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System Identification and Optimal Control for COVID-19 Epidemiological Dynamics at Amazonas State, Brazil.

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Abstract: This work aims to identify and to obtain an optimal control strategy for an epidemiological model of the COVID-19 pandemic at the State of Amazonas. Firstly, it was identified a mathematical model that describes the dynamics of coronavirus propagation at the state. In order to identify the model, it was chosen a SIRD type, whose parameters were estimated using the Least Squares Method for different scenarios: from August to November 2020 and from January to March 2021. After the parameters' estimation, the Optimal Control Problem was formulated and a performance index was chosen to minimize the cost associated with infection cases, deaths and pandemic control actions over the population. The characterization of the optimal solution was accomplished by using the Pontryagin Principle approach, restricting the final time of the control horizon. Finally, numerical solutions of state and co-state equations were obtained applying the forward and backward sweep method.

Keywords: Parameter Estimation, Inverse Problem, Pontryagin Principle, Optimal Control , COVID-19 in Amazonas

INTRODUCTION

One of the main concerns about the transmission of coronavirus at Amazonas State is the capacity of the health system both from the capital city and from the interior region to support demand load, restricted by the lack of material resources and the geographic distances. Thus, understanding the behavior of the spread of COVID-19 in the State of Amazonas becomes essential to support public policies, control strategies and to explain how the virus spread occurs. An alternative to model the spread of infectious diseases is using epidemiological models. These models divide the population into compartments, *Susceptible* $S(t)$ - *Infected* $I(t)$ - *Removed* $R(t)$, describing its behavior over time in order to analyze the infection transmission rate and the basic reproduction number R_0, determined by the ratio between infection transmission rate and infection recovery rate (Luiz, 2012). Throughout the text, a will be the transmission rate and b the recovery rate.

Marinov and Marinova (2020) investigate the dynamics of COVID-19 by first solving an inverse problem to estimate the parameters (transmission rate and recovery rate) of the SIR model from real data. Then, the estimated parameters are used to calculate the evolution of the disease in different countries. Batista (2020) aims to estimate the final size of the coronavirus epidemic. For this, initially, the parameters of the SIR model and its initial values are estimated by minimizing the difference between the number of predicted and current cases. Both studies apply the Least Squares Method (LSM) for parameter estimation. This method presents admissible results for the curve fitting of the SIR model. Based on this, other compartment configurations can be proposed, such as the SIRD model, which adds compartment D representing the deaths from the disease in the population. This model can be seen in Comunian *et al.* (2020). Once the model is identified, control through vaccination can be studied. The objective of control by vaccination is to reduce the number of susceptible individuals and, consequently, reduce the number of those infected.

In search of finding the best alternative to synthesize this control strategy, researches using Optimal Control Theory are found in the literature. The Optimal Control Theory is a study branch within modern control, whose objective is to solve an Optimal Control Problem (OCP). To solve an OCP, several approaches were developed, including the Pontryagin Principle, which provides a necessary condition for the system to be optimal (Grass, 2008). Elhia *et al.*(2013) introduce a time-delayed optimal control strategy for both state and control variables. The article also presents a solution to the system of equations applying the numerical method of forward and backward scanning, which is of great relevance to Pontryagin's Principle where two coupled systems of equations are obtained, but one has boundary conditions at t_0 and another at t_f. In Libotte *et al.* (2020), an optimal control strategy through vaccination is determined using actual data from the COVID-19 pandemic in China. Initially, inverse problems are used to estimate the parameters of the SIR model and then two strategies are proposed. The first seeks to minimize only the total number of infected, and the second minimizes both the number of infected and vaccination doses.

This work consists of identifying a model for COVID-19 at the State of Amazonas from compartmental models and solving the Optimal Control Problem for the identified model. The dynamic system adopted has its behavior described by the compartmental model SIRD. By identifying the model, it is possible to analyze and compare the result of the parameters for different scenarios, evaluating the duration over which the disease spreads, the peak of the infected curve, total accumulated cases and deaths, etc. The OCP will be solved from the initial time and the parameters of the most recent model among the proposed identification scenarios. With the numerical result obtained, the results between the estimated curves and the optimized curves will be presented and discussed.

EPIDEMIOLOGICAL MODELS

One of the epidemiological models that stood out the most was the SIR (Susceptible, Infected, Removed) model proposed by Kemarck and McKendrick in 1927, which became known as compartmental model. An important characteristic of these compartments is the fact that they are disjoint (Almeida, 2014). In other words, it is not possible for a population to belong to more than one compartment. In this work, we chose to use the SIRD model (Suscetible, Infected, Removed, Deaths). To describe the dynamics of each of these populations and considering that the population of each group varies over time, it is called S, the number of susceptible, I, the number of infected, R, the number of recovered individuals, D, the number of deaths and the total population is N.

The hypothesis adopted in this model are:

1. Constant and homogeneous total population: each individual in the population must be in one of the adopted compartments and there is no distinction between different groups within the population.;
2. Absence of vital dynamics: births and deaths from general causes will not be included in the model;
3. All susceptible populations are not immune to infection;
4. Those infected who recover acquire immunity;
5. The interaction between the population occurs uniformly: there is no variation in the population's behavior in relation to social distancing.

Thus, the dynamics of the model is given by the contact of susceptible individuals with infected individuals at a transmission rate a, these individuals recover at a recovery rate b and die at a mortality rate c. Figure 1 shows the representation of the SIRD model through the block diagram.

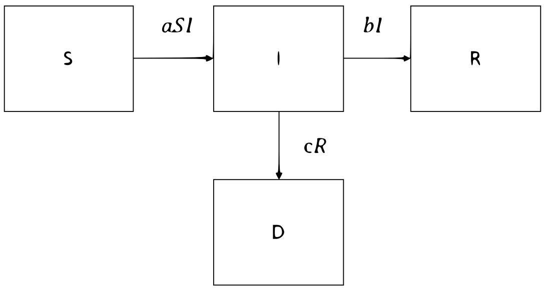

Figure 1 – SIRD model diagram.

The system of differential equations for the SIRD model is:

$$\begin{cases} \dfrac{dS}{dt} = -\dfrac{aS(t)I(t)}{N} \\ \dfrac{dI}{dt} = \dfrac{aS(t)I(t)}{N} - bI(t) - cI(t) \\ \dfrac{dR}{dt} = bI(t) \\ \dfrac{dD}{dt} = cI(t) \end{cases} \tag{1}$$

where a, b and c are positive constants within the range $[t_0, t_f]$ parsed. From SIRD model, it is obtained that $\dfrac{a}{(b+c)}\dfrac{S_0}{N}$ is the reproduction rate R_o and meets the following criteria:

- $R_o = 1$: there is an epidemic balance, infected people infect the same number of susceptible individuals;
- $R_o > 1$: there is an increasing spread of the number of infected;
- $R_o < 1$: disease tends to disappear in the population.

Parameter estimation

It is possible to find methods to estimate parameters of the SIR epidemiological model for COVID-19 through inverse problems in Marinov and Marinova (2020) and Batista (2020), which consists in using the real result of some measurements to infer the values of the parameters that characterize the system (Tarantola, 2005). The authors use the Least Squares Method (LSM) for it. The purpose of LSM is to determine parameters to fit a curve to real data, minimizing the error between this data and the estimated data. Considering the system of equations of the SIRD model represented by Eq. (1) and that $S_{est}, I_{est}, R_{est}$ and D_{est} denote the vector of data estimated over time from the discretization and S, I, R and D denote the real data vector over time, the squared error between these terms is given by

$$\phi = \sum(\varepsilon^2 + \delta^2 + \zeta^2 + \eta^2), \tag{2}$$

such that

$$\varepsilon = S_{est} - S, \tag{3}$$

$$\delta = I_{est} - I, \tag{4}$$

$$\zeta = R_{est} - R, \tag{5}$$

$$\eta = D_{est} - D. \tag{6}$$

Equations (3), (4), (5) and (6) correspond to the residuals referring to S, I, R and D respectively.

OPTIMAL CONTROL PROBLEM (OCP)

The main objective of the Optimal Control Problem (OCP) is to determine control signals that will cause a given system to satisfy physical constraints while extremize a functional or performance index (Kirk, 2004). Suppose that the state of a given system at time t is described by a n-dimensional state vector $\mathbf{x}(t) = [x_1(t), x_2(t), \ldots x_n(t)]^T$ and the control of this system given by a m-dimensional vector $\mathbf{u}(t) = [u_1(t), u_2(t), \ldots, u_m(t)]^T$.

An optimal control problem is defined as:

$$\min \left\{ J = F\left(\mathbf{x}(t_f), t_f\right) + \int_{t_0}^{t_f} G\left(\mathbf{x}(t), \mathbf{u}(t), t\right) dt \right\} \tag{7}$$

Subject to

$$\dot{\mathbf{x}}(t) = \mathbf{f}\left(\mathbf{x}(t), \mathbf{u}(t), t\right), t \in [t_0, t_f] \tag{8}$$

$$\mathbf{x}(t_0) = \mathbf{x_0} \tag{9}$$

$$x_i(t_f) = x_i^{t_f} \tag{10}$$

$$x_i(t_f) \geq x_i^{t_f} \tag{11}$$

$$x_i(t_f) \text{ free} \tag{12}$$

$$\mathbf{u}(t) \in \Omega\left(\mathbf{x}(t), t\right), \forall\, t \in [t_0, t_f] \tag{13}$$

- J is defined as the cost function, where $\mathbf{F}: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ and $\mathbf{G}: \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$;
- $\mathbf{f}: \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}$ is a vector function $\mathbf{f} = [f_1, f_2 \ldots, f_n]^T$ where for every $i = 1, \ldots, n$, there is a corresponding $f_i(x, u, t)$;
- $x_i^{t_f}$ represents the state variable x_i at instant t_f;
- Ω is the set of all admissible controls of the system in the given control horizon.

Finding admissible $(\mathbf{x}^*(t), \mathbf{u}^*(t))$ by minimizing the cost J shown in Eq. (7) is what characterized as optimal control. $\mathbf{x}^*(t)$ and $\mathbf{u}^*(t)$ are the optimal points for the state and control vectors. The restrictions imposed on the epidemiological model in this work will be t_f fixed, $0 \leq u(t) < U_{ad}$ and $U_{ad} < 1$ where U_{ad} is the maximum allowable value for $u(t)$.

Pontryagin's Principle

One of the approaches to solve the OCP is through Pontryagin's Principle. Pontryagin's Principle provides necessary conditions that an optimal solution $(\mathbf{x}^*(t), \mathbf{u}^*(t))$ must satisfy. Assuming that H represents the Hamiltonian defined by Eq. (14):

$$H(\mathbf{x}(t), \mathbf{u}(t), \rho(t), t) = G(\mathbf{x}(t), \mathbf{u}(t), t) + \rho(t)^T \cdot f(\mathbf{x}(t), \mathbf{u}(t), t). \tag{14}$$

The optimal solution is obtained by solving:

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial \rho_j}, \tag{15}$$

$$\frac{d\rho_j}{dt} = -\frac{\partial H}{\partial x_j}, \tag{16}$$

$$\frac{\partial H}{\partial u} = 0, \tag{17}$$

where $j = 1, ..., n$, ρ is called the system co-state, also known as an adjoint variable or Lagrange multiplier.

Optimal Control in SIRD Model

The SIRD model with control through vaccination is described according to the following system of differential equations:

$$\begin{cases} \dfrac{dS}{dt} = -\dfrac{aS(t)I(t)}{N} - u(t)S(t) \\ \dfrac{dI}{dt} = \dfrac{aS(t)I(t)}{N} - bI(t) - cI(t) \\ \dfrac{dR}{dt} = bI(t) + u(t)S(t) \\ \dfrac{dD}{dt} = cI(t) \end{cases}. \tag{18}$$

For the SIRD model described by Eq. (18), the performance index J_{SIRD} seeks to minimize the cost of vaccination and also minimize the total number of infected and deaths according to Eq. (19):

$$J_{SIRD} = \int_{t_0}^{t_f} \alpha I^2(t) + \beta D^2(t) + \gamma u^2(t) dt. \tag{19}$$

The adopted values for α, β and γ were, respectively, 1, 1 and 0.5, so that the weight of the cost of infected and death is more relevant for the index. Then the Hamiltonian H_{SIRD} is defined by

$$\begin{aligned} H_{SIRD} =& I^2(t) + D^2(t) + \frac{1}{2}u^2(t) + \rho_1(t)\left[-\frac{aS(t)I(t)}{N} - u(t)S(t)\right] + \rho_2(t)\left[\frac{aS(t)I(t)}{N} - bI(t) - cI(t)\right] + \\ &+ \rho_3(t)\left[bI(t) + u(t)S(t)\right] + \rho_4(t)cI(t). \end{aligned} \tag{20}$$

Therefore, to obtain the optimal control equation $u^*(t)$, it has to minimize H_{SIRD} in relation to u

$$\frac{\partial H}{\partial u} = u(t) - \rho_1(t)S(t) + \rho_3(t)S(t) = 0, \tag{21}$$

$$u(t) = S(t)\left(\rho_1(t) - \rho_3(t)\right). \tag{22}$$

Equation (22) represents the optimal value of u for the performance index J_{SIRD} to be minimized. Thus, by finding $S(t)$, $\rho_1(t)$ and $\rho_2(t)$, it is possible to determine the optimal vector $u^*(t)$. From the Pontryagin's Principle, it is possible to determine the system of differential equations of co-state for the SIRD model, the system takes the following form:

$$\begin{cases} \dfrac{d\rho_1}{dt} = -[-aI(t)\rho_1(t) - u(t)\rho_1(t) + aI(t)\rho_2(t) + u(t)\rho_3(t)] \\ \dfrac{d\rho_2}{dt} = -[-2I(t) - aS(t)\rho_1(t) + (aS(t) - b - c)\,\rho_2(t) + b\rho_3(t) + c\rho_4(t)] \\ \dfrac{d\rho_3}{dt} = 0 \\ \dfrac{d\rho_4}{dt} = 2D(t) \end{cases} . \tag{23}$$

RESULTS

Parameter Estimation

The database provides the accumulated number of cases, the accumulated number of recovered and the accumulated number of deaths. One of the hypothesis when adopting the SIRD model is that the population must be homogeneous and its parameters are constants. In this way, it is necessary to analyze data from COVID-19 in Amazonas that would provide the best curve fit. Through the identification algorithm, it was possible to notice that, when using a time interval in which behavior of the population changes, it would affect the data in such a way that the error between the estimated data and the database used for validation increased.

From this, it is understood that all intervention points in the population dynamics (social distancing, closing and reopening of commerce, changes in case measurement, etc) generate variation in the model's parameters. Thus, the parameters were estimated in three scenarios. Figures 2, 3 and Table 1 show the curves and parameters estimated from the SIRD model. In the curves of $I(t)$, it is possible to see that the peak of infection in scenarios 1 and 3 coincides, as well as the transmission rate. On the other hand, the result of the curve $D(t)$ in scenarios 1 and 3 does not follow the same trend.

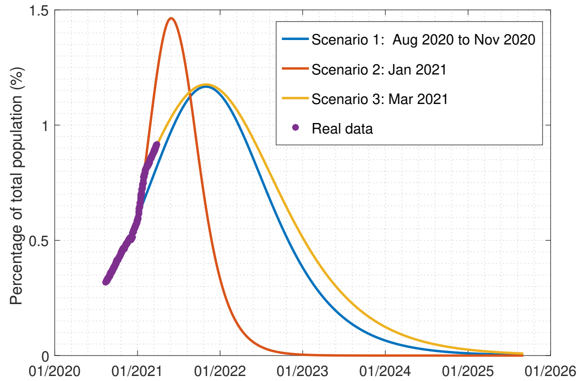

Figure 2 – Comparison between the estimated curves $I(t)$ of each established scenario and the real data.

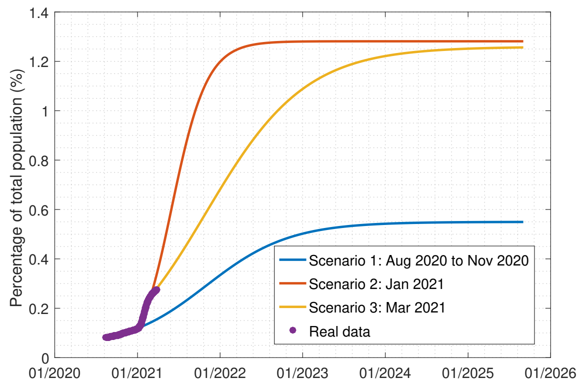

Figure 3 – Comparison between the estimated curves $D(t)$ of each established scenario and the real data.

Table 1 – Estimated parameters under different scenarios.

Parameters	Aug/2020 to Nov/2020	Jan/2021	Mar/2021
$\boldsymbol{a}$	0.0395	0.0852	0.0331
$\boldsymbol{b}$	0.0329	0.0675	0.0268
$\boldsymbol{c}$	0.0006	0.0029	0.0013
$R_o = a/(b+c)$	1.179	1.209	1.177

Table 2 – Comparison between the amount of cases and deaths for each scenario.

	Cases		**Deaths**	
	Abs.	**%**	**Abs;**	**%**
Scenario 1: Aug 2020 to Nov 2020	1.198.200	28.48%	23.120	0.55%
Scenario 2: Jan 2021	1.346.400	31.99%	53.911	1.28%
Scenario 3: Mar 2021	1.195.700	28.42%	52.661	1.26%

In Table 1, the difference between the mortality rate of the different scenarios can be seen, and in Table 2, there is the absolute total value of the amount of cases and deaths. The final total cases for the model estimated in scenarios 1 and 3 are approximately equal, however there is a difference between the proportion of deaths and cases.

Model validation

To quantify the validity of the model, the fit index based on the Normalized Mean Square Error (NMSE) between real and estimated validation data was used. Reaffirming that, for this validation, a different data from those provided for the parameter estimation were used. In other words, from August 14 to November 30, the first 40 days were used to estimate the parameters and the other 68 days to validate the curve found. Table 3 shows the estimated parameters used. The fit index (FI) can range between $-\infty$ and 1, with $-\infty$ representing a bad fit and 1 representing a perfect fit. It is calculated according to Eq. (24):

$$FI\% = \left[1 - \frac{||\mathrm{X}_{real} - X_{est}||^2}{||\mathrm{X}_{real} - \bar{X}||^2}\right] \times 100\%, \tag{24}$$

where X_{real} represents the vector of the problem's real data, X_{est} represents the vector of estimated values, and $\bar{X}$ is the vector whose coordinates correspond to the mean of X_{est} and X_{real}.

Table 3 – Estimated parameters under the validation period.

a	b	c	$\mathbf{R_0}$
0,0395	0,0329	0,0006	1,179

Figures 4 and 5 show the comparison of the estimated curve and the real data. The fit indix based on the NMSE for the compartments of SIRD model can be seen in Table 4.

Table 4 – Fit index based on NMSE between estimated data and actual data.

FI%			
S	**I**	**R**	**D**
97.34%	95.29%	97.25%	97.48%

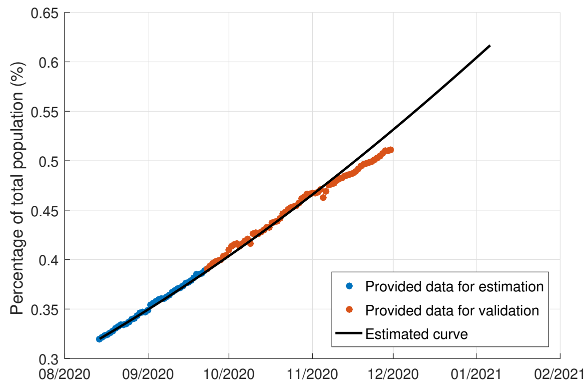

Figure 4 – SIRD model validation - $I(t)$ curve

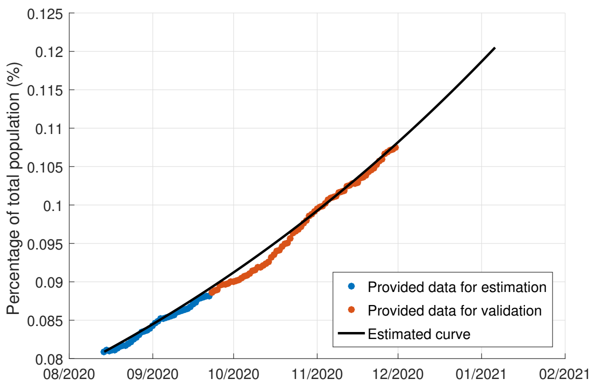

Figure 5 – SIRD model validation - $D(t)$ curve

Optimal vaccination strategy

To find the optimal control (optimal vaccination) for SIRD model, it was applied the forward and backward sweep method (Lenhart and Workman, 2007). The constants used are shown in the Table 5, where transmission, recovery and mortality rates were chosen according to scenario 3. T corresponds to the control horizon of the system, n is the number of subdivisions of the interval $[t_i, t_{i+1}]$, N is the total population of Amazonas and t_0 is the initial time. This scenario was chosen because it represents the most recent model identified among the studied scenarios.

Table 5 – Constants used in the OCP.

Constants	
$\boldsymbol{a}$	0,0331
$\boldsymbol{b}$	0,0268
$\boldsymbol{c}$	0,0013
$\boldsymbol{T}$	365
n	100
N	4207714
t_0	01/03/2021

Figures 6 and 7 show the curve $I(t)$ and $D(t)$ without any control strategy and with optimal control based on the assumption that vaccination has an efficacy of 100%, that is, all vaccinated individuals would become immunized.

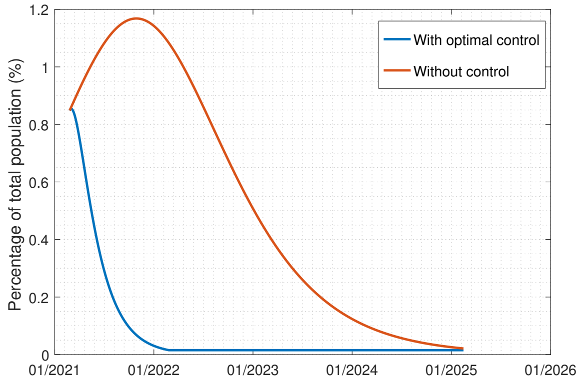

Figure 6 – Comparison between $I(t)$ curve with optimal control and without control.

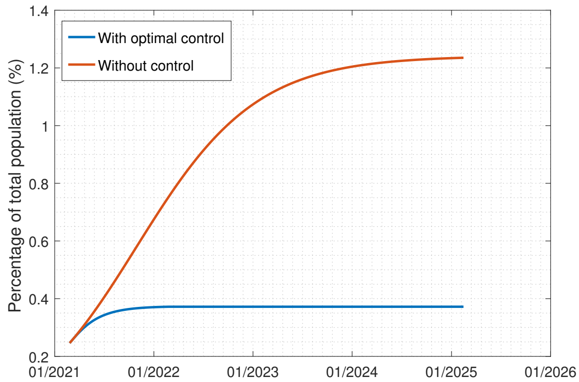

Figure 7 – Comparison between $D(t)$ curve with optimal control and without control.

For the SIRD model, the results can be seen in Table 6. Table 7 shows the amount of people vaccinated at the end of the control horizon

Table 6 – Comparison between the values of the SIRD model without control and with optimal control defined in a control horizon of 365 days.

	Without control	With optimal control
Final value of cases	28.29%	8.64%
Final value of deaths	1.24%	0.37%
Peak of infection	1.17%	0.85%
Final value of immune population - R	27,04%	52,38%

Table 7 – Final size of the vaccinated population.

Vaccinated population	
1.856.900	44.13%

In Table 8, the associated cost for each component of the performance index is found, calculated according to the Eqs. 25, 26, 27 and 28:

$$J_I = \int_{t_0}^{t_f} I^2(t) \approx \sum_{t_0}^{t_f} I_i^2, \tag{25}$$

$$J_D = \int_{t_0}^{t_f} D^2(t) \approx \sum_{t_0}^{t_f} D_i^2, \tag{26}$$

$$J_I = \int_{t_0}^{t_f} 0.5u^2(t) \approx \sum_{t_0}^{t_f} 0.5u_i^2, \tag{27}$$

$$J = J_I + J_D + J_u. \tag{28}$$

Table 8 – Performance index

J_I	J_D	J_u	J
0.0053	0.0043	0.0025	0.0121

Figures 8 and 9 show the curve of vaccinated individual and cases in the theoretical control strategy and in the real strategy until December 1st, 2020. For the vaccinated individuals, only data from those who completed the immunization cycle taking single-dose or two-dose vaccines are used.

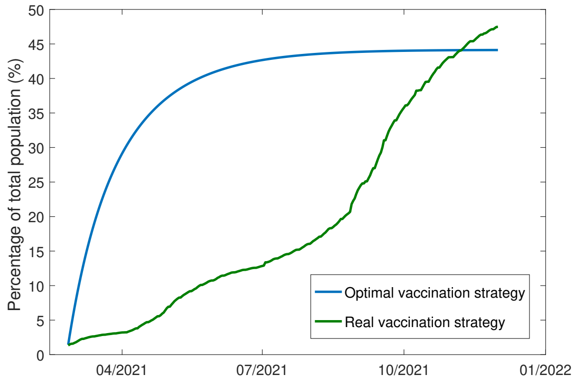

Figure 8 – Population vaccinated in the theoretical scenario and in the real scenario.

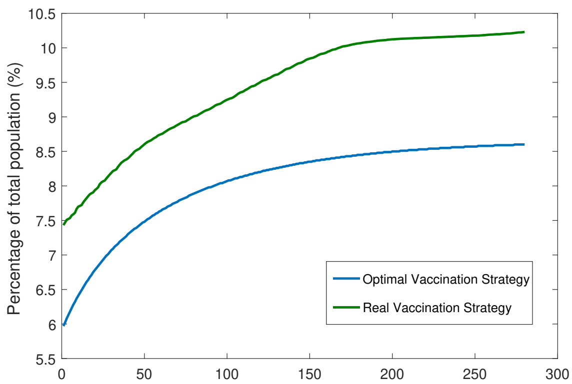

Figure 9 – Cases in the theoretical scenario and in the real scenario.

CONCLUSION

The results presented were replied to all compartments established in this study. The results of the parameters presented above and the method used showed a satisfactory curve fit for the scenarios in which they were estimated. This was possible through the use of the Least Squares Method, which is configured as a gray-box identification as it works directly with real data to estimate the parameters. By adopting compartmental models in their simple form (without vital dynamics and other terms that would affect the complexity of the model), a key step was to analyze the context in which the state's population was passing through, verify periods in which there was an increase or decrease in social isolation and all events that also contributed to changes in population behavior and interaction.

The application of the Optimal Control Theory in epidemiological models proved to be of great advantage to reduce the duration of the epidemic, reduce the number of infected individuals and also to obtain the lowest possible cost represented by the performance index J. Regarding the proposed control (vaccination) and OCP formulated, it was obtained through the simulations that vaccinating 44.13% of the population is the optimal solution only for control horizon established. On the other hand, the solution cannot be implemented in a trivial way, since several factors must be taken into account, such as the vaccine's efficacy, State's vaccination capacity and time. In addition, the control presented focuses on the vaccination of susceptible individuals. Currently, due to the emergence of new variants of COVID-19 and the loss of immunity in recovered individuals, there is no distinction in the vaccination of who is susceptible or not. In cases where there is a need for more than one dose to guarantee immunity, planning using the optimal strategy must also take this factor into account and also the time that an individual remains immunized.

In order to continue the research, addressing aspects not studied in this work or to improve the formulations presented, some suggestions and considerations for future work are presented below:

1. Adaptive estimation of parameters of a SIRD model from the introduction of new real data, making the transmission, recovery and mortality rates not constant;

2. Optimal control in a SIRD model with time delay in the control variable due to the time required for susceptible individuals to become immunized;

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