Direct estimation of SIR model parameters through second-order finite differences

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SIR model is widely used for modeling the infectious diseases. This is a system of ordinary differential equations (ODEs). The numbers of susceptible, infectious, or immunized individuals are the compartments in these equations and change in time. Two parameters are the factor of differentiating these models. Here, we are not interested in solving the ODEs describing a certain SIR model. Given the observed data, we try to estimate the parameters that determine the model. For this, we propose a least squares approach using second-order centered differences for replacing the derivatives appeared in the ODEs. Then we arrive at a simple linear system that can be solved explicitly and furnish the approximations of the parameters. Numerical results over various artificial data verify the simplicity and accuracy of the new method.

KEYWORDS
COVID-19, finite differences, least squares, SIR epidemic model

MSC CLASSIFICATION
92C60; 65L12; 65F20

1 INTRODUCTION

The epidemic SIR model was introduced with the pioneering work by Kermack and McKendrick.\textsuperscript{1} In the classical model, we assume as follows:

- We neglect the populations’ age structure, inhomogeneities, and group behavior.
- We divide the population into the three homogeneous sections: the susceptible people $s$, the infectious people $i$, and recovered people $r$. To explain that the number of susceptible, infectious, and removed persons differ over time (even though the total size of the population remains constant), we represent the exact numbers as function of time $t$, namely, $s(t)$, $i(t)$, and $r(t)$.
- We ignore births and deaths within the population. Thus, the population size $N$ is constant in time $t$, that is, $N = s(t) + i(t) + r(t)$. 

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Then SIR system can be expressed by the following set of ordinary differential equations:

\[
\frac{ds(t)}{dt} = -\frac{\beta}{N} \cdot i(t)s(t), \quad \frac{di(t)}{dt} = \frac{\beta}{N} \cdot i(t)s(t) - \gamma \cdot i(t), \quad \frac{dr(t)}{dt} = \gamma \cdot i(t).
\]  

(1)

The parameter \(\beta\) is the transmission rate, while \(\gamma\) is the recovery rate. Notice that

\[
\frac{ds(t)}{dt} + \frac{di(t)}{dt} + \frac{dr(t)}{dt} = 0,
\]

and consequently,

\[
s(t) + i(t) + r(t) = N = s(0) + i(0) + r(0).
\]

SIR model as well as many others derived from it (e.g., SIS, SIRD, MSIR, SEIR, SEIS, MSEIR, MSEIRS, and SIR with vaccination) fall in the general category of quadratic ODEs.

2 | FINITE DIFFERENCES

We are given a real function, say \(f(t)\). We also know various values of \(f\) at distinct points, \(t_1 < t_2 < \ldots < t_n\). We name for simplicity \(f_1 = f(t_1), f_2 = f(t_2),\) and so forth.

Finite differences answer the question of approximating the derivatives of \(f\) at various points \(t_k \in [t_1, t_n]\); for example, by the so-called “backward differences,” we get

\[
f'(t_k) \approx f'_{(t_k+1)} = \frac{f(t_{k+1}) - f(t_k)}{t_{k+1} - t_k} = f'_k.
\]  

(2)

As long as \(t_{k+1}\) tends to \(t_k\), the above expression approximates the true value of \(f'(t_k)\) better. This comes for the very definition of derivative since

\[
f'(t_k) = \lim_{t_{k+1} \to t_k} \frac{f(t_{k+1}) - f(t_k)}{t_{k+1} - t_k}.
\]

We concentrate in the case of equidistant points; that is, \(h = t_2 - t_1 = t_3 - t_2 = \ldots\). Then we have considerable simplifications and derive various approximations, for example,

\[
f'_k = \frac{f_{k+1} - f_k}{h}, \quad f''_k = \frac{f_{k+1} - 2f_k + f_{k-1}}{h^2},
\]  

(3)

or even

\[
f''_k = \frac{\frac{1}{12} f_{k-2} - \frac{2}{5} f_{k-1} + \frac{2}{3} f_{k+1} - \frac{1}{12} f_{k+2}}{h}.
\]  

(4)

All these expressions can be verified through Taylor expansions. Thus

\[
f'_k - f'(t_k) = \frac{1}{2} f''(t_k)h^1 + O(h^2),
\]

and approximation (2) is said to be of first order.

For (3), we have

\[
f' k - f'(t_k) = \frac{1}{k+1} f'''(t_k)h^2 + O(h^3),
\]

and we get a second-order approximation.

Finally for (4), we have

\[
f'' k - f''(t_k) = \frac{1}{30} f^{(4)}(t_k)h^4 + O(h^5),
\]

and this is a fourth-order difference. Differences (3) and (4) fall in the special class of the “centered differences.”

Here, we focus on differences (2) and (3). We will use them in order to approximate \(\beta\) and \(\gamma\) from (1) after we are given values at various points.
3 | EXTRACTING FORMULAS FOR THE PARAMETERS

We proceed setting $h = 1$. If $t_1 = 0$, then we have $s_1 = s(0), s_2 = s(1), s_3 = s(2), \ldots, i_1 = i(0), i_2 = i(1), \ldots$, and so forth. Of course we may begin with $t_1 = 100$ and adjust the various values; that is, $s_1 = s(100), s_2 = s(101)$, and so forth.

3.1 | First-order backward differences

In the sense of least squares, we approximate the three derivatives in (1) with first-order backward differences and set the following sum:

$$l = \sum_{j=1}^{n-1} \left\{ \left( s_{j+1} - s_j + \frac{\beta}{N} i_{j+1} s_{j+1} \right)^2 + \left( i_{j+1} - i_j - \frac{\beta}{N} i_{j+1} s_{j+1} + \gamma \cdot i_{j+1} \right)^2 + \left( r_{j+1} - r_j - \gamma \cdot i_{j+1} \right)^2 \right\}$$

We are interested in minimizing $l$ with respect to the parameters $\beta$ and $\gamma$. Thus, we differentiate and arrive at

$$\frac{\partial l}{\partial \beta} = \frac{4}{n^2} \sum_{j=2}^{n-1} i_j^2 s_j - \frac{2}{n} \sum_{j=2}^{n-1} i_j s_j \sum_{j=2}^{n-1} i_j \sum_{j=2}^{n-1} \left( i_{j-1} i_j s_j - i_j s_{j-1} s_j - i_j^2 s_j + i_j s_j^2 \right) = 0,$$

$$\frac{\partial l}{\partial \gamma} = -\frac{2}{n} \beta \sum_{j=2}^{n-1} i_j^2 s_j + 4 \gamma \sum_{j=2}^{n-1} i_j^2 - 2 \sum_{j=2}^{n-1} \left( i_j i_{j+1} - i_{j+1} r_j + i_{j+1} r_{j+1} \right) = 0.$$

This is a simple linear system with two equations. We solve it explicitly for

$$\beta = \frac{-\frac{8}{n} \sum_{j=2}^{n-1} \left( i_{j-1} i_j s_j - i_j s_{j-1} s_j - i_j^2 s_j + i_j s_j^2 \right) \cdot \sum_{j=2}^{n-1} i_j^2}{16 \frac{n^2}{n} \sum_{j=2}^{n-1} i_j^2 s_j \cdot \sum_{j=2}^{n-1} i_j^2 - 4 \left( \sum_{j=2}^{n-1} i_j^2 s_j \right)^2},$$

and

$$\gamma = \frac{\frac{8}{n^2} \sum_{j=2}^{n-1} i_j^2 s_j \cdot \sum_{j=2}^{n-1} \left( i_{j-1} i_j s_j - i_{j-1} s_j - i_{j+1} r_j + i_{j+1} r_{j+1} \right)}{16 \frac{n^2}{n} \sum_{j=2}^{n-1} i_j^2 s_j \cdot \sum_{j=2}^{n-1} i_j^2 - 4 \left( \sum_{j=2}^{n-1} i_j^2 s_j \right)^2}.$$

In order to avoid problems in denominator, the following expression

$$\left| \frac{4 \sum_{j=2}^{n-1} i_j^2 s_j \cdot \sum_{j=2}^{n-1} i_j^2 - \left( \sum_{j=2}^{n-1} i_j^2 s_j \right)^2}{4 \sum_{j=2}^{n-1} i_j^2 s_j \cdot \sum_{j=2}^{n-1} i_j^2} \right|^2$$

has to be far enough from zero.

3.2 | Second-order differences

Now, we may proceed using second-order centered differences and construct the sum.

$$l = \sum_{j=2}^{n-1} \left\{ \left( \frac{s_{j+1} - s_{j-1}}{2} \right)^2 + \left( \frac{i_{j+1} - i_{j-1}}{2} - \frac{\beta}{N} i_j s_j + \gamma \cdot i_j \right)^2 + \left( \frac{r_{j+1} - r_{j-1}}{2} - \gamma \cdot i_j \right)^2 \right\}$$
Differentiating, we get

\[
\frac{\partial l}{\partial \beta} = \frac{4}{n^2} \beta \sum_{j=2}^{n-1} j^2 s_j^2 - \frac{2}{n} \gamma \sum_{j=2}^{n-1} j^2 s_j + \frac{1}{n} \sum_{j=2}^{n-1} (i_{j-1} s_{j-1} - i_j s_{j-1} s_j + i_j s_{j+1} s_j) = 0, \\
\frac{\partial l}{\partial \gamma} = -\frac{2}{n} \beta \sum_{j=2}^{n-1} j^2 s_j + 4\gamma \sum_{j=2}^{n-1} j^2 - \sum_{j=2}^{n-1} (i_j r_{j+1} - i_j r_{j-1}) - i_1 t_2 + i_{n-1} t_n = 0.
\]

Again, this simple system has a unique solution

\[
\beta = \frac{-\frac{4}{n} \sum_{j=2}^{n-1} (i_{j-1} s_{j-1} - i_j s_{j-1} s_j + i_j s_{j+1} s_j) \cdot \sum_{j=2}^{n-1} j^2}{\frac{16}{n^2} \sum_{j=2}^{n-1} j^2 s_j^2 \cdot \sum_{j=2}^{n-1} j^2 - \frac{4}{n^2} \left( \sum_{j=2}^{n-1} j^2 s_j \right)^2}, \\
\gamma = \frac{-\frac{2}{n} \beta \sum_{j=2}^{n-1} j^2 s_j \sum_{j=2}^{n-1} \left( i_{j-1} s_{j-1} - i_j s_{j-1} s_j - i_j s_{j-1} s_j + i_{j+1} s_{j+1} s_j \right)}{\frac{16}{n^2} \sum_{j=2}^{n-1} j^2 s_j^2 \cdot \sum_{j=2}^{n-1} j^2 - \frac{4}{n^2} \left( \sum_{j=2}^{n-1} j^2 s_j \right)^2}. 
\]

For this case, using the same length of data, we get a better approximation of the parameters at no extra cost. Restriction (5) holds for this case too.

### 3.3 Parameters varying with time

When dealing with real data, we experience parameters varying with time. Thus, we actually have also corresponding series $\beta_j$ and $\gamma_j$ instead of constants $\beta$ and $\gamma$ through the whole interval of integration of (1). A way to circumvent this phenomenon is to continuously recalculate the parameters based only on some of the past data.

### 4 Numerical Tests

Runge–Kutta pairs are widely used for addressing IVPs. In consequence are ideal for use in SIR models. Here, we will test the two approaches over some artificially produced data. These data were taken after solving numerically (1) for some fixed values of the parameters. There are various methods for this numerical approximations. Runge–Kutta pairs are the most common ones. Especially the pair given in Tsitouras is accompanied with a dense output formula. Thus, we may get solutions at any point we wish. We are interested in getting solutions at integer points, $t_1 = 0, t_2 = 1, t_3 = 2, \ldots$.
We will use MATLAB\textsuperscript{8} for performing our tests. There we may find function \texttt{ode45} that implements the celebrated Runge–Kutta pair given in Dormand and Prince.\textsuperscript{9} Solution at distinct points is available when using \texttt{ode45}.

\subsection*{4.1 First set}

We choose $\beta = 0.25$ and $\gamma = 0.1$ with initial conditions $s_1 = s(t_1) = s(0) = 999$, $i_1 = i(0) = 1$, and $r_1 = r(0) = 0$. Then we get the values of $s$, $i$, and $r$ for $t_2$, $t_3$, $t_4$, $t_5$, and $t_6$, by the following lines in the command window of MATLAB.

\begin{verbatim}
>> beta = 0.25; gamma = 0.1; n = 1000;
>> fcn = @(x,y) [-beta*y(1)*y(2)/n; beta*y(1)*y(2)/n - gamma*y(2); gamma*y(2)];
>> [tout, yout] = ode45(fcn, (0:1:6)', [999 1 0]);
\end{verbatim}

\noindent \texttt{yout} contains three columns where the values for $s$, $i$, and $r$ are placed, respectively. Thus, we have

\begin{align*}
  s_1 &= s(0) = 999.0000, \quad s_2 = s(1) = 998.7306, \quad s_3 = s(2) = 998.4178, \\
  s_4 &= s(3) = 998.0547, \quad s_5 = s(4) = 997.6332, \quad s_6 = s(5) = 997.1439, \\
  s_7 &= s(6) = 996.5762, \\
  i_1 &= i(0) = 1.0000, \quad i_2 = i(1) = 1.1615, \quad i_3 = i(2) = 1.3490, \quad i_4 = i(3) = 1.5666, \\
  i_5 &= i(4) = 1.8192, \quad i_6 = i(5) = 2.1122, \quad i_7 = i(6) = 2.4521, \\
  r_1 &= r(0) = 0, \quad r_2 = r(1) = 0.1079, \quad r_3 = r(2) = 0.2332, \quad r_4 = r(3) = 0.3787, \\
  r_5 &= r(4) = 0.5477, \quad r_6 = r(5) = 0.7439, \quad r_7 = r(6) = 0.9717.
\end{align*}

Then we may use the function given in Appendix A for estimating $\beta$ and $\gamma$.

\begin{verbatim}
>> [b, g] = sir([999.0000 998.7306 998.4178 998.0547 997.6332 997.1439 996.5762],...
   [1.0000 1.1615 1.3490 1.5666 1.8192 2.1122 2.4521],...
   [0 0.1079 0.2332 0.3787 0.5477 0.7439 0.9717])
\end{verbatim}

\noindent \texttt{b} =

\begin{verbatim}
0.2509
\end{verbatim}

\noindent \texttt{g} =

\begin{verbatim}
0.1004
\end{verbatim}

We observe an error in the fourth decimal place.

Using the backward differences approach, we get $\beta = 0.2323$ and $\gamma = 0.0929$, which is a rather worse result since the errors are present in second decimal digit.

\subsection*{4.2 Second set}

We proceed with the same problem as above. After solving for $t \in [0, 60]$, we get the following results:

\begin{verbatim}
t   s     i     r
-   -     -     -
50  371.1083 232.7817 396.1100
51  350.2012 230.5229 419.2759
52  330.7208 227.1286 442.1507
53  312.6500 222.7176 464.6323
54  295.9431 217.4256 486.6313
55  280.5250 211.4041 508.0708
56  266.3082 204.8103 528.8815
57  253.2516 197.7514 548.9970
58  241.2734 190.3401 568.3865
59  230.2902 182.6820 587.0278
\end{verbatim}
Then we may confirm error at only fourth decimal digit.

$$\beta = 0.2598 \quad \text{and} \quad \gamma = 0.1012; \text{ that is, the error is about } 10^{-2}.$$

### 4.3 Third set

We choose $\beta = 0.1$ and $\gamma = 0.09$ with initial conditions $s_1 = s(t_1) = s(0) = 99$, $i_1 = i(0) = 1$, and $r_1 = r(0) = 0$. Then we integrate in the interval $t \in [0, 100]$ and get output at the integer points by typing the following lines in the command window of MATLAB.

```matlab
>> [b,g]=sir(s,i,r)
b =
0.2499
g =
0.0999
```

Again, using backward differences approach, we get $\beta = 0.1001$ and $\gamma = 0.0901$; that is, the error is about $10^{-4}$. Again the second-order centered differences offered two more digits of accuracy.

### 4.4 Fourth set: Real data for COVID-19

The U.S. time-series data of confirmed, recovered, and death cases were retrieved from COVID-19 time series for US. There we may find information on a daily basis at GMT 0:00, converted to a CSV format. We used approximately $N = 3.31 \times 10^8$. Small fluctuations of $N$ affect extremely slightly the outcome. The produced series of $\beta_j$ and $\gamma_j$ were based each time in the previous 14 observations (days). The number of cases reduces at weekends. Thus, a multiplier of seven is a good choice. An important quantity, called reproduction number at time $j$ and given as

![FIGURE 1](R_0 for the United States from 23 June 2020 to 21 September 2020 using a 14-day window [Colour figure can be viewed at wileyonlinelibrary.com])
is plotted in Figure 1 for the last 90 days (i.e., 23 June–20 September 2020). There we observe a maximum value at the end of June, and since, then we have a declining.

The number of cases should be as accurate as possible. Using 14 days backwards (or more) smooths the data. However, there are countries that they report recovered cases every 1–2 months! Then it’s impossible to apply this model.

Another issue in this case is the number of days to be used. In Figure 2, we present again $R_0$ for the U.S. data, but now, $\beta_j$ and $\gamma_j$ were based each time in the previous 21 days. We observe almost the same behavior. But the latter implementation is showing a little slower reaction. Smoothing the data before entering them in the model could be another treatment for this case.

5 | CONCLUSION

We presented a method for explicitly estimating the two parameters appearing in the classical SIR model. Having at hand the values $s, i,$ and $r$ at distinct points, we form a least squares sum after replacing the derivatives with centered differences. This sum is quadratic in the parameters. Thus, we may directly get formulas for the parameters since the minimization of the least squares sum concludes to a linear system of two equations.

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CONFLICT OF INTEREST

This work does not have any conflicts of interest.

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APPENDIX A

The MATLAB function `sir` implements the centered differences approach. $b$ stands for $\beta$, and $g$ stands for $\gamma$. This is as simplified as it can be. Thus, no checks or other issues were included. The readers have to take care themselves on the length of the inputs, the solvability of the data, and so forth.

```matlab
function [b, g] = sir(s, i, r);
    n = s(1) + i(1) + r(1);
    le = length(s);
    ss = s(2:le-1);
    ii = i(2:le-1);
    rr = r(2:le-1);
    mat = [4/n^2*sum((ii.^2).*ss.^2), -2/n*sum(ii.^2).*ss; ... 
           -2/n*sum(ii.^2)*ss, 4*sum(ii.^2)];
    cons = [1/n*sum(ii(1:le-2).*ss) - 1/n*sum(ii.*i(3:le).*ss) ... 
            -1/n*sum(ii.*s(1:le-2).*ss) + 1/n*sum(ii.*ss.*i(3:le));
            -sum(ii.*r(3:le)) + sum(ii.*r(1:le-2)) - i(1)*i(2) + i(1)*i(1)];
    res = mat \ cons; b = res(1); g = res(2);
    return
```