Estimating *SIR* model parameters from data using differential evolution: an application with COVID-19 data

Sergio Rica
Universidad Adolfo Ibáñez
Facultad de Ingeniería y Ciencias
Santiago, Chile
sergio.rica@uai.cl

Gonzalo A. Ruz
Universidad Adolfo Ibáñez
Facultad de Ingeniería y Ciencias.
Center of Applied Ecology and Sustainability (CAPES)
Santiago, Chile
gonzalo.ruz@uai.cl

***Abstract*—The problem of fitting parameters of a dynamical system appears to be relevant in many areas of knowledge, like weather forecasting, system biology, epidemiology, and financial markets. In this paper, we analyze the Susceptible-Infected-Recovered (SIR) epidemiological model. We first derive an alternative representation of the SIR model, reducing it to one differential equation that models the cumulative number of infected cases in function of time. Then we present a differential evolution approach to estimate the parameters of this dynamical model from data. We illustrate the proposed approach with COVID-19 data from Santiago, Chile. The goodness of fit, obtained by the differential evolution algorithm outperformed ten times the results obtained by a random search strategy used in previous works.**

***Index Terms*—Dynamical System, SIR model, Differential Evolution, COVID-19 data.**

I. Introduction

Dynamical systems are transversally used to describe a variety of dynamical behaviour from disparate areas of knowledge. In short, let us assume we have a dynamical system given by a set of ordinary differential equations (o.d.e.), that contain d variables $\boldsymbol{u}(t) = \{u_1(t), u_2(t), \dots u_d(t)\}$ that depend explicitly on time, and a set of parameters $\{\boldsymbol{\mu}\} = \{\mu_1, \mu_2, \dots \mu_p\}$:

$$\frac{d}{dt}\boldsymbol{u}(t) = f_{\{\boldsymbol{\mu}\}}(\boldsymbol{u}(t); t),$$

with a set of initial conditions

$$\boldsymbol{u}(t = t_0) = \boldsymbol{u}^{(0)}.$$

In this paper, we focus on the problem of fitting the parameters of a given dynamical system to obtain the best fit between the data and the solution given by the dynamical system.

Then, the parameters to be determined are $\mathcal{P} = \{t_0, u_1^{(0)}, u_2^{(0)}, \dots u_d^{(0)}, \mu_1, \mu_2, \dots \mu_p\}$, thus the total number of parameters to determine is $D = d+p+1$. The problem is the following, given a dataset of discrete values of the variables at some discrete times:

$$(t_n, \boldsymbol{u}_n), \quad \text{for} \quad n = 1, 2, \dots N$$

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which values for the parameters $\{\boldsymbol{\mu}\}$ and the initial conditions $\boldsymbol{u}^{(0)}$ best fit the dataset in the sense that the norm:

$$\sum_{n=0}^{N-1} ||\boldsymbol{u}(t_n) - \boldsymbol{u}_n||^2,$$

is minimum.

This kind of optimization problems appear in many fields such as physics, engineering, biology, and finance. In many cases, practical problems have objective functions that are non-differentiable, non-continuous, non-linear, noisy, flat, multi-dimensional or have many local minima, constraints or stochasticity, making these problems difficult (if not impossible) to solve analytically.

More precisely, we address this question to the *SIR* epidemiological model. Almost a hundred years ago, Kermack and McKendrick [1] introduced a mathematical model for epidemics, which is known today as the *SIR* model for infectious deseases. Later in the seventies this epidemiological model was introduced to understand the temporal evolution of the 1960's racial riots in different cities of USA as Los Angeles, Detroit and Washington DC [2]. The *SIR* epidemiological model appears to describe satisfactorily riots as the one happened in France in 2005 [3] or in Chile in 2019 [4].

The problem of estimating parameters to fit as best as possible the model with the number of riots events in time, provided by authorities, was developed in [4]. Using a simple random search algorithm the results appears to be satisfactory, nevertheless a more systematic approach is desirable for this class of problem.

Evolutionary computation approaches have also been used for parameter estimation in ordinary differential equations. For example, in Simos, *et al.* [5], particle swarm optimization was used to fit an epidemic model to data. A genetic algorithm was used to find parameter sets using available time-series data from the introduction of cholera in Haiti [6]. Instead of working with o.d.e., [7] performs a simulation of epidemics using cellular automata and differential evolution, showing that despite their simplicity, they are able to contribute significantly to an understanding of the spread of real epidemics. The SEIR

with Social Distancing model was analyzed in [8]. The estimation of the SEIR–SD model parameters with data from Covid-19 from Italy, was carried out through the use of differential evolution. Other approaches like [9], [10], consider modeling epidemic networks, where evolutionary computation is used to locate likely epidemic networks for different epidemic profiles (simulated using the SIR model over the network).

In this paper, due to its real value parameter search characteristics, we formulate a differential evolution algorithm [11] to estimate the parameters of the *SIR* model from the COVID-19 data for the city of Santiago, Chile. We also use the random search approach described in [4] for comparison. Overall, we show the effectiveness of the use of differential evolution for this problem.

The rest of the paper is organized as follows. Section II defines the *SIR* model and develop briefly its main characteristics, then, we summarize the basis of the *differential evolution* algorithm. The application of the SIR model fitted with COVID-19 data for the city of Santiago, Chile is presented in Section III. Results and analysis of the simulations are shown in Section IV. Final conclusions and future directions are discussed in Section V.

II. Background

A. The SIR model.

The model is governed by three variables: $I(t)$ represents the number of "infected" individuals as a function of time, $S(t)$ is the number of individuals susceptible to the disease and may be "infected" at time t, and $R(t) = N - S(t) - I(t)$ is the number of recovered individuals at time t, that only follows the dynamics of $I(t)$ and $S(t)$, because N, the total population, is constant. Then the equations for susceptible and infected individuals of the *SIR* model reads [1]

$$\frac{d}{dt}I(t) = -\alpha I(t) + \beta S(t)I(t) \quad (1)$$

$$\frac{d}{dt}S(t) = -\beta S(t)I(t) \quad (2)$$

where α is a decaying rate of the infected population and the nonlinear term $\beta S(t)I(t)$ represents a transmission rate at which a susceptible individual becomes infected. The two parameters α, with units of $(\text{time})^{-1}$, and β with units of $(\text{individuals})^{-1}\times(\text{time})^{-1}$ represent the exit rate from the infected class and the transmission rate per individual.

Finally, this set of ordinary differential equations is complemented by the initial conditions:

$$I(t_0) = I_0 \quad \& \quad S(t_0) = S_0.$$

A first consequence of the model, one has that the number of susceptible individuals, decrease strictly in time, therefore the asymptotic dynamics is: $I(t) \to 0$ as $t \to \infty$ and $S(t) \to S_\infty$, as well. Second, the dynamics depends crucially on the initial value S_0, in particular, if it is greater or smaller than α/β. Therefore, it appears useful to use a dimensionless variable instead of $S(t)$, namely a kind of *dynamic reproduction number*

$$\xi(t) = \frac{1}{\nu}S(t),$$

where we define the shorthand notation

$$\nu = \frac{\alpha}{\beta}.$$

Thus equations (1) and (2) read

$$\frac{d}{dt}I(t) = \alpha\left(-1 + \xi(t)\right)I(t), \quad (3)$$

$$\frac{d}{dt}\xi(t) = -\frac{\alpha}{\nu}\xi(t)I(t). \quad (4)$$

We have explicitly not included α in a dimensionless temporal scale because, its selected value by the data has a fundamental interpretation, therefore it is better to keep it with the natural units. As before, equations (3) and (4) must be solved together with the initial conditions:

$$I(t_0) = I_0 \quad \& \quad \xi(t_0) = \xi_0.$$

Usually the parameter ξ_0 is named the reproduction number [12], [13]. If $\xi_0 < 1$ the evolution of $I(t)$ is a decreasing function. Indeed, if initially $\xi_0 < 1$, and because $\xi(t)$ is a decreasing function, then the right hand side of eqn. (3) is always negative so that $I(t)$ is a strictly decreasing function of time, moreover $I(t) \to 0$ exponentially in time. However, if initially $\xi_0 > 1$, then, the right hand side of eqn. (3) is positive so that $I(t)$ increases in time after a maximum value, $I_{\max}$, that is reached whenever $\xi(t_{\max}) = 1$. Afterwards, this sign becomes negative and thus $I(t)$ decreases exponentially in time. This simple dynamics is represented in Fig. 1 (b & c). Therefore, $\xi_0 > 1$ acts as a trigger that ignites an epidemic event.

In the following we reduce the ordinary differential equations (3) and (4) set to a single variable. Although this is a particular property of the *SIR* model, the general method rules formally speaking in the same way to an arbitrary number of o.d.e. Integrating (4) one gets [14]

$$\xi(t) = \xi_0 e^{-\frac{\alpha}{\nu}\int_{t_0}^{t} I(t')\,dt'}, \quad (5)$$

and defining

$$v(t) = \int_{t_0}^{t} I(t')\,dt', \quad (6)$$

so that $v'(t) = I(t)$ and $v(t_0) = 0$, and, introducing $\xi(t)$ from (5) into (3) one gets

$$\frac{d^2}{dt^2}v(t) = -\alpha\frac{d}{dt}v(t) + \alpha\xi_0 e^{-\frac{\alpha}{\nu}v(t)}\frac{d}{dt}v(t),$$

which can be integrated once:

$$\frac{d}{dt}v(t) = -\alpha v(t) + \nu\xi_0\left(1 - e^{-\frac{\alpha}{\nu}v(t)}\right) + I_0. \quad (7)$$

Here we have used that $v(t_0) = 0$, and $v'(t_0) = I_0$.

Although, one may integrate directly (7), and thus it is exactly solvable, we shall work directly with the time dependent ordinary differential equation (7) because the aim of this paper is to show how to adjust the prediction of a dynamical rule in time with the available data.

B. Differential evolution

Optimization problems appear in many fields such as physics, engineering, biology, and finance. In many cases, practical problems have objective functions that are non-differentiable, non-continuous, non-linear, noisy, flat, multi-dimensional or have many local minima, constraints or stochasticity, making these problems difficult (if not impossible) to solve analytically. Here, evolutionary computation can be used to find an approximate solution, in particular, we will describe a class of evolutionary algorithm called differential evolution.

Differential evolution is a stochastic, population-based optimization algorithm introduced by Storn and Price [11] for optimizing functions with real-valued parameters (solution space). The general problem formulation is as follows: for an objective function $f : X \subseteq \mathbb{R}^D \to \mathbb{R}$ where the feasible region $X \neq \emptyset$, the minimization problem is to find:

$$x^* \in X \text{ such that } f(x^*) \leq f(x)\ \forall x \in X$$

where $f(x^*) \neq -\infty$. To solve this problem, differential evolution follows a standard evolutionary algorithm procedure composed of the following four stages:

1) Initialization,
2) Mutation,
3) Recombination,
4) Selection.

The algorithm loops (generations) between stages 2), 3), and 4) until a satisfactory solution is found. More details of each stage is as follows.

Let us start with some notations. Suppose we want to optimize a function with D real parameters. The user must define the size of the population $popsize$ (it must be at least four). The parameter vectors have the form:

$$x_{i,G} = [x_{1,i,G}, x_{2,i,G}, \ldots, x_{D,i,G}] \quad i = 1, 2, \ldots, popsize$$

where G is the generation number.

1) Initialization: The user must define upper and lower bounds for each parameter ($G = 1$):

$$x_j^L \leq x_{j,i,1} \leq x_j^U \quad j = 1, \ldots, D.$$

Then, randomly select the initial parameter values uniformly on the intervals $\left[x_j^L, x_j^U\right]$. Each of the $popsize$ parameter vectors undergoes mutation, recombination and selection.

2) Mutation: The purpose of the mutation stage is to expand the search space. For a given parameter vector $x_{i,G}$, the algorithm randomly selects three vectors $x_{r_1,G}$, $x_{r_2,G}$, and $x_{r_3,G}$ such that the indices i, r_1, r_2 and r_3 are distinct. Then the weight difference of two of the vectors is added to the third:

$$v_{i,G+1} = x_{r_1,G} + F(x_{r_2,G} - x_{r_3,G})$$

where $0 \leq F \leq 2$ is a constant, called the *mutation factor* and $v_{i,G+1}$ is called the *donor vector*.

3) Recombination: Recombination incorporates successful solutions from the previous generation. The *trial vector* $u_{i,G+1}$ is developed from the elements of the *target vector*, $x_{i,G}$, and the elements of the donor vector, $v_{i,G+1}$. Elements of the donor vector enter the trial vector with probability CR

$$u_{j,i,G+1} = \begin{cases} v_{j,i,G+1} & \text{if } \text{rand}_{j,i} \leq CR \quad \text{or} \quad j = \text{I}_{\text{rand}} \\ x_{j,i,G} & \text{if } \text{rand}_{j,i} > CR \quad \text{and} \quad j \neq \text{I}_{\text{rand}} \end{cases}$$

$$i = 1, 2, \ldots, popsize; j = 1, 2, \ldots, D$$

where $\text{rand}_{j,i} \sim U[0, 1]$ and I_{rand} is a random integer from $[1, 2, \ldots, D]$. I_{rand} ensures that $v_{i,G+1} \neq x_{i,G}$.

4) Selection: The target vector $x_{i,G}$ is compared with the trial vector $v_{i,G+1}$ and the one with the lowest function value is admitted to the next generation:

$$x_{i,G+1} = \begin{cases} u_{i,G+1} & \text{if } f(u_{i,G+1}) \leq f(x_{i,G}) \\ x_{i,G} & \text{otherwise} \end{cases}$$

$$i = 1, 2, \ldots, popsize$$

The mutation, recombination and selection stages continue until some stopping criterion is reached.

III. Methods

A. Parameters of the SIR-model to be estimated

To fit the data with the solution of the system of ordinary differential equation (7), we need to fit the parameters α, ν together with an initial condition, $\{t_0, I_0, \xi_0\}$; that is, we need to find the best fit varying five parameters of a dynamical problem. Naturally, because (7) does not depend explicitly on time any modification on t_0 just shifts the solution on the time axis, therefore, it allows to better adjust by a simple transformation of the data. In any case, in the current application we do not consider this particular invariance so that the algorithm chooses itself the best value of t_0 regardless of any assumption. In the following we describe the raw data, then we provide the results and discuss it.

B. The data

We use the official *on-line* available data [15]. More precisely, the data contains the date as time in units of [days], and the cumulative number of infected people to date, for the sixteen different administrative regions, that is $v(t)$ for different regions. Initially, we focus on the Metropolitan Santiago-area which has the largest number of infected people. The data runs from March 3rd, 2020 ($t = 0$) up to date. However, for the analysis we consider a window from March 3rd up to June 16th ($t = 106$). Subsequently an extra 30000 infected people was added to the records on June 17th. This data is shown in Fig. 1 (a).

Using the presented algorithm we estimate the parameters of the *SIR* model by minimizing the following objective functional which is a sort of mean squared error:

$$f[v] = \frac{1}{N} \sum_{n=0}^{N-1} \left(\frac{v(t_n)}{v_n} - 1 \right)^2,$$

where N is the number of elements of the dataset, $v(t)$ is the numerical solution of the o.d.e. (7) using the obtained parameters, thus, $v(t_n)$ is this solution evaluated at t_n. On the other hand, v_n is the value of the cumulative infected people from the data at day t_n.

C. Differential evolution implementation

We used the differential evolution implementation available from SciPy [16] optimize built on the NumPy library of Python. We used the default differential evolution parameter values: $popsize = 15$, $F = U[0.5, 1]$ (sampled for each generation), $CR = 0.7$, and $maxiter = 1000$ (the maximum number of generations). The parameter vector of our problem has de form: $[\alpha, \nu, t_0, I_0, \xi_0]$. The upper and lower bounds for each parameter used in this work for the differential evolution are shown in Table I.

TABLE I
PARAMETER RANGE

Parameter	Range
α	$[0.001, 0.1]$
ν	$[1000, 30000]$
t_0	$[1, 50]$
I_0	$[0, 30]$
ξ_0	$[1, 7]$

The fitness function that was fed into the *differential_evolution* function of SciPy optimize, consisted in a function that first obtained a numerical solution $v(t)$ of the o.d.e. (7) using the current parameter vectors (candidate solutions), then we proceeded evaluating in the error function described above. For the case studied (106 points) the execution time is only a few seconds (see Table II).

IV. RESULTS AND ANALYSIS

Applying the algorithm for the dataset of $N = 106$ different days one gets the parameters summarized in Table II. Briefly, the differential evolution method finds an optimal value for solution of the o.d.e. which is 10 time more precise, that a random method. The random method requires an initial estimations of the parameters. In the current situation, we can estimate easily one parameter by noticing the following: equation (7) provides us an interesting relation among I and v,

$$I = -\alpha v + \nu\xi_0 \left(1 - e^{-\frac{\alpha}{\nu}v}\right) + I_0. \tag{8}$$

One notices that for small v, a linear relation ($\approx I_0 + \alpha(\xi_0 - 1)v, + \dots$) among these variables holds. This provides us with a relation between α and the reproduction number ξ_0. From the data one gets $\alpha(\xi_0 - 1) \approx 0.075$, moreover varying the parameters we can easily fit the data with the previous relation. We used this as a first guess. Then we explored randomly 10^4 trials around this initial guess for a better set of parameters, i.e., parameters that yield smaller error. The random search is limited to a finite size domain. Next, this random process is iterated and the size is reduced by half for instance at each step. After a number of iterations, the search converges to a better set of parameters. The results using this random search are presented in the Table II. As we can see the differential evolution is almost 10 times more precise.

TABLE II
PARAMETER RESULTS

Class	Parameters of the SIR model	
	Diff. Evol.	***Random Search***
α [1/day]	$3.03176239 \times 10^{-2}$	3.87501×10^{-2}
ν [ind]	7.01702615×10^{3}	4.40952×10^{3}
t_0 [day]	28.243323	10.3795
I_0 [ind]	$7.61079388 \times 10^{-2}$	18.3495
ξ_0	3.27161825	3.08074
$v(t_0)$ [a]	1420	0
$\tau = 1/\alpha$ [day]	32.9841	25.8064
$\beta = \alpha/\nu$ [b]	4.32058×10^{-6}	8.78783×10^{-6}
error $f[\cdot]$	$6.7385429751 \times 10^{-3}$	4.41214×10^{-2}
Execution time	6.5 secs [c]	457.6 secs [d]

[a] This value is added at the end.
[b] Units of [ind$^{-1}\times$ day^{-1}].
[c] In an iMac Pro (2017).
[d] In an iMac Pro (2017); 3.76×10^3 in a MacBookAir 2014.

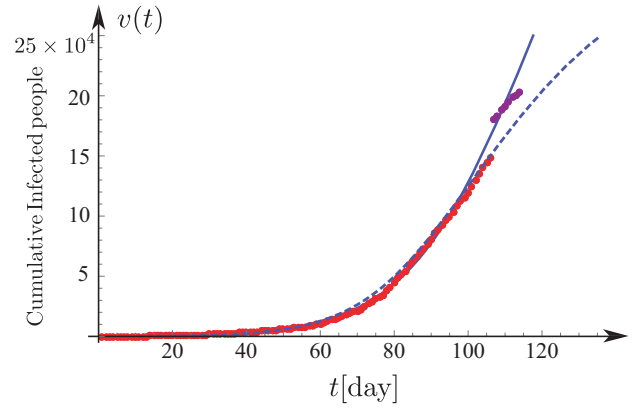
From the data we see that the fundamental parameters are roughly $\alpha = 3.03 \times 10^{-2}$ [1/day], therefore the typical time scale is of the order of $\tau = 1/\alpha = 33$ [days], therefore, if the parameters keeps their value, the epidemic will be reduced by a factor 20 in almost 3 months. The transmission rate per individual $\beta = 4.32 \times 10^{-6}$ [ind^{-1} day^{-1}]. Although this number looks to be very small, it must be interpreted by equation (5), as follows: during the infected period $\tau \sim 1/\alpha$, an infected individual may transmit the disease with a rate $\beta \times \tau \sim 1/\nu \approx 1.4 \times 10^{-4}$ [ind^{-1}], that is, it is enough that 7000 of susceptible individuals propagate with probability 1 (in average) the disease. This can be seen via the reproduction number $\xi_0 = 3.27$ which is above the unit critical value.

Figure 1 (a) shows the analyzed data for visual comparison of the solutions of the model by using the parameters from the differential evolution method (continuous lines in all plots) and from the random search (segmented lines in all plots). As said previously, we made the estimation with a dataset of 106 days.

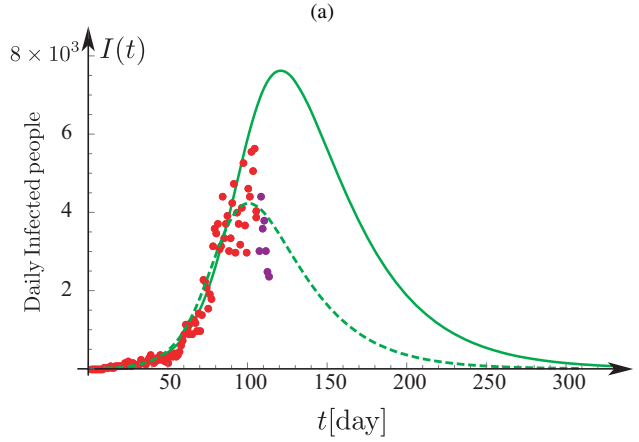
Figure 1 (b) shows the daily number of infected individual $I_n = v_n - v_{n-1}$ from the data as a function of time. This data is compared with the solution of the o.d.e. via equation (8) for comparison.

The dynamic reproduction number $\xi(t) = \xi_0 e^{-\beta v(t)}$ is a good indicator of the current state of dissemination probability, Fig. 1 (c) shows the dynamic reproduction number $\xi(t)$ as a function of time, today ($t = 115$ day), its value is close to the unit, showing, if data is trustable, that the disease may decay in the following month. The maximum daily infected people is expected to occur at the day 121, that is roughly 4 months after March 3^{rd} or early July.

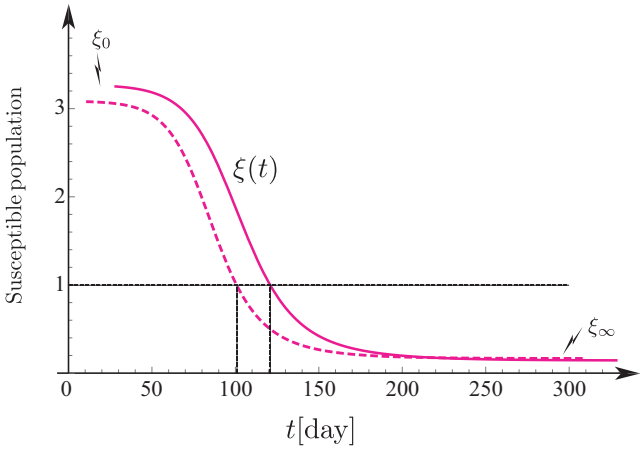
On June 16, the Ministry of Health (MINSAL) of Chile announced that they would be adding more than 30000 new



(a)



(b)



(c)

Fig. 1. (a) Plot of $v(t)$ vs. t, with the time in [days]. The red dots correspond to the data that we used to estimate the parameters. The blue continues line is the result of the numerical calculation of the solutions of the o.d.e. using the estimation of parameters via the differential evolution method (the parameters given in Table II). The blue segmented line for a numerical calculation of the solution of the o.d.e. with the parameters obtained via the random search (the parameters are also given in Table II). The purple dots represents data collected post the day $t = 106$, therefore not used in the estimations. (b) Plot of the daily infected people $I(t)$ vs t. This result shows that maximum daily infected population is reached at a time $t = 120.7$ [day]. (c) Plot of the dynamic reproduction number $\xi(t)$. In all plots the continuous curves follow after the differential evolution protocol and the segmented ones follow after the random search.

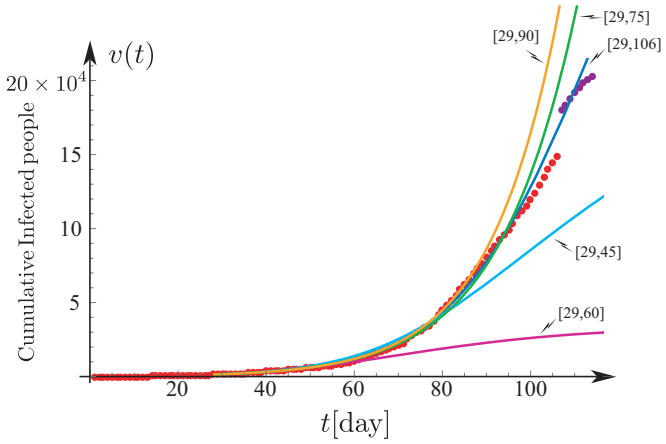


Fig. 2. Projection of $v(t)$ with models fitted with different amount of data points (days). The different fits correspond to the following time intervals: (cyan) $t \in [29, 45]$, (pink) $t \in [29, 60]$, (green) $t \in [29, 75]$, (orange) $t \in [29, 90]$, and (blue) $t \in [29, 106]$.

cases (on June 17). This measure was explained by the authorities pointing out that the national counting system had been subjected to stress, and had detected a significant number of people, who had not been notified of their status, had not been updated. Thus, there are people who took a PCR test, came out positive and the count was not performed. According to MINSAL, that number reached 31412 cases, which were fundamentally in the Metropolitan Region and are distributed throughout the entire pandemic period. The operation of the counting system is fed by the notifications that doctors make when diagnosing and then updated with the information provided by the corresponding laboratory. In the midst of the pandemic, there had been delays in these two actions. For our analysis, these additional cases, appear as a "jump" (discontinuity) from day 107 onwards as can be seen in Fig. 1 (a). Both the model fitted using the random search and the differential evolution approach were fitted with data until day 106. It is interesting to notice, that when performing projections with the models, we notice that the model fitted via differential evolution predicted better the "miscount".

In fact, the SIR model can only be used for short-range predictive purposes, since the dynamic can vary significantly depending of the amount of data that is used to fit the model. Also, the growth speed of the new infected cases, changes depending on the control actions, like quarantines, which can not be captured rapidly by the SIR model. Fig. 2 shows projections of $v(t)$ using differential evolution with different number of data points (days) to fit the model.

V. Conclusion

In this paper we have presented the problem of estimating the parameters of a dynamical system with data using differential evolution. As an application, we show this approach considering an alternative SIR model, which can be formulated in one differential equation, modeling the cumulative number of infected cases as a function of time. The results showed

that using differential evolution for parameter estimation, outperformed significantly the results obtained by a previously employed random search approach [4]. Moreover, fine-tuning of the parameters of the differential evolution algorithm was not conducted, instead we used the default values of the SciPy [16] optimize library. Future research will consider the impact on the results (if any) of fine-tuning the differential evolution parameters such as $popsize$, CR and, F.

It is important to point out that methodological changes in how the pandemic is managed during the actual event, changes the patterns/dynamics of the data, therefore, predictions using the SIR model analyzed in this paper, cannot be used for long-range predictions, since these types of models do not consider external factors that modify the dynamics of the data.

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