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Using chaos indicators to determine vaccine influence on epidemic stabilization

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Virus outbreaks have the potential to be a source of severe sanitarian and economic crisis. We propose a new methodology to study the influence of several parameter combinations on the dynamical behavior of simple epidemiological compartmental models. Using this methodology, we analyze the behavior of a simple vaccination model. We find that for susceptible-infected-recovered (SIR) models with seasonality and natural death rate, a new vaccination can reduce the chaoticity of epidemic trajectories, even with nonvaccinated adults. This strategy has little effect on the first infection wave, but it can stop subsequent waves.

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I. INTRODUCTION

The COVID-19 pandemic caused a sanitarian and economic crisis across the planet. For this reason, the prediction of new epidemics and fast response strategies are fundamental to prevent potentially catastrophic events [1]. Vaccination, when available, is a powerful method to fight epidemics caused by virus outbreaks [2]. Unfortunately, vaccination campaigns can be slowed down for several factors, like politics, popular hesitance, and speed of production, among others. These factors can prevent all the population to get vaccinated and therefore become immune to the virus. Public agents must take into account these limitations and provide the best vaccination strategy to the population. With this goal in mind, the behavior of epidemics must be understood in detail.

Compartmental models, such as susceptible-infected-recovered (SIR) and its variations, can be described by a few quantities that can be statistically estimated and combined into a single parameter called the basic reproduction number R_0. These models can be adapted to consider additional effects as natural death and seasonality with the inclusion of new parameters, as the natural death rate μ and the degree of seasonality δ. Nevertheless, these models must be studied in detail, as even simple ones can be chaotic, losing their predictive power [3–5]. Several authors have focused on the dynamical properties of these nonlinear equations using standard tools of the field. Several authors, like Zhang *et al.* [6] and Kamo and Sasaki [7], study the dynamical behavior of such systems using standard tools as Lyapunov exponents and bifurcation diagrams. These works show that the influence of the degree of seasonality δ can lead to chaos.

Methods from different areas can provide new information on epidemics caused by virus outbreaks. We propose to use grid classification, a technique used to explore the dynamics of orbital motion in celestial dynamics [8]. This method provides a fast way to study the epidemic evolution according to the parameters involved in the model. Also, the color-coded basin diagrams are useful to analyze the possible outcome from response strategies employed to fight present or future diseases.

The development of vaccines is an essential component of any virus-control strategy, as pointed out by Paltiel *et al.* [9] Vaccines reduce susceptibility among the uninfected and viral spread in those who are infected, providing direct and indirect protection. Regarding an epidemic situation, the question is how vaccination impacts the trajectory of disease progression. These trajectories are strongly dependent on different factors, such as the biological response, production, and distribution time, among others.

In this work, we employ a SIR model with natural death rate and seasonality and complement the model introducing vaccination. Our goal is to understand the influence of vaccination on the stabilization and mitigation of epidemics. We investigate how vaccination can reduce the quantity of chaotic epidemics trajectories and the maximum number of infected individuals. The SIR model is very simple and uses assumptions that are not valid for several real cases. Nevertheless, although we chose a very simple model, grid classification is a powerful method that can be adapted for more complex models with any number of parameters.

II. MODEL AND METHODS

In this work, we use an adapted SIR models to study seasonality and vaccine benefits for different epidemics. The

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original SIR model proposed by Kermack and McKendrick [10] is one of the more simple compartmental models in epidemiology. In this model, the population, composed of a total of N individuals, is divided into three classes, or compartments, called "susceptible," "infective," and "recovered." The classic epidemic model is given by the following set of differential equations:

$$\frac{dS}{dt} = -\beta\frac{IS}{N}, \tag{1}$$

$$\frac{dI}{dt} = \beta\frac{IS}{N} - \gamma I, \tag{2}$$

$$\frac{dR}{dt} = \gamma I, \tag{3}$$

where S, I, and R are respectively the number of susceptible, infected, and recovered individuals; β is the transmission rate; and γ is the recovery rate. This model does not consider any deaths, so $S(t) + I(t) + R(t) = N$ is constant.

We denote the fraction of N on each compartment respectively by $s = S/N$, $i = I/N$, and $r = R/N$. The parameters β and γ can be combined into a single quantity known as the basic reproduction number $R_0 = \beta/\gamma$. Performing a time scaling $t_{\text{new}} = \gamma t_{\text{old}}$, the classical model is now given by

$$\frac{ds}{dt} = -R_0 is, \tag{4}$$

$$\frac{di}{dt} = R_0 is - i, \tag{5}$$

$$\frac{dr}{dt} = i, \tag{6}$$

where $s(t) + i(t) + r(t) = 1$.

The original SIR model can be complemented to accommodate several effects such as natural death and seasonality. We will adapt the procedure from Aron and Schwartz [11] for the susceptible-exposed-infected-recovered (SEIR) model. In this case, other parameters are introduced: the natural death rate μ and the degree of seasonality δ. The equations are given by

$$\frac{ds}{dt} = -R_0[1 + \delta\sin(2\pi\omega t)]is - \mu s + \mu, \tag{7}$$

$$\frac{di}{dt} = R_0[1 + \delta\sin(2\pi\omega t)]is - i - \mu i, \tag{8}$$

$$\frac{dr}{dt} = i - \mu r, \tag{9}$$

where $\omega = 1/\gamma$ is the inverse of the mean infection time. In this model, we are following the work by Aron and Schwartz and considering the seasonality period as the original time unit. This model also considers that the number of individuals N is constant, so the number of deceased individuals is compensated by the same number of newborns. We assume that these newborns start as susceptible individuals, even if their parents are infected. The number of deaths is an important factor to be considered in the first phases of new epidemics like COVID-19. Several countries reported excess deaths when comparing with the same period before and after this virus outbreak. Even in a normal situation, the assumption that N is constant can be disputed due to fluctuations in the total number of individuals caused by external factors. Some time after the first outbreak the population reaches a new equilibrium, as the remaining individuals are more resistant, which does not mean that the virus is gone. There is a possibility that the disease becomes endemic, and new infection waves can occur. In this work, we will consider such new waves caused by an endemic disease.

The quantity R_0 does not have a minimum value but in general is considered to be larger than 1, as epidemic trajectories with $R_0 \leqslant 1$ tend to disappear. There is also no upper limit for R_0, but from all known diseases, like measles, the larger values are $R_0 \approx 12$–18. We consider R_0 in the interval [1,40]. Nowadays there are no known diseases with such large R_0. On the other hand, several types of virus, including coronavirus, are very likely to suffer mutations, and several new variants are the object of concern as they present a larger R_0, spreading more rapidly. Even if it is unlikely, it is possible that we may have a virus with high R_0.

For the natural death rate, we shall use $\mu = 0.01$ as used by Kamo and Sasaki [7]. The degree of seasonality, used to introduce a time variation in the reproduction number, must lie in the range [0,1).

There are several propositions to include vaccination on SIR models [12,13]. For this work, we chose a simple but realistic one to study the influence of this virus-control method on the system dynamics. That models use includes a fourth compartment for vaccinated individuals, with the fraction v of the population given by v. The equations depend on a fixed vaccination rate, denoted by p. The equations are given by

$$\frac{ds}{d\tau} = -R_0[1 + \delta\sin(2\pi\omega t)]is - \mu s + (1 - p)\mu, \tag{10}$$

$$\frac{di}{d\tau} = R_0[1 + \delta\sin(2\pi\omega t)]is - i - \mu i, \tag{11}$$

$$\frac{dr}{d\tau} = i - \mu r, \tag{12}$$

$$\frac{dv}{d\tau} = p\mu - \mu v. \tag{13}$$

It is important to observe that in this model only newborns are vaccinated, so the vaccination rate must range in the interval [0,1]. In the case $p = 0$ no individuals get vaccinated, and we get the original SIR model. In this case, $p = 1$ all newborns are vaccinated, so they are no longer exposed to the disease. Nevertheless, the original population is always susceptible. The deceased individuals are then replaced by the same number of newborns that can be vaccinated or not. Not vaccinated newborns are counted as susceptible.

The study of dynamical behavior for epidemiological systems consists of the analysis of the influence of different parameters on the dynamics. Usually, every parameter is studied separately, considering all the others fixed. Although this approach is correct, it can miss interesting features from different parameter combinations. To study the influence of different combinations of parameters it is useful to consider multi-dimensional displays. We propose the use of grid classification [8], in which different trajectories are classified according to their properties and the results are plotted on a two-dimensional display. In this approach, we perform the numerical integration of several epidemic trajectories using a different combination of the parameters involved in the model. All trajectories are integrated using the same set of initial conditions. For this work we consider $s_0 = 0.9999$, $i_0 = 0.0001$, $r_0 = 0$, and $v_0 = 0$ (for vaccination), representing a population with a very small fraction of infected individuals. We also consider a fixed natural death rate of $\mu = 0.01$ and a mean infection rate such that $\omega = 0.02$. The other parameters are studied in their range to investigate their influence on the system dynamics.

One important property for SIR models is stability. To classify if the system based on a determined set of parameters is chaotic, there are several methods available. In this work, we use smaller alignment index (SALI) [14] to perform the classification, as it is reliable and faster than other methods, such as Lyapunov exponents. According to this method, the system is chaotic if SALI $< 10^{-8}$ and regular if SALI $> 10^{-4}$. For $10^{-8} \leqslant$ SALI $\leqslant 10^{-4}$ the results are inconclusive and further numerical integration is needed. The SIR model with seasonality and the normal death rate is described by three parameters, namely the basic reproduction number R_0, the degree of seasonality δ, and the natural death rate μ. We investigate the influence of R_0 and δ on the system dynamics and perform a classification according to the chaoticity.

Another important feature is the maximum number of infected individuals of a given epidemic trajectory. According to the SIR models, the number of infected individuals reaches a maximum that depends on the parameters involved in the model. Grid classification can be used to classify different epidemic trajectories according to this number. In this work, we perform the classification using the first wave of infection according to subsequent waves. The first wave is more severe, with a great number of infected individuals. The following infection waves, in SIR models, are much lower. We generate grid classification diagrams and investigate the influence of these quantities on vaccination rate p and reproduction number R_0.

Although the SIR model is a standard in epidemiology, this model has severe limitations [15]. It makes several simplifying assumptions about the population, such as homogeneous mixing, absence of migration, and so on. Also, the parameters do not allow for the quantification of uncertainty in model parameters. As the parameters are not known with any precision, more complex models can demonstrate the uncertainty in projections. The actual effect of social distancing, for example, is often unknown. The vaccination model incorporated in the SIR model is also a simplification. It simply removes from the susceptible compartment vaccinated individuals, assuming that they can never be infected. It does not take into account the effectiveness or the validity period of the vaccine. These parameters can be incorporated into more complex models [9].

III. RESULTS

In Fig. 1 we show the stability classification for different combinations of the parameter R_0 in the interval [1,40] and δ in the interval [0,0.2]. It is possible to observe that the diagram structure is nontrivial. The main chaotic region lies in the region with high R_0 and low δ, including larger values of δ as R_0 increases. Nevertheless, there are also several chaotic "islands" outside of this main region. These small regions become larger as R_0 increases, and have very small SALI, indicating great sensibility to initial conditions.

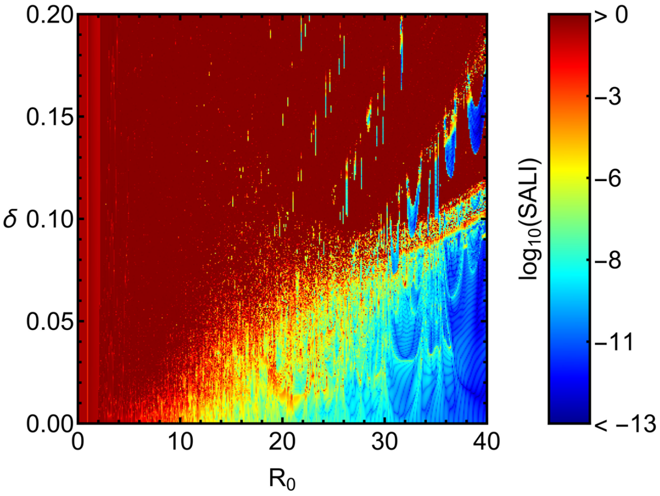

FIG. 1. SIR model with natural death rate and seasonality. R_0 is the basic reproduction number and δ is the seasonality degree. SALI $< 10^{-8}$ regions correspond to chaotic systems. For this diagram we use $\mu = 0.01$ and $\omega = 0.02$.

The influence of vaccination can be found in Fig. 2. Each diagram is generated considering a different vaccination rate, $p = 0.1$, $p = 0.3$, $p = 0.5$, and $p = 0.7$. As the vaccination rate increases the chaotic "islands" become smaller, as the main chaotic region for small δ. This result implies that several epidemic trajectories that were chaotic become stable when newborn vaccination is included. So the introduction of vaccination provides a stabilization of this SIR model.

The classification based on the maximum number of infected individuals $i_{\max}$ for the first and subsequent epidemic waves can be found in Fig. 3. In Fig. 3(a) the equal color line inclination show that, in addition to the well-known dependency on R_0, as δ increases $i_{\max}$ also increases. In Fig. 3(b) a different pattern can be observed. It indicates that now smaller values of R_0 have larger $i_{\max}$ and have the same dependency on δ.

The introduction of vaccination brings some interesting information on the maximum number of infected individuals, as can be seen in Fig. 4. Figure 4(a) shows that this number depends on R_0 as expected, but it does not have a visible dependency on p, as the lines with equal colors are vertical. For the subsequent waves in Fig. 4(b) it is possible to observe that there is a nontrivial dependence on p. In particular, it is possible to observe that, when the vaccination reaches a threshold value for each R_0 subsequent waves are fully contained.

IV. DISCUSSION

Evidently, most of the real-known diseases do not present chaotic behavior in this model, as they have low R_0. But there are diseases such as measles [16] that can have $R_0 = 18$, and unknown diseases can have an even lager reproduction number. These diseases can present chaotic behavior depending on the seasonality degree. The structure of the chaotic region

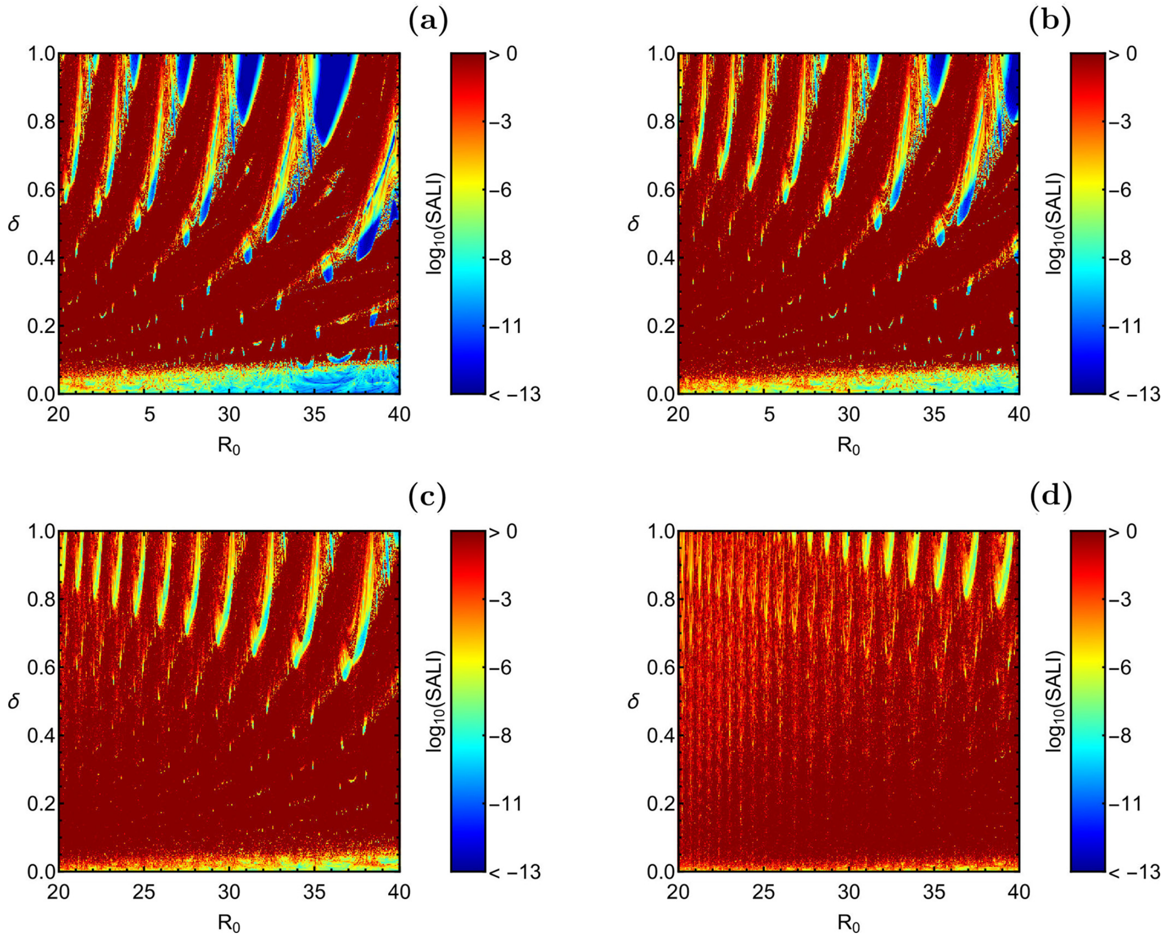

FIG. 2. Vaccination effect on stability of SIR models for different combinations of R_0 and δ, for vaccination rates (a) $p = 0.1$, (b) $p = 0.3$, (c) $p = 0.5$, and (d) $p = 0.7$. As p increases, the systems become more stable. For all these diagrams we use $\mu = 0.01$ and $\omega = 0.02$.

in the SIR model is nontrivial, as can be seen in Fig. 1, so the study of the two parameters separately can lead to wrong conclusions. In addition to the chaotic region with high R_0 and low δ, there are several "islands" in that parameter space corresponding to chaotic epidemic trajectories.

When we introduce vaccination several formerly chaotic regions become stable, as can be seen in Fig. 2. Even the isolated "islands" of chaos tend to vanish when vaccination is introduced. We can conclude that in the context of this simplified model that vaccination of newborns is able to control

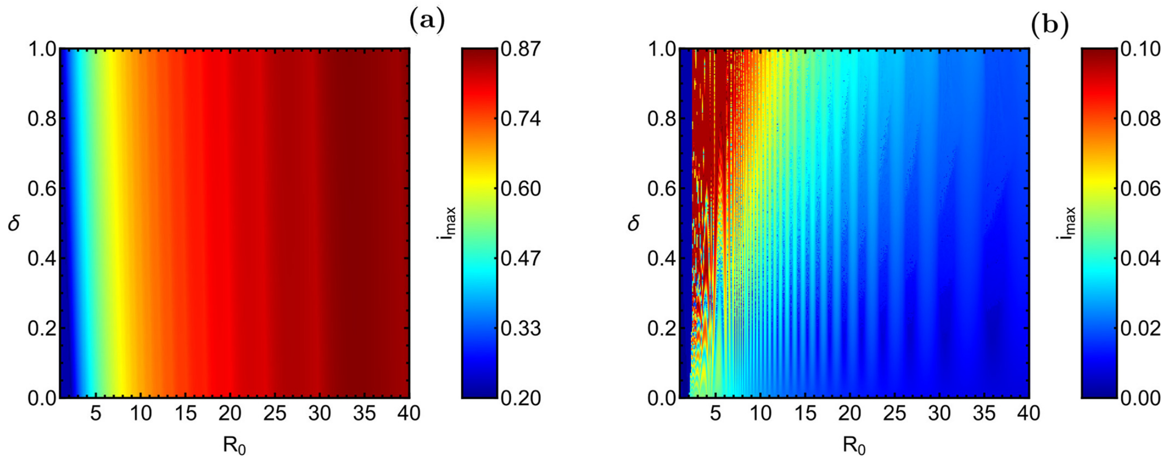

FIG. 3. Maximum number of infected individuals for (a) the first wave and (b) subsequent waves of epidemic infection without vaccination. In these diagrams we consider $\mu = 0.01$ and $\omega = 0.02$.

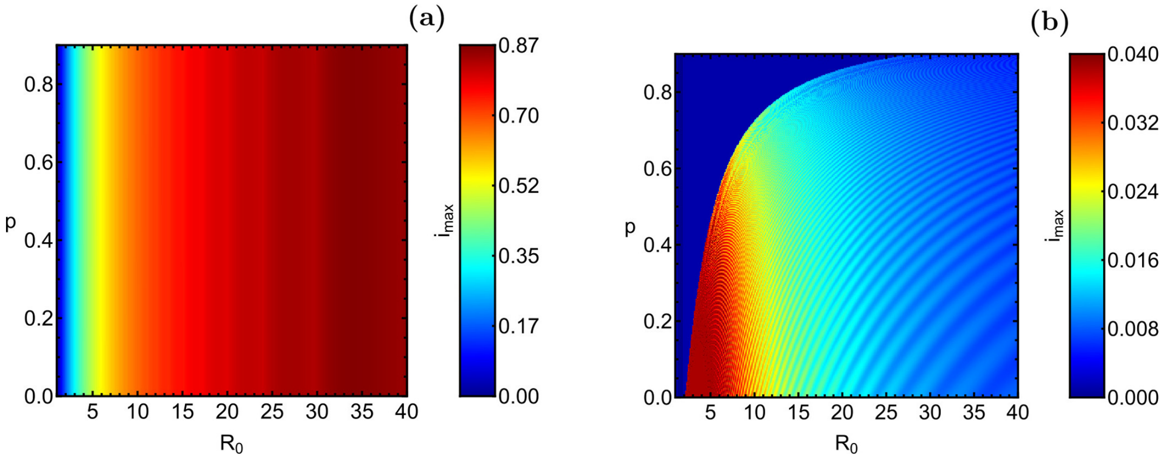

FIG. 4. Maximum number of infected individuals for (a) the first wave and (b) the subsequent waves of the epidemics for $\delta = 0.05$. Note that the number is independent of the vaccination rate p for the first wave, but for subsequent waves there is a nontrivial influence of p. In these diagrams we consider $\mu = 0.01$ and $\omega = 0.02$ and $\delta = 0.05$.

chaos in most of the epidemic trajectories. The less chaotic, the more predictable the models are, as they lose their sensibility to initial conditions. This is an unexpected benefit from a vaccination as a strategy of epidemics control. The vaccination influence on stabilization of epidemics was the object of several studies, but the grid classification provides a more complete analysis for different scenarios. This is essential for models that depend on several parameters.

Considering the maximum number of infected individuals, it is clear from Fig. 3 that R_0 controls the dynamics, but the degree of seasonality δ has an influence on the number of individuals that get infected by the disease. This is expected as the effect of seasonality is to change the effective value of the reproduction number. As δ increases, the reproduction number achieves larger values and more individuals get infected. Also, we can see that the maximum number of infections for subsequent waves is greater for smaller reproduction numbers. This is explained by the fact the for large R_0 most of the individuals are infected in the first wave.

The introduction of vaccination has little effect on the first wave of infection, as can be seen in Fig. 4(a). This is also expected as our model assumes only the vaccination of newborns, which occur at a much smaller rate than the number of new infections. On the other hand, when we study subsequent infection waves, as in Fig. 4(b), we obtain a very different picture. We can see a very clear influence of vaccination, as the number of subsequent infections becomes zero for sufficiently large values of the vaccination rate p. For larger R_0, a higher fraction of newborns must be vaccinated in order to control the epidemic. In this case, the grid classification allows obtaining the threshold value for the vaccination rate in order to contain further infection waves for each epidemic.

In conclusion, we show that vaccination, when available, is a key strategy for the control of epidemics caused by virus outbreaks. The benefits of the vaccination go beyond controlling the number of infections. It is also useful so the epidemic becomes predictable and other control strategies can be combined. This is an essential matter for any policy of public health.

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