Backcasting COVID-19: A Physics-Informed Estimate for Early Case Incidence

G.A. Kevrekidis\textsuperscript{a,d}, Z. Rapti\textsuperscript{b}, Y. Drossinos\textsuperscript{c}, P.G. Kevrekidis\textsuperscript{d}, M.A. Barmann\textsuperscript{d}, Q.Y. Chen\textsuperscript{d}, J. Cuevas-Maraver\textsuperscript{e,f}

\textsuperscript{a}Department of Applied Mathematics and Statistics, Johns Hopkins University, Baltimore, MD 21218, USA
\textsuperscript{b}Department of Mathematics and Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign
\textsuperscript{c}European Commission, Joint ResearchCentre, I-21027 Ispra (VA), Italy
\textsuperscript{d}Department of Mathematics and Statistics, University of Massachusetts Amherst, Amherst, MA 01003, USA
\textsuperscript{e}Grupo de Física No Lineal, Departamento de Física Aplicada I, Universidad de Sevilla. Escuela Politécnica Superior, C/Virgen de África, 7, 41011-Sevilla, Spain
\textsuperscript{f}Instituto de Matemáticas de la Universidad de Sevilla (IMUS). Edificio Celestino Mutis. Avda. Reina Mercedes s/n, 41012-Sevilla, Spain

Abstract

It is widely accepted that the number of reported cases during the first stages of the COVID-19 pandemic severely underestimates the number of actual cases. We leverage delay embedding theorems of Whitney and Takens and use Gaussian Process regression to estimate the number of cases during the first 2020 wave based on the second wave of the epidemic in several European countries, South Korea, and Brazil. We assume that the second wave was more accurately monitored and hence that it can be trusted. We then construct a manifold diffeomorphic to that of the implied original dynamical system, using fatalities or hospitalizations only. Finally, we restrict the diffeomorphism to the reported cases coordinate of the dynamical system. Our main finding is that in the European countries studied, the actual cases are under-reported by as much as 50\%. On the other hand, in South Korea - which had an exemplary and proactive mitigation approach - a far smaller discrepancy between the actual and reported cases is predicted, with an approximately 17\% predicted under-estimation. We believe that our backcasting framework is applicable to other epidemic outbreaks where (due to limited or poor quality data) there is uncertainty around the actual cases.

Keywords: COVID-19, Embedding Theorems, Epidemics, Time Series, Gaussian Process

1. Introduction

During the early stages of COVID-19 (and in fact of any emerging disease) even estimating the basic reproduction number $R_0$ was a challenge \cite{2, 25, 37, 50} due to lack of information and the absence or poor quality of data. $R_0$ is defined as the number of secondary infections an infectious individual can generate in a population of susceptible individuals. It is quite important for epidemiologists and public health officials to have an accurate estimate of its magnitude. The clinical characteristics of the disease - latency period, period of infectiousness, incubation period - were not known, so differing estimates of $R_0$ existed (ranging from 1.4-6.49) \cite{30} that largely depended on the models that were used to estimate them and the corresponding assumptions made. At the same time, limited testing capacity obscured the true size of the epidemic and the actual growth rate. Varying estimates of symptomatic and asymptomatic cases also exist \cite{20, 40, 45}. These inadequacies, in turn, caused serious handicaps in mounting an appropriate response by public health authorities. While our understanding of the relevant models and both their benefits and weaknesses has
greatly progressed [17, 19, 21], there is still significant room for improvement of our understanding of both
the first and subsequent waves of the epidemic.

As the epidemic progresses and more data become available - daily new cases, number of tests performed,
daily new hospital admissions, daily new deaths, etc. - these too should be taken with a grain of salt. It is
now widely known, and generally accepted, that COVID-19 reported data are neither reliable nor complete,
and that the best practice is to base mathematical models on hospitalization and fatality time series data
[19]. Reported-case count time series are unreliable due to the limited number of tests available initially,
and the large number of cases that are asymptomatic [40] and/or go unreported [29]. A recent systematic
review and data meta-analysis concluded that 35.1% [95% CI: 30.7 - 39.9%] were asymptomatic infections
[45].

It is then natural that various methods and studies exist attempting to reconstruct the true number of
case counts and fatalities. In [42] a backcasting approach based on fatalities and a Gamma distribution of
the time from infection to death was used to study the epidemic in 15 countries. It was estimated that
the number of infected people is 6.2 [95% CI: 4.3 – 10.9] times higher than reported. This echoes a study
of the epidemic in the US [54], where probabilistic bias analysis was used to approximate the true case
counts. They found that 89% of infections were undocumented. Indeed, the US Centers for Disease Control
indicated an under-reporting of infections by a factor of 2 to 13 times in [13], illustrating the gravity and
relevance of the issue. In Brazil, it was estimated [38] that the actual case counts are three times and the
deaths twice as many as those reported.

A study of the epidemic dynamics around the globe [44] using a Bayesian Gaussian Process model found
large disparities in the degree of under-reporting among countries. Cumulative infection data from several
European countries were studied using the so-called capture-recapture methods [4] and it was found that
the ratio of calculated total over observed (i.e., reported) cases was around 2.3. In [9] we chose to neglect
infection data and instead focused on fatalities, for a study of the epidemic in Mexico. Fitting the model
to the infection time series produced unreliable predictions of future deaths, due to the under-reporting of
infections.

While fatalities are believed to be more reliable than case counts [9], care should still be taken when using
them as a benchmark due to different ways of measuring and reporting the data among countries [3]. For
instance, excess deaths, rather than reported deaths, during the first wave in the northern part of Italy
were embedded in a differences-in-differences regression model. One of the findings of the study was that
deaths may be under-reported by as much as 60% [8]. The reason for the discrepancy is that only hospital
deaths are included in the official reports. The excess mortality in the first months of the epidemic was
estimated to be 28% higher than the reported COVID-19 fatalities. Another pertinent point is that delays
in death counts may be as long as a year in some cases [52]. This limits our ability to produce accurate,
real-time forecasts if recent data are not reliable; but if the vast majority of the data is eventually counted
and correctly revised, then this situation lends well to a retrospective analysis after, say, a year.

In the present study, we develop and apply a method that can be used to extrapolate from the second
(and generally latter) wave, the fatalities and the COVID-19 infections. We assume that during the second wave
both reported infections and reported fatalities are accurate and are used together with the fatalities during
the first wave (also assumed to be accurate) to backcast the reported infections during the first wave. This
method can be applied to countries whose COVID-19 time series are characterized by a first peak, succeeded
by a period of very low daily incidence during the summer months (i.e., between the first and the second
wave), followed by a second peak in the fall. Using the second-wave time series as training sets for our
algorithm, we carry out this program for a substantial number of countries, principally from Europe, but
also from Asia and America, obtaining a consistent under-reporting of the relevant diagnostics.

Our presentation is structured as follows. First we provide the mathematical background for our analysis
in Section 2.1. Subsequently, we present the relevant data and their structure in Section 2.2, comment on
uncertainty in diagnosed cases in 2.3, and we present a schematic of our methodology in 2.4. In Section 3 we
present our numerical findings, and Section 4 wraps up the manuscript with some conclusions and directions.
for future work. The Supplementary Material contains further information on our methodology, describes model parameters, and addresses issues concerning data uncertainty and hyperparameter tuning.

2. Method

2.1. Theory: Delay embedding

Our operating assumption is that we are given the time series of Reported Cases ($C$) and Reported Fatalities (Deaths) ($D$) per day in a geographical region over time. More specifically, we denote

\[
D = \{d_t\}_{t \geq 0}^T \tag{1}
\]

\[
C = \{c_t\}_{t \geq 0}^T \tag{2}
\]

where $d_t, c_t$ denote the fatalities and officially diagnosed cases on day $t$, for $t = 0, 1, 2, \ldots, T$. We further assume that $D$ is accurate for all $t$ while $C$ is only accurate after time $t \geq T^*$ and inaccurate for $t < T^*$, where $T^*$ is a time point chosen between the first and second waves, chosen as explained in the following section.

Suppose that $d_t$ and $c_t$ are discrete observations of two corresponding quantities $D(t)$, $C(t)$ that satisfy an $n$-dimensional system of coupled deterministic ordinary differential equations whose dynamics feature a unique attractor. Then, the state of the system at any given time can be represented by an $n$-dimensional vector and the overall behavior of the system can be represented on a manifold $\mathcal{M} \subset \mathbb{R}^n$.

According to the delay embedding theorems of Whitney and Takens [10, 35, 46, 49], we are able to use only $d_t$ to construct a manifold $\mathcal{M}_D \subset \mathbb{R}^k$ that is diffeomorphic to $\mathcal{M}$. Such a manifold is guaranteed to exist whenever the embedding dimension $k$ satisfies $k \geq 2n + 1$: that is, there exists a differentiable invertible transformation (diffeomorphism) $f : \mathcal{M}_D \to \mathcal{M}$. Since $c_t$ is known after time $T^*$ we can use that part of the data set to learn (using regression) the restriction of $f$ to the “reported-cases” coordinate

\[
\hat{f} \sim f|_C : \mathcal{M}_D \to C(t), \quad t \geq T^* \tag{3}
\]

We proceed to evaluate $\hat{f}$ on the points of the reconstructed manifold $\mathcal{M}_D$ observed for $t \leq T^*$ in order to estimate $c_t$ during the early stages of the pandemic.

2.2. Data

In Supplementary Material (SM), Appendix A, we summarize the sources of our data and we comment on their quality. In addition, we address issues of data uncertainty, we comment on the reliability of the time series used and on the embedding and Gaussian Process parameters.

2.2.1. Structure and $T^*$

The framework proposed in Section 2.1 is very general in that it only requires two time series of the observed quantities ($C$, $D$) and some knowledge of the time $T^*$.

$T^*$ is the time after which $C$ can be considered accurate, and it may be hard to define. The naive definition of accurate and inaccurate is true and false respectively, meaning that we take all information after time $T^*$ at face value. It is arguably more natural to think of the accuracy of the considered data as a continuously varying quantity as opposed to a Boolean variable. In principle, it may be possible to incorporate additional statistics such as (but not limited to) the amount of testing [18] and vaccination rates [34] to quantify the uncertainty of the data. However, this process would complicate our analysis since the availability, quality, and adequacy of additional markers is not certain, and their consideration would result in a more complex but less applicable model.

Fortunately, there is structure in many time series at the country and local level that can be exploited. Several countries in Europe experienced a first peak in the observed cases and fatalities, as shown in Figures
1a and 1b, respectively. This was followed by a decline during the summer months, before the second peak in the fall. Thus, a heuristic definition of $T^*$ can be described as the time when mortality falls close to zero for a long period, which coincides, in many countries, with the summer months of 2020. The leads to an almost boolean $T^*$ occurring sometime within this period.

Figure 1: Seasonal structure of the (a) case and (b) death time series for the UK and the three most populous countries in the EU (Germany, France, Italy) during the first months of 2020. (The UK officially exited the EU after the 31st of January, 2020). Few diagnosed cases and deaths were observed during the summer months.

We note that our backcasting results are not sensitive to such a $T^*$, as long as its choice is reasonable, namely falls within the period of low mortality and not close to the second peak (see Section 3.1 for the effect of the choice of $T^*$ on backcasting results for Italy). A compromise in the characterization of accuracy can be reached by assuming that the data after $T^*$ are not necessarily true, but can be trusted enough to make an estimate of the true number of infections after $T^*$, which is further explored in Section 2.3.

An additional complication arises due to varying mortality rates as the epidemic progressed. For instance, a study for Sweden [48] spanning data from March to September 2020 found that mortality in hospitalized patients decreased as the pandemic progressed. This may be attributed to improvements in treatment protocols, the availability of new treatments [e.g. remdesivir, monoclonal antibodies], differences in the virulence of circulating variants [27], or differing age distribution of those infected in the first versus second wave [22]. The inability to address these issues fully is why our results are qualified as approximate estimates of the true case incidence.

2.3. Uncertainty in Diagnosed Cases

We are interested in building an uncertainty estimate around the diagnosed cases we use during our calibration period, which will, in turn, correspond to uncertainty around the backcasted result. We turn to the literature to obtain a “hidden-case” estimator that preserves some of the integrity of our current data.

The Capture-Recapture (CRC) method presented in [4] estimates that if the diagnosed cases at time $t$ are $c_t$, then the true number of cases at time $t$ is a random variable $\hat{c}_t$, where [4], [55]:

$$E[\hat{c}_t] = c_t + \frac{(c_t)^2}{c_{t-1} - d_t}$$

$$V[\hat{c}_t] = \frac{(c_t)^4}{(1 + c_{t-1} - d_t)^3} + \frac{4(c_t)^3}{(1 + c_{t-1} - d_t)^2} + \frac{(c_t)^2}{1 + c_{t-1} - d_t}.$$  

(4)

(5)

Thus, the case time series after $T^*$ can be adjusted (accompanied by a 95% confidence interval) using case and fatality observations after $T^*$. This estimator only depends on our available time-series information, and does not take into account any external prior knowledge (such as serial interval distribution, etc). This
is desirable because we believe that post-$T^*$ diagnosed case counts are of much higher fidelity than early ones, and we would like our estimates to be based on them, since they are true observables of the system behavior we are trying to capture.

Our results show that this estimate cannot be used reliably in this problem framework without backcasting, since $\hat{c}_t$ still depends on the validity of $c_t$, which is not close to the true number of cases before $T^*$. We choose to present the main part of our numerical results using CRC to quantify uncertainty, aside from Figures 5 and 6 in Section 3.1 where we also present the incorporated Gaussian-Process (GP) uncertainty estimates. The uncertainty estimation method, however, is arbitrary, and one can choose it independently as part of the backcasting algorithm.

2.4. The Backcasting Algorithm

Figure 2: Flowchart of the proposed Backcasting Algorithm. The acronyms are: FNN: False-Nearest-Neighbors; GP: Gaussian Process (regression); CRC: Capture-Recapture (method).

Figure 2 summarizes the algorithm we used to backcast the number of cases, given two time series. We chose the time series of reported number of cases and number of fatalities. First, the embedding dimension $k$ was determined via the False-Nearest-Neighbors (FNN) [1] (or alternatively Average False Neighbors (AFN) [6]) algorithm as implemented in the Python nonlinear time series module nolitsa\(^1\) [32], [33]. Then, we used Gaussian Process (GP) regression (see SM, Appendix B) to obtain $f_{GP}$, a process that requires learning the case time series after time $T^*$ and then using it to backcast the number of case before $T^*$. We used the sklearn\(^2\) Python library [39] to perform the Gaussian Process regression. Lastly, we quantified uncertainty estimates using the capture-recapture method of Ref. [4]. We note in passing that further work on the use of GP for learning dynamical system behavior in the same manner can be found in [28].

Importantly, each step of the proposed algorithm is independent. One may use GP if other reliable uncertainty estimates are not available, but may also use another regression method to learn the estimated function. Similarly one may also use a separate uncertainty method specific to the country or data set the algorithm is applied to. This is impractical when working with multiple countries, but it will lead to more accurate results when optimizing these choices for a specific data set. The theory behind the validity of the algorithm is valid regardless of the method applied.

In SM, Appendix A.3, we provide further information on the definition and use of the embedding parameters (the delay time $\tau$ and the embedding dimension $k$) along with Gaussian Process parameters and the corresponding kernels used.

\(^1\)https://github.com/manu-mannattil/nolitsa
\(^2\)https://scikit-learn.org/stable/modules/gaussian_process.html
3. Numerical Results

3.1. Italy: A Case Study

We analyze the time series of a single country as a prototypical case example: Italy.

In Figure 3 we present the normalized time series for Italy from the beginning of the pandemic. While the fatalities in the two waves beginning at approximately \( t = 30 \) and \( t = 250 \), respectively, are of the same magnitude, we note that the diagnosed cases during the first wave are much lower than the second wave would suggest. In this case, a nominal \( T^* \) is identified, but it could be specified to be at any point where the incidence of both cases and fatalities is very low (i.e., during the summer months).

Because the disparity between the mortality rates of the two waves suggested by Figure 3 is not trustworthy, and since the data satisfy the structure presented in Section 2.2.1, we claim that this is a good candidate time series to backcast. Using the FNN algorithm we estimate the embedding dimension for the fatality time series to be \( k = 10 \) (see Figure 4 where the percentage of false neighbors drops to 0 at that dimension). In addition, we arbitrarily, but consistently, as discussed, pick \( T^* = 160 \) occurring during the period of low case incidence.

Given the embedding dimension we construct \( \mathcal{M}_D \) such that \( \mathbf{d}_t = \{d_{t-9}, ..., d_t\} \in \mathcal{M}_D \), proceeding to fit our GP estimator:

\[
\hat{f}_{\text{GP}}(\mathbf{d}_t) = c_t, \quad \forall t \geq 160
\]

and then backcast to the initial cases \( \hat{c}_t \):

\[
\hat{c}_t = \hat{f}_{\text{GP}}(\mathbf{d}_t), \quad \forall t \in [10, 160]
\]

We obtain the result shown in Figs. 5-6. A remarkable feature of Fig. 5 is that at the peak of the first wave, the number of reported daily cases was found to be less than 10,000, while any selection of the kernel in our backcasting scenarios suggests that there were approximately 40,000 cases at that time. Even adjusting for the trusted observations in Fig. 6, we still find a substantial disparity between the number of cumulative cases observed and the ones predicted by our backcasting analysis. The uncertainty interval of this and similar figures is computed based on the uncertainty of the corresponding daily cases, and is > 95% based on the sub-additivity of standard deviation. As we consider more data, the disparity (as a ratio) between
observed and estimated cases will necessarily decrease because the result is cumulative and the increments agree after $T^*$. Comparing cumulative cases at $T^*$ gives a more accurate picture of the beginning stages of the pandemic, while comparing at a later time can be used to understand the long-term effect of that early (unreported) spike in cases; see, for example, the results presented in Tables 2 and 3.

We demonstrate the effect of changing the time window on the backcasting result in Figure 7a, whereas the effect of varying the $T^*$ is shown in Figure 7b. In the latter it can be seen that variations of $T^*$ do not change the qualitative picture described above. In the former, we can see that $k = 13$ may lead to potential overfitting, while already $k = 10$ yields an adequate qualitative representation of the number of cases.

The uncertainty estimate associated with the GP implementation is not necessarily accurate, since the obtained uncertainty intervals can be tuned using the kernel parameters. To avoid additional computation,
we circumvent this issue using the same $T^* = 160$ and time window $k = 10$, but apply the CRC method to adjust cases and their uncertainty after $T^*$ (as described in Section 2.3). The associated backcasted results are presented in Figure 8. Moreover, the cumulative number of cases based on the CRC-adjusted backcasting is shown in Figure 9a. Figure 9b, instead, shows backcasting results using the hospitalization time series in place of the fatalities time series as the predictor for cases. It is important to realize that the CRC adjustment of the cases can only be relied upon for $t \geq T^*$ and not where the estimated number of cases is unrealistic. We note similar behavior to Figure 6 but with a much narrower uncertainty envelope due to the smaller uncertainty after the CRC adjustment.

3.2. Comparative Results

We extend our considerations to Spain, Sweden (where official policies related to COVID-19 were notably very different from those in other EU countries), Germany, United Kingdom, France and South Korea, as well as Brazil, with the last two representing rather extremely opposite-end examples of mitigation approaches towards the pandemic, as discussed below. These countries (with the exception of Brazil) fit the time-series profile described in Section 2.2.1: they have a first peak, followed by a period over the summer of 2020 where reported cases ebbed and then a subsequent second peak during the fall months of 2020.

Among these countries, Sweden has the distinction of not ordering a nationwide lockdown during the first wave of the pandemic, as the other European countries considered in this work did [12]. Instead, among the mandated measures adopted were self isolation, social distancing, banning of public events and partial school closures. South Korea adopted a proactive approach and started developing testing capabilities almost two weeks before the first case in the country [36], established contact tracing protocols as early as mid-February of 2020, enforced social distancing from March 22 to April 15, demanded tests for all incoming travelers and quarantine for travelers from selected countries, and lastly, redistributed resources at hospitals and emphasized the use of personal protective equipment by health care workers.

In sharp contrast, the lack of coordination at the federal level and delays in the implementation of mitigation measures in Brazil have been well documented [5, 7]. Testing capacity in the country was very limited, with test kits being available for the first time in March 2020, whereas the first phase of the epidemic in Brazil
started in the middle of February 2020. Additionally, there were regions with extremely low ICU bed capacity, such as Amazonas, where the capacity was 11 beds for 100,000 people. As a result, Manaus, the capital city of Amazonas, was one of the regions that were affected particularly intensely. For instance, fatalities per 100,000 people due to COVID-19 in this region exceeded by a factor of two the fatalities in the country overall.

All country time series (except that of Brazil, as previously mentioned) satisfy the structure of Section 2.2.1 (see, also, Figures 1a and 1b) and this structure extends to the corresponding hospitalization data, when available. In the results shown in Figure 10 we use both $D$ and $H$ as predictors, with the uncertainty estimated using the capture-recapture process [4]. The embedding dimension $k$ was again estimated using the False Nearest Neighbor algorithm, with the results presented in Table 1. We find that the predicted, cumulative number of cases in the four countries illustrated in Figure 10 was larger by a factor typically between 1.3 and 2 when evaluated at the end time of our data set (April 4, 2021). However, the same factors vary greatly when computed at time $T^*$, at which point the estimate is purely through the backcasted result.

For Germany, Spain, South Korea, and Brazil, daily hospital occupancy is not readily available in our data set, and we only include the prediction based on the corresponding fatalities. Figure 11 presents the
Figure 8: Demonstration of the capture-recapture (CRC) approach [4] to estimate uncertainty in the diagnosed cases. The CRC adjustment (presented in 2.3) to the number of cases is insufficient when the estimated number of cases is not realistic, which can be seen in comparison to the backcasted estimate of Figure 5. However, they may be considered a reasonable estimate of the true number of missed cases later on (\(c_t\) for \(t \geq T^*\)).

![Graph showing CRC approach]

Figure 9: Backcasting for Italy using the CRC case estimate and uncertainty after \(T^* = 160\). Here \(T^* = 160, k = 10\). The left panel uses the data for deaths to perform the backcasting, while the right panel uses that for hospitalizations. While the results are not identical they are reasonably consistent.

![Graph showing backcasting]

Table 1: Estimates of the embedding dimension \(k\) of the death time series for each country.

| Country     | Embedding dimension (Estimate, FNN) | Start Date (dd/mm/yy) |
|-------------|------------------------------------|-----------------------|
| Brazil      | 5                                  | 26/02/20              |
| France      | 8                                  | 24/01/20              |
| Germany     | 9                                  | 27/01/20              |
| Italy       | 10                                 | 31/01/20              |
| South Korea | 12                                 | 21/01/20              |
| Spain       | 5                                  | 01/02/20              |
| Sweden      | 7                                  | 01/02/20              |
| United Kingdom | 6                              | 31/01/20              |

backcasted cumulative number of cases (in analogy to the left panel of Figure 10), whereas Table 3 presents
Figure 10: Backcasting of the cumulative number of cases using deaths (left) and hospitalizations (right) as predictors. For all of the countries we use $T^\star = 160$ and the corresponding embedding dimension estimated in Table 1, as well a delay time of one day.

Table 2: Summary of the Fig. 10 backcasting predictions for the cumulative number of diagnosed cases at time $T^\star$ (July 9, 2020) and at the end of the considered period (April 4, 2021). Two different predictors were used: Death or hospitalization times series, both coupled with capture-recapture (CRC) uncertainty estimates.

| Country        | Reported number of cases $\times 10^6$ | Death backcasting number $\times 10^6$ | Backcasted to reported | Hospitalization backcasting number $\times 10^6$ | Backcasted to reported |
|----------------|----------------------------------------|----------------------------------------|------------------------|-----------------------------------------------|------------------------|
|                | Backcasted cumulative number of cases ($> 95\%$ CI) | Backcasted cumulative number of cases ($> 95\%$ CI) | Backcasted cumulative number of cases ($> 95\%$ CI) | Backcasted cumulative number of cases ($> 95\%$ CI) |
| Italy          | 0.24                                   | 1.68 (1.61, 1.75)                      | 7.91 (6.73, 7.29)      | 1.46 (1.40, 1.52)                             | 4.89 (4.70, 5.08)      |
| France         | 0.20                                   | 1.89 (1.82, 1.96)                      | 9.27 (8.93, 9.61)      | 2.17 (2.09, 2.25)                             | 10.66 (10.27, 11.04)   |
| Sweden         | 0.08                                   | 0.61 (0.56, 0.66)                      | 7.97 (7.35, 8.58)      | 0.48 (0.44, 0.53)                             | 6.33 (5.80, 6.87)      |
| United Kingdom | 0.28                                   | 2.20 (2.13, 2.28)                      | 7.73 (7.46, 8.01)      | 1.57 (1.50, 1.64)                             | 5.51 (5.28, 5.74)      |
|                |                                        |                                        |                        |                                               |                        |
|                | 04/04/2021                              |                                        |                        |                                               |                        |
| Italy          | 3.59                                   | 5.13 (5.03, 5.33)                      | 1.43 (1.37, 1.48)      | 4.89 (4.70, 5.08)                             | 1.36 (1.31, 1.42)      |
| France         | 4.70                                   | 6.54 (6.31, 6.77)                      | 1.39 (1.34, 1.44)      | 6.84 (6.60, 7.08)                             | 1.45 (1.40, 1.51)      |
| Sweden         | 0.80                                   | 1.35 (1.25, 1.46)                      | 1.69 (1.56, 1.82)      | 1.22 (1.12, 1.32)                             | 1.53 (1.40, 1.65)      |
| United Kingdom | 4.36                                   | 6.40 (6.17, 6.62)                      | 1.47 (1.42, 1.52)      | 5.75 (5.54, 5.96)                             | 1.32 (1.27, 1.37)      |

the results of our calculations at $t = 400$ and compares them to the reported number of cases (analogously with Table 2).

Two other studies that performed backcasting of cases are [4] and [12]. According to [4], which used a capture-recapture method, the ratio of total to reported cases for Italy, Germany, Spain and the UK, were 2.23, 2.30, 2.21 and 2.37, respectively. Instead, according to the results shown in Tables 2 and 3, we find that the ratio of backcasted cumulative number of cases to the reported number is 1.43 (Italy), 1.85 (Germany), 2.00 (Spain), and 1.47 (United Kingdom). These numbers are smaller than those reported in [4], but they are
Figure 11: Backcasting results for countries where daily hospitalization records are not (or are partially) available. For all the countries we use $T^* = 160$ and a window, embedding dimension, of 15 days, and the same kernel for the Gaussian Process (Matérn kernel).

Table 3: Summary of the Fig. 11 backcasting predictions for the cumulative number of diagnosed cases at time $T^*$ (July 9, 2020) and at the end of the considered period (April 4, 2021). The death times series coupled with capture-recapture (CRC) uncertainty estimates was used as a predictor.

| Country    | Reported number of cases $\times 10^6$ | Backcasted cumulative number of cases ($> 95\%$ CI) | Death backcasting $\times 10^6$ | Backcasted to reported |
|------------|----------------------------------------|-----------------------------------------------------|--------------------------------|------------------------|
|            |                                        | 09/07/2020 – $T^*$                                   |                                 |                        |
| Germany    | 0.19                                   | 1.03 (0.98, 1.08)                                   | 5.30 (5.03, 5.58)               |                        |
| South Korea| 0.01                                   | 0.03 (0.02, 0.4)                                    | 2.64 (1.83, 3.46)               |                        |
| Spain      | 0.29                                   | 2.12 (2.03, 2.21)                                   | 7.38 (7.06, 7.70)               |                        |
|            |                                        | 04/04/2021 – Final Date                              |                                 |                        |
| Germany    | 2.84                                   | 3.79 (3.62,3.96)                                   | 1.33 (1.27, 1.40)               |                        |
| South Korea| 0.10                                   | 0.13 (0.09, 0.16)                                   | 1.22 (0.91, 1.53)               |                        |
| Spain      | 3.28                                   | 5.17 (4.95, 5.38)                                   | 1.57 (1.51, 1.64)               |                        |

consistent with the overall observation that the number of reported cases during the first epidemic wave is significantly smaller than the actual number of infected individuals. In [12], backcasting was performed from observed deaths based on a Bayesian mechanistic model; they found that until May 4, 2020, the percentage of population infected in Italy, France, UK, Germany, Sweden and Spain was 4.6 %, 3.4%, 5.1%, 0.85%, 3.7% and 5.5%, respectively. These far exceed the reported infections in each of these countries.

In comparison, our results in the same order are 2.8 %, 2.8%, 3.3%, 1.2%, 5.9%, 4.5%. We note that these results are in the same ballpark as those of [12], although there are differences due to the detailed assumptions of each setting.

We also include the backcasting projection for Brazil: the number of daily cases is shown in Figure 12a, whereas the cumulative number of cases is presented in Figure 12b. There, the data do not satisfy the distinct wave structure of the previous examples. Irrespective of that, we found similar features as in the previously reported examples. In particular, we found that the diagnosed cases for $t \leq T^*$ were under-reported although by a substantially smaller fraction than in other countries. Specifically, the proposed backcasting method predicts a higher and earlier peak in cases than observed, but it notably fails when trying to extrapolate outside of the range of the given data: early predictions, when cases and deaths due to Covid-19 are near zero, should yield a similar result. The left tail should therefore be considered inaccurate. We only include this example to demonstrate why the backcasting result may not be trustworthy if the structure of the data is not consistent with Section 2.2.1, even if it seems plausible.
Figure 12: Backcasting results for Brazil with a time window of 5 days. The left panel includes results for two different choices of kernel (Exponential and RBF) for the GP regression. After time $T^* = 160$, the predicted cases (pink) are close to the observed cases (blue) since the model has been trained at those points. The right panel only presents one of the results (RBF) for the sake of clarity.

4. Discussion-Conclusion

We developed a computational framework that uses as input the case and fatality incidence in the second wave of the COVID-19 epidemic in various regions to evaluate the magnitude of case incidence of the first wave, assuming the incidence of fatalities is accurate. The framework is based on algorithms that leverage the Takens-Whitney delay-embedding theorems [46, 49, 53], use the method of False Nearest Neighbors [1] to estimate the embedding dimension, and employ Gaussian Processes (GP) to perform nonlinear regression (as well as to quantify the resulting uncertainty). Uncertainty is also quantified using the capture-recapture approach of [4].

The method requires a minimal number of external parameters, besides those hyperparameters internal to the GP algorithm. These parameters include the embedding dimension $k$, the parameter $T^*$, and the time delay $\tau$, which for the 7-day averaged time series was taken to be one day. The parameter $k$ is the number of lagged observations required to construct the manifold $M_D$ diffeomorphic to $M$. The time parameter $T^*$ separates (somewhat artificially) the data into a segment past $T^*$, after which the data are considered to be accurate (typically a low incidence time during the summer). Assuming the accuracy of fatalities (or hospitalizations) the aim is to backcast the incidences during the first wave, i.e., during the early stages of the pandemic, based on the trends between cases and fatalities. The relatively small number of parameters and hyperparameters sets the current methodology apart from other ODE or PDE based approaches, for which a significant effort is required to resolve parameter identifiability issues [9, 24].

The framework was used with data from various European countries, which adopted disparate mitigation strategies, as well as with data from South Korea and Brazil, which also followed antipodal approaches to curtail the burden of the pandemic. Among the findings of this study is that in the six European countries studied (Italy, France, United Kingdom, Sweden, Germany and Spain) the first wave was, as widely suspected, considerably larger than reported. Specifically, at the end of the period considered, the ratio of predicted (backcasted) cumulative number of infections to those reported was found to be 1.43 (Italy), 1.39 (France), 1.47 (UK), 1.69 (Sweden), 1.33 (Germany), and 1.57 (Spain), i.e., the predicted number of cases was consistently greater by over 30% than the reported number. In South Korea, however, where the epidemic was controlled, the discrepancy between predicted and observed cases is substantially smaller; we found the ratio of predicted to reported to be 1.20, a discrepancy of 20%. This is a case example, as was explained in the text, where a significantly different (and far more proactive) mitigation strategy was brought to bear, which is apparently reflected in our results.

There are numerous technical issues and further possibilities to consider along this line of efforts. Backcasting can be implemented between other time series, e.g., between deaths and hospitalizations. A
relevant time series that has received considerable attention is that of “excess deaths”. This has been a traditional way to gauge the uncertainty around the death toll of exceptional events, such as the current pandemic [52] or extreme heat waves [14]. Excess deaths measure the deviation of the observed death toll from the expected death toll during a period of time, where the expected death toll is often a function (if not the direct average) of the death toll of the previous few years.

While this is an accurate measure of the overall impact of the pandemic, it takes into account increases or decreases in mortality due to other causes as well. Because of the disruptive nature of the pandemic, it is almost certain that the excess deaths seen are not all attributed to the virus itself: for example, the diversion of most medical resources to the care for COVID-19 patients, decreased their availability for the care of patients with other chronic illnesses or with non-COVID-19 acute symptoms. There are also countries that have not seen a rise in excess deaths despite confirmed deaths due to the coronavirus [23]. Australia and New Zealand recorded lower mortality than in recent years, which is attributed to social distancing measures that decreased mortality for reasons other than COVID-19, e.g., due to low incidence of seasonal flu. Uruguay and Norway, also reported negative excess deaths.

Trying to isolate true COVID-19 fatalities missed in the official numbers is a daunting (if not impossible) task, and that is acknowledged in the relevant literature as well [3]. Statistically, (and if we disregard the concerns of the above paragraph) we can perform regression between the observed and excess deaths to find what percent of deaths was missed. This is a process that must be done individually for each country, and its accuracy depends on the availability and quality of data sets, accumulated over several years.

An alternative method to quantify the magnitude of the true number of cases, which has been put in practice in various regions, is to monitor the viral load carried in sewer waste [41, 47]. It would be useful to examine the relevant correlations in subsequent waves vs. the measurements during the first wave. In a scenario where significant testing takes place (as, e.g., is the case in South Korea among our selected examples) or was subsequently developed, perhaps one can use the correlation between fatalities, symptomatic and asymptomatic cases, in order to infer the fractions of infections that stem from symptomatic vs. asymptomatic cases. This is an interesting aspect of such epidemiological models for which presently there is considerable uncertainty with very different asymptomatic fractions being reported in different studies [29].

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References

[1] H. D. I. Abarbanel and M. B. Kennel. Local false nearest neighbors and dynamical dimensions from observed chaotic data. *Physical Review E*, 47:3057–3068, 1993.

[2] C. Anastassopoulou, L. Russo, A. Tsaliris, and C. Siettos. Data-based analysis, modelling and forecasting of the COVID-19 outbreak. *PLoS ONE*, 15(3):e0230405, 2020.

[3] T. Beaney, J. M. Clarke, V. Jain, A. K. Golestaneh, G. Lyons, D. Salmon, and A. Majeeed. Excess mortality: the gold standard in measuring the impact of COVID-19 worldwide? *Journal of the Royal Society of Medicine*, 113(9):329–334, 2020.

[4] D. Bohning, I. Rocchetti, A. Maruotti, and H. Holling. Estimating the undetected infections in the COVID-19 outbreak by harnessing capture–recapture methods. *International Journal of Infectious Diseases*, 97:197–201, 2020.

[5] L. F. Buss, C. Prete Jr, C. M. M. Abraham, A. Mendrone Jr, T. Salomon, C. de Almeida-Neto, R. F. O. Franca, M. C. Belotti, M. P. S. S. Canvalho, A. G. Costa, M. A. E. Crispim, S. C. Ferreira, N. A. Fraili, S. Gurzenda, C. Whittaker, L. T. Kamaura, P. L. Takecian, P. da Silva Peixoto, M. K. Okawa, A. S. Sishiya, V. Rocha, N. A. Salles, A. de Souza Santos, M. A. da Silva, B. Custer, K. V. Parag, M. Barral-Netto, M. U. G. Kraemer, R. H. M. Pereira, O. G. Pybus, M. P. Busch, M. C. Castro, C. Dye, V. H. Nascimento, N. R. Faria, and E. Sabino. Three-quarters attack rate of SARS-CoV-2 in the Brazilian Amazon during a largely unmitigated epidemic. *Science*, 371:288–6292, 2021.

[6] Liangyue Cao. Practical method for determining the minimum embedding dimension of a scalar time series. *Physica D: Nonlinear Phenomena*, 110(1-2):43–50, 1997.

[7] M. C. Castro, S. Kim, L. Berberia, A. F. Ribeiro, S. Gurmenda, K. B. Ribeiro, E. Abbott, J. Blossom, B. Rache, and B. H. Singer. Spatiotemporal pattern of COVID-19 spread in Brazil. *Science*, 372:821–826, 2021.

[8] G. Ciminelli and S. Garcia-Mandico. COVID-19 in Italy: An analysis of death registry data. *Journal of Public Health*, 42(4):730–730, 2020.

[9] J. Cuevas-Maraver, P.G. Kevrekidis, Q.Y. Chen, G.A. Kevrekidis, Víctor Villalobos-Daniel, Z. Rapti, and Y. Drossinos. Lockdown measures and their impact on single- and two-age-structured epidemic model for the COVID-19 outbreak in Mexico. *Mathematical Biosciences*, 346:108590, 2021.

[10] E. R. Deyle and G. Sugihara. Generalized theorems for nonlinear state space reconstruction. *PLoS ONE*, 6(3):e18295, 2011.

[11] Ensheng Dong, Hongru Du, and Lauren Gardner. An interactive web-based dashboard to track COVID-19 in real time. *The Lancet infectious diseases*, 20(5):533–534, 2020.

[12] S. Flaxman, S. Mishra, A. Gandy, H. J. T. Unwin, T. A. Mellan, H. Coupland, C. Whittaker, H. Zhu, T. Berah, J. W. Eaton., M. Monod, Imperial College COVID-19 Response Team, A. C. Ghani, C. A. Donnelly, S. Riley, M.A.C. Vollmer, N.M. Ferguson, L. Okell, and S Bhatt. Estimating the effects of non-pharmaceutical interventions on COVID-19 in Europe. *Nature*, 584:257–261, 2020.

[13] Center for Disease Control and Prevention. Commercial laboratory seroprevalence surveys. https://www.cdc.gov/coronavirus/2019-ncov/cases-updates/commercial-lab-surveys.html.

[14] A. Fouillet, G. Rey, V. Wagner, K. Laaidi, P. Empereur-Bissonnet, A. Le Tertre, P. Frayssinet, P. Bessemoulin, F. Laurent, P. De Crouy-Chanel, E. Jougla, and D. Henmon. Has the impact of heat waves on mortality changed in France since the European heat wave of summer 2003? a study of the 2006 heat wave. *International Journal of Epidemiology*, 37:309–317, 2008.

[15] A. M. Fraser and H.L. Swinney. Independent coordinates for strange attractors from mutual information. *Physical Review A*, 33:1134–1140, 1986.

[16] William Gilpin. Deep reconstruction of strange attractors from time series. *arXiv preprint arXiv:2002.05909*, 2020.

[17] Iain H. Holmzahl and C. Buckee. Wrong but useful: what COVID-19 epidemiological models can and cannot tell us. *The New England Journal of Medicine*, 383(4):305–305, 2020.

[18] A. J. Ing, C. Cocks, and J. P. Green. COVID-19: in the footsteps of Ernest Shackleton. *Thorax*, 75:693–694, 2020.

[19] Lyndon P. James, Joshua A. Salomon, Caroline O. Buckee, and Nicolas A. Menzies. The use and misuse of mathematical modeling for infectious disease policymaking: Lessons for the COVID-19 pandemic. *Medical Decision Making*, 41(4):379–385, 2021. PMID: 35358899.

[20] N. James, M. Menzies, and P. Radchenko. COVID-19 second wave mortality in Europe and the United States. *Chaos*, 31:031105, 2021.

[21] C. Anastassopoulou, L. Russo, A. Tsaliris, and C. Siettos. Data-based analysis, modelling and forecasting of the COVID-19 outbreak. *PLoS ONE*, 15(3):e0230405, 2020.
COVID-19 complications among Massachusetts healthcare workers: a cohort study. *Pathogens and Global Health*, 115(1):4–6, 2021.

[28] Seungjoon Lee, Felix Dietrich, George E Karniadakis, and Ioannis G Kevrekidis. Linking Gaussian process regression with data-driven manifold embeddings for nonlinear data fusion. *Interface Focus*, 9(3):20180083, 2019.

[29] R. Li, S. Pei, B. Chen, Y. Song, T. Zhang, W. Yang, and J. Shaman. Substantial undocumented infections facilitates the rapid dissemination of novel coronavirus (SARS-CoV-2). *Science*, 368:489–493, 2020.

[30] Y. Liu, A. A. Gayle, A. Wilder-Smith, and Rocklov J. The reproduction number of COVID-19 is higher compared to SARS coronavirus. *Journal of Travel Medicine*, 2020.

[31] Y. Mammeri. A reaction-diffusion system to better comprehend the unlockdown: Application of SEIR-type model with diffusion to the spatial spread of COVID-19 in France. *Computational and Mathematical Biophysics*, 8:102–113, 2020.

[32] Manu Mannattil, Himanshu Gupta, and Sagar Chakraborty. Revisiting evidence of chaos in X-Ray light curves: The case of GRS 1915+105. *The Astrophysical Journal*, 833(2):208, dec 2016.

[33] Manu Mannattil, Ambirish Pandey, Mahendra K Verma, and Sagar Chakraborty. On the applicability of low-dimensional models for convective flow reversals at extreme Prandtl numbers. *The European Physical Journal B*, 90(12):1–9, 2017.

[34] E. Mathieu, H. Richie, E. Ortiz-Opsina, M. Roser, J. Hasell, C. Appel, C. Giattino, and L. Rodés-Guirao. A global database of COVID-19 vaccinations. *Nature Human Behaviour*, 2021.

[35] L. Noakes. The Talens embedding theorem. *International Journal of Bifurcation and Chaos*, 1(4):867–872, 1991.

[36] J. Oh, J.-K. Lee, D. Schwarz, H. L. Ratcliffe, J. F. Markins, and L. R. Hirschhorn. National response to COVID-19 in the Republic of Korea and lessons learned for other countries. *Health Systems and Reform*, 6:e1753464, 2020.

[37] R. Omori, K. Mizumoto, and G. Chowell. Changes in testing rates could mask the novel coronavirus disease (COVID-19) growth rate. *International Journal of Infectious Diseases*, 94:116–118, 2020.

[38] B. Paizao, L. Baroni, M. Pedroso, R. Sales, L. Escobar, R. de Sousa, C. and de Freitas Saldanha J. Soares, R. Coutinho, F. Porto, and E. Ogasawara. Substantial underestimation of SARS-CoV-2 infection in the United States. *New Generation Computing*, 2021.

[39] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

[40] M. Peirline, K. Linka, F. Sahli Costabal, J. Bhattacharya, E. Bendavid, J. A. P. Ioannidis, and E. Kuhl. Visualizing the invisible: The effect of asymptomatic transmission on the outbreak dynamics of COVID-19. *Computer Methods in Applied Mechanics and Engineering*, 2020.

[41] M. Petala, M. Kostoglou, Th. Karapantzos, C.I. Dovas, Th. Lytras, D. Praslevis, E. Roilides, A. Koutsoliotou-Senabakhi, G. Panagiotakopoulos, V. Syspa, S. Metallidis, A. Papa, E. Stylianidis, A. Papadopoulos, S. Tsiodras, and N. Papaioannou. Relating SARS-CoV-2 shedding rate in wastewater to daily positive tests data: A consistent model based approach. *Science of the Total Environment*, 807:150838, 2022.

[42] S. J. Phipps, R. Q. Grafton, and T. Kompas. Robust estimates of the true (population) infection rate for COVID-19: a backtracking approach. *Royal Society Open Science*, 7:200909, 2020.

[43] C. E. Rasmussen and C. K. I. Williams. Gaussian Processes for Machine Learning. In T. Dietterich, editor, *Adaptive Computation and Machine Learning*. MIT Press, 55 Hayward Street, Cambridge, MA 02142, 2006.

[44] T. W Russell, N. Golding, J. Hellewell, S. Abbott, L. Wright, C. A. B. Pearson, K. van Zandvoort, C. I. Jarvis, H. Gibbs, V. Liu, R. M. Eggo, W. J. Edmunds, A. J. Kucharski, and CMMID COVID-19 working group. Reconstructing the early global dynamics of under-ascertained COVID-19 cases and infections. *BMC Medicine*, 18:322, 2020.

[45] Pratha Sah, Meagan C. Fitzpatrick, Charlotte F. Zimmer, Elaheh Abdollahi, Lyndon Juden-Kelly, Seyed M. Moghadas, Burton H. Singer, and Alison P. Galvani. Asymptomatic SARS-CoV infection: A systematic review and meta-analysis. *Proceedings of the National Academy of Sciences (U.S.A).* 118(34):e2109229118, 2021.

[46] T. Sauer, J. A. Yorke, and M. Casdagli. Embedology. *Journal of Statistical Physics*, 61:181–221, 1990.

[47] L. C. Scott, A. Aubee, L. Babahaji, K. Vigil, S. Tims, and T. G. Aw. Targeted wastewater surveillance of SARS-CoV-2 on a university campus for COVID-19 outbreak detection and mitigation. *Environmental Research*, 200:111374, 2021.

[48] K. Stralin, E. Wahlstrom, S. Walther, A. M. Bennet-Bark, M. Heurgen, T. Lindén, J. Holm, and H. Hanberger. Mortality trends among hospitalised COVID-19 patients in Sweden: A nationwide observational cohort study. *The Lancet Regional Health-Europe*, 4:100054, 2021.

[49] F. Talens. Detecting strange attractors in turbulence. *Lecture Notes in Mathematics*, 808:366–381, 1980.

[50] G. Viceconte and N. Petrosillo. COVID-19 Bt: Magic number or conundrum? *Infectious Disease Reports*, 12:8516, 2020.

[51] A. Viguie, G. Lorenzo, F. Auricchio, D. Baroli, T. J. R. Hughes, A. Patton, A. Reali, T. E. Yankelov, and A. Veneziani. Simulating the spread of COVID-19 via a spatially-resolved susceptible–exposed–infected–recovered–deceased (SEIRD) model with heterogeneous diffusion. *Applied Mathematics Letters*, 111:106617, 2021.

[52] D. M. Weinberger, J. Chen, T. Cohen, F. W. Crawford, F. Mostashari, D. Olson, V. E. Pitzer, N. G. Reich, M. Russi, L. Simonsen, A. Watkins, and C. Viboud. Estimation of excess deaths associated with the COVID-19 pandemic in the United States, March to May 2020. *JAMA Internal Medicine*, 180(10):1336–1344, 2020.

[53] H. Whitney. Differentiable manifolds. *Annals of Mathematics*, 37:645–680, 1936.

[54] S. L. Wu, A. N. Mertens, Y. S. Crider, A. Nguyen, N. N. Pokpongkiet, S. Dajadji, A. Seth, M. S. Hsiang, A. Colford Jr., J. M.and Reingold, B. F. Arnold, A. Hubbard, and J. Benjamin-Chung. Substantial underestimation of SARS-CoV-2 infection in the United States. *Nature Communications*, 11:5407, 2020.

[55] daSum, Qianlin Lin, Jingyu Liu, Guangyu Yang, Weiming Wang, Yijun Lou, Daozouhao Gao, Lin Yang, Daihai He, et al. Preliminary estimation of the basic reproduction number of novel coronavirus (2019-nCoV) in China, from 2019 to 2020: A data-driven analysis in the early phase of the outbreak. *International journal of infectious diseases*, 2020.
92:214–217, 2020.
Appendix A. Data

Appendix A.1. Source and Quality

The data used in the Numerical Results, Section 3 in the main text, come from a single source for consistency. We use the publicly available data set by Our-World-In-Data (OWID)\(^3\) that aggregates information from other trustworthy sources (for confirmed cases and deaths the JHU database [11] is used, while hospitalizations are sourced from several government websites). This means that availability and quality of some data categories are different across countries (for example, Germany does not readily publish daily hospitalization data and Spain has days on which the reported cases are negative, functioning as adjustments to previous reports). In turn, comparisons between statistics across countries is not always possible, and even if it is, may not be trustworthy.

Due to these and related issues, our estimates are dependent on data quality and trustworthiness. To avoid large disparities in reporting strategies and healthcare we have focused on a few selected countries. Furthermore, we address data uncertainty in the following section.

The latest version of the data set used was downloaded on April 4, 2021. We consider data after the Spring of 2021 to correspond to a very different dynamical system, in which a large part of the population (of countries for which results are presented) almost discontinuously obtained immunity due to vaccine roll-out. Thus, we do not consider later data in this work.

Our model is centered around learning the relationship between diagnosed cases \((c_t)\) and reported fatalities \((d_t)\). Assuming that there is enough trustworthy information (past the selected \(T^*\)), we can extrapolate backwards to points in time where we do not believe the available information. However, even though COVID-19 monitoring has been improving continuously, it would be naïve to entirely trust even the most recent information. We therefore attempt to address uncertainties that may surround the two types of time series we work with.

Appendix A.2. Addressing Data Uncertainty

Our model is centered around learning the relationship between diagnosed cases \((c_t)\) and reported fatalities \((d_t)\). Assuming that there is enough trustworthy information (past the selected \(T^*\)), we can extrapolate backwards to points in time where we do not believe the available information. However, even though COVID-19 monitoring has been improving continuously, it would be naïve to entirely trust even the most recent information. We therefore attempt to address uncertainties that may surround the two types of time series we work with.

Appendix A.2.1. Reliability of Time Series

Of all the pandemic markers available to us, fatalities and hospitalizations are possibly the most reliable data sets, as we have also discussed at some length in earlier work [9]. Since the method developed in Section 2.1 (main text) is valid for arbitrary time series, as long as these two are coupled in the dynamical system, we can replace the role of the death time series \((D)\) by a hospitalization time series \((H)\), under the reasonable assumption that the number of hospitalized patients should also be an observable quantity of the pandemic.

In principle, one can use either time series (and any other similar observable, such as ICU admissions) to backcast the numbers of cases. This can be used as a tool to increase the certainty of a prediction by repeating the computational experiment using different time series. However, hospitalization data are less readily available world-wide, and for countries with low hospital capacity the time series may not be as predictive, since there is no way to quantify the severity of an outbreak solely on these records after capacity is reached; after that point, capacity saturation yields misleading results regarding the number of cases.

It is important to note that our estimates of the true case incidence include a mixture of symptomatic and asymptomatic cases. This is because early on tests were scarce and not available to the broader public, while

\(^3\)https://github.com/owid/covid-19-data
Appendix A.3. Hyperparameters

The hyperparameters needed to perform the relevant computations, i.e., parameters that control the learning process but do not necessarily have an interpretable physical meaning, can be split in two groups:

1. Those associated with the reconstruction of the diffeomorphic manifold (namely the embedding dimension $k$ and the delay time $\tau$).
2. Those given to the GP regressor (i.e., specifying the kernel).

In this section we explain how these hyperparameters are set and their relevance to physical quantities and characteristics of the observed data, where relevant.

(1) Embedding Parameters

$\tau$ is the delay time between subsequent observations of $d_t$ needed when performing the $M_D$ manifold reconstruction (Appendix C). It is meant to capture a natural variance that may occur in the dynamical system over a shorter time scale, and can be estimated using empirical methods (e.g., based on mutual information, as in [15]). However, because of the weekly fluctuation in our data (both in recorded cases and fatalities, which decrease substantially during the weekends), it is a priori natural to smoothen the data using a 7-day rolling average. This has the effect of making $\tau = 1$ day for all of our data sets which become mostly smooth, meaning that we can use sequential observations of $d_t$ when constructing $M_D$. Note that using the smoothed data is not a prerequisite for the proposed method.

The embedding dimension $k$ is the number of sequential observations of $d_t$ needed to reconstruct $M_D$, i.e., the dimension of $M_D$. It can be estimated using empirical algorithms such as False Nearest Neighbors (FNN) [1] and Average False Neighbors (AFN) [6]. This parameter need not be optimal: The theory presented in Section 2.1 (main text) guarantees that an embedding dimension of at most $2n+1$ is sufficient to embed in Euclidean space, where $n$ is the dimension of the original manifold. If $k^*$, the minimal embedding dimension, is sufficient, reconstructions using $k > k^*$ points will still be diffeomorphic to $M$ (in the absence of noise).

Still, it is important, that $n$ is small enough so that the available data are adequate for the reconstruction: e.g., for $n = 5$ we can take $k = 11$ and a point $d_t = \{d_{t-10}, ..., d_t\} \in M_d \subset \mathbb{R}^{11}$. Then we will require that $\hat{f}_{GP}(d_t) = c_t$ to be the cases at time $t$ (where $\hat{f}_{GP}$ is the transformation based on the GP estimator, see, also, Section 3.1). Thus, having a large $n$ corresponds to needing a longer time series to reconstruct the corresponding manifold. Furthermore, using a larger $k$ than necessary may lead to overfitting ([26], [16]).

We may refer to the embedding dimension as the "time-window" which defines the dimension of a point in $M_D$.

(2) Gaussian Process Parameters

Herein, we describe broadly a mathematical framework that justifies the use of regression to learn the relationship between observed cases of and deaths due to COVID-19, in contrast to other methods. We use Gaussian Process regression to obtain the transformation $\hat{f}_{GP}$. The choice of GP for regression is made because of the integrated uncertainty estimates the method offers.

The GP Kernel is the family of functions used to fit the data, and thereby obtain $\hat{f}_{GP}$. We use the Matérn (SM, B.3) kernel which is a generalization of the Radial Basis Function kernel (RBF) (SM, B.2). This choice is made empirically based on the characteristics of the data. For COVID-19 series we observe relatively smooth trajectories with no periodic features and some noise. (This would not be the case if the data were not smoothed a priori, as weekly periodicity in the un-smoothed data would warrant the addition of a periodic kernel). Though we only include results of another kernel (RBF) in Section 3.1, we consistently observe that the choice of kernel need not be unique, and the backcasting projection is mainly dependent on
the relationship between the observed data and not on the choice of kernel (assuming the latter is reasonable). For the equations and specific kernel parameters see Appendix A.

While we may use the terms “parameter” and “hyperparameter” interchangeably in this text, we note that their choice does not raise identifiability issues, since it is indeed possible to recover the same accuracy of a resulting estimator with different choices of hyperparameters, and parameter uniqueness is not required by the nature of our problem (the pandemic). This is in contrast to closed form ODE/PDE models in which the values of corresponding parameters are fundamentally significant in interpreting results of such a model [24, 31, 51].

Appendix B. Gaussian Processes

Gaussian process regression is a non-parametric and supervised learning methodology that can be used to make predictions and simultaneously quantify uncertainty. Prior knowledge about the system is encoded in the probability kernels used and regression is performed by specifying distributions over an infinite number of possible functions passing through the observation points.

A Gaussian process [43] is specified by its mean \( m \) and covariance \( k \) functions. If \( c = f(d) \) is the real process then:

\[
\begin{align*}
m(d_t) &= \mathbb{E}[f(d_t)] \\
k(d_t, d_{t'}) &= \mathbb{E}[f(d_t) - m(d_t)]\mathbb{E}[f(d_{t'}) - m(d_{t'})]
\end{align*}
\]

and

\[
f(d_t) \sim \mathcal{GP}(m(d_t), k(d_t, d_{t'}))
\] (B.1)

In the sklearn implementation of the method the covariance matrix specified by the kernel function \( k \) has a zero diagonal value, denoted by the parameter \( \alpha \). There are numerical advantages to having a nonzero such value which makes the matrix positive definite. In the results of Section 3 we use the default \( \alpha = 1e^{-10} \).

Overall we make use of two kernels: the Radial Basis Function Kernel (RBF) given by

\[
k_{\text{RBF}}(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2l^2}\right)
\] (B.2)

and the Matérn Kernel.

\[
k_M(x_i, x_j) = \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}}{l}\|x_i - x_j\|_2\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}}{l}\|x_i - x_j\|_2\right)
\] (B.3)

where \( l > 0 \) is a real-valued length scale parameter, \( \Gamma(\cdot) \) is the Gamma function, \( K_\nu(\cdot) \) is a modified Bessel function, and \( \nu \) is a parameter determining the smoothness of the kernel [39]. They were combined with a Constant Kernel and a White Noise Kernel to account for variance in the mean and possible small amounts of noise respectively. In the results of Section 3 only the Matérn kernel was used with \( \nu \) chosen to be 7/2. The remaining kernel hyperparameters are tuned during fitting by maximizing the log-marginal-likelihood using the L-BFGS algorithm. The implementation is performed entirely using Python’s sklearn library.

For a detailed presentation of Gaussian Process Regression see [43].
Appendix C. Embedding Theorems

The delay embedding theorems of Whitney and Takens guarantee that for any manifold \( S \subset \mathbb{R}^n \) parameterized by time, it is possible to construct a manifold \( S^* \) that is diffeomorphic to \( S \): there exists a differentiable bijective function \( f : S \rightarrow S^* \) such that its inverse is differentiable as well. The reconstruction can be achieved using the time series of a one-dimensional observable that is coupled to all components of the dynamical system. An upper bound on the embedding dimension \( k \) (number of delay observations of the one coordinate that is needed to construct \( S^* \)) is \( 2n + 1 \) (i.e. \( S^* \subset \mathbb{R}^{2n+1} \)).

These theorems are powerful and, in fact, suitable to address much more complicated problems, like chaotic dynamics. While in our problem we anticipate the dynamics to be much simpler, their appeal is their ability to uncover information about the system whose explicit dynamics are unknown, especially doing so through the use of a single observed variable (and its delays) as opposed to a larger number of observed quantities.

The Whitney embedding theorem [53] can be restated as

**Whitney Embedding Theorem, 1936** Any \( n \)-dimensional, differentiable (of class \( C^r \)) manifold \( M \) can be embedded in \( \mathbb{R}^{2n+1} \) through a \( C^r \) function.

Takens [49] focused on dynamical systems for which an observable exists and proved the following delay embedding theorem. Assume \( M \) is an \( n \)-dimensional compact manifold. Let \( X \) be a vector field on \( M \) and \( y : M \rightarrow \mathbb{R} \) be a smooth function (observable). Moreover, let \( \phi \) denote the flow of \( X \) on \( M \) (smooth diffeomorphism).

**Takens Delay Embedding Theorem, 1981** For pairs \((\phi, y)\), \( \phi : M \rightarrow M \), it is a generic property that the map \( \Phi_{(\phi, y)} : M \rightarrow \mathbb{R}^{2n+1} \) defined by

\[
\Phi_{(\phi, y)}(x) = (y(x), y(\phi(x)), \ldots, y(\phi^{2n}(x)))
\]  

is an embedding.

While the Takens theorem pertains to smooth attractors, it was later generalized to apply to attractors of any box-counting dimension [46]. Another generalization is for more than one observables [10].