $\mathbf{y}_0 + \hat{\mathbf{y}}_0$ and $\mathbf{F}_N(t,\mathbf{y}_N(t)) + \mathbf{M}$ are positive for all $t \geq 0$. In addition, if we consider the function

$$\mathbf{y}_N^{\pm}(t,x) = \mathbf{y}_N(t,x) \pm \mathbf{M}t \pm \tilde{\mathbf{y}}_0, \tag{3.11}$$

we observe that it satisfies system (3.9), and, of course, the equation (3.10). We notice that $\mathbf{y}_N(t,x) = \mathbf{y}_N^-(t,x) + \mathbf{M}t + \tilde{\mathbf{y}}_0 \leq \mathbf{M}t + \tilde{\mathbf{y}}_0$, since $\mathbf{y}_N^-$ is negative. Then, from (3.10) and (3.11), we get the following bound:

$$\left\|\mathbf{y}_N(t,\cdot)\right\|_{L^\infty(\Omega)} \leq \overline{M}t + \left\|\mathbf{y}_0\right\|_{L^\infty(\Omega)}, \tag{3.12}$$

or equivalently $\mathbf{y}_N \in L^\infty(Q_T)$ with the bound $\overline{M}T + \left\|\mathbf{y}_0\right\|_{L^\infty(\Omega)}$, which does not depend on N.

In order to prove the positivity of $\mathbf{y}_N$, we rewrite (3.8) as the system

$$\partial_t \mathbf{y}_N(t,x) = \Delta \mathbf{y}_N(t,x) + \mathbf{F}_N(t,\mathbf{y}_N(t,x)) \quad \text{on } Q_T, \tag{3.13}$$

$$\nabla \mathbf{y}_{N,1}\cdot\eta = \nabla \mathbf{y}_{N,2}\cdot\eta = \nabla \mathbf{y}_{N,3}\cdot\eta = 0 \quad \text{on } \Sigma_T, \tag{3.14}$$

$$\mathbf{y}_N(0,x) = \mathbf{y}_0(x), \quad \text{on } \Omega. \tag{3.15}$$

Then, using the notation $\mathbf{y}_{N,i}^{\top} = \sup\left\{\mathbf{y}_{N,i}, 0\right\}$ and $\mathbf{y}_{N,i}^{\perp} = -\inf\left\{\mathbf{y}_{N,i}, 0\right\}$, for $i = 1,2,3$, we deduce some estimations for (3.13)–(3.15), which implies the positivity of the solution of the truncated problem (3.8). In order to get the desired estimates, if we multiply the i-th equation of (3.13) by $\mathbf{y}_{N,i}^{\perp}$ and integrate on $[0,t]\times\Omega$, we deduce that

$$\int_0^t \int_\Omega \partial_s \mathbf{y}_{N,i}^{\perp}\mathbf{y}_{N,i}^{\perp} dxds = \int_0^t \int_\Omega \Delta \mathbf{y}_{N,i}^{\perp}\mathbf{y}_{N,i}^{\perp} dxds + \int_0^t \int_\Omega \mathbf{F}_N(s,\mathbf{y}_N)\cdot \mathbf{y}_N^{\perp} dxds.$$

Using the identity $\partial_s(\mathbf{y}_{N,i}^2) = 2\partial_s \mathbf{y}_{N,i}\mathbf{y}_{N,i}$, the Green's identity, and the boundary conditions (3.14), we have that

$$\int_\Omega \left[\mathbf{y}_{N,i}^{\perp}(t,x)\right]^2 dx = \int_\Omega \left[\mathbf{y}_{N,i}^{\perp}(0,x)\right]^2 dx - 2\int_0^t \int_\Omega \left|\nabla \mathbf{y}_{N,i}^{\perp}(s,x)\right|^2 d\mathbf{x}ds$$

$$+2\int_0^t\int_\Omega \mathbf{F}_{N,i}(s,\mathbf{y}_N(s,x))\mathbf{y}_{N,i}^{\perp}(s,x)dxds.$$

Now, using assumption (H2), we have that $\mathbf{y}_{N,i}^{\perp}(0,x)=0$, and using (H3), we deduce the bound

$$\int_\Omega \left|\mathbf{y}_{N,i}^{\perp}(t,x)\right|^2 dx \leq K_i \int_0^t\int_\Omega \left|\mathbf{y}_{N,i}^{\perp}(t,x)\right|^2 dxds,$$

for some positive constants K_i. If we apply the integral Gronwall's inequality, we deduce that $\int_\Omega \left|\mathbf{y}_{N,i}^{\perp}(t,x)\right|^2 dx \leq 0$, or equivalently $\mathbf{y}_{N.i}^{\perp}(t,x)=0$ on $[0,t]\times\Omega$ for each $i=1,2,3$. Hence, we have that $\mathbf{y}_{N,i}(t,x)=\mathbf{y}_{N,i}^{\top}(t,x)$ on $[0,t]\times\Omega$ for all $t\geq 0$, or equivalently the components of $\mathbf{y}_N$ are strictly positive on Q_T.

The existence and uniqueness of a positive local solution of the system (1.13)–(1.16) is deduced by the following arguments. If we select $N>2\cdot\left\|\mathbf{y}_0\right\|_{L^\infty(\Omega)}$ to define the truncated problem, we observe that $\overline{M}\theta+\left\|\mathbf{y}_0\right\|_{L^\infty(\Omega)}\leq N/2$ is satisfied for some $\theta\in[0,T]$. From (3.12), we have that $\left|\mathbf{y}_{N,i}(t,x)\right|\leq N$ on $[0,\theta]\times\Omega$ for , $i=1,2,3$. Then, from (3.7), we have that $\mathbf{F}_N=\mathbf{F}$ for $t\in]0,\theta]$, and, consequently, $\mathbf{y}_N$ is a solution of (1.12)–(1.16) on $[0,\theta]\times\Omega$.

Step (ii). *The local solution is a global solution.* To achieve this purpose it is sufficient to prove that $\mathbf{y}_N$ is bounded on $[0,\theta]\times\Omega$. From (3.8), by adding the equations of the system, we have that

$$\begin{aligned}
&\partial_t(\mathbf{y}_{N,1}+\mathbf{y}_{N,2}+\mathbf{y}_{N,3})-\Delta(\mathbf{y}_{N,1}+\mathbf{y}_{N,2}+\mathbf{y}_{N,3})=0, && \text{in} \quad]0,\theta[\times\Omega,\\
&\nabla(\mathbf{y}_{N,1}+\mathbf{y}_{N,2}+\mathbf{y}_{N,3})\cdot\eta=0, && \text{on} \quad]0,\theta[\times\partial\Omega,\\
&(\mathbf{y}_{N,1}+\mathbf{y}_{N,2}+\mathbf{y}_{N,3})(x,0)=(S_0+I_0+R_0)(x), && \text{in} \quad \Omega.
\end{aligned}$$

The positivity of $\mathbf{y}_{N,i}$ on $[0,\theta]\times\Omega$ (proved in Step (i)) and the weak maximum principle (see [41]) imply that $0\leq(\mathbf{y}_{N,1}+\mathbf{y}_{N,2}+\mathbf{y}_{N,3})(x,t)\leq\|S_0+I_0+R_0\|_{L^\infty(\Omega)}$ on $[0,\theta]\times\Omega$, i.e., $\mathbf{y}_N$ is is bounded on $[0,\theta]\times\Omega$. Moreover, by the regularity of the local solution resulting from the application of Theorem 2.1, we conclude that the solution of system (1.13) and (1.14) is positive on Ω and has the regularity $(S,I,R)\in L^\infty(Q_T)^3\cap W^{1,2}(0,T;L^2(\Omega))^3$ and $(S,I,R)\in L^2(0,T,H^2(\Omega))^3$, which prove (3.1).

Step (iii). *Proof of the estimates* (3.2)–(3.4). From (1.13), by squaring both sides and integrating on $\Omega\times(0,t)$, we get

$$\begin{aligned}
&\int_0^t\int_\Omega\Big(-\beta(x)f(S,I)-u(t)g(S)\Big)^2dxds=\int_0^t\int_\Omega\Big(\partial_tS-\Delta S\Big)^2dxds\\
&=\int_0^t\int_\Omega|\partial_tS|^2\,dxds-2\int_0^t\int_\Omega\partial_tS\,\Delta S\,dxds+\int_0^t\int_\Omega|\Delta S|^2\,dxds\\
&=\int_0^t\int_\Omega|\partial_tS|^2\,dxds-2\left[\int_0^t\int_{\partial\Omega}\partial_tS\,\nabla S\cdot\eta d\sigma ds-\int_0^t\int_\Omega\nabla(\partial_tS)\cdot\nabla S\,dxds\right]+\int_0^t\int_\Omega|\Delta S|^2\,dxds\\
&=\int_0^t\int_\Omega|\partial_tS|^2\,dxds-2\left[-\int_0^t\int_\Omega\frac{1}{2}\partial_t\left(|\nabla S|^2\right)dxds\right]+\int_0^t\int_\Omega|\Delta S|^2\,dxds\\
&=\int_0^t\int_\Omega|\partial_tS|^2\,dxds+\int_\Omega|\nabla S|^2\Big|_0^t\,dx+\int_0^t\int_\Omega|\Delta S|^2\,dxds
\end{aligned}$$

$$= \int_0^t \int_\Omega |\partial_t S|^2 \, dxds + \int_0^t \int_\Omega |\Delta S|^2 \, dxds + \int_\Omega |\nabla S|^2 \, dx - \int_\Omega |\nabla S_0|^2 \, dx.$$

This identity implies (3.2) by using assumptions (H2)–(H4), and the fact that S and I are bounded and positive. The estimates on (3.3) and (3.4) are deduced by similar arguments by starting from (1.13) and (1.14). □

4. Analysis of the optimal control problem

In this section, we analyze the optimal control problem (1.19), getting the existence of solutions and the characterization of the optimal solutions.

4.1. Existence of the solution to the optimal control problem

In this section, we analyze the existence of solutions to the optimal control problem (1.19). More precisely, we have the following result.

Theorem 4.1. *Consider that the assumptions (H1)–(H3) and (H5) are satisfied. Then, the optimal control problem* (1.19) *admits at least one solution.*

Proof. Let us consider $J_0 = \inf\left\{J(S,I,R,\beta,\gamma,u) : (S,I,R,\beta,\gamma,u) \in E\right\}$. We notice that (S,I,R) is the solution of the direct problem (1.12)–(1.16) corresponding to $(\beta,\gamma,u) \in \mathcal{U}_{ad}$. By the definition of J and the regularity of the state equation solution of the we follow that J is bounded, consequently, J_0 is finite. It follows that there exists a sequence $(S_n, I_n, R_n, \beta_n, \gamma_n, u_n)_{n\in\mathbb{N}}$ belong to E such that

$$J_0 \le J(S_n, I_n, R_n, \beta_n, \gamma_n, u_n) \le J_0 + \frac{1}{n} \tag{4.1}$$

and $M(S_n, I_n, R_n, \beta_n, \gamma_n, u_n) = 0$. We observe that $M(S_n, I_n, R_n, \beta_n, \gamma_n, u_n) = 0$ means that (S_n, I_n, R_n) satisfies system (1.12)–(1.16) with (β_n, γ_n, u_n) instead of (β, γ, u), or, more precisely,

$$\partial_t S_n - \Delta S_n = -\beta_n(x) f(S_n, I_n) - u(t) g(S_n), \quad \text{in} \quad Q_T, \tag{4.2}$$
$$\partial_t I_n - \Delta I_n = p\beta_n(x) f(S_n, I_n) - \gamma_n(x) I_n, \quad \text{in} \quad Q_T, \tag{4.3}$$
$$\partial_t R_n - \Delta R_n = (1-p)\beta_n(x) f(S_n, I_n) + \gamma_n(x) I_n + u(t) g(S_n), \quad \text{in} \quad Q_T, \tag{4.4}$$
$$\nabla S_n \cdot \eta = \nabla I_n \cdot \eta = \nabla R_n \cdot \eta = 0, \quad \text{on} \quad \Sigma_T, \tag{4.5}$$
$$(S_n, I_n, R_n)(0,x) = (S_0, I_0, R_0)(x), \quad \text{in} \quad \Omega. \tag{4.6}$$

Then, applying Theorem 3.1 to the system (4.2)–(4.6), it is obtained that

$$(S_n, I_n, R_n) \in \left[L^2(0,T;H^2(\Omega))^3 \cap L^\infty(0,T;H^1(\Omega))^3\right], \quad \|\partial_t(S_n, I_n, R_n)\|_{L^2(Q_T)^3} \le K, \tag{4.7}$$
$$\|(S_n, I_n, R_n)\|_{L^2(0,T;H^2(\Omega))^3} \le K, \quad \|(S_n, I_n, R_n)(t,\cdot)\|_{H^1(\Omega)^3} \le K, \quad \|(S_n, I_n, R_n)\|_{L^\infty(Q_T)^3} \le K, \tag{4.8}$$

where K is a generic positive constant (independent of n and $(S_n, I_n, R_n, \beta_n, \gamma_n, u_n)$).

We can prove that (S_n, I_n, R_n) is compact in $C([0,T];L^2(\Omega))^3$ by applying integration by parts and developing some estimates as specified below. Testing Eqs (4.2)–(4.4) with S_n, I_n, and R_n, respectively, integrating over $\Omega \times [0, t]$, using the boundary and the initial conditions (4.5) and (4.6), we deduce the identities

$$\int_\Omega |S_n(x,t)|^2 dx = \int_\Omega |S_0(x)|^2 dx - \int_0^t \int_\Omega |\nabla S_n(x,s)| dx ds$$
$$- \int_0^t \int_\Omega \Big[-\beta_n(x) f(S_n(x,\tau), I_n(x,\tau)) - u(\tau) g(S_n(x,\tau)) \Big] S_n(x,\tau) dx d\tau,$$
$$\int_\Omega |I_n(x,t)|^2 dx = \int_\Omega |I_0(x)|^2 dx - \int_0^t \int_\Omega |\nabla I_n(x,\tau)| dx d\tau$$
$$- \int_0^t \int_\Omega \Big[p\beta_n(x) f(S_n(x,\tau), I_n(x,\tau)) - \gamma_n(x) I_n(x,\tau) \Big] I_n(x,\tau) dx d\tau,$$
$$\int_\Omega |R_n(x,t)|^2 dx = \int_\Omega |R_0(x)|^2 dx - \int_0^t \int_\Omega |\nabla R_n(x,\tau)| dx d\tau$$
$$- \int_0^t \int_\Omega \Big[(1-p)\beta_n(x) f(S_n(x,\tau), I_n(x,\tau)) + \gamma_n(x) I_n(x,\tau) + u(\tau) g(S_n(x,\tau)) \Big] R_n(x,\tau) dx d\tau.$$

We observe that the previous expressions hold for all $t > 0$. Similar identities are valid if we consider $s > 0$ instead of t. Then, subtracting the corresponding expressions for s and t, using estimations (4.7) and (4.8) and assumptions (H3)–(H4), it follows that

$$\left| \int_\Omega (S_n)^2(t,x) dx - \int_\Omega (S_n)^2(s,x) dx \right| \le K\,|t-s|\,,$$
$$\left| \int_\Omega (I_n)^2(t,x) dx - \int_\Omega (I_n)^2(s,x) dx \right| \le K\,|t-s|\,,$$
$$\left| \int_\Omega (R_n)^2(t,x) dx - \int_\Omega (R_n)^2(s,x) dx \right| \le K\,|t-s|\,.$$

Hence, by application of the Ascoli-Arzela theorem ([62, Theorem A.2.1, p. 296]), we deduce that (S_n, I_n, R_n) is compact in $C([0,T]; L^2(\Omega))^3$, and using (4.7) and (4.8) together with the compact embedding of $H^1(\Omega)$ in $L^2(\Omega)$, we also deduce that $(S_n, I_n, R_n)(t,\cdot)$ is compact in $L^2(\Omega)^3$.

From the compactness results for the sequence $(S_n, I_n, R_n)_{n\in\mathbb{N}}$, estimates (4.7) and (4.8), and the definition of $\mathcal{U}_{ad}$, we have the existence of $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u}) \in E$ and a subsequence of the minimizing sequence $(S_n, I_n, R_n, \beta_n, \gamma_n, u_n)_{n\in\mathbb{N}}$, also denoted by $(S_n, I_n, R_n, \beta_n, \gamma_n, u_n)_{n\in\mathbb{N}}$, such that

$$(S_n, I_n, R_n) \longrightarrow (\overline{S}, \overline{I}, \overline{R}) \text{ in } L^2(\Omega)^3 \text{ uniformly with respect to } t,$$
$$\Delta(S_n, I_n, R_n) \rightharpoonup \Delta(\overline{S}, \overline{I}, \overline{R}) \text{ in } L^2(Q_T)^3,$$
$$\partial_t(S_n, I_n, R_n) \rightharpoonup \partial_t(\overline{S}, \overline{I}, \overline{R}) \text{ in } L^2(Q_T)^3,$$
$$(S_n, I_n, R_n) \rightharpoonup (\overline{S}, \overline{I}, \overline{R}) \text{ in } L^2(0,T; H^2(\Omega))^3,$$
$$(\beta_n, \gamma_n, u_n) \rightharpoonup (\overline{\beta}, \overline{\gamma}, \overline{u}) \text{ in } L^\infty(\Omega)^2 \times L^\infty([0,T]).$$

Here we have used the fact that the boundedness of $\Delta(S_n, I_n, R_n)$ in $L^2(Q_T)^3$ implies the weak convergence. Therefore, passing to the limit in (4.2)–(4.6), it follows that $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u})$ satisfies the system (1.12)–(1.16), i.e., $M(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u}) = 0$, and consequently $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u}) \in \mathcal{D}$. From (4.1), it is concluded that $J_0 = (\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u})$. □

4.2. Definition and analysis of the adjoint system

Let us consider that $(\overline{S},\overline{I},\overline{R},\overline{\beta},\overline{\gamma},\overline{u}) \in \mathcal{D}$ is a solution of the optimal control problem (1.18). We notice that $M(\overline{S},\overline{I},\overline{R},\overline{\beta},\overline{\gamma},\overline{u}) = 0$ means that $(\overline{S},\overline{I},\overline{R})$ satisfies the system (1.12)–(1.16) with $(\overline{\beta},\overline{\gamma},\overline{u})$ instead of (β,γ,u).

$$
\begin{aligned}
\partial_t w_1 + \Delta w_1 &= \overline{\beta}(x)\partial_1 f(\overline{S},\overline{I})\Big(w_1 - pw_2 - (1-p)(w_3+k_5)\Big) + \overline{u}(t)g'(\overline{S})(w_1 - w_3) \\
&\quad - k_4\overline{u}(t)\Big(c'(\overline{S})g(\overline{S}) + c(\overline{S})g'(\overline{S})\Big), && \text{in } Q_T, \quad (4.9)\\
\partial_t w_2 + \Delta w_2 &= \overline{\beta}(x)\partial_2 f(\overline{S},\overline{I})\Big(w_1 - pw_2 - (1-p)(w_3+k_5)\Big) + \overline{\gamma}(x)(w_2 - w_3) - k_3, && \text{in } Q_T, \quad (4.10)\\
\partial_t w_3 + \Delta w_3 &= 0, && \text{in } Q_T, \quad (4.11)\\
\nabla w_1\cdot\eta &= \nabla w_2\cdot\eta = \nabla w_3\cdot\eta = 0, && \text{on } \Sigma_T, \quad (4.12)\\
(w_1,w_2,w_3)(x,T) &= \Big(k_1(\overline{S}-S^d), k_1(\overline{I}-I^d) + k_7, k_1(\overline{R}-R^d)\Big)(x), && \text{in } \Omega. \quad (4.13)
\end{aligned}
$$

For system (4.9)–(4.13), we have the following result. For details on the deduction of the adjoint systems on optimal control problems, we refer to [64].

Theorem 4.2. *Consider that the assumptions of Theorem 4.1 are satisfied, and assume that* $(\overline{S},\overline{I},\overline{R},\overline{\beta},\overline{\gamma},\overline{u}) \in \mathcal{D}$ *is a solution of the optimal control problem* (1.19). *Then, the adjoint system* (4.9)–(4.13) *has at least one solution such that* $(w_1,w_2,w_3) \in \Big[W^{1,2}(0,T;L^2(\Omega))\Big]^3$.

The proof of Theorem 4.2 can be developed by reformulating the end backward boundary value problem (4.9)–(4.13) as an initial boundary value problem by introducing the change of variables $s = T - t$ and $\mathbf{w}^\star(s,x) = \mathbf{w}(T-s,x)$ and using the standard theory for linear parabolic systems [41]. Moreover, using the regularity of $(\overline{S},\overline{I},\overline{R})$ obtained by the application of Theorem 3.1 and assumptions (H1)–(H5), we deduce the proof of the theorem. Alternatively, the proof follows by an argument similar to that of the one presented in the proof of Theorem 3.1.

4.3. Differentiability of J and M, and cones (descent, tangent, and its dual) to J

To apply Theorem 2.3, we shall determine the cones of direction of descent, $K_d(J,(S,I,R.\beta,\gamma,u))$ and tangent $K_t(\mathcal{D},(S,I,R.\beta,\gamma,u))$, or K_d and K_t for short.

Theorem 4.3. *Consider J is the cost function defined in* (1.17) *and the operator M defined on the equations* (1.20)–(1.25)*, defining the constraint set of the optimization problem given in* (1.19). *Then, J is Frechet differentiable with derivative*

$$
\begin{aligned}
J'_G &:= J'(S,I,R,\beta,\gamma)(\tilde{S},\tilde{I},\tilde{R},\tilde{\beta},\tilde{\gamma})\\
&= k_1\int_\Omega \Big((S(x,T)-S^d(x))\tilde{S}(x,T) + (I(x,T)-I^d(x))\tilde{I}(x,T) + (R(x,T)-R^d(x))\tilde{I}(x,T)\Big)dx\\
&\quad + k_2\int_\Omega \Big(\nabla\beta(x)\nabla\tilde{\beta}(x) + \nabla\gamma(x)\nabla\tilde{\gamma}(x)\Big)dx + k_3\iint_{Q_T}\tilde{I}(x,t)dxdt\\
&\quad + k_4\iint_{Q_T}\Big(c'(\tilde{S}(x,t))g(S(x,t)) + c(S(x,t))g'(\tilde{S}(x,t))\Big)\tilde{S}(x,t)u(t) + c(S(x,t))g(S(x,t))\tilde{u}(t)dxdt\\
&\quad + k_5\iint_{Q_T}(1-p)\beta(x)\Big(\partial_1 f(\tilde{S}(x,t),I(x,t))\tilde{S}(x,t) + \partial_2 f(S(x,t),\tilde{I}(x,t))\tilde{I}(x,t)\Big)dxdt
\end{aligned}
$$

$$+ k_6 \int_0^T \tilde{u}(t)dt + k_7 \int_\Omega \tilde{I}(x,T)\, dx, \tag{4.14}$$

and the following properties are satisfied:

(a) The descent and dual cones of J, K_d and K_d^*, are given by the sets

$$K_d = \Big\{(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) \in E \ : \ J'_G < 0\Big\}, \text{ and } K_d^* = \Big\{ -\lambda J'_G : \lambda \geq 0\Big\}. \tag{4.15}$$

(b) M is Gâteaux differentiable with derivative M'_G satisfying the identity

$$M'_G(S, I, R, \beta, \gamma)(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) = (\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3, \tilde{\psi}_4, \tilde{\psi}_5, \tilde{\psi}_6), \tag{4.16}$$

for any $(S, I, R, \beta, \gamma) \in E$ if and only if

$$\partial_t \tilde{S} - \Delta \tilde{S} + \tilde{\beta}(x) f(S, I) + \beta(x) \nabla f(S, I) \cdot (\tilde{S}, \tilde{I}) + \tilde{u}(t) g(S) + \tilde{S} u(t) g'(S) = \tilde{\psi}_1, \quad \text{in } Q_T, \tag{4.17}$$

$$\partial_t \tilde{I} - \Delta \tilde{I} - \tilde{\beta}(x) f(S, I) - p\beta(x) \nabla f(S, I) \cdot (\tilde{S}, \tilde{I}) + \tilde{\gamma}(x) I + \gamma(x) \tilde{I} = \tilde{\psi}_2, \quad \text{in } Q_T, \tag{4.18}$$

$$\begin{aligned}\partial_t \tilde{R} - \Delta \tilde{R} - (1-p)\tilde{\beta}(x) f(S, I) - (1-p)\beta(x) \nabla f(S, I) \cdot (\tilde{S}, \tilde{I}) - \tilde{\gamma}(x) I \\ - \gamma(x)\tilde{I} - \tilde{u}(t) g(S) - \tilde{S} u(t) g'(S) = \tilde{\psi}_3, \quad \text{in } Q_T,\end{aligned} \tag{4.19}$$

$$\nabla \tilde{S} \cdot \eta = \nabla \tilde{I} \cdot \eta = \nabla \tilde{R} \cdot \eta = 0, \quad \text{in } \Gamma_T, \tag{4.20}$$

$$(\tilde{S}, \tilde{I}, \tilde{R})(x, 0) = (\tilde{\psi}_4, \tilde{\psi}_5, \tilde{\psi}_6), \quad \text{on } \Omega. \tag{4.21}$$

(c) M is strictly differentiable and its derivative is a surjective operator.

(d) The tangent cone to the set $\mathcal{D}$ at $(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma})$, K_t, and its dual, K_t^*, are given by the sets

$$K_t = \Big\{(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) \in E \ : \ M'(S, I, R, \beta, \gamma)(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) = 0\Big\}, \tag{4.22}$$

$$K_t^* = \Big\{\mathcal{L} \in E' \ : \ \mathcal{L}(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) = 0, \ \forall (\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) \in K_t\Big\}. \tag{4.23}$$

Additionally K_t is a vector space.

Proof. [(a)] Using the definition of J given in (1.17), it is straightforward to deduce that J is Gâteaux differentiable and continuous, and so consequently it is Frechet differentiable, and its derivative is defined by the expression given in (4.14). We notice that J'_G is a convex and continuous operator. Then, from the results presented in [58], we deduce that if J is regularly decreasing for all $(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}) \in E$, the descent cone and its dual are defined by the sets given in (4.15), and we refer to [58, Theorem 10.2, p. 69] for details.

[(b)] Using the definition of M given in (1.20)–(1.25), by evaluating the operator M at the points $(S + k\tilde{S}, I + k\tilde{I}, R + k\tilde{R}, \beta + k\tilde{\beta}, \gamma + k\tilde{\beta})$ and (S, I, R, β, γ) and developing the difference of the results, we get that $\delta\mathbf{M} := M(S + k\tilde{S}, I + k\tilde{I}, R + k\tilde{R}, \beta + k\tilde{\beta}, \gamma + k\tilde{\beta}) - M(S, I, R, \beta, \gamma)$ with

$$\begin{aligned}\delta\mathbf{M}_1 =& k\partial_t \tilde{S} - k\Delta\tilde{S} + (\beta + k\tilde{\beta})(x) f(S + k\tilde{S}, I + k\tilde{I}) - \beta(x) f(S, I) \\ &+ (u + k\tilde{u})(t) g(S + k\tilde{S}) - u(t) g(S), \\ \delta\mathbf{M}_2 =& k\partial_t \tilde{I} - k\Delta\tilde{I} - p(\beta + k\tilde{\beta})(x) f(S + k\tilde{S}, I + k\tilde{I}) + p\beta(x) f(S, I) \\ &+ (\gamma + k\tilde{\gamma})(x)(I + k\tilde{I}) - \gamma(x) I,\end{aligned}$$

$$\begin{aligned}\delta\mathbf{M}_3 =& k\partial_t\tilde{R} - k\Delta\tilde{R} - (1-p)(\beta + k\tilde{\beta})(x)f(S+k\tilde{S}, I+k\tilde{I})\\ &+ (1-p)\beta(x)f(S,I) - (\gamma + k\tilde{\gamma})(x)(I+k\tilde{I}) + \gamma(x)I\\ &- (u+k\tilde{u})(t)g(S+k\tilde{S}) + u(t)g(S),\\ \delta\mathbf{M}_4 =& k\tilde{S}(x,0), \quad \delta\mathbf{M}_5 = k\tilde{I}(x,0), \quad \delta\mathbf{M}_6 = k\tilde{R}(x,0).\end{aligned}$$

Then, using the fact that

$$\begin{aligned}&(\beta + k\tilde{\beta})(x)f(S+k\tilde{S}, I+k\tilde{I}) - \beta(x)f(S,I)\\ &\quad = k\tilde{\beta}(x)f(S+k\tilde{S}, I+k\tilde{I})\\ &\qquad + k\beta(x)\left[\frac{f(S+k\tilde{S}, I+k\tilde{I}) - f(S, I+k\tilde{I})}{(S+k\tilde{S})-S}\right]\tilde{S} + k\beta(x)\left[\frac{f(S, I+k\tilde{I}) - f(S,I)}{(I+k\tilde{I})-I}\right]\tilde{I},\\ &(u+k\tilde{u})(t)g(S+k\tilde{S}) - u(t)g(S) = k\tilde{u}(t)g(S+k\tilde{S}) + ku(t)\left[\frac{g(S+k\tilde{S}) - g(S)}{(S+k\tilde{S})-S}\right]\tilde{S},\\ &(\gamma + k\tilde{\gamma})(x)(I+k\tilde{I}) - \gamma(x)I = k\tilde{\gamma}(x)(I+k\tilde{I}) + k\gamma(x)\tilde{I},\end{aligned}$$

and the definitions of $\hat{\psi}_i$ given on (4.17)–(4.21), we get

$$\begin{aligned}&\frac{\delta\mathbf{M}_1}{k} - \tilde{\psi}_1 = \tilde{\beta}(x)\left[f(S+k\tilde{S}, I+k\tilde{I}) - f(S,I)\right]\\ &+ \beta(x)\left\{\left[\frac{f(S+k\tilde{S}, I+k\tilde{I}) - f(S, I+k\tilde{I})}{(S+k\tilde{S})-S}\right]\tilde{S} + \left[\frac{f(S, I+k\tilde{I}) - f(S,I)}{(I+k\tilde{I})-I}\right]\tilde{I} - \nabla f(S,I)\cdot(\tilde{S},\tilde{I})\right\}\\ &+ \tilde{u}(t)\left[g(S+k\tilde{S}) - g(S)\right] + u(t)\left\{\left[\frac{g(S+k\tilde{S}) - g(S)}{(S+k\tilde{S})-S}\right] - g'(S)\right\}\tilde{S},\\ &\frac{\delta\mathbf{M}_2}{k} - \tilde{\psi}_2 = -p\tilde{\beta}(x)\left[f(S+k\tilde{S}, I+k\tilde{I}) - f(S,I)\right]\\ &- p\beta(x)\left\{\left[\frac{f(S+k\tilde{S}, I+k\tilde{I}) - f(S, I+k\tilde{I})}{(S+k\tilde{S})-S}\right]\tilde{S} + \left[\frac{f(S, I+k\tilde{I}) - f(S,I)}{(I+k\tilde{I})-I}\right]\tilde{I} - \nabla f(S,I)\cdot(\tilde{S},\tilde{I})\right\} + k\tilde{I},\\ &\frac{\delta\mathbf{M}_3}{k} - \tilde{\psi}_3 = -(1-p)\tilde{\beta}(x)\left[f(S+k\tilde{S}, I+k\tilde{I}) - f(S,I)\right]\\ &- (1-p)\beta(x)\left\{\left[\frac{f(S+k\tilde{S}, I+k\tilde{I}) - f(S, I+k\tilde{I})}{(S+k\tilde{S})-S}\right]\tilde{S} + \left[\frac{f(S, I+k\tilde{I}) - f(S,I)}{(I+k\tilde{I})-I}\right]\tilde{I} - \nabla f(S,I)\cdot(\tilde{S},\tilde{I})\right\}\\ &- k\tilde{I} - \tilde{u}(t)\left[g(S+k\tilde{S}) - g(S)\right] - u(t)\left\{\left[\frac{g(S+k\tilde{S}) - g(S)}{(S+k\tilde{S})-S}\right] - g'(S)\right\}\tilde{S},\\ &\frac{\delta\mathbf{M}_4}{k} - \tilde{\psi}_4 = \frac{\delta\mathbf{M}_5}{k} - \tilde{\psi}_5 = \frac{\delta\mathbf{M}_6}{k} - \tilde{\psi}_6 = 0.\end{aligned}$$

Moreover, we note that

$$\begin{aligned}&\lim_{k\to 0}\left\|\left(\frac{f(S+k\tilde{S}, I+k\tilde{I}) - f(S, I+k\tilde{I})}{(S+k\tilde{S})-S}, \frac{f(S, I+k\tilde{I}) - f(S,I)}{(I+k\tilde{I})-I}\right) - \nabla f(S,I)\right\|_{\tilde{E}} = 0\\ &\lim_{k\to 0}\left\|\frac{g(S+k\tilde{S}) - g(S)}{(S+k\tilde{S})-S} - g'(S)\right\|_{\tilde{E}} = 0.\end{aligned}$$

Hence, we can deduce that $||\delta\mathbf{M}/k - (\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3, \tilde{\psi}_4, \tilde{\psi}_5, \tilde{\psi}_6)||_{\tilde{E}} \to 0$ when $k \to 0$, and, consequently, by the Gâteaux derivative definition, we conclude the proof of [(b)].

[(c)] In order to prove that M' is a surjective operator, we choose an arbitrary $(\tilde{\xi}_1, \tilde{\xi}_2, \tilde{\xi}_3, \tilde{\xi}_4, \tilde{\xi}_5, \tilde{\xi}_6) \in \tilde{E}$ and using the methodology used to prove Theorem 3.1, we get that the solution of the system (4.17)–(4.21) belongs to $(\tilde{S}, \tilde{I}, \tilde{R}) \in W^{1,2}(0, T; H)^3$. We observe that $(S, I, R, \beta, \gamma) \mapsto M'_G(S, I, R, \beta, \gamma)$ is continuous, since, by using the continuous Sobolev inclusion $H^2(\Omega) \subset L^\infty(\Omega)$, we deduce that $M'_G(S, I, R, \beta, \gamma)$ is bounded in the norm of $\tilde{E}$. Then, M is strictly differentiable.

[(d)] From items (b) and (c), we get that M is is Gâteaux differentiable and M'_G is continuous and surjective. Then, from Theorem 2.4, we deduce that $\mathcal{D}$ at (S, I, R, β, γ) is the kernel of the operator M'_G and is given by the set K_t defined in (4.22). In particular, K_t is a vector space, since is the kernel of a linear operator. Meanwhile, the proof of (4.23) is deduced by using the definition of dual cone. □

4.4. First–order optimality conditions

In this section, we present the necessary conditions for optimality of the constrained optimization problem (1.19).

Theorem 4.4. *Consider that assumptions (H1)–(H6) are satisfied. Let* $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u}) \in \mathcal{D}$ *be a solution of* (1.19) *and* (w_1, w_2, w_3) *a solution of the adjoint* (4.9)–(4.13). *Then, the inequality*

$$\begin{aligned}
&\iint_{Q_T} \tilde{\beta}(x)\nabla f(\overline{S}, \overline{I}) \cdot (\overline{S}, \overline{I})\Big(- w_1 + p w_2 + (1-p)(w_3 + k_5)\Big) dxdt \\
&\quad + k_2 \int_\Omega \Big(\nabla\overline{\beta}(x)\nabla(\tilde{\beta} - \overline{\beta})(x) + \nabla\overline{\gamma}(x)\nabla(\tilde{\gamma} - \overline{\gamma})(x)\Big)dx + k_3 \iint_{Q_T} \tilde{I}(x,t)dxdt \\
&\quad + k_4 \iint_{Q_T} \Big[\overline{u}(t)\Big(c'(\tilde{S}) - c'(\overline{S})\Big)g(\overline{S})\tilde{S} + \overline{u}(t)c(\overline{S})\Big(g'(\tilde{S}) - g'(\overline{S})\Big)\tilde{S} + c(\overline{S})g(\overline{S})(\tilde{u} - \overline{u})(t)\Big]dxdt \\
&\quad + k_6 \int_0^T (\tilde{u} - \overline{u})(t)dt + k_7 \int_\Omega \tilde{I}(x, T)dx \geq 0
\end{aligned} \tag{4.24}$$

is satisfied for any $(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}, \tilde{u}) \in \mathcal{D}$.

Proof. Let us consider the notation introduced in Theorem 4.3. If $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u})$ is a solution of the optimal problem (1.19), we deduce that the descent and tangent cone at $(\overline{S}, \overline{I}, \overline{R}, \overline{\beta}, \overline{\gamma}, \overline{u})$ are disjoint, i.e. we have that $K_d \cap K_t = \emptyset$. Then, by Theorem 2.3, we follow the existence of two continuous functionals $G_1 \in K_d^*$ and $G_2 \in K_t^*$, not both identically zero, such that

$$G_1 + G_2 = 0. \tag{4.25}$$

It is called the Euler-Lagrange equation.

To prove (4.24), we proceed as follows: We begin by assuming that $(\tilde{S}, \tilde{I}, \tilde{R}, \tilde{\beta}, \tilde{\gamma}, \tilde{u}) \in E$ is a solution of the following system:

$$\partial_t\tilde{S} - \Delta\tilde{S} + \tilde{\beta}(x)f(\overline{S}, \overline{I}) + \overline{\beta}(x)\nabla f(\overline{S}, \overline{I}) \cdot (\tilde{S}, \tilde{I}) + \tilde{u}(t)g(\overline{S}) + \tilde{S}\overline{u}(t)g'(\overline{S}) = 0, \quad \text{in } Q_T, \tag{4.26}$$

$$\partial_t\tilde{I} - \Delta\tilde{I} - \tilde{\beta}(x)f(\overline{S}, \overline{I}) - p\overline{\beta}(x)\nabla f(\overline{S}, \overline{I}) \cdot (\tilde{S}, \tilde{I}) + \tilde{\gamma}(x)\overline{I} + \overline{\gamma}(x)\tilde{I} = 0, \quad \text{in } Q_T, \tag{4.27}$$

$$\partial_t\tilde{R} - \Delta\tilde{R} - (1-p)\tilde{\beta}(x)f(\overline{S},\overline{I}) - (1-p)\overline{\beta}(x)\nabla f(\overline{S},\overline{I})\cdot(\tilde{S},\tilde{I}) - \tilde{\gamma}(x)\overline{I}$$
$$- \overline{\gamma}(x)\tilde{I} - \tilde{u}(t)g(\overline{S}) - \tilde{S}\overline{u}(t)g'(\overline{S}) = 0, \quad \text{in } Q_T, \tag{4.28}$$
$$\nabla\tilde{S}\cdot\eta = \nabla\tilde{I}\cdot\eta = \nabla\tilde{R}\cdot\eta = 0, \quad \text{in } \Gamma_T, \tag{4.29}$$
$$\tilde{S}(x,0) = \tilde{I}(x,0) = \tilde{R}(x,0) = 0, \quad \text{on } \Omega. \tag{4.30}$$

The analysis of existence of solutions for the initial–boundary value problem (4.26)–(4.30) follows by the arguments used in the proof of Theorem 4.2, since (4.26)–(4.28) is a linear system. Moreover, we notice two facts. First $(\tilde{S},\tilde{I},\tilde{R},\tilde{\beta}-\overline{\beta},\tilde{\gamma}-\overline{\gamma},\tilde{u}-\overline{u}) \in K_t$, which implies that $G_2(\tilde{S},\tilde{I},\tilde{R},\tilde{\beta}-\overline{\beta},\tilde{\gamma}-\overline{\gamma},\tilde{u}-\overline{u}) = 0$. Second, from (4.15) and the definition of J'_G given in (4.14), we have that

$$G_1(\tilde{S},\tilde{I},\tilde{R},\tilde{\beta}-\overline{\beta},\tilde{\gamma}-\overline{\gamma},\tilde{u}-\overline{u})$$
$$= \lambda k_1 \int_\Omega \Big[\big(\overline{S}(x,T) - S^d(x)\big)\tilde{S}(x,T) + \big(\overline{I}(x,T) - I^d(x)\big)\tilde{I}(x,T) + \big(\overline{R}(x,T) - R^d(x)\big)\tilde{R}(x,T)\Big]dx$$
$$+ \lambda k_2 \int_\Omega \big(\nabla\overline{\beta}(x)\nabla(\tilde{\beta}-\overline{\beta})(x) + \nabla\overline{\gamma}(x)\nabla(\tilde{\gamma}-\overline{\gamma})(x)\big)dx + \lambda k_3 \iint_{Q_T} \tilde{I}(x,t)dxdt$$
$$+ \lambda k_4 \iint_{Q_T} \Big[\overline{u}(t)c'(\tilde{S})g(\overline{S})\tilde{S} + \overline{u}(t)c(\overline{S})g'(\tilde{S})\tilde{S} + c(\overline{S})g(\overline{S})(\tilde{u}-\overline{u})(t)\Big]dxdt$$
$$+ \lambda k_5 \iint_{Q_T} (1-p)\overline{\beta}(x)\Big[\partial_1 f(\tilde{S},\overline{I})\tilde{S} + \partial_2 f(\overline{S},\tilde{I})\tilde{I}\Big]dxdt$$
$$+ \lambda k_6 \int_0^T (\tilde{u}-\overline{u})(t)dt + \lambda k_7 \int_\Omega \tilde{I}(x,T)\,dx \geq 0,$$

for some nonnegative λ. It is clear that $\lambda \neq 0$, since, if we assume that $\lambda = 0$, we have that $G_1 = 0$, and from (4.25), we deduce that $G_2 = 0$. It is a contradiction with the fact that G_1 and G_2 are not both identically zero, which was deduced by Theorem 2.3. Then, without loss of generality, we can consider $\lambda = 1$ such that

$$k_1 \int_\Omega \Big[\big(\overline{S}(x,T) - S^d(x)\big)\tilde{S}(x,T) + \big(\overline{I}(x,T) - I^d(x)\big)\tilde{I}(x,T) + \big(\overline{R}(x,T) - R^d(x)\big)\tilde{R}(x,T)\Big]dx$$
$$+ k_2 \int_\Omega \big(\nabla\overline{\beta}(x)\nabla(\tilde{\beta}-\overline{\beta})(x) + \nabla\overline{\gamma}(x)\nabla(\tilde{\gamma}-\overline{\gamma})(x)\big)dx + k_3 \iint_{Q_T} \tilde{I}(x,t)dxdt$$
$$+ k_4 \iint_{Q_T} \Big[\overline{u}(t)c'(\tilde{S})g(\overline{S})\tilde{S} + \overline{u}(t)c(\overline{S})g'(\tilde{S})\tilde{S} + c(\overline{S})g(\overline{S})(\tilde{u}-\overline{u})(t)\Big]dxdt$$
$$+ k_5 \iint_{Q_T} (1-p)\overline{\beta}(x)\Big[\partial_1 f(\tilde{S},\overline{I})\tilde{S} + \partial_2 f(\overline{S},\tilde{I})\tilde{I}\Big]dxdt$$
$$+ k_6 \int_0^T (\tilde{u}-\overline{u})(t)dt + k_7 \int_\Omega \tilde{I}(x,T)\,dx \geq 0. \tag{4.31}$$

Testing Eqs (4.9)–(4.11) with $\tilde{S}$, $\tilde{I}$, and $\tilde{R}$, respectively, we get

$$\int_\Omega (w_1\tilde{S})(x,T)dx - \int_\Omega (w_1\tilde{S})(x,0)dx - \iint_{Q_T} w_1\big(\partial_t\tilde{S} - \Delta\tilde{S}\big)dxdt$$
$$= \iint_{Q_T} \Big[\overline{\beta}(x)\partial_1 f(\overline{S},\overline{I})\big(w_1 - pw_2 - (1-p)(w_3 + k_5)\big) + \overline{u}(t)g'(\overline{S})(w_1 - w_3)$$

$$- k_4\overline{u}(t)\Big(c'(\overline{S})g(\overline{S}) + c(\overline{S})g'(\overline{S})\Big)\Big]\tilde{S}\,dxdt,$$

$$\int_\Omega (w_2\tilde{I})(x,T)dx - \int_\Omega (w_2\tilde{I})(x,0)dx - \iint_{Q_T} w_2\Big(\partial_t\tilde{I} - \Delta\tilde{I}\Big)dxdt$$

$$= \iint_{Q_T} \Big[\overline{\beta}(x)\partial_2 f(\overline{S},\overline{I})\Big(w_1 - pw_2 - (1-p)(w_3 + k_5)\Big) + \overline{\gamma}(x)(w_2 - w_3) - k_3\Big]\tilde{I}dxdt,$$

$$\int_\Omega (w_3\tilde{R})(x,T)dx - \int_\Omega (w_3\tilde{R})(x,0)dx - \iint_{Q_T} w_3\Big(\partial_t\tilde{R} - \Delta\tilde{R}\Big)dxdt = 0.$$

Then, replacing the end conditions for (w_1, w_2, w_3), using system (4.26)–(4.30) and adding the results, we have

$$k_1 \int_\Omega \Big((\overline{S}(x,T) - S^d(x))\tilde{S}(x,T) + (\overline{I}(x,T) - I^d(x))\tilde{I}(x,T) + (\overline{R}(x,T) - R^d(x))\tilde{R}(x,T)\Big)dx$$

$$= -\iint_{Q_T} \tilde{\beta}(x)\nabla f(\overline{S},\overline{I})\cdot(\overline{S},\overline{I})\Big(w_1 - pw_2 - (1-p)w_3\Big)dxdt + k_4\iint_{Q_T} \overline{u}(t)\Big(c'(\overline{S})g(\overline{S}) + c(\overline{S})g'(\overline{S})\Big)dxdt$$

$$- k_5\iint_{Q_T} (1-p)\overline{\beta}(x)\nabla f(\overline{S},\overline{I})\cdot(\tilde{S},\tilde{I})dxdt. \tag{4.32}$$

Replacing (4.32) in (4.31), we deduce (4.24). □

5. Numerical simulations

5.1. Some theoretical basis

In this section, we consider the numerical approximation of the optimal control problem by following the ideas detailed in [63] (see also [64]). The construction of the numerical approximation is a procedure which involves the following three steps. First, we develop a numerical approximation of the state equation in the appropriate space where the initial-boundary problem is well posed. Second, we construct a numerical approximation of the objective function. Third, the continuous optimal control problem is reduced to a finite-dimensional representation using the numerical approximation of the state equation and the cost function. Particularly, for the third step, we consider at least three possible forms of controls to be determined: (I) constant controls; (II) control with some specific functional forms with some unknown parameters in terms of the spatial variable, temporal variable, and the state; and (III) controls belong a general function space depending of the spatial variable, temporal variable, and the state. In case (III), the general function space should be a finite-dimensional approximations of the admissible set. Moreover, from a practical point of view, Case (I) does not differ from Case (II), and Case (III) is more complex as the approximation requires more advanced approach. Hence, we focus on cases (I) and (II).

5.2. Discretization of the state Eqs (1.12)–(1.16)

In this section we consider that $\Omega =]0,1[$, $\partial\Omega = \{0,1\}$, $Q_T = (0,1)\times[0,T]$, and $\Sigma_T = \{0,1\}\times[0,T]$. The discretization of the system (1.12)–(1.16) is given by a semi-implicit finite difference scheme. We begin by introducing the standard discretization of Q_T. We select $M, N \in \mathbb{N}$ such that the discretization of Ω is given by $x_j = j\Delta x$ for $j = 0,\ldots,M$ with $\Delta x = L/(M+1)$, and the discretization of $[0,T]$ is given by $t_n = n\Delta t$ for $n = 0, \dots, N$ with $\Delta t = 1/N$. Moreover, we consider that the approximation of a given function $\Psi : \overline{Q}_T$ at (x_j, t_n) is denoted by Ψ^n_j. Similarly, the approximation of the functions $\overline{\Psi} : \overline{\Omega} \to \mathbb{R}$ and $\underline{\Psi} : [0,1] \to \mathbb{R}$ at x_j and t_n are denoted by $\overline{\Psi}_j$ and by $\underline{\Psi}^n$, respectively. In order to introduce a numerical method for approximating the optimization problem, we develop the calculus of a discrete gradient using the discretize-then-optimize approach: We begin by introducing a numerical method approximating the state Eqs (1.12)–(1.16), and then we introduce a discrete version of the optimization problem. More precisely, we consider that the system (1.12)–(1.16) is approximated by the following finite difference scheme:

$$\frac{S^{n+1}_j - S^n_j}{\Delta t} - \frac{S^{n+1}_{j+1} - 2S^{n+1}_j + S^{n+1}_{j-1}}{(\Delta x)^2} = -\beta_j f(S^n_j, I^n_j) - u^n g(S^n_j), \qquad j = 1, \dots, M-1, \tag{5.1}$$

$$\frac{I^{n+1}_j - I^n_j}{\Delta t} - \frac{I^{n+1}_{j+1} - 2I^{n+1}_j + I^{n+1}_{j-1}}{(\Delta x)^2} = p\beta_j f(S^n_j, I^n_j) - \gamma_j I^n_j, \qquad j = 1, \dots, M-1, \tag{5.2}$$

$$\frac{R^{n+1}_j - R^n_j}{\Delta t} - \frac{R^{n+1}_{j+1} - 2R^{n+1}_j + R^{n+1}_{j-1}}{(\Delta x)^2} = (1-p)\beta_j f(S^n_j, I^n_j) + \gamma_j I^n_j + u^n g(S^n_j), \qquad j = 1, \dots, M-1, \tag{5.3}$$

$$\frac{S^{n+1}_j - S^{n+1}_{j-1}}{\Delta x} = \frac{I^{n+1}_j - I^{n+1}_{j-1}}{\Delta x} = \frac{R^{n+1}_j - R^{n+1}_{j-1}}{\Delta x} = 0, \qquad j \in \{0, M\}, \tag{5.4}$$

$$S^0_j = S_0(x_j), \quad I^0_j = I_0(x_j), \quad R^0_j = R_0(x_j), \qquad j \in j = 0, \dots, M, \tag{5.5}$$

where $n = 0, \dots, N-1$. We use the notation $(S_\Delta, I_\Delta, R_\Delta)$ for the numerical approximation obtained by the scheme (5.1)–(5.5) with numerical coefficients $(\beta_\Delta, \gamma_\Delta, u_\Delta)$.

5.3. Discretization of cost function (1.17) *and finite-dimensional approximation of* (1.18)

We consider the discretization of (1.18) when the controls are parametric dependent functional forms. Let us consider that the functions β, γ, and u are parametrized by a finite number of parameters denoted by $\mathbf{e} = (e_1, e_2, \dots, e_m)$ and the optimal control problem (1.18) is approximated by the optimization problem

$$\left.\begin{array}{l} \text{Find } \mathbf{e} \in \mathbb{R}^m \text{ minimizing the cost function } \mathcal{J}_\Delta(\mathbf{e}) = J_\Delta(S_\Delta, I_\Delta, R_\Delta, \beta_\Delta, \gamma_\Delta, u_\Delta) \\ \text{subject to } (S_\Delta, I_\Delta, R_\Delta, \beta_\Delta, \gamma_\Delta, u_\Delta) \text{ solution of (5.1)–(5.5) with } \beta, \gamma \\ \text{and } u \text{ parametrized by } \mathbf{e}, \text{ i.e. } \beta_\Delta = \beta_\Delta(\cdot, \mathbf{e}),\ \gamma_\Delta = \gamma_\Delta(\cdot, \mathbf{e}),\ u_\Delta = u_\Delta(\cdot, \mathbf{e}), \end{array}\right\} \tag{5.6}$$

where J_Δ is the discretization of the cost function (1.17) is given by

$$\begin{aligned} J_\Delta(S_\Delta, I_\Delta, R_\Delta, \beta_\Delta, \gamma_\Delta, u_\Delta) &= \frac{k_1 \Delta x}{2} \sum_{j=0}^{M} \Big[(S^N_j - S^d_j)^2 + (I^N_j - I^d_j)^2 + (R^N_j - R^d_j)^2 \Big] \\ &+ \frac{k_2 \Delta x}{2} \sum_{j=0}^{M} \Big[(\beta'_j)^2 + (\gamma'_j)^2 \Big] + k_3 \Delta x \Delta t \sum_{j=0}^{M} \sum_{n=0}^{N} I^n_j + k_4 \Delta x \Delta t \sum_{j=0}^{M} \sum_{n=0}^{N} c(S^n_j) u^n g(S^n_j) \\ &+ k_5 \Delta x \Delta t \sum_{j=0}^{M} \sum_{n=0}^{N} (1-p)\beta_j f(S^n_j, I^n_j) + k_6 \Delta t \sum_{n=0}^{N} u^n + k_7 \Delta x \sum_{j=0}^{M} I^N_j. \end{aligned} \tag{5.7}$$

We observe that $(S_\Delta, I_\Delta, R_\Delta)$ depends on $\mathbf{e}$, but the notation is not included explicitly.

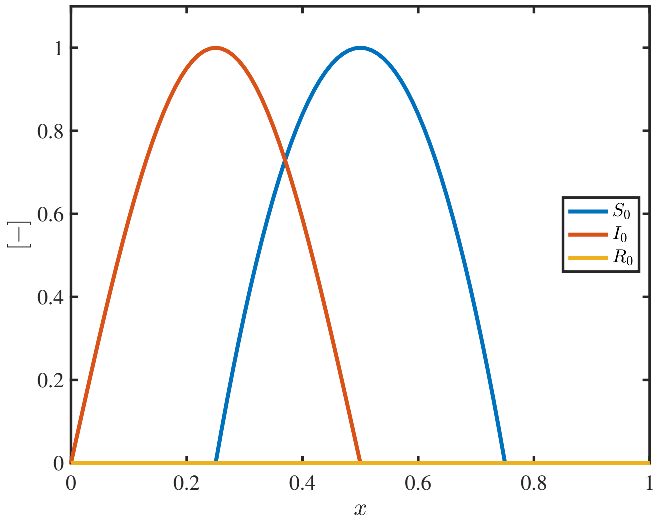


Figure 3. The initial conditions defined in (5.8) and (5.9) are used for numerical simulations of the state equations and for the optimal control problem solutions, where S_0 and I_0 are defined in (5.8) and (5.9), respectively. We notice that $R_0(x) = 0$.

5.4. Numerical examples

In the numerical examples, we consider that the initial condition are defined by

$$S_0(x) = \begin{cases} (1-4x)(4x-3), & x \in [1/4, 3/4], \\ 0, & \text{otherwise}, \end{cases} \tag{5.8}$$

$$I_0(x) = \begin{cases} \sin(2\pi x), & x \in [0, 1/2], \\ 0, & \text{otherwise}, \end{cases} \tag{5.9}$$

and $R_0(x) = 0$. We fix that $f(S, I) = SI$, $g(S) = S$, $p = 0.05$, and $c(S) = 1 - S$. We show the graphs of the initial condition in Figure 3. Moreover, to solve the optimization problem (5.6), we have used the `optimiset` routine of MATLAB.

5.4.1. Example 1: Constant function β, γ and u

In this example, we consider that the coefficients of the reaction terms $\beta, \gamma : \overline{\Omega} \to (0, 1)$ and $u : [0, T] \to (0, 1)$ are constant functions to be determined. More precisely, we assume that the parameters to determine by the optimal control problem are $\mathbf{e} = (e_1, e_2, e_3)$, such that $\beta(x; \mathbf{e}) = e_1$, $\gamma(x; \mathbf{e}) = e_2$ and $u(t; \mathbf{e}) = e_3$. We construct the measurement profiles by developing a numerical simulation of (1.12)–(1.16) with the finite difference scheme (5.1)–(5.5) with $\Delta t = 1.0E - 7$ and $\Delta x = 2.0E - 4$. We assume that the initial guess $\mathbf{e}^{obs} = (0.1, 0.1.0.1)$ and get that the identified functions are defined by the parameters $\mathbf{e}^{\infty} = (0.00166, 0.00559, 0.20440)$. The numerical identification is developed by considering $M = 100$ and $N = 500$. The comparison of the observed, identified, and initial guess profiles are shown in Figure 4.

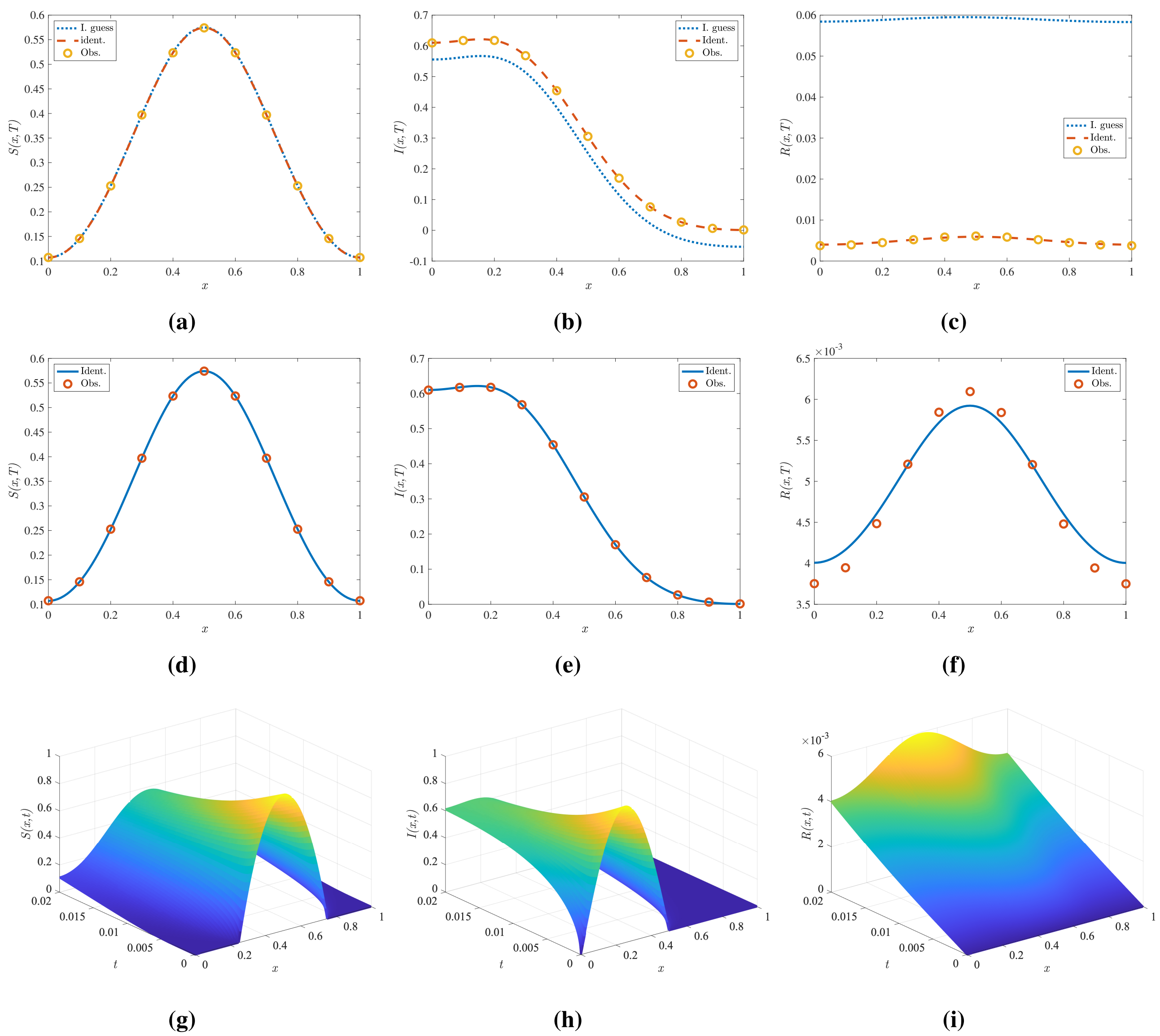


Figure 4. Identification results for Example 1. (a)–(c) Comparison of end profiles for observed, initial guess, and identified for susceptible, infected, and recovered state variables, respectively. (d)–(f) Comparison of end profiles for observed and identified for susceptible, infected, and recovered state variables, respectively. (g)–(i) Simulation of (1.12)–(1.16) with the finite difference scheme (5.1)–(5.5) with identified parameters.

Table 1. Parameters for Example 2 and defining the functions given in (5.10).

	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8
$\mathbf{e}^{obs}$	0.0010	100.0000	50.0000	0.0010	1000.0000	0.2500	0.2500	0.5000
$\mathbf{e}^{ig}$	0.1000	200.0000	100.0000	0.1000	2000.0000	0.1000	0.1000	0.1000
$\mathbf{e}^{\infty}$	0.0001	50.8658	21.8599	0.0051	1883.6000	0.2386	0.1637	0.4515

5.4.2. Example 2: Non-constant functions β, γ and u

In this example, we assume that the functions $\beta, \gamma : \overline{\Omega} \to (0, 1)$ and $u : [0, T] \to (0, 1)$ are parametric functions defined in terms of $\mathbf{e} = (e_1, \ldots, e_8)$ as follows:

$$\beta(x; \mathbf{e}) = e_1 \operatorname{sech}(e_2 x - e_3), \quad \gamma(x; \mathbf{e}) = e_4 \exp(-e_5(x - e_6)^2), \quad u(t; \mathbf{e}) = e_7 t + e_8. \tag{5.10}$$

We construct the measurements profiles by solving (1.12)–(1.16) with the numerical scheme (5.1)–(5.5) by considering the parameters given in $\mathbf{e}^{obs}$ in Table 1. The optimization problem is solved by considering the initial guess $\mathbf{e}^{ig}$, and we get that the identified parameters are $\mathbf{e}^{\infty}$. The numerical identification is developed by considering $M = 100$ and $N = 1000$. The comparison of the observed, identified, and initial guess profiles and coefficients are shown in Figures 5 and 6, respectively.

6. Conclusions

This paper analyzes the control and reaction identification in a mathematical model for carrier-borne epidemics. Firstly, a mathematical model of carrier-borne epidemics with a general transmission function and vaccination was established. The mathematical model was deduced by extending the assumptions considered in [24] for the case of the spatial movement of the populations on the spatial domain, obtaining a reaction-diffusion system as a governing equation of the epidemics. The boundary conditions consider that the populations are isolated during the process, or, equivalently, there is no emigration or immigration. The infection force is considered to satisfy the assumptions introduced in [8]. An existence and uniqueness result for the initial boundary value problem was introduced and proved by applying semigroup theory. Second, reaction identification and optimal control problems are formulated as constrained optimization problems. The cost function considers two parts: two terms for least squares and regularization, and five terms for minimizing the infected population, the control, and the economic loss. The optimal control problem is studied by applying the Dubovitskii and Milyutin formalism, obtaining the main results of the existence of solutions, the existence of solution for the adjoint state, and a first-order optimality condition. Moreover, the paper presents numerical examples of the control-parameter identification problem.

The analysis of parameter identification and control problems for epidemiological models has gained significant momentum in recent years [42]. This increase in activity is reflected in the growing number of published articles on the subject, particularly in the context of the COVID-19 pandemic [65–67]. As a result, there are considerable challenges in the areas of mathematical analysis, numerical methods, and specific applications. In this context, we have identified the following issues as requiring further in-depth research:

(i) *Generalization to more complex compartmental models.* In this paper, we have considered that the carriers are given by a constant fraction $p \in [0, 1]$, which can be generalized to a compartmental model by incorporating a new compartment for an asymptomatic class of individuals. In the line of complex compartmental models, system (1.12)–(1.16) can be further extended to include other classes of individuals (e.g., hospitalized, quarantined, vaccinated), and additional properties of the coefficients and interaction functions (e.g., heterogeneity, non-local behavior interactions, time delays, stochastic effects, seasonality, and age structure).

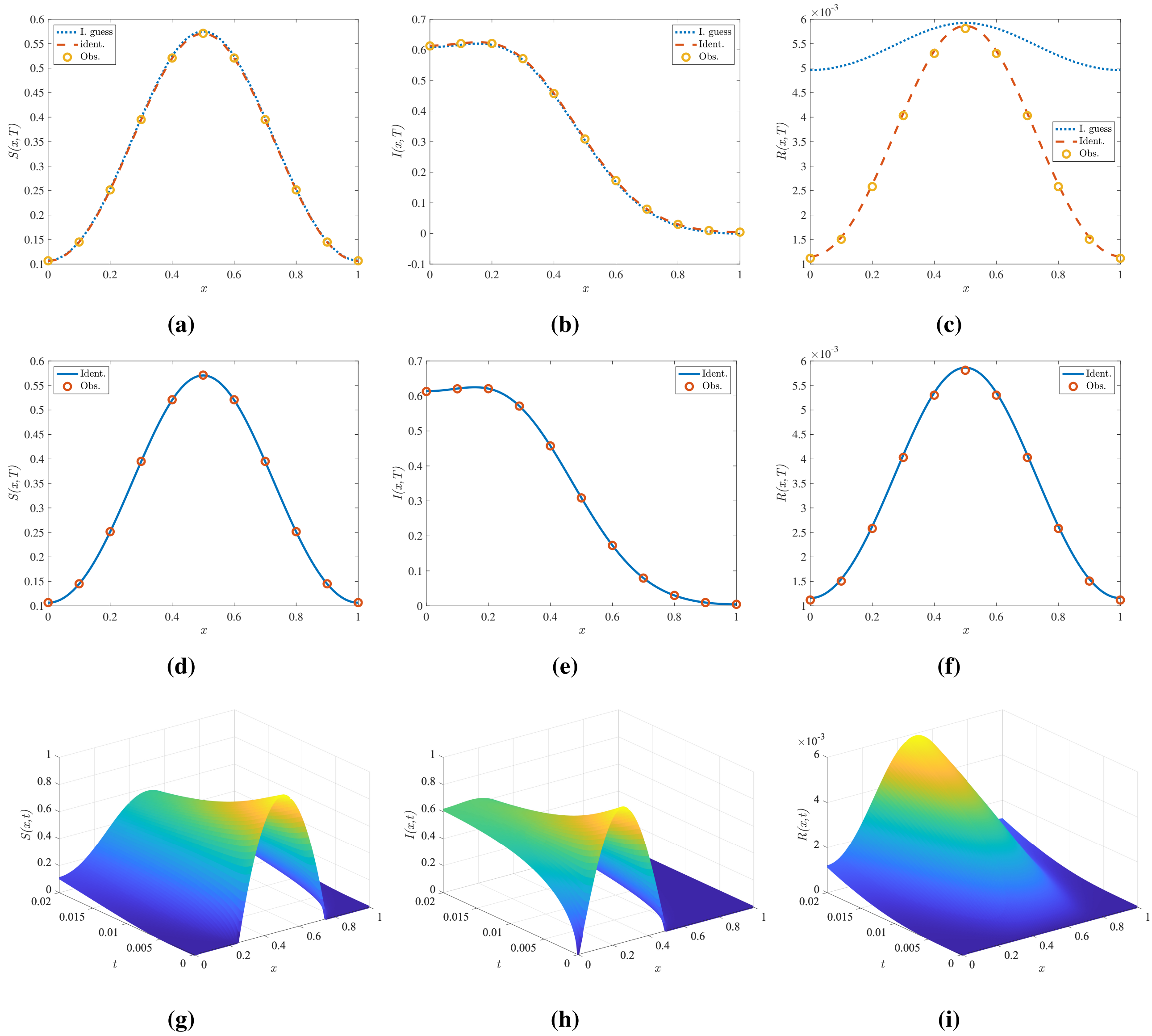
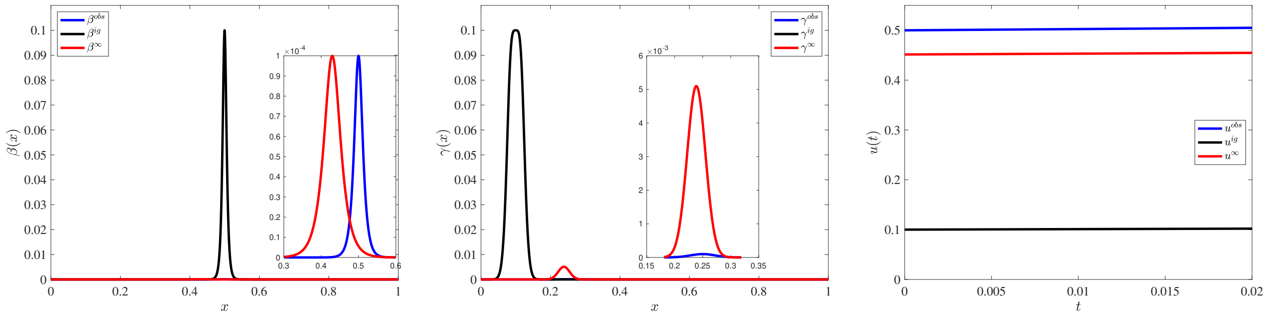


Figure 5. Identification results for Example 2. The parameters are given on Table 1. (a)–(c) Comparison of end profiles for observed, initial guess, and identified for susceptible, infected, and recovered state variables, respectively. (d)–(f) Comparison of end profiles for observed and identified for susceptible, infecte, and recovered state variables, respectively. (g)–(i) Simulation of (1.12)–(1.16) with the finite difference scheme (5.1)–(5.5) with identified parameters.



(a) **(b)** **(c)**

Figure 6. The observed, initial guess, and identified functions in Example 5.4.2: (a) β, (b) γ and (c) u.

(ii) *Analysis of other cost functions.* The cost function examined in this work generalizes the formulation initially proposed by [8] in the case of ordinary differential equation models. Nevertheless, further research is needed to develop and analyze more appropriate cost functions that arise in the context of some specific infectious disease transmission and control. Moreover, we need to research the characterization of bang-bang controls in the case of linear cost functions constrained to reaction-diffusion systems, as demonstrated in [24] for ordinary differential equation models.

(iii) *Advanced numerical methods.* The proposal of advanced numerical methods to solve the optimal control problems is required. It is necessary to develop numerical methods based on numerical adjoint states or sensitivity analysis, utilizing a discretization of the Dubovitskii-Milyutin formalism. Particularly, it is required to perform the numerical approximations of bang-bang type controls when the cost functions are linear. Furthermore, advanced studies on the numerical performance, convergence, and error estimates of these approximations should be conducted.

(iv) *Applications to experimental data.* In the context of epidemiological models governed by ordinary differential equations, there exists extensive literature (see, for example, [65–67]). However, studies focused on parameter identification for models based on partial differential equations are relatively scarce [42]. Additionally, the design of cost functions in epidemiological modeling demands thorough analysis. Boundary conditions and local domain observations often serve as critical components in defining appropriate objective functions.

(v) *Analysis of the reproduction number in control problems.* By applying similar ideas to [68], we deduce that

$$R_0 = \sup\left\{ \frac{N\int_\Omega \beta\phi^2 dx}{\int_\Omega \left[|\nabla\phi|^2 + (\gamma + ug)\phi^2 \right] dx} \mid \phi \in H^1(\Omega); \phi \neq 0 \right\}$$

defines the reproduction number of the system (1.12)–(1.14). The relationship between the reproduction number and the qualitative behavior of the solution for the forward problems has been studied by several authors [42]. The parameter R_0 is used to characterize the stability in ordinary differential and reaction-diffusion systems. Meanwhile, in the case of parameter identification problems, it is used to characterize the sensitivity of the state equations with respect to the parameters defining the coefficients. However, to the best of our knowledge, a characterization of the parameter identification, as well as the optimal control problem solutions, in terms of R_0

remains unknown.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare there is no conflicts of interest.

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