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Explicit Representation of Periodic Solutions and Parameter Estimation Problem of Predator-Prey System

Jehan Mohammed Khudhir

Department of Mathematics, College of Science, University of Basrah, Basrah, Iraq.

Email: jehan.khudhir@uobasrah.edu.iq

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1-Introduction

Many Mathematical methods for solving parameter estimation problems have been developed over the date, such that splines [24], sensitivity functions [18], adaptive observers [4], [21], [14] and [15] and shooting methods [5]. All these methods simulate modelled trajectories or state variables to fit empirical data. Particularly, however, it is difficult to apply such methods because of many issues include the issue of the necessity to access derivatives of the state variable of models, nonlinear parametrization, slow convergence, unwell conditioned problems, etc [2]. Many active mathematical researches for decades [11], [12] and [13] are related to state and parameter estimation of linear and nonlinear equations especially the research area of using the adaptive observer systems. Adaptive observers provide an estimation of the initial values of state variables and the unknown (constant) parameters of system of equations.

ABSTRACT

It is known that some dynamical systems have not analytical solution which is impossible or sometime difficult to find. In fact, undertaking a manual simulation or using complicated methods (need to find derivatives such that Newton method) of such systems is a difficult task due to the complexity of the computations. Therefore, a computerized simulation is frequently required to find accurate results in fast execution time especially for solving biological problems like Predator Prey model. This paper aims to find integral representation solutions for Predator Prey model using the new method proposed by Mohammed, J. & Tyukin, I in [16]. These integral representation solutions are periodic and depend on parameters of the Predator Prey model explicitly, then, however, it requires to estimate these parameters. Application of the method to solve parameter estimation problem of predator–prey model is illustrated in details with constructing the solutions for state and parameter estimation.

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^{*}Corresponding author : Jehan Mohammed Khudhir

Email addresses: jehan.khudhir@uobasrah.edu.iq

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Predator-prey model is one of the active systems from the interaction life in ecology and evolutionary biology which has been extensively studied by many researchers over the last few decades, for example [3],[9] and [23]. Mathematical models have played an important role in understanding the complex scenarios of such problems. Most of the predator-prey models are usually assumed that the predators impact the population of prey through direct killing or, however, predator presence may change the behavior of prey which could affect the prey population more than direct predation [19] and [7]. A simple example could be the changes of predation [22], [10] and [25]:

$$\dot{x} = \beta_1 x - \frac{\beta_1 x^2}{\beta_2} - \frac{\beta_3 z x}{\beta_4 + x}$$

$$\dot{q} = -\beta_6 q + \frac{\beta_5 q x}{\beta_4 + x}$$

$$\tag{1}$$

where the variables x and q represent the population density of prey and predator, respectively, and $\beta = (\beta_1, \beta_2, ..., \beta_6)$ are parameters which are subjected to evolutionary modifications. It is supposed that the values of these parameters correspond to the unique stable limit cycle, and assume that the system evolves on the cycle for simplicity. Now, the question is how the consequences process of predicting evolutionary changes in such relevant systems can make solving the parameters and state variables estimation problem of (1) from available measurement data faster. Our data is restricted for samples of the predator x(t) rather than the prey q(t). Mohammed, J. & Tyukin, I in [16] proposed a method for fast evaluation of periodic solutions of systems of ordinary differential equations for set of known and unknown parameter values and initial conditions. The method represents the periodic solution of systems as sums of elementary function and computable integrals dependent on parameters and initial conditions faster (see [16] and [2]), even, however, many methods for finding solutions to inverse problems have been developed to date such that interval analysis [20] and particle filters and Bayesian inference methods [1] as computerized simulation which required for accurate results and fast execution time.

The work in this research is organized as follows: section two gives the problem statement and will review the integral formula proposed by Mohammed, J. & Tyukin, I [16] for class of systems for which the representation of periodic solutions is possible according to some general assumptions. In Section 3 we investigate the model of predator prey in (1) and the possibility of transforming it to the form that enable us to apply the method for parameters and states estimation. This includes main results of the estimations illustrated numerically and in figures.

2- Problem Statement and Integral representation of Periodic Solutions of ODEs

Consider the system of equations in the form [16]:

$$\dot{x} = \psi(t, y)x + \Phi(t, y)\theta + G(t, y, z, \lambda)$$

$$\dot{z} = v(t, y, \lambda)z + w(t, y, \lambda)$$

$$y = x_1; \quad x(t_0) = x_0, \ z(t_0) = z_0$$
(2)

where $x \in \mathbb{R}^n$ and $z \in \mathbb{R}^m$ are the state variables, and $y \in \mathbb{R}$ is the output of the system, $\psi(t, y) \in \mathbb{R}^{n \times n}$ is a known matrix dependent on the output variable y and the independent variable t; and $\lambda \in \mathbb{R}^k$ and $\theta \in \mathbb{R}^r$ are unknown parameters.

It is assumed that the solution of system (2) is defined in the period of time $[t_0, t_0 + T]; T > 0$ and it is T –periodic, the function F is continuous, bounded, the function $\Phi: \mathbb{R} \times \mathbb{R} \to \mathbb{R}^{n \times r}$ is defined in $L_{\infty}[t_0, \infty) \cap C^0$, the function $G: \mathbb{R} \times \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^k \to \mathbb{R}$ is defined in $L_{\infty}[t_0, \infty) \cap C^1$. Moreover, it is assumed all the functions $\psi(\cdot, y(\cdot)), z(\cdot, y(\cdot), \lambda)$ and $G(\cdot, y(\cdot), z(\cdot), \lambda)$ are T –periodic, and $v(\cdot, y(\cdot), \lambda)$ and $w(\cdot, y(\cdot), \lambda)$ are continuous functions. The last assumption is that the observability Gramian matrix

$$Gr(T,t_0) = \int_{t_0}^{t_0+T} M_A(\tau,t_0) C_1 C_1^T M_A(\tau,t_0)^T d\tau; \qquad C_1 = col(1,0,\dots,0)$$

is of full rank and $Rank(Gr(T, t_0)) = n + r$; where $M_A(t, t_0)$ is the fundamental solution matrix of

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$$\dot{X} = A(t, y(t))X; \quad A(t, y(t)) = \begin{pmatrix} \psi(t, y(t)) & \Phi(t, y(t)) \\ 0 & 0 \end{pmatrix}$$
(3)

such that $M_A(t_0, t_0) = I_{n+r}$.

From (2), the parameter estimation system to solve for the state variables x, z and the parameter θ is considered as follow:

$$\begin{aligned} \dot{x} &= \psi(t, y)x + \Phi(t, y)\theta + G(t, y, z, \lambda) \\ \dot{\theta} &= 0 \\ \dot{z} &= v(t, y, \lambda)z + w(t, y, \lambda) \\ y &= x_1; \quad x(t_0) = x_0, \ z(t_0) = z_0, \ \theta(t_0) = \theta_0 \end{aligned}$$

Therefore, the state variable *X* of following system combines the state variable *x* and parameters θ entering the right-hand-side of equations in (1); *i.e. X* = (*x*, θ):

$$\dot{X} = A(t, y(t))X + \begin{pmatrix} G(y(t), \lambda', t) \\ 0 \end{pmatrix}$$

$$\dot{z} = v(t, y, \lambda)z + w(t, y, \lambda)$$

$$y = CX; \quad X(t_0) = X_0, \quad z(t_0) = z_0$$
(4)

here the matrix A(t, y(t)) is defined in (3) and $C = (1, 0, ..., 0) \in \mathbb{R}^{n+r}$.

The following observer system is considered for the dynamical system of equations in (4):

$$\dot{\hat{X}} = A(t, y(t))\hat{X} + \begin{pmatrix} G(t, y(t), \lambda') \\ 0 \end{pmatrix} + R^{-1}C(C^T\hat{X} - y)$$

$$\dot{R} = -\left(\alpha + A(t, y(t))^T\right)R - RA(y(t), t) + CC^T$$

$$\hat{X}(t_0) = \hat{X}_0 \in \mathbb{R}^{n+r} \text{ and } R(t_0) \in \mathbb{R}^{(n+r) \times (n+r)}$$
(5)

where \hat{X} is the state variable of the observer system, R is a positive definite symmetric matrix, and α is a real positive parameter. Solutions of the observer system (5) are defined and periodic for all $t \ge t_0$ as assumed for the system of equations in (3), and then R(t) is defined in [8] by the following equation:

$$R(t) = e^{-\alpha(t-t_0)} M_{\rm A}(t_0, t)^T R(t_0) M_{\rm A}(t_0, t) + \int_{t_0}^t e^{-\alpha(t-s)} M_{\rm A}(s, t)^T R(t_0) M_{\rm A}(s, t) ds$$
(6)

R(t) is symmetric, positive-definite and non-singular for all $t \ge t_0$. Furthermore, R(t) is bounded since the value of the parameter α is chosen to satisfy

$$\left\| e^{-\alpha(t-t_0)} \mathbf{M}_{\mathbf{A}}(t_0, t)^T \right\| \le K e^{-\gamma(t-t_0)}, \quad \gamma > 0$$
⁽⁷⁾

and $R(t_0)$ is a unique symmetric chosen for ensuring that the function R(t) defined by (6) is T -periodic (see Lemma3 in [16]).

In addition to the observer observed periodic trajectory x(t), the variable z admits the closed form solution:

$$z(t, y(t), \lambda) = e^{\int_{t_0}^t v(s, y(s), \lambda) ds} z(t_0, y(t_0), \lambda) + e^{\int_{t_0}^t v(s, y(s), \lambda) ds} \int_{t_0}^t e^{-\int_{t_0}^s v(\tau, y(\tau), \lambda) d\tau} w(s, y(s), \lambda) ds$$
$$= e^{\int_{t_0}^t v(s, y(s), \lambda) ds} z(t_0, y, \lambda) + \int_{t_0}^t e^{\int_s^t v(\tau, y(\tau), \lambda) d\tau} w(s, y(s), \lambda) ds$$
(8)

where

$$z(t_0, y, \lambda) = \left(1 - e^{-\int_{t_0}^{t_0+T} v(s, y(s), \lambda) ds}\right)^{-1} \int_{t_0}^{t_0+T} e^{\int_{s}^{t_0+T} v(\tau, y(\tau), \lambda) d\tau} w(s, y(s), \lambda) ds$$

We have that system (4) is uniquely identifiable on the period of time $[t_0, t_0 + T]$ (see the proof in [16]) in which it is assumed that for every $\lambda \in \mathbb{R}^k$, the set of different parameters $\varepsilon(\lambda)$ that satisfy the error dynamical system of (5) consists of just one element.

The observed periodic solution of system (4) is considered by the next theorem.

Theorem [2],[16] :Consider system (4) and suppose that the assumptions for equations of system (2) are satisfied and system (4) is uniquely identifiable. In addition, suppose that condition (6) holds and the values of α and the initial condition $R(t_0)$ in (4) are chosen such that R(t) > 0 is T –periodic.

$$\hat{X}(t,\lambda') = C^{T}(M(t,t_{0})\hat{X}_{0} + M(t,t_{0})\int_{t_{0}}^{t}M(t_{0},\tau)\left(R^{-1}(\tau)Cy(\tau)\begin{pmatrix}G(\tau,y(\tau),\lambda')\\0\end{pmatrix}\right)d\tau$$
(9)

Where

 $\hat{X}_{0} = \left(I_{n+r} - M(t_{0} + T, t_{0})\right)^{-1} M(t_{0} + T, t_{0}) \int_{t_{0}}^{t_{0} + T} M(t_{0}, \tau) \left(R^{-1}(\tau)Cy(\tau) + \begin{pmatrix}G(\tau, y(\tau), \lambda')\\0\end{pmatrix}\right) d\tau$

Then

$$\hat{y}(t,\lambda') = C^T X(t,\lambda) \text{ or } \hat{X}(t,\lambda') = X(t,\lambda) \quad \forall t \in [t_0, t_0 + T] \quad \leftrightarrow \quad \lambda' = \lambda$$

The proof of theorem is provided in details in [16].

3- Integral Formula of Periodic Solutions and Parameter Estimation Problem of Predator Prey System

Consider predator prey system of equations in (1). The values of parameters are considered as follows [22]:

$$\beta_1 = 1, \ \beta_2 = 1.3, \ \beta_3 = 1, \ \beta_4 = 1, \ \beta_5 = 3, \ \beta_6 = 0.1$$
 (10)

and the initial conditions:

$$x_0 = x(t_0) = 0.0053$$
 and $q_0 = q(t_0) = 0.2536$; $t_0 = 0$ (11)

We can notice that the predator prey system is not in the form of system (2) which should, however, lead us to apply the main theorem (Theorem 3.6 [16]), thus it could be transformed into that system of class (2). Suppose that the transformation is introduced by the following new variable [2]:

$$z = x + \frac{\beta_3}{\beta_5} q \quad ; \quad \beta_3, \beta_5 \neq 0 \tag{12}$$

Thus, by substituting $q = \frac{\beta_5}{\beta_3}(z - x)$ in (1):

$$\dot{x} = \beta_1 x - \frac{\beta_1 x^2}{\beta_2} - \frac{\beta_5 x}{\beta_4 + x} (z - x)$$

and

$$\frac{\beta_5}{\beta_3}(\dot{z}-\dot{x}) = \left(-\beta_6 + \frac{\beta_5 x}{\beta_4 + x}\right) \left(\frac{\beta_5}{\beta_3}(z-x)\right)$$

implies to

$$\dot{z} = \left(-\beta_6 + \frac{\beta_5 x}{\beta_4 + x}\right)(z - x) + \beta_1 x - \frac{\beta_1 x^2}{\beta_2} - \frac{\beta_5 x}{\beta_4 + x}(z - x)$$

Then the equations of the system transformed in the new coordinates as follow:

$$\dot{x} = \beta_1 x - \frac{\beta_1 x^2}{\beta_2} - \frac{\beta_5 x}{\beta_4 + x} (z - x)$$

$$\dot{z} = -\beta_6 z + \beta_1 x - \frac{\beta_1 x^2}{\beta_2} + \beta_6 x$$
(13)

In addition to the output of the system, $y(t) = C_1 x(t)$, and the initial conditions $x(t_0) = x_0$, $z(t_0) = z_0$.

The phase plane of the predator-prey model and the solution curves for x and z shown in Figure (1) have been demonstrated by using numerical simulations in MATLAB programming with the values of parameters in (10) and initial conditions in (11). The figures show that the solution curve of the system is periodic which could be theoretically considered and solved by the representation form in (9).



Figure (1): the figure in the left panel shows the periodic oscillations of predator *x* (blue curve) and prey (red curve) populations and the figure in the right panel shows the phase plane diagram represents the stable limit cycle around its interior equilibrium.

Equations in the system (13) become in the form of equations in (2) which can be written in the matrix form includes the vectors of the unknown parameters and known parameters, by means of the following equation form for the variable z:

$$z(t,\beta_{1},\beta_{2},\beta_{6}) = e^{\int_{t_{0}}^{t}(-\beta_{6})dt} z_{0}(\beta_{1},\beta_{2},\beta_{6}) + e^{\int_{t_{0}}^{t}(-\beta_{6})dt} \int_{t_{0}}^{t} e^{-\int_{t_{0}}^{s}(-\beta_{6})ds} \left(\beta_{1}x(\tau) - \frac{\beta_{1}x^{2}(\tau)}{\beta_{2}} + \beta_{6}x\right)d\tau$$
$$= e^{\beta_{6}(t_{0}-t)} z_{0}(\beta_{1},\beta_{2},\beta_{6}) + e^{\beta_{6}(t_{0}-t)} \int_{t_{0}}^{t} e^{\beta_{6}(s-t_{0})} \left(\beta_{1}x(\tau) - \frac{\beta_{1}x^{2}(\tau)}{\beta_{2}} + \beta_{6}x\right)d\tau$$
$$z_{0}(\beta_{1},\beta_{2},\beta_{6}) = z(t_{0},\beta_{1},\beta_{2},\beta_{6})$$
$$= \left(1 - e^{-\beta_{6}T}\right)^{-1} e^{-\beta_{6}T} \int_{t_{0}}^{t_{0}+T} e^{\beta_{6}(s-t_{0})} \left(\beta_{1}x(\tau) - \frac{\beta_{1}x^{2}(\tau)}{\beta_{2}} + \beta_{6}x\right)d\tau$$
(14)

The observer variable of the system (13), $x(\cdot)$, is periodic with $t_0 = 0$ and T = 34.05 implies that we have 34057 values of data, however, $x(\cdot)$ can be denoted by x(t) or $x(t; \beta_1, \beta_2, \beta_5, \beta_6); \beta_6 \neq 0$.

Then dynamics of *x* includes $z(t, \beta_1, \beta_2, \beta_6)$:

$$\dot{x} = \beta_1 x - \left(\frac{\beta_1}{\beta_2} - \frac{\beta_5}{\beta_4 + x}\right) x^2 - \frac{\beta_5}{\beta_4 + x} z(t, \beta_1, \beta_2, \beta_6)$$
(15)

which is in the form of class of system (1) with the vector $\lambda = (\beta_1, \beta_2, \beta_4, \beta_5, \beta_6)$. We notice that, however, by using the transformation in (12), the number of unknown parameters is reduced to 5 parameters comparing to the 6 unknown parameters in the original problem (1). Moreover, both equations in (13) could be defined with λ even some of the parameters $\beta_1, \beta_2, \beta_4, \beta_5, \beta_6$ are not appeared in the right-hand side of the equations.

Notice that there is not θ parameters in system (13) which means $\Phi(t, y) = 0$, and $\psi(t, y) = 0$ implies to A(t, y) = 0, therefore, here the representation of periodic solution is defined for X = x and by the end of the solution we get $x_0 = X_0$, $C = C_1 = 1$, and $G(t, y(t), \lambda) = \beta_1 x - \left(\frac{\beta_1}{\beta_2} - \frac{\beta_5}{\beta_4 + x}\right) x^2 - \frac{\beta_5}{\beta_4 + x} z(t, \beta_1, \beta_2, \beta_6)$.

Now, Theorem (1) can be applied and the observed periodic trajectory of x(t) or $x(t; \beta_1, \beta_2, \beta_5, \beta_6)$. of the predator prey system (13) can be represented as in the explicit integral formula (9).

The corresponding expression of the observed periodic solution $\hat{X}(t, \lambda')$ is:

$$\begin{split} \hat{X}(t,\lambda') &= \\ M(t,t_0)\hat{X}_0 + \\ \int_{t_0}^t M(t_0,\tau) \left(R^{-1}(\tau)Cy(\tau) + \beta_1 y(\tau) - \left(\frac{\beta_1}{\beta_2} - \frac{\beta_5}{\beta_4 + y(\tau)}\right) y(\tau)^2 \right. \\ &\left. \frac{\beta_5}{\beta_4 + y(\tau)} z(t,\beta_1,\beta_2,\beta_6) \right) d\tau \end{split}$$

where

$$\begin{aligned} \hat{X}_0 &= \left(I_{n+r} - M(t_0 + T, t_0) \right)^{-1} M(t_0 + T, t_0) \int_{t_0}^{t_0 + T} M(t_0, \tau) \left(R^{-1}(\tau) \mathcal{C} y(\tau) + \beta_1 y(\tau) - \left(\frac{\beta_1}{\beta_2} - \frac{\beta_5}{\beta_4 + y(\tau)} \right) y(\tau)^2 - \frac{\beta_5}{\beta_4 + y(\tau)} z(t, \beta_1, \beta_2, \beta_6) \right) d\tau \end{aligned}$$

To illustrate how the method works for this class of system, suppose that $y(t_i) = x(t_i; t_0; (x_0; z_0); \beta)$; i = 0,1,...,N be the measured data. Numerical evaluation of integrals and solutions of all auxiliary differential equations was performed on N = 1000 data points with the step size of $t_{i+1} - t_i = 0.0001$ for all i = 0,1,...,N-1 within the integral interval [0, 34.05] and the periodicity of the solutions x(t) and q(t) should be satisfied at that period of time.

The data values of $y(t_i)$; i = 0, 1, ..., N are simulated numerically by using improved Euler method. To measure how far the values of $\hat{y}(\cdot, \lambda') = \hat{x}(\cdot, \lambda')$ are close to the output data $y(\cdot)$ we use the sums of least square errors equation between $\hat{y}(\cdot)$ and $y(\cdot), \sum_{i=0}^{N} (y(t_i) - \hat{y}(t_i, \lambda'))^2$. The fundamental solution matrices $M(t_i, t_0)$; i = 0, 1, ..., N, are computed for the linear system $\dot{x} = -R^{-1}x$, $\dot{R} = -\alpha R + 1$ by the Runge-Kuta method for [0, 34.05] with step size 0.01 and the value of $\alpha = 1$. The value of $R(t_0)$ was chosen to satisfy which is called Sylvester equation [6], $h_1^{-1}R(t_0) - R(t_0)h_2 = h_1^{-1}H$ where the matrices h_1, h_2, H are defined from equation (6), for more details see Lemma3 in [16].

Figure 2 shows the relative error, $E(t_i) = (y(t_i) - \hat{y}(t_i, \lambda'))/||y||_{\infty,[t_0,t_0+\infty]}$ for nominal parameter values. Table 1 provides the results of using parameterized representations in combination with the nonlinear simplex method that is called Nelder-Mead algorithm [17] to estimate the values of parameters $\beta_1, \beta_2, \beta_4, \beta_5, \beta_6$. Figure 2 shows the results of estimation the parameters through the iterations of implementing the steps of Nelder-Mead algorithm where after 1560 steps the estimates are close to the true values of parameters, where the values 1, 2, and 0.5 of reflection, expansion, and contraction coefficients in the algorithm, respectively. This particular simulation spent 20:3056 minutes in Matlab R2020.

β_1	β_2	β_4	β_5	β_6
1	1.3	1	3	0.1
0.01	0.1	0.1	0.2	0.0001
0.9999	1.29998	1	2.99988	0.1

Table 1: Rows 1, 2 and 3 show the true, initial and estimated values of β_1 , β_2 , β_4 , β_5 , β_6 , respectively.

To evaluate the computational advantage of the integral representation form of equation (9), the time required for 1000 calculations of y(t) by equation (9) comparing with one time of using Runge-Kuta method over the interval $[t_0, t_0 + T]$ but we used the identical parameter values in both methods. This experiment shows that evaluation of the integral representation, equation (9), in Matlab, on CPU is on average 5 times faster than Runge-Kuta integration as shown in Table 2.



Table 2: Time spent for	1000 calculations o	of $y(t)$ for $t \in$	$[t_0, t_0 + T].$
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Figure 2: right panel shows the values of $y(t) = x(t, x_0, \lambda)$ (blue curve), as a function of $\lambda = (\beta_1, \beta_2, \beta_4, \beta_5, \beta_6)$ and the real initial condition x_0 , obtained by numerical integration of (1) by Euler method, and the values of $\hat{y}(t_i, \lambda')$ (red curve) have been computed from representation (9) numerically as a function of the estimated values of parameters λ' and then obtain the estimated initial value \hat{x}_0 , and left panel shows the relative error $E(t_i) = (y(t_i) - \hat{y}(t_i, \lambda'))/||y||_{\infty,[t_0,t_0+\infty]}$ as a function of t.

The real trajectories y(t) and the approximated trajectories $\hat{y}(t_i, \lambda')$ of predator x shown in Figure 2 (right panel) are nearly coincide with least square error 10^{-5} due to the differences in calculation errors of numerical integration. This result of estimations is more accurate than using another integral formula of periodic solutions of ODE system proposed in [22] where the least square error approximately equals 10^{-4} .

4- Conclusion

In this paper, we presented the method of integral representation of periodic solutions of system of ordinary differential equations which formulate, however, parameter estimation and inverse problems proposed by Mohammed, J. & Tyukin, I in [16]. We considered this method since it enables us to find an explicit integral representation of the periodic solutions of problems which do not have analytical solutions and also to illustrate the possibility of reducing the number of unknown parameters in the form of the integral representation. Predator prey model illustrated how to use and apply the method in case that some of systems are not in the required statement form and then use a particular transformation for such systems to start using the method. Applying the method reduced the dimensionality of the problem to 5 by using the transformation instead of solving the inverse problem for 6 parameters and it could provide more reductions of dimensionality of parameters entering the model nonlinearly and computed as a part of the representation. The results show that the estimated values of parameters were coincide the real values with very small error.

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