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Unraveling the Influence of the Objective Functional on Epidemic Optimal Control: Insights from the SIR Model *

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Abstract

In the application of optimal control theory to medical and biological problems, the dependence of the objective functional on the control variable is often subject to uncertainty. This study examines the effects of this dependency on the outcomes of optimal control problems in the context of disease control using the SIR model. We formulate two distinct optimal control problems: one for the control of disease spread through prophylactic vaccination, and another for the treatment of infected individuals. For each scenario, we propose four variations of the objective functional to capture the cost of control interventions, namely, quadratic state-independent, quadratic state-dependent, linear state-independent, and linear state-dependent. We also conduct numerical simulations to compare optimal control solutions across different weight parameters. While some qualitative characteristics of the control profiles are similar in certain scenarios, there are also notable differences suggesting that the choice of objective functional can substantially alter the resulting control profiles. Consequently, when there is uncertainty regarding the functional form of the objective and its relationship to the control parameter, it is recommended to evaluate multiple objectives and subsequently identify which solution is most suitable for practical implementation.

Keywords: Epidemic model, Optimal control, Objective functional, Disease control, SIR model

1 Introduction

Optimal control theory is a mathematical framework that helps in determining the best control strategies to optimize a given objective in complex systems [20, 55]. Optimal control theory can potentially bring significant benefits in medicine and epidemiology by providing a systematic and quantitative approach to optimizing control strategies, treatment regimens, resource allocation, and public health policies to improve health outcomes and address public health challenges effectively, e.g., [2, 4, 10, 33, 45, 48, 53]. While optimal control theory can offer valuable insights and solutions to optimization problems in various fields, real-life systems are often highly complex and subject to significant uncertainty, especially in biology and medicine [48]. Modeling these systems accurately and incorporating all relevant factors into the optimal control problem can be challenging. Hence, even if simplifying assumptions are necessary and commonly made when formulating mathematical optimization models, modelers should be careful as some assumptions may not always reflect the true complexity of real-life systems, potentially leading to inaccuracies and limitations in the optimization results [31].

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In optimal control problems for biological applications, a common source of uncertainty is the functional form of the objective that defines the optimization criterion [18, 26, 31, 46]. In particular, the exact nature of the objective functional and how it relates to the control parameter is often unclear and difficult to define accurately. Hence, as a simplification, many studies assume that the objective is directly related to a sum of the weighted squares of the control term e.g., [1, 5, 12, 14, 16, 21, 27, 35, 39, 44, 42, 51, 49, 52, 54, 56]. These objective functionals are typically called L_2 -objectives. Such formulation is mathematically convenient, as in this case, the optimal controls can be characterized as explicit functions of the state and adjoint variables via the necessary conditions provided by Pontryagin’s maximum principle. Then, the optimal control problem can be straightforwardly reduced to a two-point boundary value problem suitable for numerical solving [36, 33]. So, the main advantage of objective functionals with a quadratic term in the control is its mathematical simplicity. However, in biomedical and epidemiological applications, interpreting such L_2 -objectives is not always clear and their use is often difficult to justify from a biological perspective. For instance, [31] argued that L_1 -objectives, that is, objective functionals with a linear dependence on the control, may capture the cost of an intervention policy more accurately than L_2 -objectives but one has to take into consideration that optimal control problems under the L_1 -formulation usually involve singular and bang-bang controls and are generally less amenable to mathematical analysis [6, 11, 22, 24, 30, 38]. The linear dependency on the control might also not be the most realistic option, as some form of nonlinearity of the cost is likely to occur, for example, due to the overload of the health service. Another related problem is the functional dependency of the objective on the state variables and the impact of this on the optimal control. For instance, if the control $u(t)$ represents a time-dependent vaccination rate administered in the susceptible population $S(t)$, then it is plausible to assume that control costs are proportional to the number of vaccinated individuals given by $u(t)S(t)$ [18, 47, 50]. Nonetheless, the cost is usually represented by u or by u^2 without considering the number of people being vaccinated. These points highlight the importance of conducting additional research to explore how the choice of objective functional influences the solutions of optimal control problems. Understanding this relationship is essential to identify an objective function that accurately reflects the biological problem at hand and is therefore relevant for decision-makers.

In this paper, we further investigate the role played by different objectives on optimal control outcomes. Four different types of functions are suggested to represent the cost of control interventions in the objective functional: (i) quadratic state-independent (QSI) cost, (ii) quadratic state-dependent (QSD) cost, (iii) linear state-independent (LSI) cost, and (iv) linear state-dependent (LSD) cost. This leads to four optimal control problems whose quantitative analysis is a nontrivial problem by itself. Aiming to obtain analytical results, we perform our analysis using the classical SIR epidemic model with demography. We remark that optimal control problems for the SIR epidemic model have garnered interest since many decades ago. One of the earliest contributions was by Morton and Wickwire [37], who explored optimal immunization strategies for the deterministic SIR model without demography. They used an integral cost functional in which the control appeared linearly and did not depend on the state variables (LSI cost). Their results suggested that the optimal control policies were of the bang-bang type. Wickwire [59] also studied the SIR model without demography to examine optimal isolation strategies, employing an LSD integral cost functional that aims to minimize the total number of infected individuals. His findings revealed that the optimal approach was to either implement full control throughout the entire epidemic or to apply no control at all. The studies [37, 59] assumed that transmission was governed by the mass action incidence. Bobisud [8] and Behncke [7] extended the results of Morton and Wickwire considering more general contact rates. More recently, Hansen and Day [25] revisited the SIR model without demography and mass action transmission rate to address a time-optimal control problem. They aimed to optimize both isolation and vaccination strategies simultaneously while considering isoperimetric constraints. Sharbayta et al. [51] considered the optimal control of social distancing in a behavioral SIR model using an L_2 -objective. The novelty of our study lies in providing a detailed comparison of optimal control outcomes for the SIR model with demography, using four of the most widespread objectives in the literature. To the best of the authors’ knowledge, there has been very little mathematical research in this area, such as [29, 31]. Furthermore, we also explore how the weight parameters in the objective affect the qualitative properties of optimal control outcomes.

The rest of the study is organized as follows: In the next section, we formulate the optimal vaccination problem for the SIR model. In subsection 2.1, we apply Pontryagin’s maximum principle to

derive the first-order necessary conditions. Subsection 2.2 presents the numerical approximation of the optimal vaccination profiles. The optimal treatment problem is formulated in Section 3, and the numerical approximation of the treatment control profiles is provided in subsection 3.1. Finally, the results are thoroughly analyzed in the discussion section 4.

2 Optimal vaccination for the SIR epidemic model

We consider the *SIR* epidemic model to describe the spread of an infectious disease in a population of size $N(t) = S(t) + I(t) + R(t) = 1$ for all t . Herein, $S(t)$, $I(t)$, and $R(t)$ denote the proportions of susceptible, infectious, and recovered individuals at time t , respectively. The population is assumed to be in demographic equilibrium, where the birth and death rates are equal and are denoted by a positive constant μ . The parameters β and γ are positive constants representing the transmission and the recovery rates, respectively. We extend the SIR model by introducing a time-dependent control, $v(t)$, which represents a prophylactic vaccine administered to healthy individuals to prevent infection. We assume that the immunity induced by the vaccine is permanent. This leads to the following modified SIR model with control:

$$\begin{aligned} \frac{dS}{dt} &= \mu - \beta SI - (\mu + v(t))S, & S(0) &= S_0 > 0, \\ \frac{dI}{dt} &= \beta SI - (\gamma + \mu)I, & I(0) &= I_0 > 0. \end{aligned} \tag{1}$$

Due to the constant population size assumption, one equation in the SIR model is redundant so we omitted the equation for the recovered class R . Observe that if $I(0) = 0$ then $I(t) = 0$ for all $t > 0$, hence, for relevant epidemiological cases we need to assume positive initial conditions for the susceptible and the infectious compartments. The biologically relevant region for system (1) is

$$\Omega = \{(S, I) \in \mathbf{R}_+^2 : S > 0, I > 0, S + I \leq 1\}.$$

For model (1) it is well-known that region Ω is positively invariant and unique solutions exist for all $t > 0$, so system (1) is mathematically and epidemiologically well-posed.

Public health authorities wish to minimize both the cost of infection and the cost of implementing the control during a finite time interval $[0, t_f]$. Therefore, we consider the following objective functional:

$$J_i(v(t)) = \int_0^{t_f} \varphi(I(t)) + \sigma_i(v(t), S(t)) dt. \tag{2}$$

Here, function $\varphi(I)$ represents the cost of the reduction in health and well-being, that is, the cost of infection or morbidity costs. The function $\sigma_i(v, S)$ represents the costs of the control action (vaccination cost in our model). We assume that the cost of infection is proportional to the size of the infected class, hence $\varphi(I(t)) = A_1 I(t)$. This simplification allows us to focus on the impact of the cost function $\sigma_i(v, S)$ in the form of the optimal control solution. Following the ideas introduced by [18], we consider the following forms for the cost function $\sigma_i(v, S)$:

$$\begin{aligned} \sigma_1(v, S) &= A_2 v^2, & \text{quadratic state-independent (QSI) cost,} \\ \sigma_2(v, S) &= A_2 v^2 S, & \text{quadratic state-dependent (QSD) cost,} \\ \sigma_3(v, S) &= A_2 v, & \text{linear state-independent (LSI) cost,} \\ \sigma_4(v, S) &= A_2 v S, & \text{linear state-dependent (LSD) cost.} \end{aligned} \tag{3}$$

It is important to note that in both the QSI and LSI cases, the cost of vaccination does not depend on the number of people being vaccinated, which is clearly unrealistic from a biological perspective. Despite this, the QSI and LSI formulations are surprisingly common in optimal control applications within epidemiology [1, 3, 5, 6, 9, 12, 16, 19, 23, 21, 27, 32, 35, 39, 40, 41, 49, 52, 54, 56]. As such, we have included these cases aiming to compare optimal control outcomes.

The coefficients $A_i > 0$ ($i = 1, 2$) are positive weights that influence the optimal control solution by determining the relative importance or priority given to different aspects of the control problem. Adjusting the weights is necessary to balance the monetary cost of disease and the cost of the control measures (for more details see Section 2.2). Given economic or logistical constraints, it is clear that

the vaccination rate $v(t)$ should be bounded. Additionally, it is crucial to recognize that in our model, $v(t)$ represents a rate rather than a fraction. Therefore, while stating $0 < v(t) < 1$ might be considered technically correct, it lacks precision. A constant vaccination rate v can be approximated using the formula $C(\tau) = 1 - \exp(-v\tau)$ or $v = -\ln(1 - C(\tau))/\tau$, where $C(\tau)$ is the immunization coverage at time τ [43]. For example, to achieve a 90% immunization coverage in 100 days, the constant vaccination rate should be approximately $v = 0.023$. Hence, it is assumed that the daily vaccination rate satisfies $v \leq v_{\max} = 0.023$, so the set of admissible controls is

$$\mathcal{V} = \{v : [0, t_f] \rightarrow [0, v_{\max}] \subseteq [0, 1] \text{ Lebesgue measurable}\}. \quad (4)$$

Let $x = (S, I)^T$ and denote the right-hand side of system (1) as the vector function $F(t, x, v)$. The optimal control problem is

$$\min_{v \in \mathcal{V}} J_i(v) = \min_{v \in \mathcal{V}} \int_0^{t_f} L_i(t, x, v) dt \quad \text{subject to system (1)}, \quad (5)$$

where $L_i(t, x, v) = A_1 I + \sigma_i(v, S)$ and the functions $\sigma_i(v, S)$ ($i = 1, 2, 3, 4$) are given by (3). The proof of the existence of an optimal control $v^*(t)$ and corresponding optimal states $x^* = (S^*, I^*)^T$ for each of our control problems is given in A.

2.1 Necessary conditions for optimality

Pontryagin's maximum principle allows us to convert the optimal control problem (5) into a problem of minimizing pointwise a Hamiltonian H_i ($i = 1, 2, 3, 4$) with respect to the control function $v(t)$. The Hamiltonian is defined in terms of the integrand $L_i(t, x, v)$ of the objective functional and the right-hand side $F(t, x, v)$ of the control model (1) as follows:

$$H_i(t, x, v, \lambda) = \lambda_0 L_i(t, x, v) + \langle \lambda(t), F(t, x, v) \rangle \quad (6)$$

where $\lambda_0 \geq 0$ and $\lambda(t) = (\lambda_S, \lambda_I)^T$ is a piecewise differentiable adjoint vector function which is usually interpreted as the marginal valuation of the associated state variable at time t . From the maximum principle, we obtain the following necessary conditions for the optimality of a controlled trajectory [55].

Proposition 1. *Let $v^*(t)$ and $x^*(t)$ be the optimal control and the corresponding optimal states for the optimal control problem (5). Then there exists a non-negative scalar λ_0 and a piecewise differentiable adjoint variable $\lambda(t)$ such that the vector $(\lambda_0, \lambda(t))$ is not the zero vector for all $t \in [0, t_f]$ and*

$$H_i(t, x^*, v^*, \lambda) \leq H_i(t, x^*, v, \lambda) \quad (7)$$

holds for any $t \in [0, t_f]$ and all controls $v \in \mathcal{V}$ ($i = 1, 2, 3, 4$). Furthermore, except at the points of discontinuities of v^ , the adjoint variable $\lambda = (\lambda_S, \lambda_I)^T$ satisfies the equations*

$$\frac{d\lambda_j}{dt} = -\frac{\partial H_i(t, x^*, v^*, \lambda)}{\partial x_j}, \quad \lambda_j(t_f) = 0, \quad (j = S, I).$$

Please note that the scalar λ_0 cannot vanish for this problem because, if it did, the transversality condition $\lambda_j(t_f) = 0$, ($j = S, I$) will contradict the non-triviality of the multipliers and hence $\lambda_0 > 0$. Without loss generality, we assume $\lambda_0 = 1$. For the quadratic cost functions $\sigma_i(v, S)$ ($i = 1, 2$), the application of the first-order necessary conditions coming from the maximum principle (Proposition 1) allows the explicit characterization of the optimal control as a function dependent on the state and adjoint variables. Generally, for these L_2 -type objectives, the resultant optimal control is a continuous function. In the case of the linear cost functions $\sigma_i(v, S)$ ($i = 3, 4$), the optimization problem often gives rise to singular and bang-bang (piecewise constant) controls. Consequently, the characterization of the optimal control in such instances is challenging, making the overall problem more complex to manage. Before going further, we need to remark on two important consequences of the maximum principle.

Remark 1. *If the Hamiltonian is not an explicit function of t , that is, $H_i(t, x, v, \lambda) = H_i(x, v, \lambda)$, then $H_i(x, v, \lambda)$ is constant with minimum value along the optimal solution. Hence, for our problem $H_i(t, x^*, v^*, \lambda) = H_i(x^*, v^*, \lambda) = \text{const}$.*

Remark 2. If a minimum of $H_i(t, x^*, v, \lambda)$ is found through (7) at v^* then the following first-order optimality condition

$$\frac{\partial H_i}{\partial v}(t, x^*, v^*, \lambda) = \frac{\partial \sigma_i}{\partial v}(v^*, S^*) - \lambda_S S^* = 0 \quad (8)$$

must be satisfied so the Hamiltonian has a minimum in the set of admissible controls. Furthermore, if $H_i(t, x^*, v, \lambda)$ is twice continuously differentiable with respect to v , then

$$\frac{\partial^2 H_i}{\partial v^2}(t, x^*, v^*, \lambda) \geq 0. \quad (9)$$

The condition (9) is the classical Legendre-Clebsch condition [55].

2.1.1 Quadratic state-independent case

For the cost function $\sigma_1(v, S) = A_2 v^2$, the Hamiltonian takes the next form

$$H_1(x, v, \lambda) = A_1 I + A_2 v^2 + \lambda_S (\mu - \beta S I - (\mu + v)S) + \lambda_I I (\beta S - \gamma - \mu).$$

Hence, the system for the adjoint variables is

$$\begin{aligned} \frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu + v^*) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - \mu), \end{aligned}$$

and the optimality condition (8) for this case reduces to

$$\frac{\partial H_1(x^*, v^*, \lambda)}{\partial v} = 2A_2 v^* - \lambda_S S^* = 0.$$

Solving the above equation considering the constraints (4), we obtain the following characterization for the QSI optimal control:

$$v_{QSI}^*(t) = \min \left\{ v_{\max}, \max \left\{ 0, \frac{1}{2A_2} \lambda_S(t) S^*(t) \right\} \right\}.$$

Observe that condition (9) is satisfied, so a minimum occurs at v_{QSI}^* .

2.1.2 Quadratic state-dependent case

For the cost function $\sigma_2(v, S) = A_2 v^2 S$, the Hamiltonian is given by the following equation:

$$H_2(x, v, \lambda) = A_1 I + A_2 v^2 S + \lambda_S (\mu - \beta S I - (\mu + v)S) + \lambda_I I (\beta S - \gamma - \mu).$$

The adjoint system is thus as follows

$$\begin{aligned} \frac{d\lambda_S}{dt} &= -A_2 (v^*)^2 + \lambda_S (\beta I^* + \mu + v^*) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - \mu). \end{aligned}$$

The optimality condition for this case becomes

$$\frac{\partial H_2(x^*, v^*, \lambda)}{\partial v} = 2A_2 v^* S^* - \lambda_S S^* = 0.$$

Solving the above equation considering the constraints (4), we have the following characterization for the QSD optimal control:

$$v_{QSD}^*(t) = \min \left\{ v_{\max}, \max \left\{ 0, \frac{1}{2A_2} \lambda_S(t) \right\} \right\}.$$

The second derivative of the Hamiltonian H_2 with respect to v is positive, so v_{QSD}^* is a minimizer. Comparing the unbounded control solution $v_{QSI}^* = \frac{1}{2A_2} \lambda_S S^*$ with the unbounded control solution $v_{QSD}^* = \frac{1}{2A_2} \lambda_S$, we see that the main difference is that v_{QSI}^* depends on the susceptible class whereas this class does not appear in the expression for v_{QSD}^* . It is also worth noting that the λ_S appearing in v_{QSI}^* is different from the one appearing in v_{QSD}^* as they are given by the solution of two different adjoint systems (for simplicity, we have avoided a case-specific notation in the adjoint systems).

2.1.3 Linear state-independent case

For the cost function $\sigma_3(v, S) = A_2v$, the Hamiltonian is

$$H_3(x, v, \lambda) = A_1I + A_2v + \lambda_S (\mu - \beta SI - (\mu + v)S) + \lambda_I I (\beta S - \gamma - \mu)$$

and the adjoint system satisfies

$$\begin{aligned} \frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu + v^*) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - \mu). \end{aligned}$$

In this case, the optimality condition is

$$\frac{\partial H_3(x^*, v^*, \lambda)}{\partial v} = A_2 - \lambda_S S^* = 0. \quad (10)$$

Since the Hamiltonian H_3 is linear on the control, the optimality condition (10) does not depend on v and we cannot directly obtain the control characterization as we did for the QSI and QSD cases. Nevertheless, defining

$$\psi(t) = A_2 - \lambda_S(t)S^*(t), \quad (11)$$

the necessary conditions for optimality give the following optimal control solution:

$$v_{LSI}^*(t) = \begin{cases} 0, & \text{if } \psi(t) > 0, \\ v_{\max}, & \text{if } \psi(t) < 0, \\ \text{singular}, & \text{if } \psi(t) = 0. \end{cases} \quad (12)$$

Hence ψ is commonly known as a switching function. Observe that at times t_1 such that $\psi(t_1) = 0$ all the controls trivially satisfy (10). So all admissible controls are candidates for optimality. Extremal controls for which the switching function vanishes over an open interval $(t_1, t_2) \subset [0, t_f]$ are called singular [28]. The order of the singularity of the control u on (t_1, t_2) is defined [17] as the least integer κ such that

$$\frac{\partial}{\partial u} \frac{d^{2\kappa}}{dt^{2\kappa}} \psi \neq 0.$$

If $\psi = 0$ on (t_1, t_2) , then all the derivatives of ψ must also vanish on the singular interval (t_1, t_2) . So even if the optimality condition does not guide us in characterizing the control, we can use the fact that all the derivatives of the switching function vanish to obtain the singular part of the control. For a single input system that is linear in the control variable, it is well-known that the control can appear for the first time only in an even-numbered derivative of the switching function [28]. Let us assume that $\psi = 0$ on (t_1, t_2) , then $\lambda_S = A_2/S^* > 0$. To find the singular control, we need to compute at least the first two derivatives of the switching function. Using $\lambda_S S^* = A_2$ and the chain rule, we obtain (hereafter the $*$ in the optimal control and states is omitted to ease notation)

$$\frac{d\psi}{dt} = - \left(\frac{d\lambda_S}{dt} S + \frac{dS}{dt} \lambda_S \right) = \lambda_I \beta SI - \mu \lambda_S = 0.$$

This allows us to express the adjoint variable λ_I in terms of the state variables as $\lambda_I = \mu \lambda_S / \beta SI$. Since S and I are positive in Ω and $\lambda_S > 0$ then $\lambda_I > 0$. After lengthy computations, we obtain the second derivative of the switching function as

$$\frac{d^2\psi}{dt^2} = \beta SI(-A_1 + \beta A_2) + 2\mu[\beta \lambda_I I - \lambda_S(\beta I + \mu + v)] = 0 \quad (13)$$

The last expression implies $\frac{\partial}{\partial v} \frac{d^2\psi}{dt^2} \neq 0$. Therefore, the order of the singularity κ of the control is $\kappa = 1$. The generalized Legendre-Clebsch conditions (GLCC) establish [28] that if v is singular of order κ , then

$$(-1)^\kappa \frac{\partial}{\partial v} \frac{d^{2\kappa}}{dt^{2\kappa}} \psi \geq 0, \quad (14)$$

for the control to be minimizing. For our model $-\frac{\partial}{\partial v} \frac{d^2\psi}{dt^2} = 2\mu A_2/S > 0$, so condition (14) is satisfied and we cannot disregard the possibility of singular controls via the GLCC. Solving (13) for the control function v , we obtain

$$v_{sing}^{LSI}(t) = \beta I[S(-A_1 + \beta A_2) + 2\mu(\lambda_I - \lambda_I S - \lambda_S)]/2\mu\lambda_S,$$

under the admissibility condition $0 \leq v_{sing}^{LSI}(t) \leq v_{\max}$. Observe that $v_{sing}^{LSI}(t)$ is well-defined because $\lambda_S > 0$ on (t_1, t_2) . Therefore, we have proven the following result.

Theorem 1. *The optimal vaccination rate $v_{LSI}^*(t)$ for the LSI control problem satisfies*

$$v_{LSI}^*(t) = \begin{cases} 0, & A_2 > \lambda_S(t)S^*(t), \\ v_{\max}, & A_2 < \lambda_S(t)S^*(t), \\ v_{sing}^{LSI}(t), & A_2 = \lambda_S(t)S^*(t) \end{cases}$$

2.1.4 Linear state-dependent case

For the cost function $\sigma_4(v, S) = A_2 v S$, the Hamiltonian is given by the following equation:

$$H_4(x, v, \lambda) = A_1 I + A_2 v S + \lambda_S (\mu - \beta S I - (\mu + v) S) + \lambda_I I (\beta S - \gamma - \mu)$$

and the adjoint system is

$$\begin{aligned} \frac{d\lambda_S}{dt} &= -A_2 v + \lambda_S (\beta I^* + \mu + v^*) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - \mu). \end{aligned}$$

In this case, the optimality condition is

$$\frac{\partial H_4(x^*, v^*, \lambda)}{\partial v} = (A_2 - \lambda_S) S^* = 0.$$

Since $S(t) > 0$ in Ω , the switching function (hereafter the $*$ in the optimal control and states is omitted to ease notation) is $\psi(t) = A_2 - \lambda_S(t)$. Hence, the necessary conditions for optimality give

$$v_{LSD}^*(t) = \begin{cases} 0, & \text{if } \psi(t) > 0, \\ v_{\max}, & \text{if } \psi(t) < 0, \\ \text{singular}, & \text{if } \psi(t) = 0. \end{cases} \quad (15)$$

Next, we prove that the optimal control profile for $v_{LSD}^*(t)$ is purely bang-bang, that is, the switching function ψ only vanishes at isolated points. Suppose that $\psi = 0$ on an open interval $(t_1, t_2) \subset [0, t_f]$, then all the derivatives of ψ also vanish in this interval. Moreover, $\psi = 0$ yields $\lambda_S(t) = A_2$ so $\lambda_S(t)$ is a positive constant on (t_1, t_2) . Therefore, the first derivative of the switching function can be easily obtained as

$$\frac{d\psi}{dt} = A_2 v + \beta I \lambda_I - (\beta I + \mu + v) \lambda_S = \beta I (\lambda_I - \lambda_S) - \mu \lambda_S = 0.$$

Therefore,

$$\begin{aligned} \frac{d^2\psi}{dt^2} &= \beta \frac{dI}{dt} (\lambda_I - \lambda_S) + \beta I \frac{d\lambda_I}{dt} \\ &= \beta [(\lambda_I - \lambda_S)(\beta S I - (\gamma + \mu) I + I(-A_1 + \beta S \lambda_S + (\gamma + \mu) \lambda_I - \beta S \lambda_I))] \\ &= \beta I [A_2 (\gamma + \mu) - A_1] = 0, \end{aligned}$$

which yields $A_1/A_2 = \gamma + \mu$. However, the ratio A_1/A_2 can take different values depending on the cost of infection and vaccination which implies a contradiction and gives the following result.

Theorem 2. *The optimal vaccination rate $v_{LSD}^*(t)$ does not present a singular arc. Instead, the control profile follows a bang-bang structure*

$$v_{LSD}^*(t) = \begin{cases} 0, & \text{if } A_2 > \lambda_S(t), \\ v_{\max}, & \text{if } A_2 < \lambda_S(t). \end{cases}$$

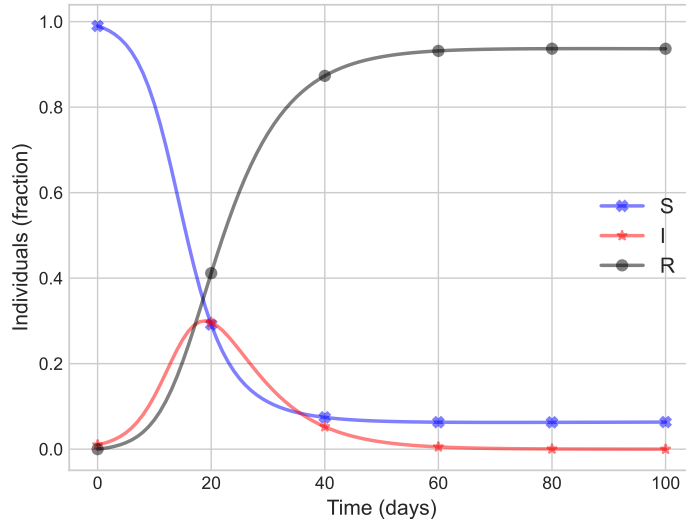


Figure 1: Dynamics of model (1) in the uncontrolled case. The model parameters are $\mu = 1/(70 \times 365)$ (days^{-1}), $\gamma = 1/7$ (days^{-1}), and $\beta = 2.7/7$ (days^{-1}) with initial conditions $S(0) = 0.99$, $I(0) = 0.01$.

2.2 Numerical approximation of the optimal vaccination for the SIR model

The numerical solution of the optimal control problem relies on BOCOP 2.2.1 [57]. BOCOP is part of the development of the INRIA-Saclay initiative for open source optimal control toolbox and is supported by the team Commands <http://www.bocop.org>. In BOCOP, the optimal control problem is approximated by a finite-dimensional optimization problem. This is done by a discretization in time applied to the state and control variables, as well as the dynamics equation. The finite-dimensional optimization problem is solved using a large-scale nonlinear programming method called IPOPT (Interior Point OPTimizer) [58]. These methods are usually less precise than indirect methods (e.g. the forward-backward sweep method [36]) based on the maximum principle, but more robust concerning the initialization.

The model parameters for the numerical simulations are taken from the measles model presented in [13] and are given by $\mu = 1/(70 \times 365)$ (days^{-1}), $\gamma = 1/7$ (days^{-1}), and $\beta = 2.7/7$ (days^{-1}). We consider the early phase of the outbreak assuming initial conditions $S(0) = 0.99$, $I(0) = 0.01$. The final time for our simulations is $t_f = 100$ days. The basic reproduction number R_0 for model (1) is given by $R_0 = \beta/(\gamma + \mu)$ and hence for our parameter values $R_0 \approx 2.7 > 1$. Therefore, in the uncontrolled case model (1) presents supercritical dynamics and converges to the endemic equilibrium where the I class is $I = \mu(R_0 - 1)/\beta$ (see Fig. 1). Observe that although it seems that the value of I^* tends to zero instead of going to an endemic equilibrium, this is correct because μ is close to zero so the value of $I = \mu(R_0 - 1)/\beta = 0.00018$ is also small.

The weight parameters $A_i > 0$ ($i = 1, 2$) are relevant variables of choice for the optimal control problem [31, 46, 53]. By adjusting the weights, one can prioritize certain objectives over others, leading to a tailored optimal control solution that aligns with specific optimization criteria. The ratio A_1/A_2 is of particular importance in the qualitative properties of the optimal control outcomes. For instance, $A_1/A_2 \ll 1$ implies that the unitary morbidity cost is less than the unitary cost of the control. This might limit in excess the use of control. On the other hand, if $A_1/A_2 \gg 1$ then the use of control could be inexpensive, leading to an excessive use of control with almost no penalization. For many real-life scenarios, the costs of a healthcare intervention or therapy are often small compared to the potential losses that an epidemic can inflict [46]. Therefore, we start assuming that $A_1/A_2 = 5$. The resulting optimal control profiles and their associated optimal states are shown in the left and right columns in Fig. 2, respectively.

Fig. 2 shows (see the left column) that the control profiles for the quadratic formulations, $v_{QSI}^*(t)$ and $v_{QSD}^*(t)$, share very similar qualitative characteristics. However, in quantitative terms the $v_{QSI}^*(t)$ solutions implies that the control should be used at its maximum capacity for approximately 57 days whereas $v_{QSD}^*(t)$ implies maximum vaccine deployment for almost 80 days. This difference is significant

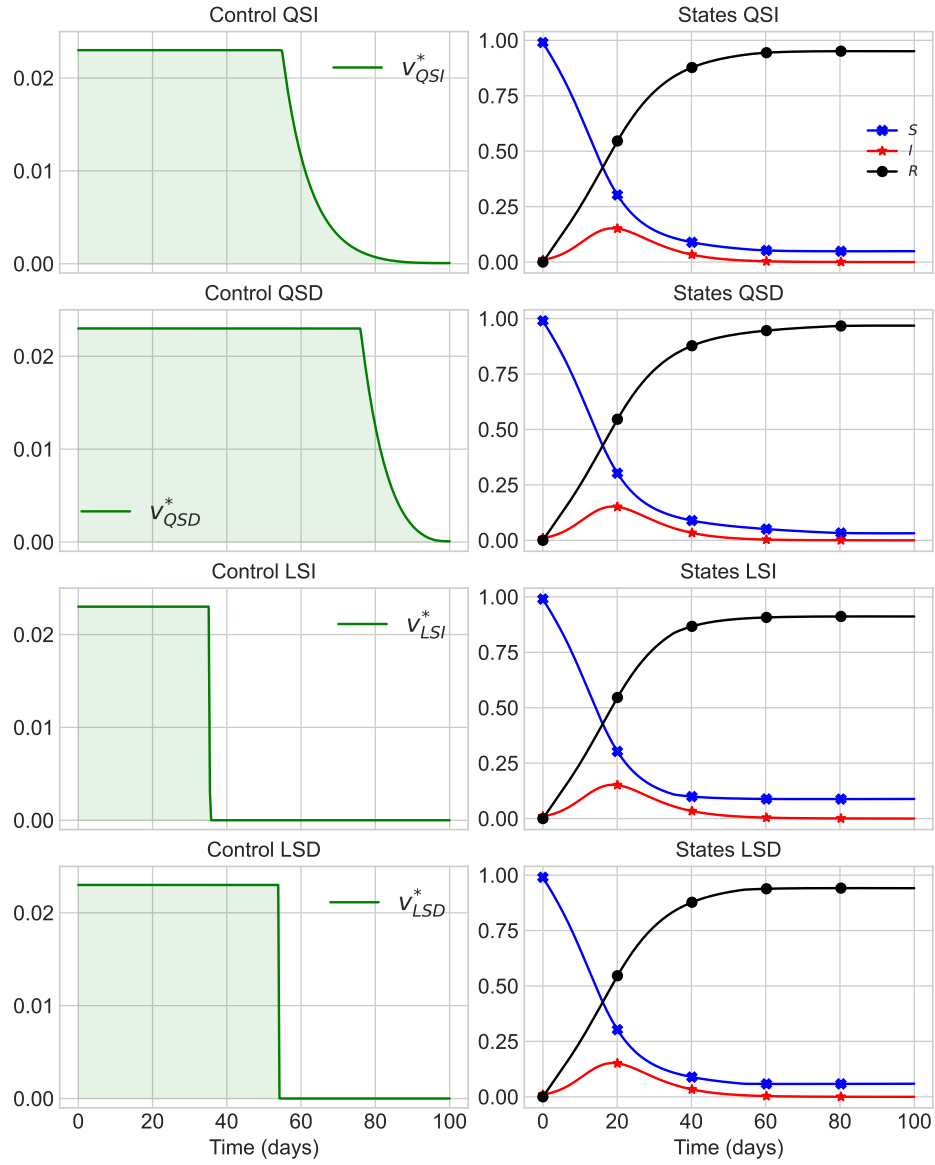


Figure 2: Numerical approximation of the vaccination profile (left column) and associated states (right column) for the SIR control model (1). The weight parameters are $A_1 = 5$, $A_2 = 1$.

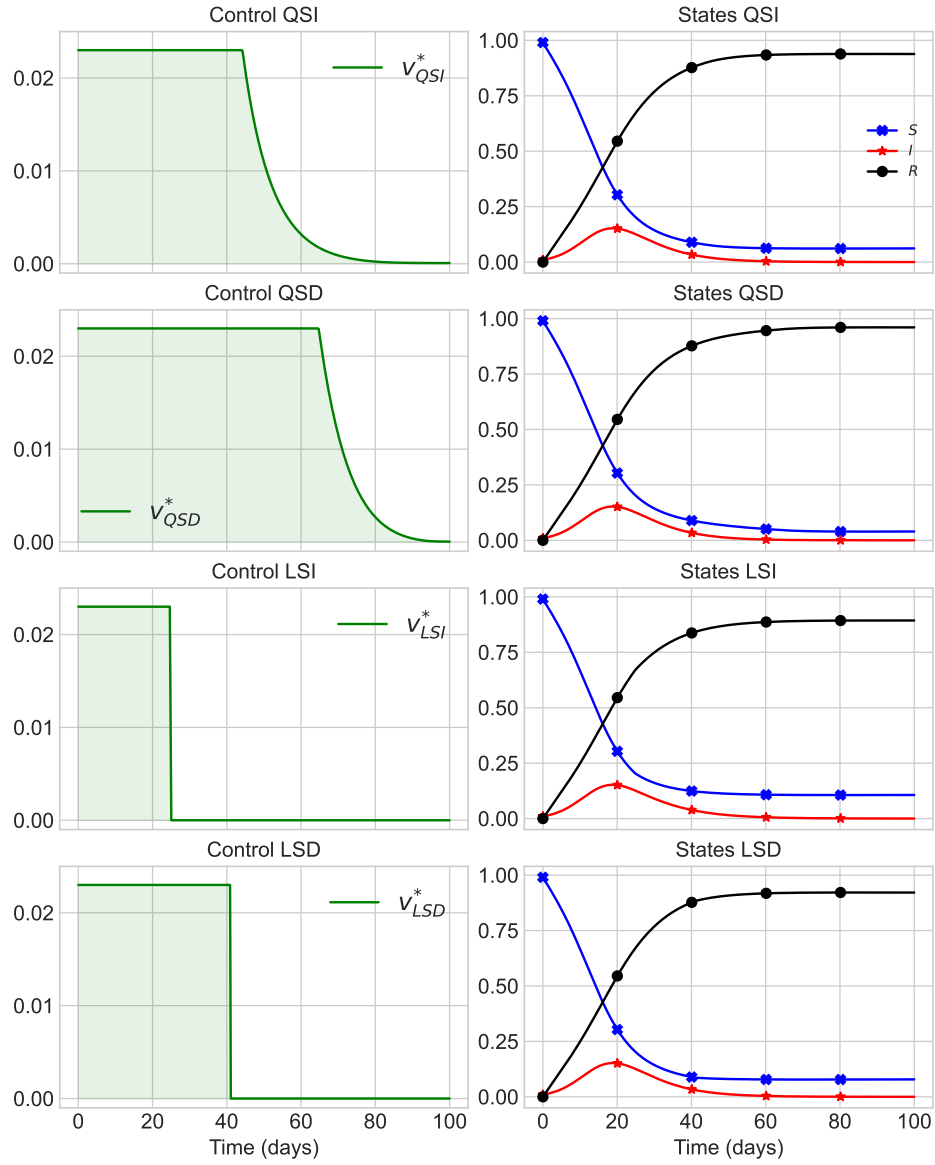


Figure 3: Numerical approximation for the vaccination profile (left column) and associated states (right column) for the SIR control model (1). The weight parameters are $A_1 = 1$, $A_2 = 1$.

for a time horizon of 100 days. Likewise, the control profiles for the linear formulations, $v_{LSI}^*(t)$ and $v_{LSD}^*(t)$, exhibit comparable patterns presenting a bang-bang structure. In quantitative terms, $v_{LSI}^*(t)$ suggest 38 days of maximum vaccine deployment while $v_{LSD}^*(t)$ suggest 55 days. A comparison between the quadratic and linear control profiles reveals that the quadratic formulations recommend a greater deployment of vaccines. A reasonable explanation is that for our model the linear cost is more expensive than the quadratic cost as the maximum vaccination rate v_{\max} satisfies $0 \leq v^2 \leq v \leq v_{\max} < 1$. We notice a similar trend when examining the quadratic (linear) density-dependent control $v_{QSD}^*(t)$ ($v_{LSD}^*(t)$) in comparison to the quadratic (linear) density-independent control $v_{QSI}^*(t)$ ($v_{LSI}^*(t)$), where the density-dependent profiles indicate a greater deployment of vaccines. Since the state variables represent fractions of the population, we have $v(t)S(t) < v(t)$ and $v(t)^2S(t) < v(t)^2$ for all t , so the control costs for density-dependent formations is less costly. Overall, although the four optimal control profiles share some qualitative properties (such as initial maximum vaccine deployment), in quantitative terms there are significant differences, for instance, the profile $v_{QSD}^*(t)$ maintains the maximum control effort for almost twice the time compared with the profile $v_{LSI}^*(t)$. On the other hand, the associated states are almost the same for the four problems (see the right column in Fig. 2) with the epidemic peak on day 20. We also considered a scenario in which the weights A_1 and A_2 are equal ($A_1 = A_2 = 1$) so the costs of vaccination and infection are similar. The results for this case are depicted in Fig. 3. The optimal control profiles shown in Fig. 3 present the same qualitative features as those in Fig. 2. Therefore, relatively small changes in the cost of vaccination do not significantly change the vaccination strategy.

3 Optimal treatment for the SIR epidemic model

In the previous section, we proposed an optimal control problem to optimize a time-dependent vaccination rate. To provide further insights into how different objective functionals influence optimal control outcomes in epidemic models, we expand our investigation by considering an optimal control problem to optimize a time-dependent control $u(t)$ that represents the per capita treatment rate of infected individuals. The model is governed by the following system of differential equations:

$$\begin{aligned} \frac{dS}{dt} &= \mu - \beta SI - \mu S, & S(0) &= S_0 > 0 \\ \frac{dI}{dt} &= \beta SI - \gamma I - u(t)I - \mu I, & I(0) &= I_0 > 0. \end{aligned} \tag{16}$$

In model (16), the treatment function $u(t)$ accelerates the recovery of the infectious individuals. The rest of the parameters are the same as in the *SIR* model (1) and the total population size satisfies $N(t) = S(t) + I(t) + R(t) = 1$ for all t (the equation for the R class is omitted).

In practice, it is reasonable to expect that multiple interventions, such as social distancing, lockdowns, and mask use, would be implemented simultaneously to control most diseases. Therefore, focusing only on treating infected individuals as a control method is an oversimplification. However, it is important to note that for some diseases, like tuberculosis (TB), prevention largely depends on treatment. Although TB has a vaccine (Bacille Calmette-Guerin), it is not highly effective in adults and does not prevent all forms of TB [15]. Additionally, implementing social distancing can be difficult in regions with high TB prevalence, especially in overcrowded living conditions.

The optimal control problem aims to minimize the cumulative number of infectious individuals and the control effort, hence, the objective functional is defined as follows:

$$\Gamma_i(u(t)) = \int_0^{t_f} A_1 I(t) + C_i(u(t), I(t)) dt. \tag{17}$$

The term $A_1 I(t)$ in the objective (17) represents the monetary costs of having, at each time, $I(t)$ infectious individuals, whereas the function $C_i(u(t), I(t))$ represents the treatment costs. We consider four different cost function $C_i(u, I)$ ($i = 1, 2, 3, 4$) defined as follows:

$$\begin{aligned} C_1(u, I) &= A_2 u^2, & \text{QSI cost,} \\ C_2(u, I) &= A_2 u^2 I, & \text{QSD cost,} \\ C_3(u, I) &= A_2 u, & \text{LSI cost,} \\ C_4(u, I) &= A_2 u I, & \text{LSD cost.} \end{aligned} \tag{18}$$

The time-dependent treatment rate is bounded and satisfies $0 \leq u(t) \leq u_{\max} \leq 1$ for all t . The maximum value, u_{\max} , will depend on the infection under study. Nevertheless, considering a mean recovery time $1/\gamma$ equal to τ days, for an optimistic case in which the maximum treatment rate doubles the speed of recovery, then $1/(\gamma + u_{\max}) = \tau/2$ which implies $u_{\max} = \gamma$. For most diseases, more than one day is needed for recovery so $u_{\max} = \gamma \leq 1$. Hence, the set of admissible controls is

$$\mathcal{U} = \{u : [0, t_f] \rightarrow [0, u_{\max}] \subseteq [0, 1] \text{ Lebesgue measurable}\}. \quad (19)$$

The optimal control problem consists of finding an optimal treatment function $u^*(t)$, such that

$$\Gamma_i(u^*) = \min_{u \in \mathcal{U}} \Gamma_i(u(t)) = \min_{u \in \mathcal{U}} \int_0^{t_f} A_1 I(t) + C_i(u(t), I(t)) dt, \quad (20)$$

subject to SIR model with treatment (16). The existence of the optimal control solution for problem (20) is established by following the same argument as the proof provided in Theorem 5, and is therefore omitted. As before, the maximum principle converts the optimal control problem (20) into a problem of minimizing pointwise a Hamiltonian \hat{H}_i given by

$$\hat{H}_i(x, u, \lambda) = A_1 I + C_i(u, I) + \lambda_S (\mu - \beta SI - \mu S) + \lambda_I I (\beta S - \gamma - u - \mu).$$

The derivation of the first-order necessary conditions for optimality is given next.

3.0.1 Quadratic state-independent case

For the cost function $C_1(u, I) = A_2 u^2$, the Hamiltonian takes the next form

$$\hat{H}_1(x, u, \lambda) = A_1 I + A_2 u^2 + \lambda_S (\mu - \beta SI - \mu S) + \lambda_I I (\beta S - \gamma - u - \mu).$$

Hence, the system for the adjoint variables is

$$\begin{aligned} \frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - u^* - \mu), \end{aligned}$$

and the optimality condition reduces to

$$\frac{\partial \hat{H}_1(x^*, u^*, \lambda)}{\partial u} = 2A_2 u^* - \lambda_I I^* = 0.$$

Hence, we obtain the following characterization for the QSI optimal control:

$$u_{QSI}^*(t) = \min \left\{ u_{\max}, \max \left\{ 0, \frac{1}{2A_2} \lambda_I(t) I^*(t) \right\} \right\}.$$

Observe that the second derivative of the Hamiltonian \hat{H}_1 with respect to u is positive, so a minimum occurs at u_{QSI}^* .

3.0.2 Quadratic state-dependent case

For the cost function $C_2(u, I) = A_2 u^2 I$, the Hamiltonian is given by the following equation:

$$\hat{H}_2(x, u, \lambda) = A_1 I + A_2 u^2 I + \lambda_S (\mu - \beta SI - \mu S) + \lambda_I I (\beta S - \gamma - u - \mu).$$

The adjoint system is thus as follows

$$\begin{aligned} \frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 - A_2 (u^*)^2 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - u^* - \mu). \end{aligned}$$

The optimality condition for this case becomes

$$\frac{\partial \hat{H}_2(x^*, u^*, \lambda)}{\partial u} = 2A_2 u^* I^* - \lambda_I I^* = 0.$$

Therefore, we have the following characterization for the QSD optimal control:

$$u_{QSD}^*(t) = \min \left\{ u_{\max}, \max \left\{ 0, \frac{1}{2A_2} \lambda_I(t) \right\} \right\}.$$

The second derivative of the Hamiltonian \hat{H}_2 with respect to u is positive, so u_{QSD}^* is a minimizer.

3.0.3 Linear state-independent case

For the cost function $C_3(u, I) = A_2 u$, the Hamiltonian is

$$\hat{H}_3(x, u, \lambda) = A_1 I + A_2 u + \lambda_S (\mu - \beta S I - \mu S) + \lambda_I I (\beta S - \gamma - u - \mu)$$

and the adjoint system satisfies

$$\begin{aligned} \frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - u^* - \mu). \end{aligned} \quad (21)$$

In this case, the optimality condition is

$$\frac{\partial \hat{H}_3(x^*, u^*, \lambda)}{\partial u} = A_2 - \lambda_I I^* = 0. \quad (22)$$

Let us define the switching function

$$\psi(t) = A_2 - \lambda_I(t) I^*(t). \quad (23)$$

Since $\psi(t)$ does not explicitly depend on the control $u(t)$, the possibility of singular control arises and hence:

$$u_{LSI}^*(t) = \begin{cases} 0, & \text{if } \psi(t) > 0, \\ u_{\max}, & \text{if } \psi(t) < 0, \\ \text{singular}, & \text{if } \psi(t) = 0. \end{cases}$$

To investigate the singular solution, we suppose $\psi = 0$ on an interval $(t_1, t_2) \subset [0, t_f]$ which implies that all the derivatives of ψ vanish in this interval. First, note that $\psi = 0$ implies $\lambda_I I^* = A_2 > 0$. Using this equality and the chain rule, we obtain the first derivative of the switching function as (hereafter the $*$ in the optimal control and states is omitted to ease notation)

$$\frac{d\psi}{dt} = -\{I[-A_1 + \lambda_S \beta S - \lambda_I (\beta S - \gamma - u - \mu)] + \lambda_I I (\beta S - \gamma - u - \mu)\} = I(A_1 - \lambda_S \beta S) = 0.$$

Since $I(t) > 0$ in Ω , we have $\lambda_S \beta S = A_1 > 0$. Hence the second derivative of the switching function is

$$\begin{aligned} \frac{d^2\psi}{dt^2} &= -\beta I [S(\lambda_S (\beta I + \mu) - \lambda_I \beta I) + \lambda_S (\mu - \beta S I - \mu S)] \\ &= \beta I [\lambda_I \beta S I - \lambda_S \mu] = \beta I [A_2 \beta S - \lambda_S \mu] = 0, \end{aligned}$$

therefore $\lambda_S \mu = A_2 \beta S > 0$. Since the first two derivatives of the switching function are independent of the control, we also need to compute the third and fourth derivatives. The third derivative of the switching function is

$$\begin{aligned} \frac{d^3\psi}{dt^3} &= \beta I [A_2 \beta (\mu - \beta S I - \mu S) - A_2 \beta (\beta S I + \mu S) + A_2 \beta \mu] \\ &= \beta I [2A_2 \beta \mu - 2A_2 \beta (\beta S I + \mu S)] \\ &= 2A_2 \beta^2 I [\mu - (\beta S I + \mu S)] = 0, \end{aligned}$$

hence $\mu - \beta SI - \mu S = 0$. Using this result, we obtain the following expression for the fourth derivative of the switching function

$$\begin{aligned}\frac{d^4\psi}{dt^4} &= -2A_2\beta^2 I[\beta S'I + \beta SI' + \mu S'] \\ &= -2A_2\beta^2 I[(\mu - \beta SI - \mu S)(\beta I + \mu) + \beta SI(\beta S - \gamma - u - \mu)] \\ &= -2A_2\beta^3 SI^2(\beta S - \gamma - u - \mu) = 0.\end{aligned}$$

The last expression implies $\frac{\partial}{\partial u} \frac{d^4\psi}{dt^4} \neq 0$. Therefore, the order of the singularity of the control is $\kappa = 2$. For our model $\frac{\partial}{\partial u} \frac{d^4\psi}{dt^4} > 0$, so condition (14) is satisfied and we cannot disregard the possibility of singular controls via the GLCC. Since $S, I > 0$ in Ω , the above equality implies that $\beta S - \gamma - u - \mu = 0$. Solving this equation for the control function u we obtain its singular part

$$u_{sing}^{LSI}(t) = \beta S(t) - \gamma - \mu,$$

under the admissibility condition $0 \leq u_{sing}^{LSI}(t) \leq u_{\max}$. However, $\mu - \beta SI - \mu S = 0$ and $\beta S - \gamma - u - \mu = 0$ imply that S and I are constant in the interval (t_1, t_2) with the following values:

$$S = \frac{1}{\beta} \sqrt{\frac{\mu A_1}{A_2}}, \quad I = \frac{\mu}{\beta} \left(\frac{1 - S}{S} \right).$$

Therefore $u(t)$ is also constant in (t_1, t_2) and the Hamiltonian becomes $\hat{H}_3 = A_1 I + A_2 u$. By remark 1, the Hamiltonian is constant with minimum value along the optimal solution, hence $u(t) = 0$ but this is only possible if $\psi > 0$, which contradicts the original assumption for the control to be singular. Therefore, we have proven the following result.

Theorem 3. *The optimal treatment rate $u_{LSI}^*(t)$ does not present a singular arc. Instead, the control profile for $u_{LSD}^*(t)$ is given by*

$$u_{LSI}^*(t) = \begin{cases} 0, & A_2 > \lambda_I(t) I^*(t) \\ u_{\max}, & A_2 < \lambda_I(t) I^*(t) \end{cases}$$

3.0.4 Linear state-dependent case

For the cost function $C_4(u, I) = A_2 u I$, the Hamiltonian is given by the following equation:

$$\hat{H}_4(x, u, \lambda) = A_1 I + A_2 u I + \lambda_S (\mu - \beta SI - \mu S) + \lambda_I I (\beta S - \gamma - u - \mu)$$

and the adjoint system is

$$\begin{aligned}\frac{d\lambda_S}{dt} &= \lambda_S (\beta I^* + \mu) - \lambda_I \beta I^*, \\ \frac{d\lambda_I}{dt} &= -A_1 - A_2 u + \lambda_S \beta S^* - \lambda_I (\beta S^* - \gamma - u^* - \mu).\end{aligned}\tag{24}$$

In this case, the optimality condition is

$$\frac{\partial \hat{H}_4(x^*, u^*, \lambda)}{\partial u} = (A_2 - \lambda_I) I^* = 0,\tag{25}$$

Since $I(t) > 0$ in Ω , the switching function (hereafter the * in the optimal control and states is omitted to ease notation) is $\psi(t) = A_2 - \lambda_I(t)$. Hence, the necessary conditions for optimality give

$$u_{LSD}^*(t) = \begin{cases} 0, & \text{if } \psi(t) > 0, \\ u_{\max}, & \text{if } \psi(t) < 0, \\ \text{singular}, & \text{if } \psi(t) = 0. \end{cases}$$

We can assume that $\psi = 0$, that is, $\lambda_I = A_2 > 0$ on an open interval $(t_1, t_2) \subset [0, t_f]$ to investigate the singular solution using the derivatives of ψ . A simple computation verifies that

$$\frac{d\psi}{dt} = A_1 - \lambda_S \beta S + A_2 (\beta S - \gamma - \mu) = 0,$$

hence $A_1 + \beta S(A_2 - \lambda_S) - A_2(\gamma + \mu) = 0$, and the second derivative of the switching function is

$$\begin{aligned}\frac{d^2\psi}{dt^2} &= \beta[(\mu - \beta SI - \mu S)(A_2 - \lambda_S) - \lambda_S(\beta SI + S\mu) + A_2\beta SI] \\ &= \mu\beta(A_2(1 - S) - \lambda_S) = 0.\end{aligned}$$

Therefore $\lambda_S = A_2(1 - S) > 0$. Differentiating once more the switching function and simplifying, we have the following expression for the third derivative

$$\frac{d^3\psi}{dt^3} = 2\mu\beta A_2(\beta SI + \mu S - \mu) = 0,$$

this implies $\beta SI + \mu S - \mu = -S' = 0$ and hence S is constant in the singular interval. The fourth derivative reads as follows

$$\frac{d^4\psi}{dt^4} = 2\mu\beta A_2(S'(\beta I + \mu) + \beta I'S) = -2\mu\beta^2 A_2 SI(\beta S - \gamma - u - \mu) = 0,$$

which implies $\beta S - \gamma - u - \mu = 0$ so $I' = 0$ and I is constant in the interval (t_1, t_2) . In particular, S and I have the following constant values:

$$S = \sqrt{\frac{A_2(\gamma + \mu) - A_1}{A_2\beta}}, \quad I = \frac{\mu}{\beta} \left(\frac{1 - S}{S} \right).$$

Since, we are looking to minimize the Hamiltonian $\hat{H}_4 = A_1 I + A_2 u I = \text{const}$, then $u(t) = 0$, however this implies $\psi > 0$. This contradiction shows that a singular control does not exist; hence, we have the following result.

Theorem 4. *The optimal treatment rate $u_{LSD}^*(t)$ does not present a singular arc. Instead, the control profile for $u_{LSD}^*(t)$ is given by*

$$u_{LSD}^*(t) = \begin{cases} 0, & \text{if } A_2 > \lambda_I(t), \\ u_{\max}, & \text{if } A_2 < \lambda_I(t). \end{cases}$$

3.1 Numerical approximation of the optimal treatment for the SIR model

We start our numerical analysis assuming that the cost of treatments is significantly less than the cost of infection so $A_1/A_2 = 5$. Fig. 4 indicates (see the left column) that the control profiles $u_{QSD}^*(t)$ and $u_{LSD}^*(t)$ follow the same structure indicating that the control should be used at its maximum capacity for the whole time interval decreasing to zero only at the final time. On the other hand the control profiles, $u_{QSI}^*(t)$ and $u_{LSI}^*(t)$, do not suggest maximum control deployment for the full interval. Instead, the control $u_{QSI}^*(t)$ is maintained at the maximum level for approximately 60 days and then decreases slowly maintaining positive values during the whole period reaching zero only at the final time. The control $u_{LSI}^*(t)$ follows a bang-bang structure and, unlike the other three control profiles, does not recommend maximum control effort during the early phase of the outbreak. Instead, $u_{LSI}^*(t)$ prescribes maximum control effort from day 9 to day 47, after which it is set to zero. Finally, note that despite some differences in the optimal control profiles, the resulting optimal state trajectories are nearly identical for the QSI, QSD, and LSD formulations, with a peak occurring around day 23 (see the right column in Fig. 4). In contrast, for the LSI formulation, the I class reaches a higher epidemic peak, which occurs around day 11.

We also consider a scenario in which the control cost might be as expensive as the cost of infection assuming $A_1/A_2 = 1$. The results are presented in Fig. 5. Again, the control profiles $u_{QSD}^*(t)$ and $u_{LSD}^*(t)$ are the same and specify that the maximum rates should be maintained in the whole time interval. This is a surprising result as the control cost is 5 times more expensive in comparison with the previous case where $A_1/A_2 = 5$. One possible explanation for this behavior is that both the QSD and LSD cost functions $C_2(u, I) = A_2 u^2 I$ and $C_4(u, I) = A_2 u I$, the control is multiplied by the infected population and since the value of I is very close to zero then both cost functions are also very close to zero. Hence, the cost of control is cheap and the optimal policy is to use it at maximum capacity. On the other hand, the control profiles $u_{QSI}^*(t)$ and $u_{LSI}^*(t)$ present notable differences. The control

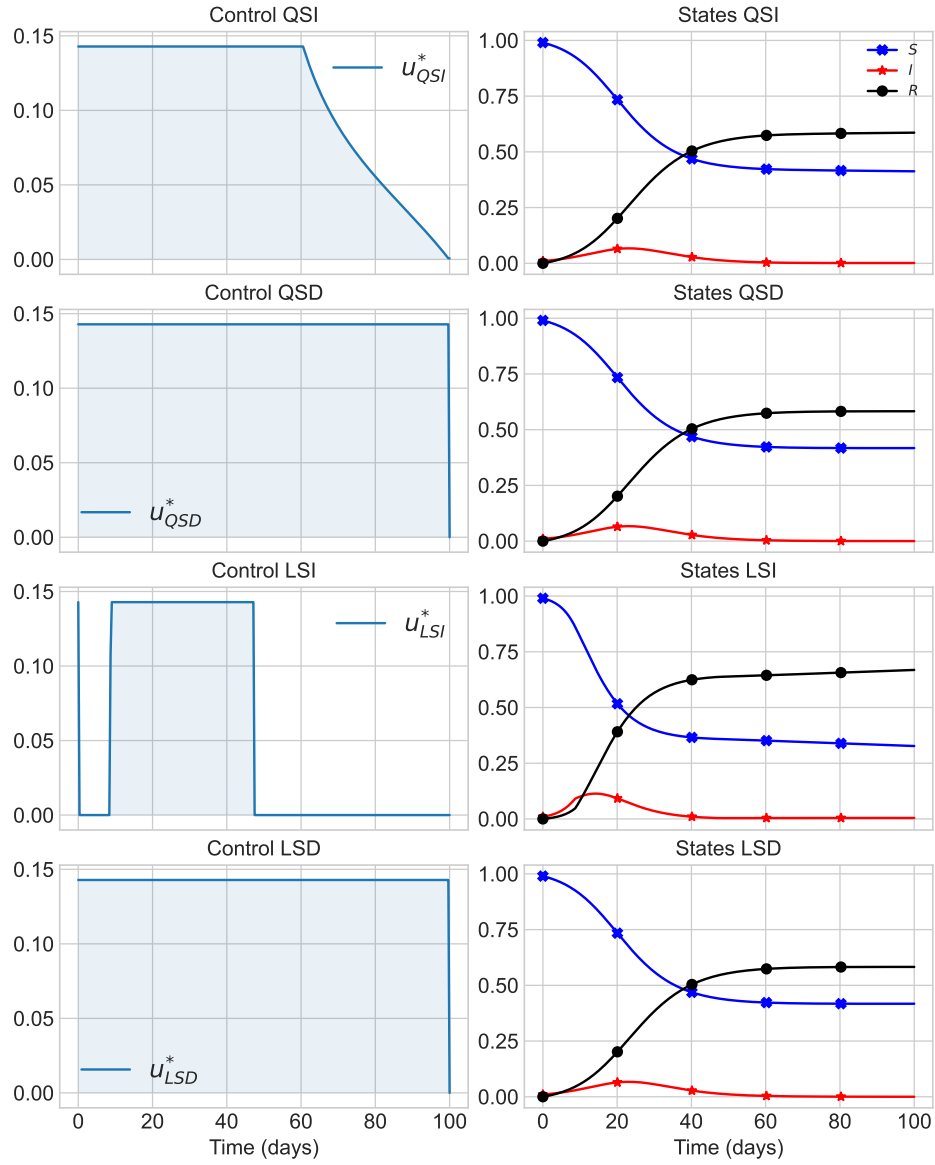


Figure 4: Numerical approximation of the treatment profile (left column) and associated states (right column) for the SIR control model (16). The weight parameters are $A_1 = 5$, $A_2 = 1$.

$u_{QSI}^*(t)$ indicates that the control effort should start with a low but positive value that is continuously increased reaching maximum control effort on day 11. The control is then maintained at its maximum value for almost 30 days and then is continuously decreased reaching zero at the end of the time interval. In contrast, the control $u_{LSI}^*(t)$ remains at zero for most of the time, with only a brief period of about 10 days at maximum capacity. Therefore, $u_{LSI}^*(t)$ is fundamentally different from the control profiles of the other three formulations. Finally, observe that the optimal states associated with the LSI problem are significantly different from the ones for the other three problems (see the right column in Fig. 5). This was expected given that the control $u_{LSI}^*(t)$ implies considerably less use of control than the other three control functions.

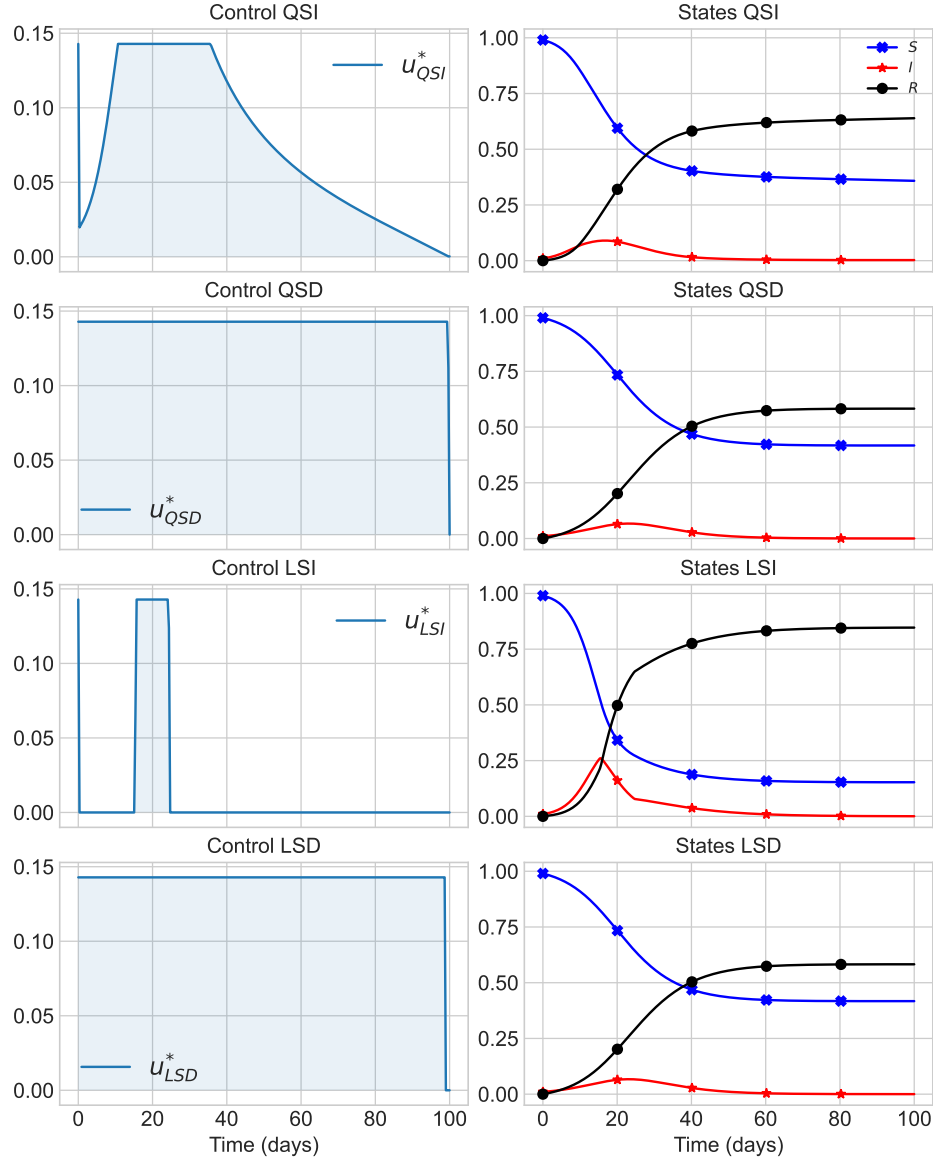


Figure 5: Numerical approximation for the treatment profile (left column) and associated states (right column) for the SIR control model (16). The weight parameters are $A_1 = 1$, $A_2 = 1$.

4 Discussion

The performance index or objective functional is a critical element in optimal control applications. Choosing a realistic objective functional ensures that the optimization process aligns with the desired

outcomes and objectives in the real-world application. The objective functional also significantly influences the mathematical properties of optimal control solutions [31, 46]. Therefore, selecting a suitable objective functional is just as important as the model used to represent the dynamics of the process being studied. In epidemiological applications, optimal control problems typically aim to minimize the disease burden while keeping a low control (such as vaccination, quarantine, or treatment) effort [26, 46]. The disease burden is often calculated by integrating the infected classes (such as the I class in the SIR model), while control costs are subjectively determined by the modeler. In many cases, the cost of a control $v(t)$ is typically defined as proportional to $v^2(t)$ in the objective functional as this leads to convexity properties that make the problem more amenable to mathematical analysis. However, this quadratic cost representation may not always be the most suitable in epidemiological and other biological scenarios [18, 26, 31, 46].

This work aimed to investigate how the choice of objective functional impacts optimal control outcomes for disease control. To this end, we developed two optimal control problems based on the classical SIR epidemic model. In the first scenario, the control represents prophylactic vaccination, while in the second scenario, it represents the treatment of infected individuals. For each scenario, we proposed four distinct objective functionals to capture the cost of control interventions: quadratic state-independent cost (QSI), quadratic state-dependent cost (QSD), linear state-independent cost (LSI), and linear state-dependent cost (LSD). It is worth noting that, in both the QSI and LSI formulations, the control cost does not depend on the actual number of individuals being vaccinated or treated, which is biologically unrealistic. Nevertheless, the QSI and LSI formulations remain surprisingly common in optimal control applications within epidemiology [1, 3, 5, 6, 9, 12, 16, 19, 23, 21, 27, 32, 35, 39, 40, 41, 49, 52, 54, 56]. As such, we have included these cases aiming to compare a large range of optimal control outcomes. The QSI and QSD cases belong to L_2 -type objectives, which usually result in continuous control profiles. On the other hand, the LSI and LSD cases are linked to L_1 -type objectives, whereby the control profiles exhibit a bang-bang structure and may include singular regimes. Additionally, selecting the right weight parameters in the objective functional is crucial for balancing trade-offs between competing targets. To illustrate this, we compared optimal control outcomes using different weight settings. Initially, the weight parameters were tuned to align the optimization process with the understanding that the cost of infection far surpasses the cost of control actions (Figs. 2 and 4) but we also considered relatively expensive controls whose costs were close to the cost of infection (Figs. 3 and 5).

For the optimal vaccination problem, the numerical experiments suggest that the control profiles for the quadratic formulations, $v_{QSI}^*(t)$ and $v_{QSD}^*(t)$, share very similar qualitative characteristics. Likewise, the control profiles for the linear formulations, $v_{LSI}^*(t)$ and $v_{LSD}^*(t)$, exhibit comparable patterns presenting a bang-bang structure. A comparison between the quadratic and linear control profiles reveals that the quadratic formulations recommend a greater deployment of vaccines. For the optimal treatment problem, the control profiles $u_{QSD}^*(t)$ and $u_{LSD}^*(t)$ are the same and specify that the maximum rates should be maintained in the whole time interval and are robust with respect to the value of the weight parameters. Whereas, $u_{QSI}^*(t)$ and $u_{LSI}^*(t)$, do not suggest maximum control deployment for the full interval and present visible differences. Overall, our numerical simulations show that while some qualitative features of the control profiles are shared in certain cases, significant differences can also be observed among them. Therefore, when faced with uncertainty about the form of the objective function and its connection to the control parameter, it is advisable to analyze the situation using multiple objectives and then determine which solution is more suitable for practical implementation. Additionally, since the QSI and LSI formulations do not account for the actual number of people vaccinated or treated, it is preferable to use the QSD or LSD formulations instead.

This study, like all modeling efforts, has a number of limitations. First, we focus on the basic SIR model because it allows us to derive a complete analytical solution for each control problem. As such, this work is primarily a theoretical modeling exercise inspired by a relevant biological problem, rather than a direct application to real-world scenarios. Additionally, we consider only a single intervention (either vaccination or treatment) at a time, whereas, in practice, multiple interventions such as social distancing, mask use, and vaccination would likely be implemented simultaneously. Another limitation is that the numerical values for the weight parameters in the objective functional are selected based on plausible mathematical assumptions, rather than on real data. Finally, our analysis is based on a finite-horizon optimal control problem with integral cost functionals, and the results may not be directly applicable to other types of optimal control settings. Despite these limitations, this investigation into

multiple objective functionals can be considered an initial endeavor toward developing theoretically enhanced strategies for optimizing control policies against communicable diseases.

CRedit authorship contribution statement

Fernando Saldaña: Conceptualization, Methodology, Software, Formal analysis, Writing – Original Draft, Writing – Review & Editing, Visualization. **Hao Wang:** Writing – Review & Editing, Supervision, Project administration. **José Ariel Camacho-Gutiérrez:** Conceptualization, Methodology, Software, Formal analysis, Writing – Review & Editing, Visualization.

Competing interests

The author declares he has no competing financial interests that could have appeared to influence the results reported in this work.

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Data availability statement

We do not analyze or generate any datasets, because our work proceeds within a theoretical and mathematical approach.

A Existence of the optimal control solution

We prove the existence of an optimal control $v^*(t)$ and corresponding optimal states $x^* = (S^*, I^*)^T$ for each of our control problems via a classical existence Theorem by Fleming and Rishel (see Theorem 4.1 and its Corollary in [20, Chapter III]). This theorem states that the following conditions are sufficient to guarantee the existence of a solution for the optimal control problem (5).

(H1) F is continuous, and there exist positive constants K_1 and K_2 such that

- (a) $|F(t, x, v)| \leq K_1(1 + |x| + |v|)$
- (b) $|F(t, \tilde{x}, v) - F(t, x, v)| \leq K_2|\tilde{x} - x|(1 + |v|)$

hold for all $t \in [0, t_f]$. Moreover, F can be written as $F(t, x, v) = f_1(t, x) + f_2(t, x)v$.

(H2) The set of admissible controls \mathcal{V} is closed and convex. Moreover, there is at least one feasible pair $(x(t), v(t))$ satisfying system (1) with $v(t) \in \mathcal{V}$.

(H3) $L_i(t, x, \cdot)$, $i = 1, 2, 3, 4$ is convex on \mathcal{V} , and $L_i(t, x, v) \geq g(v)$, where g is continuous and $|v|^{-1}g(v) \rightarrow +\infty$ as $|v| \rightarrow \infty$, $v \in \mathcal{V}$.

Theorem 5. *Consider the optimal control problem (5) with control model (1) and objective functional $J_i(v) = \int_0^{t_f} L_i(t, x, v)dt$ ($i = 1, 2, 3, 4$). Then there exists an admissible control function $v^*(t) \in \mathcal{V}$ such that $\min J_i(v)_{v \in \mathcal{V}} = J_i(v^*)$.*

Proof. Since we are considering a constant population, the solution of model (16) is bounded. In addition, $F \in C^1$, and, therefore, (a) and (b) in (H1) are ensured by suitable bounds on the partial derivatives of F and $F(t, 0, 0)$. Moreover, the state equations are linear with respect to the controls v , and, thus, $F(t, x, v) = f_1(t, x) + f_2(t, x)v$. The existence of a feasible pair is guaranteed by the Caratheodory theorem [34, pp. 182] for Cauchy problems. Moreover, for bounded controls on a finite time interval, \mathcal{V} is closed and convex, and, hence, (H2) is satisfied as well. The integrand $L_i(t, x, \cdot)$ of the objective functional is non-negative for $i = 1, 2, 3, 4$, quadratic for $i = 1, 2$ and linear for $i = 3, 4$ with respect to the controls. Therefore, $L_i(t, x, \cdot)$ is convex on \mathcal{V} . Furthermore, the set of admissible controls \mathcal{V} is bounded (this also implies that the term $|v|$ in (H1) can be omitted), and, hence, (H3) holds vacuously, completing the proof. \square

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