

Outlier and Normality Testing of the Residuals for the Morgan-Mercer-Flodin (MMF) Model Used for Modelling the Total Number of COVID-19 Cases for Brazil

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ABSTRACT

Traditionally, testing for outliers is performed by first creating a null hypothesis, H_0 , indicating that the suspected results do not differ significantly from those of other members of the data set, and then rejecting it if the likelihood of getting the experimental results is extremely low (e.g., $p=0.05$). Similarly, if H_0 can be rejected, the questionable findings may be discarded as outliers as well. If H_0 is retained in the data set, it is important to keep the dubious findings in the data set. In general, in nonlinear regression, the residuals of the curve must be normally distributed before any test for the existence of outliers is performed. This is often accomplished through the use of normalcy tests such as the Kolmogorov-Smirnov, Wilks-Shapiro, D'Agostino-Pearson, and Grubb's tests, the latter of which checks for the presence of an outlier and is the subject of this study. Normality tests for residues used in general nonlinear regression revealed that the usage of the Morgan-Mercer-Flodin (MMF) Model used for Modelling the Total Number of COVID-19 Cases for Brazil was adequate due to lack of an outlier. The critical value of Z from statistical table for Grubbs' test for a single outlier using mean and SD was 0.114 ($n=50$). The Grubbs (Alpha = 0.05) g value was 3.597. Individual Z value indicates that the residual with a value of -3 (row 3) was far from the rest and is deemed a significant outlier ($p < 0.05$). This outlier was removed, and subsequent Grubb's test show the absence of other outliers. As the Grubbs' test require for the normality of the residuals, several normality tests (Kolmogorov-Smirnov, Wilks-Shapiro, Anderson-Darling and the D'Agostino-Pearson omnibus K_2 test) were carried out and the results were found to conform to normality. In addition, a visual inspection of the model's normal probability or Q-Q plot shows a nearly straight and appeared to exhibit no underlying pattern. The resulting histogram overlaid with the ensuing normal distribution curve also reveals that the residuals were truly random and that the model used was adequately fitted.

INTRODUCTION

According to the World Health Organization (WHO), the COVID-19 pandemic is a worldwide coronavirus disease 2019 (COVID-19) pandemic caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) that was announced by the WHO in March 2020. The new virus was identified in Wuhan, China, in December of 2019; a lockdown in Wuhan and other towns in Hubei province failed to stop the epidemic, which expanded to

other parts of mainland China and throughout the world after the outbreak was detected. The outbreak was declared a Public Health Emergency of International Concern by the World Health Organization (WHO) on January 30, 2020, and a pandemic was proclaimed on March 11, 2020. The virus has been causing outbreaks in a number of countries since 2021, with the most hazardous strains being the Delta, Alpha, and Beta variants, which are the most common. As of the 22nd of July, 2021, more than 191 million cases have been documented, with more than 4.12 million

confirmed deaths due to COVID-19, making it one of the deadliest pandemics in history [1,1–5]. People are becoming increasingly conscious of the uneven distribution of SARS-COV-2 mortality among disadvantaged communities as the death toll from COVID-19 continues to rise around the world. In addition to the elderly, individuals who live in densely crowded regions, persons who have poor socioeconomic position, refugees, and members of minority groups should be taken into consideration. Almost every community is in risk of being annihilated. The infection rates in these populations are higher than those in the general population, making them more susceptible to infection and unfavourable disease effects than other groups [6,7].

In the initial period, mathematical modelling research in Wuhan City and Hubei Province total infectious cases was focused on the dynamics of the pandemic[8]. At this early stage, it has taken a significant amount of time and effort to examine surveillance data from China in order to produce parameter estimates such as the basic reproduction number (R0), case fatality rate, and incubation duration [9]. Early attempts at Susceptible-Exposed-Infectious-Recovered (SEIR) style dynamic models were 'borrowed' from what was known about other coronaviruses (SARS-CoV and MERS-CoV) and/or gained through fitting the models to monitoring data gathered during the initial outbreaks [10]. COVID-19 pandemic assessments can be carried out with the help of statistical models, including theoretical, quantitative, and simulation models. Mathematical models are then applied for other affected countries to better understand the mode and spread of infection [1,4,11–18].

Organisms growth including viral infection cases over time usually exhibit a sigmoidal growth profile that exhibits lag time (λ), acceleration to a maximal value (μ_m) and a final phase where the rate decreases and eventually reaches zero or an asymptote (A) is observed [19]. The sigmoidal curve can be fitted by different mathematical functions, such as Logistic [19,20], modified Gompertz [19,21], Richards [19,22], Schnute [19,23], Baranyi-Roberts [24], Von Bertalanffy [19,25–27], Buchanan three-phase [28,29], Huang [30–33] and Morgan-Mercer-Flodin (MMF) [34–43, 43–47]. For the analysis of the COVID-19 pandemic [8], strong predictive ability was employed models, such as updated Gompertz and Bertalanffy and logistics. The total infection case of SARS-CoV-2 in Brazil as of 15th of July 2020 to the 20th of December 2020 was modelled using several primary growth models via nonlinear regression. The MMF models found to be the best [41,42,44,46,48–51].

When linearization is used to smooth out an obviously nonlinear curve, the error structure of the data is disturbed, as is the case in this example. As a result, evaluating the uncertainty of the kinetic parameters, which are often given as a 95 percent confidence interval range, becomes more difficult. In addition, the linearization method leads in the introduction of error into the independent variable as a result of the linearization procedure [52–57]. Additionally, changes in the weights assigned to each data point can occur, which typically results in differences in the fitted parameter values between the linear and nonlinear versions of the kinetics model when compared to the linear version. Nonetheless, in nonlinear regression, the residuals of the curve must be normally distributed, and the residuals must be checked for the presence of outliers [at 95 or 99 percent confidence levels]. In most cases, normality tests such as the Kolmogorov-Smirnov, Wilks-Shapiro, and D'Agostino-Pearson, as well as the Grubb's test, which tests for the presence of an outlier, are used to do this. The Grubb's test is the subject of this study because it tests for the presence of an outlier.

METHOD

Data on the mathematical modelling of the total number of COVID-19 cases for Brazil using the MMF model (Equation 1) from our previous works [43] was utilized in this study (Fig. 6).

Residuals

Residuals are very important in assessing the health of a curve from a particular used model. Mathematically, residual for the i^{th} observation in a given data set can be defined as follows (Eqn. 1);

$$e_i = y_i - f(x_i; \hat{\beta}) \dots \dots \dots \text{(Eqn. 1)}$$

where y_i denotes the i^{th} response from a given data set while x_i is the vector of explanatory variables to each set at the i^{th} observation corresponding values in the data set.

Grubbs' Statistic

In an average value, a single data point with deformation can lead to gross error in the fitting of a nonlinear curve. Therefore, searching for an outlier is an integral aspect of curve fitting. The Grubbs test is used to evaluate the outlier in the univariate environment and the data is normally distributed [58]. The test can be applied to the maximal or minimal observed data from a Student's t distribution (Eqn. 2) and to test for both data simultaneously (Eqn. 3).

$$G_{\min} = \frac{\bar{X} - \min(X)}{s} \qquad G_{\max} = \frac{\max(X) - \bar{X}}{s} \qquad \text{(Eqn. 2)}$$

$$p_G = 2n \cdot p_t \left(G \frac{\sqrt{n(n-2)}}{n-1}, n-2, 1 \right) \qquad G_{\text{all}} = \frac{\max(\bar{X} - \min(X), \max(X) - \bar{X})}{s} \qquad p_G = n \cdot p_t \left(G \frac{\sqrt{n(n-2)}}{n-1}, n-2, 2 \right) \qquad \text{(Eqn. 3)}$$

Normality test

Residuals from the pseudo-1st order model were subjected to three normality tests- Kolmogorov-Smirnov [59,60], Wilks-Shapiro [61], Anderson-Darling [62] and the D'Agostino-Pearson omnibus K2 test [63]. Using graphical and numerical methods are two ways to search for normality. The simplest and easiest way to assess the normality of data is via graphical methods such as the normal quantile-quantile (Q-Q) plots, histograms or box plots [64]. The normality tests were carried out using the GraphPad Prism® software (Version 6.0, GraphPad Software, Inc., USA).

RESULTS AND DISCUSSION

Statistics often used in nonlinear regressions rely on the use of residual data, which is the difference between the expected and the actual values. Statistical analyses should be done to evaluate the adequacy of residues in randomness, do not include outliers, obey normality, and do not demonstrate autocorrelation. Usually, the greater the discrepancy between the expected and the observable values, the less well off the model. [65]. The Grubbs' test deals with one aspect at a time. Outliers are eliminated and test replicated before test passes without revealing any outliers. As a general rule, sample sizes of 6 or less results in biased data sets. Many variations of the same model alter the probability of

A simple strategy to identify potential outliers in testing is to include a boxplot, although more complex methodologies, such as the Chauvenet criteria in engineering and the 3-sigma criterion, coupled with the Z-score in chemometrics, are frequently employed. Despite the fact that these approaches are simple and quick, there is a considerably more effective way of employing the statistical test for outlier discovery than the methods described above. With the exception of one outlier, relevant assessments differ from the Dixon Q-test or the Grubbs ESD-test.

A variety of conditions have benefitted from the use of the Grubbs test to detect the presence of outliers [67–77]. The most significant restriction of the Grubbs test is that the thinking quantity of the outliers, denoted by the letter k, must be given explicitly. A failure to properly clarify the variable "k" can result in distorted results from the trials. A test called the Rosner Generalized Severe Studentized Deviate (ESD-test) is used when there are several outliers or when the exact number of outliers cannot be determined [78]. For example, if there is more than one outlier in a sample, the findings of the Grubbs test will be distorted, and when this occurs, the Ferguson sample skew test is more resistant to the misleading impact than the Grubbs test [79].

The number of bins and samples assessed determined the shape of the distribution. The W_2 statistic in the Wilks-Shapiro test is calculated using the anticipated values of the order statistics between identically distributed random variables as well as their independent covariance, as well as the regular normal distribution. The agreement is refused if the test statistics- W_2 have a significant impact on the outcome. According to Royston, formalised euphemism is The Kolmogorov-Smirnov statistic, when applied to data, computes the cumulative residual frequency, which is a non-parametric numerical test [61]. It evaluates the link between the model and the observed values. It can also be used to compare two sets of data to see how they differ. The p value is derived using the difference between two combined distributions as well as the sample population size.

On a more general level, the Central Limit Theorem (CLT) claims that as n approaches infinite (in actuality, $n > 30$), the probability frequency distribution tends to fit the Gaussian distribution on any continuous variable (even for discrete variables such as Binomial or Poisson distributions) [80,81]. The skewness and kurtosis of the distributions were analysed as a technique of quantifying the difference between the sample distributions and the usual distribution in order to determine the significance of the results in the D'Agostino-Pearson normality test method. Following that, the p-value of the sum of these inconsistencies or discrepancies is calculated. D'Agostino developed a variety of normality tests, the most extensively used of which is the omnibus K_2 test [63]. More and more nonlinear regression curve fitting exercise works are reporting an extensive testing for the normality of the residuals [82–90].

Graphical diagnostic of residuals normality

After removal of the outlier, the model's normal probability or Q-Q plot was nearly straight and appeared to exhibit no underlying pattern (Fig. 4). The resulting histogram (Fig. 5) overlaid with the ensuing normal distribution curve reveals that the residuals were truly random and that the model used was adequately fitted.

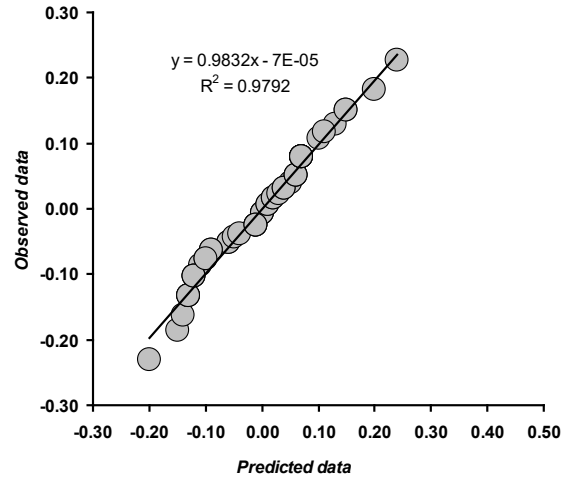


Fig 4. Normal Q-Q plot for the observed sample against theoretical quantiles after outlier removal.

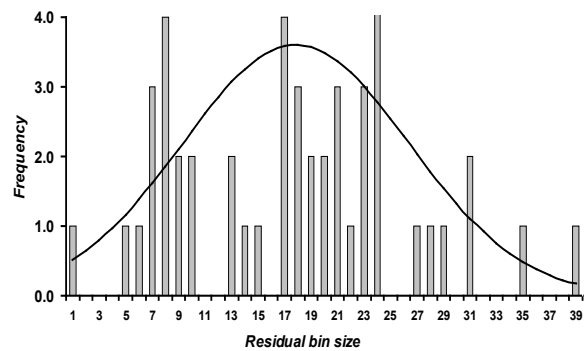


Fig 5. Histogram of residual for the pseudo-1st order model overlaid with a normal distribution (mean 0.00163 and standard deviation 0.0984).

CONCLUSION

In conclusion, the normality checks performed on the residues used in this study revealed that the use of the pseudo-1st order model in the fitting of Modelling the Total Number of COVID-19 Cases for Brazil was satisfactory due to the absence of an outlier, indicating that the model was appropriate for the data. Many studies on the application of the model used in the mathematical diagnostic of residues have been published, but it is widely known that they have not gone any farther in their exploration. In the case of a Gaussian or regular distribution, this may result in a data violation. Most of the parametric predictive estimate approaches used in nonlinear regression rely on this assumption as a necessary but not sufficient condition. On the basis of residuals that adhere to the normal distribution, methods such as the root mean square error, Pearson correlation coefficient (either standard or modified), the F-test, and the t-test are used. Type I and Type II mistakes might be avoided if these assumptions were followed. Additionally, in the event that diagnostic tests reveal that the data from the total number of COVID-19 Cases have violated any of the assumptions, the issue may be rectified in the field by implementing numerous nonparametric treatments or changing the form of the therapies in question.

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