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RESEARCH ARTICLE

Inverse Problem of Class of Delay Differential Equations and Fast Estimation of Parameters

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ABSTRACT

This article introduces an integral representation formula to solve delay nonlinear ordinary differential equations (DDEs) as an improvment to the method proposed by Tyukin I, et al. of solving a class of ordinary differential equations. The integral formula depends on the parameters of the systems explicitly as nonlinear parameterized computable functions. It features both linear and nonlinear equations and show an effective form for estimating unknown parameters. Solutions of DDEs are represented as sums of computable integrals which are implicitly dependent on the initial condition and the unknown parameters. This allows invoking parallel computational streams using Matlab tools of sums to increase the speed of calculations. On the other hand, reducing the dimension of the vector of the unknown parameters proposed by the integral representation method gives faster calculations and high accuracy in advance. Estimating the parameters appears in the model by using the least squares approach. It provides an observation model to determine the most informative data for a specific parameter, and find the best fit model. In the example of Morris-Lecar of neural cells model, the consistency of delay differential equations with the observers of cell's activation is shown by fitting the observed data to the real data within the high accuracy of estimating the parameters.

Keywords: Delay differential equations, Integral representation, Least square approach, Morris-Lecar model, Parameter estimation

Introduction

Delay differential equations (DDEs) are a class of differential equations that pay attention to modeling many real-life problems that were previously modeled as ordinary differential equations (ODEs). Class of DDEs are practically used for analyzing the delay time in systems such as population dynamics,[1] neural networks,[2] immunology,[3] physiology,[4] and epidemiology.[5] In ODEs, the functions of the systems and their derivatives are evaluated at the same time. However, the class of DDE depends on the state of the system at an earlier time. The delay can be considered as part of the time of some hidden actions, for example, in the stages of the life cycle of the tumor cells, the duration of the infectious period of a cell by tumor, the immune period,[6,7] and the duration of vaccines action in the cells.[8,9]

Employing inverse problems of DDEs to estimate unknown parameters by using the least square approaches has been addressed in many studies for practical applications,[10,11] identifiability of estimating parameters of systems[12] and biological problems[13–15] and their corresponding medical applications.[16–18] This is started by using an initial guess and then comparing the estimated values with the real ones. There are many issues the estimator may face. Estimating some of the parameters could be difficult and sometimes even impossible because DDEs or even ODEs have noisy measurements. The nonlinearity of the most relevant DDE and ODE models gives another difficulty in estimating parameters by most optimization techniques. On the other hand, other difficulties

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could affect further progress. It is, however, difficult or even impossible to find explicit known functions of parameters and initial conditions to represent some observed quantities of equations.[19] Then the estimation process cannot be reached at the same time as the numerical simulation of solutions of systems or it gives a slow process for the computational techniques used. In 2017, Tyukin I, et al.[20] proposed a method for fast and scalable evaluation of periodic solutions of systems of ordinary differential equations (ODEs) for a given set of parameter values and initial conditions of the state variables. This method is very effective for giving an explicit integral representation of solutions of the system and estimating a large number of parameters which results in accurate evaluations. In addition, it allows invoking parallel computational streams by using, however, CUDA programming to increase the speed of calculations.

Therefore, this study provides an improved technique for that proposed in 2017[20] to address the computational difficulties in solving some nonlinear differential equations and DDEs in special cases. This proposes to represent the integrals to be computable and some of the unknown parameters can be estimated explicitly within the right-hand side of the nonlinear quantities. Technical tools of adaptive observer design are employed here to provide a feasible solution for such a class of systems.

The motivation of this paper is to develop a representation framework of solutions for DDEs and to give fast and accurate parameter estimations. The next section addresses the form of DDEs, including general Assumptions regarding all terms of class of the delay systems. This is followed by proving the integral formula of solving DDEs and the main results of estimating parameters. Numerical simulations and applications to neural cell dynamics are given in the last section.

Parameterized system of DDEs

To estimate values of unknown parameters, that appear in any model equations, the inverse problem of the model should be considered. It is assumed that the collected data is given; then the unknown parameters can be determined by fitting the model equations to the data. Consider the following general form of the DDE model:

$$x'(t) = f(t, x(t), x(t-\tau); \theta), \qquad t \in [t_0, t_T] \tag{1}$$

$$y(t) = h(x)$$

where $x \in \mathbb{R}^n$ is the vector of the state variables, y is the output depends on the function $h(x)$ and θ is a vector parameter of the model. The model fitting problem is to select a value or a set of values for θ for which the function $x(t;\hat{\theta})$ provides a 'best' fit at the time $\{t_i\}$, to the output data $\{y_i\}$ for $0 \le i \le T;\ T > 0$ and $t_T = t_0 + T$. The delay term, $x(t-\tau)$, refers to a previous time in about $\tau > 0$ and represents processes and actions that take τ time to complete.

In Eq. (1), if it does not include delay, is defined for $t > t_0$ and then x refers to the current time t in the time of arguments and this is called the forward problem. Here, x refers to the state variables at previous times $t < t_0$ to show the delay effect since past states of x influence the dynamic of the current state, $x'(t)$. In this case, the initial history function $x(t-\tau)$ must be prescribed on an interval that extends before the initial time t_0 . The delay differential equation for $t > t_0$ is solved numerically, so the delay initial value problem can be only discussed as a forward problem to evaluate the dynamic systems for $x(t)$ and $x(t-\tau)$ as different state variables in the system and then the data can be numerically simulated and used to consider the form of its inverse problem.

The solution of Eq. (1) at any time $t \ge t_0$ depends on values of x from $t_0 - \tau$ to t_0, so the problem requires a history function $x_D(t)$ defined on an interval $[t_0 - \tau, t_0]$.

Now, let us define the adaptive observer design of the delay initial value problem as follows:

$$\begin{aligned}
x_J'(t) &= \mathcal{F}(y(t), t)\, x_J + \mathcal{L}(y(t), t)\, p \\
&\quad + \mathcal{K}(y(t), q(t, y(t)), q_D(t, y(t)), \vartheta, t) \\
\dot{p} &= -\mathcal{L}(y(t), t)\, p \\
q(t, y(t)) &= x_{j_1}(t),\ t \ge t_0 \\
q_D(t, y(t)) &= x_{j_2}(t),\quad t_0 - \tau \le\ t \le t_0 \\
y &= C^T x_J,\ t \ge t_0 \\
x(t) &= x_D(t),\quad t_0 - \tau \le\ t \le t_0
\end{aligned} \tag{2}$$

where $x_J(t)$ represents the vector of the nonlinear state variables, $q(t, y(t))$ and $q_D(t, y(t))$ represent linear equations and delay nonlinear equations, respectively. Then, the dimension of the system is $n = n_1 + j_1 + j_2$ The two vectors of parameters, $p \in \mathbb{R}^m$ and $\vartheta \in \mathbb{R}^r$, including the parameters of θ, *i.e.* $\theta = (p, \vartheta)$.

For system (2), let the following Assumption as follows:

Assumption 1:

1- The solution trajectoryof $x_J'(t)$ is periodic for $t \in [t_0, t_T]$.

2- The function $\mathcal{F}(y(\cdot),\cdot)$, defined $\mathcal{F}:\mathbb{R}\times\mathbb{R}\to\mathbb{R}^{n_1}$, is bounded, continuous, and periodic.
3- Real values of the parameters $p\in\mathbb{R}^m$ and $\vartheta\in\mathbb{R}^r$ are unknown.
4- Values of the output $y=C^T x(t)$, where $C=col(1,0,0,\ldots,0)\in\mathbb{R}^{n_1}$, for all $t\in[t_0,t_T]$ are available that take the data values of x_1 only.
5- The function $\mathcal{L}(y(\cdot),\cdot)$, defined $\mathcal{L}:\mathbb{R}\times\mathbb{R}\to\mathbb{R}^{n_1+m}$, is periodic, and is in the field $L_\infty[t_0,\infty)\cap\mathcal{C}^0$.
6- The function $\mathcal{K}(y(\cdot),q(\cdot,y(\cdot)),q_D(\cdot,y(\cdot)),\vartheta,\cdot)$, defined $\mathcal{K}:\mathbb{R}\times\mathbb{R}^d\times\mathbb{R}^r\times\mathbb{R}\to\mathbb{R}^{n_1}$, is periodic and is defined in $L_\infty[t_0,\infty)\cap\mathcal{C}^1$.

At the time t_0 in system (2), the derivative of the initial history function, if it exists, gives the left derivative of $x_D(t,y(t))$,

For the delay differential equations in (2) we always consider the derivative $x_J'(t)$ at the time t_0 just from the right side. Then, the left derivative of the initial history function, if it exists, represents the left derivative of $x_J(t)$:

$$\lim_{t\to t_0^-} x_D'(t,y(t)) = x_J'(t_0) = \lim_{t\to t_0^-}\frac{x_J(t)-x_J(t_0)}{t-t_0}$$

Which likely gives different derivatives from the right side:

$$\lim_{t\to t_0^+} x'(t) = \lim_{t\to t_0^+}\left(\mathcal{F}(y(t),t)\,x+\mathcal{L}(y(t),t)\,p + \mathcal{K}\left(y(t),q(t,y(t)),q_D(t,y(t)),\vartheta,t\right)\right)$$

A convenient notation for the system to have more effective estimation is combining the state variables x_J and the parameters p in a new variable X_J and system (2) becomes in the form:

$$X_J'(t)=\begin{pmatrix}\mathcal{F}(y(t),t)+\lambda C^T & \mathcal{L}(y(t),t)\\ -\mathcal{L}(y(t),t) & 0\end{pmatrix}X_J + \begin{pmatrix}\mathcal{K}\left(y(t),q(t,y(t)),q_D(t,y(t)),\vartheta,t\right)-\lambda y(t)\\ y(t)\mathcal{L}(y(t),t)\end{pmatrix} \tag{3}$$

$$Y=C_1^T X_J = C^T x_J$$

where $X_J=(x,p)^T\in\mathbb{R}^{n_1+m}$ and $C_1=col(1,0,0,\ldots,0)\in\mathbb{R}^{n_1+m}$.

Existence and uniqueness of solutions

To prove the existence and uniqueness of solutions of system (2) in the delay differential equations setting, it can be represented using its associated integral equation.

Solutions of Eq. (3) for $t\in[t_0,t_T]$ are in the form:

$$X_J(t)=\varphi(t,t_0)X_J(t_0)+\varphi(t,t_0)\int_{t_0}^{t}\varphi(s,t_0)^T \times\begin{pmatrix}\mathcal{K}\left(y(s),q(s,y(s)),q_D(s,y(s)),\hat{\vartheta},s\right)-\lambda y(s)\\ y(s)\mathcal{L}(y(s),s)\end{pmatrix}ds \tag{4}$$

where $\lambda\in\mathbb{R}^{n_1}$ and this system has normalized fundamental solution matrices $\varphi(t,t_0)$, $\forall\ t\in[t_0,t_T]$: $\varphi(t_0,t_0)=I_{n_1+m}$.

This leads us to the associated integral equation by noticing that $X_J(t_0)=X_D(t_0)$:

$$X_J(t)=\begin{cases}\varphi(t,t_0)X_J(t_0)+\int_{t_0}^{t}\varphi(t,s)\times\begin{pmatrix}\mathcal{K}\left(y(s),q(s,y(s)),q_D(s,y(s)),\hat{\vartheta},s\right)-\lambda y(s)\\ y(s)\mathcal{L}(y(s),s)\end{pmatrix}ds, & t_0\le t\le t_T\\ X_D(t), & t_0-\tau\le t\le t_0\end{cases} \tag{5}$$

Lemma 1: *If $x_J(t)$ is continuous on $[t_0-\tau,t_T]$, then $x_D(t)$ for $t_0-\tau\le t\le t_0$ is a continuous function of t on $[t_0,t_T]$.*

Proof: Since $x_J(t)$ is continuous on the compact set $[t_0-\tau,t_T]$ then it is uniformly continuous on that set. Therefore, for all $t_1,t_2\in[t_0-\tau,t_T]$ and for all $\delta>0$, there exist $\epsilon>0$ such that whenever $|t_2-t_1|<\delta$, then $|x_J(t_2)-x_J(t_1)|<\epsilon$.

Thus, for $t_1^*,t_2^*\in[t_0,t_T]$ and $|t_2^*-t_1^*|<\delta$, the norm $|x_J(t_2^*-\tau)-x_J(t_1^*-\tau)|<\epsilon$ is satisfied which implies that $|x_D(t_2^*)-x_D(t_1^*)|<\epsilon$. This, therefore, proved the continuity of $x_D(t)$ in t for $[t_0,t_T]$. □

From Lemma 1, it can be observed that the delay differential equations $q_D(t,y(t))$ are also continuous on $[t_0,t_T]$. In Eq. (5), it is concluded that $x_J(t)$ is defined for all $t\in[t_0-\tau,t_T]$, Lemma 1 includes that $x_J(t)$ is a continuous function for $t\in[t_0,t_T]$ and by Assumption 1, $\mathcal{K}(y(t),q(t,y(t)),q_D(t,y(t)),\vartheta,t)$ is continuous. Then, by the fundamental calculus theorem, it could differentiate both sides of Eq. (5) to get the initial value problem of the system (2).

It can be simply showing that system (2) is uniquely identifiable on $[t_0-\tau,t_T]$. Define the first set as

$$\gamma_1(\tilde{p},\tilde{\vartheta})=\Big\{(p',\vartheta'),\ p'\in\mathbb{R}^m,\ \vartheta'\in\mathbb{R}^r \mid L(y(t),t)^T \times(p'-\tilde{p})+K\left(y(t),q(t,y(t)),q_D(t,y(t)),\vartheta',t\right) - K\left(y(t),q(t,y(t)),q_D(t,y(t)),\tilde{\vartheta},t\right) = 0,\ \forall\ t\in[t_0,t_T]\Big\} \tag{6}$$

or

$$\gamma_1\ (\tilde{p},\tilde{\vartheta})=\Big\{(\acute{p},\acute{\vartheta}),\ p'\in\mathbb{R}^m,\ \acute{\vartheta}\in\mathbb{R}^r|x\left(t,\tilde{p},\tilde{\vartheta}\right)-x\left(t,\acute{p},\acute{\vartheta}\right)=0,\ \forall\, t\in[t_0-\tau,t_0]\Big\}\quad(7)$$

The parameterization problem of the system (2) can be indistinguishable from each other which makes the values of $x(t)$ to be known for all $t\in[t_0,\mathrm{t}_T]$ and are all included in $\gamma_1\ (\tilde{p},\tilde{\vartheta})$. This implies, from Eqs. (6) and (7), that if $x(t,\tilde{p},\tilde{\vartheta})=x(t,\acute{p},\acute{\vartheta})$ for all $t\in[t_0-\tau,\mathrm{t}_T]$ then $(\acute{p},\acute{\vartheta})\in\gamma_1\ (\tilde{p},\tilde{\vartheta})$. This also could be satisfied, in other words, if $y(t,\tilde{p},\tilde{\vartheta})=y(t,\acute{p},\acute{\vartheta})$ for all $t\in[t_0-\tau,\mathrm{t}_T]$. However, the set $\gamma_1\ (\tilde{p},\tilde{\vartheta})$ may contain various values for at least one parameter then system (2) does not have a unique solution on $[t_0-\tau,\mathrm{t}_T]$.

For simplicity, system (2) has been considered with unique solutions on $[t_0-\tau,t_T]$.

Assumption 2: The set $\gamma_1\ (\tilde{p},\tilde{\vartheta})$ contains only one vector of values for the unknown parameters.

Integral formula for solving delay differential equations

Consider the following linear system with the state variables μ_1 and μ_2:

$$\frac{d}{dt}\begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix}=\begin{pmatrix}\mathcal{F}\left(y\left(t\right),t\right)+\lambda C^T & \mathcal{L}\left(y\left(t\right),t\right)\\ -\mathcal{L}\left(y\left(t\right),t\right) & 0\end{pmatrix}\begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix}\quad(8)$$

with the fundamental solution matrices $\varphi(t,t_0),\ \forall\, t\in[t_0,t_T]$: $\varphi(t_0,t_0)=I_{n_1+m}$.

Theorem 1: *Consider system (2) and suppose that Assumptions 1 and 2 hold. Let the function $\mathcal{L}(y(t),t)$ satisfies:*

$$\int_{t_0}^{t_T}\mathcal{L}\left(y\left(s\right),s\right)\mathcal{L}\left(y\left(s\right),s\right)^T ds\geq\gamma I_{n_1+m},\ \ \gamma>0.$$

Then the following statements are equivalents:

1) $\hat{Y}(\hat{\vartheta},t)=C_1^T X_J(t;t_0,X_J(t_0),\vartheta)$, $\forall\, t\in[t_0,t_T]$; $\hat{Y}:\mathbb{R}^r\times\mathbb{R}\to\mathbb{R}$,

such that

$$\hat{Y}\left(\hat{\vartheta},t\right)=C_1^T\left[\varphi\left(t,t_0\right)\ \hat{X}_J\left(t_0\right)+\int_{t_0}^{t}\varphi\left(t,s\right)\times\begin{pmatrix}\mathcal{K}\left(y\left(s\right),q\left(s,y\left(s\right)\right),q_D\left(s,y\left(s\right)\right),\hat{\vartheta},s\right)-\lambda y\left(s\right)\\ y\left(s\right)\mathcal{L}\left(y\left(s\right),s\right)\end{pmatrix}ds\right];$$

$$t_0\leq\ t\leq t_T\quad(9)$$

or

$$\hat{Y}\left(\hat{\vartheta},t\right)=C_1^T X_D\left(t\right);\quad t_0-\tau\leq\ t\leq t_0\quad(10)$$

where

$$\hat{X}_J\left(t_0\right)=\left(I_{n+m}-\varphi\left(t_T,t_0\right)\right)^{-1}\int_{t_0}^{t_T}\varphi\left(t_T,s\right)\times\begin{pmatrix}\mathcal{K}\left(y\left(s\right),q\left(t,y\left(s\right)\right),q_D\left(s,y\left(s\right)\right),\hat{\vartheta},s\right)-\lambda y\left(s\right)\\ y\left(s\right)\mathcal{L}\left(y\left(s\right),s\right)\end{pmatrix}ds$$

2) $\vartheta=\hat{\vartheta}$

Moreover, the values of x_0 and p satisfy:

$$\hat{X}_D\left(t_0\right)=\hat{X}_J\left(t_0\right)=\begin{pmatrix}\hat{x}_J\left(t_0\right)\\ \hat{p}\end{pmatrix}\quad(11)$$

Proof: Let us first assume that 1) is satisfied. According to the theorem of proofing the unique solutions,[21] there exist positive numbers ρ,U such that:

$$\|\varphi\left(t,\tilde{t}_0\right)\|\leq Ue^{-\rho\left(t-\tilde{t}_0\right)},\quad\forall\, t\geq\tilde{t}_0;\quad t,\tilde{t}_0\in[t_0,\infty).$$

The matrix $(I_{n+m}-\varphi(t_T,t_0))^{-1}$ exists because all the matrices $I_{n+m}-\varphi(t,t_0)$, for all $t\in[t_0-\tau,\mathrm{t}_T]$, have non-zero eigenvalues.

Consider the variable, where $X=(X_1,X_2)$ is the vector of variables of the system:

$$\frac{d}{dt}\begin{pmatrix}X_1\\ X_2\end{pmatrix}=\begin{pmatrix}\mathcal{F}\left(y\left(t\right),t\right)+\lambda C^T & \mathcal{L}\left(y\left(t\right),t\right)\\ -\mathcal{L}\left(y\left(t\right),t\right) & 0\end{pmatrix}\begin{pmatrix}X_1\\ X_2\end{pmatrix}+\begin{pmatrix}\mathcal{K}\left(y\left(t\right),q\left(t,y\left(t\right)\right),q_D\left(t,y\left(t\right)\right),\vartheta,t\right)-\lambda y\left(t\right)\\ y\left(t\right)\mathcal{L}\left(y\left(t\right),t\right)\end{pmatrix}\quad(12)$$

Solutions of Eq. (12) are defined for all $t\geq t_0$, and the function $X(\cdot)=(x(\cdot,\tilde{p},\tilde{\vartheta}),\tilde{p})$ is defined in the domain of the function $x(t,\tilde{p},\tilde{\vartheta})$ extended to $[t_0,\infty)$. Solutions of Eq. (8) introduced with $\mu_1(t_0)=X_1(t_0)-x_J(t_0)$, $\mu_1(t_0)=X_1(t_0)-p$, where $\mu_1(t)$ for all $t\in[t_0,\mathrm{t}_T]$ has constant values if $\hat{y}(\tilde{\vartheta},t)=y(t)$. Since the set $\gamma_1\ (\tilde{p},\tilde{\vartheta})$, according to Assumption 1, contains just one element, then it implies that $X_2(t_0)=\tilde{p},\vartheta'=\tilde{\vartheta}$. However, the dynamics of $X_J(t)$ satisfy that $X_J=X_D(t)$ is not required to be periodic on all t in $[t_0-\tau,t_0]$. Notice that Eq. (12) is linear and has the following form of unique exponentially stable solutions:

$$X(t) = \varphi(t, t_0)\, X(t_0) + \int_{t_0}^{t} \varphi(t, s) \times \begin{pmatrix} \mathcal{K}\left(y(s), q(s, y(s)), q_D(s, y(s)), \hat{\vartheta}, s\right) - \lambda y(s) \\ y(s)\, \mathcal{L}\left(y(s), s\right) \end{pmatrix} ds, \quad \forall t \in [t_0, t_T]$$

and

$$X(t) = X_D(t), \ \forall t \in [t_0 - \tau, t_0]$$

This shows that Eqs. (9) and (10) hold.

Now, if 2) holds, let $\acute{p}, \acute{\vartheta}$ be parameters satisfy that $y(\acute{p}, \acute{\vartheta}, t) = y(t)$ for all $t \in [t_0, t_T]$ and $y(\acute{p}, \acute{\vartheta}, t) = x_D(t)$ for all $t \in [t_0 - \tau, t_0]$. For the variable χ, $\chi(t) \equiv 0$ if $X_1(t_0) = x_0$, $X_2(t_0) = \tilde{\vartheta}$ which implies that $\hat{y}(\acute{\vartheta}, t) = y(\acute{p}, \acute{\vartheta}, t) = y(t)$ for all $t \in [t_0, t_T]$. This includes that $x_D(\acute{p}, \acute{\vartheta}, t_0) = X_1(t_0)$ and $\hat{y}(\acute{\vartheta}, t) = y(\acute{p}, \acute{\vartheta}, t) = x_D(t)$ for all $t \in [t_0 - \tau, t_0]$. □

Notice that $X_D(t)$ at t_0 could be from Eq. (4) as follows:

$$X_J(t_0) = \begin{cases} \varphi(t_0, t_0)\, X_J(t_0) + \int_{t_0}^{t_0} \varphi(t_0, s) \\ \times \begin{pmatrix} \mathcal{K}\left(y(s), q(s, y(s)), q_D(s, y(s)), \hat{\vartheta}, s\right) - \lambda y(s) \\ y(s)\, \mathcal{L}\left(y(s), s\right) \end{pmatrix} ds \\ X_D(t_0) \end{cases}$$

$$= I_{n+m}\, X_D(t_0) + \int_{t_0}^{t_0} \varphi(t_0, s) \times \begin{pmatrix} \mathcal{K}\left(y(s), q(s, y(s)), q_D(s, y(s)), \hat{\vartheta}, s\right) - \lambda y(s) \\ y(s)\, \mathcal{L}\left(y(s), s\right) \end{pmatrix} ds$$

$$= I_{n+m}\, X_D(t_0) + 0$$

$$= X_D(t_0)$$

Then from the first condition of Assumption 1, the initial value gets the form:

$$X_D(t_0) = \hat{X}_J(t_0) = \left(I_{n+m} - \varphi(t_T, t_0)\right)^{-1} \int_{t_0}^{t_T} \varphi(t_T, s) \times \begin{pmatrix} \mathcal{K}\left(y(s), q(t, y(s)), q_D(s, y(s)), \hat{\vartheta}, s\right) - \lambda y(s) \\ y(s)\, \mathcal{L}\left(y(s), s\right) \end{pmatrix} ds.$$

The above theorem considers the case of solving delay differential equations and improving for the integral formula introduced by Ivan, et al.[20]

Remark 1: To consider and apply the integral formula of the inverse problem, the data are compared for N discrete points $\{t_i\}_{i=1}^{N}$ in $[t_0 - \tau, t_T]$; N_1, N_2 are the number of points at the periods of time $[t_0, t_T]$ and $[t_0 - \tau, t_0]$, respectively. This allows the formulation in Theorem 1 to include the inference problem as the least square error:

$$\begin{aligned} \tilde{\vartheta} &= \arg \min_{\vartheta \in \mathbb{R}^r} \sum_{i=1}^{N} \left[\left(\hat{y}(t_i) - y(t_i)\right)^2 + \left(\hat{x}_J(t_i - \tau) - x_J(t_i - \tau)\right)^2 \right] \\ &= \arg \min_{\vartheta \in \mathbb{R}^r} \left[\sum_{i=1}^{N_1} \left(\hat{y}(t_i) - y(t_i)\right)^2 + \sum_{i=1}^{N_2} \left(\hat{x}_D(t_i) - x_D(t_i)\right)^2 \right] \end{aligned} \tag{13}$$

In this case, discretizing the continuous-time dynamical system is not computationally required. The drawbacks of solving inverse problems of the system (2) in case of estimating the overall unknown parameters vector is (x_0, p, ϑ) is that its dimension is $n_1 + m + r$ and the original matrix $\mathcal{F}(\vartheta)$ will depend implicitly on ϑ. Then, however, the expressions of solutions of Eq. (2) will include the nonlinearly parameterized term $e^{\mathcal{F}(\vartheta)(t-t_0)}$. Therefore, the purpose of the integral formula to reduce the number of unknown parameters to r parameters has been clearly concluded here.

Example 1: *Consider Morris and Lecar's model of single neural membrane activity introduced in 1981,*[22] *and it is formed here with a time delay:*

$$\begin{aligned} \dot{x} &= g_{Ca} m_\infty(x)\left(x(t) - E_{Ca}\right) + g_K z(x)\left(x(t) + E_K\right) + g_L\left(x(t-\tau) + E_L\right) + I \\ \dot{z} &= \frac{-1}{\alpha(x)} z + \frac{w(x)}{\alpha(x)} \\ y &= x, \quad t \geq t_0 \end{aligned} \tag{14}$$

where

$$m_\infty(x) = 0.5\left(1 + \tan\left(\frac{x - v_1}{v_2}\right)\right),$$

$$w_\infty(x) = 0.5\left(1 + \tan\left(\frac{x + v_3}{v_4}\right)\right),$$

$$\alpha(x) = \varepsilon_0\left(\cosh\left(\frac{x + v_3}{2\, v_4}\right)\right)^{-1}$$

Where x and z are the measured membrane voltage and the gating variable of the neural cells' activation, respectively. Nernst potential parameters are assumed to be known as $E_{Ca} = 55.17$, $E_K = -110.14$, $E_L = 49.49$; and the other parameters will be studied as unknown parameters. To give practical results for the parameters ε_0, ν_3 and ν_4 the integral $B(t) = \int_{t_0}^{t} \frac{-1}{\alpha(s)} ds$ should be negative at $t = t_T$. Here $x(t)$ is periodic for a given period of time $[t_0, t_T]$ and it is assumed that observations are defined and studied for the solutions of Eq. (14) on the stable period. The general solution of the linear equation of z is expressed as:

$$z(t) = e^{B(t)} z_0 + \int_{t_0}^{t} e^{B(t)-B(s)} \frac{w_\infty(x(s))}{\alpha(x(s))} ds$$

$$z_0 = z(t_0) = z(t_T) = (1 - e^{B(t_T)})^{-1} \times \int_{t_0}^{t_T} e^{B(t_T)-B(s)} \frac{w_\infty(x(s))}{\alpha(x(s))} ds$$

Let us rewrite $\dot{x}$ as follow:

$$\dot{x} = (x_D(t),\ 1) \begin{pmatrix} g_L \\ I - 0.5E_L \end{pmatrix} + g_{Ca} m_\infty(x)(y(t) - E_{Ca}) + g_K\, z(x)(y(t) + E_K)$$

Then the observer system:

$$\dot{\hat{X}} = \begin{pmatrix} \lambda & X_D(t) & 1 \\ -X_D(t) & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{g}_L \\ \hat{I} - 0.5\hat{E}_L \end{pmatrix} + \begin{pmatrix} \mathcal{K}(y(t), z(y(t)), \hat{\vartheta}, t) - \lambda y(t) \\ y(t) x_D(t) \\ y(t) \end{pmatrix}$$

where $\mathcal{K}(y(t), z(y(t)), \hat{\vartheta}, t) = g_{Ca} m_\infty(x)(y(t) - E_{Ca}) + g_K\, z(x)(y(t) + E_K)$ does not depend on $X_D(t)$ but only on the measured data $y(t)$, and $\mathcal{L}(y(t), t) = (x_D(t),\ 1)$.

Neuronal transmissions are inherently affected by time delay factors. The electrical potential is generated from the chemical potential reactions inside the neural cells. The time delay between the gap of synapses of every two neurons is formed by the amount of time spent on the chemical reactions. In the model, $x_D = x(t)$ for all $t \in [t_0 - \tau, t_0]$.

The delayed interactions could lead to many interesting and even unexpected phenomena. To consider the effects of time delay, it may take time series of the inter-spike intervals as shown in Fig. 1 and the model is periodic when $\tau = 3$, see the panel (iii) in Fig. 1.

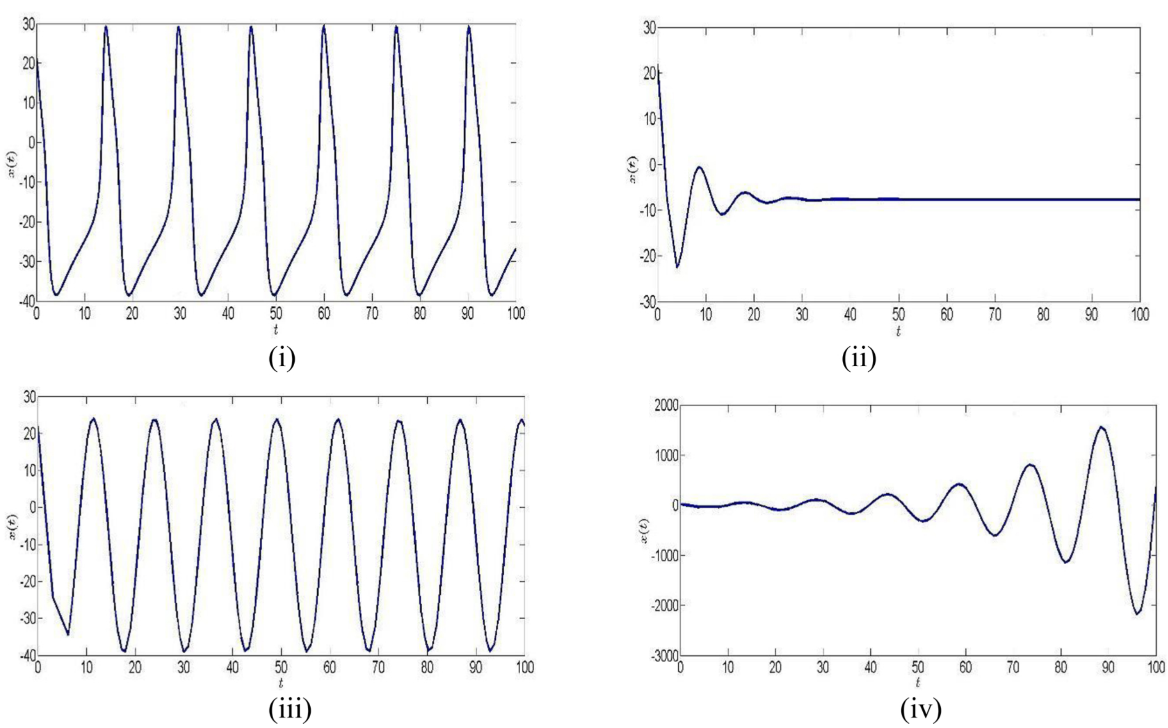

Fig. 1. Numerical solutions of system (14). The time series solutions for $x(t)$ at the true values of p and ϑ. The figures show the reconstructed voltage of the neural cells changes with different values of delay between two cells: i) no delay ii) $\tau = 2$ iii) $\tau = 3$ iv) $\tau = 4$, with the initial point $(x(t_0), z(t_0)) = (21.963877; 0.385192)$.

Table 1. First row and second row show the true and estimated values of ϑ, respectively vector $\vartheta = (v_1, v_2, v_3, v_4, \varepsilon_0, g_{Ca}, g_K)$.

v_1	v_2	v_3	v_4	ε_0	g_{Ca}	g_K
−1	15	−10	14.5	3	−1.1	−2
−1.009	14.08	−10.106	1.502	2.97	−1.09	−1.89

Eq. (14) could be presented in the form Eq. (5) with the state variable $X = (x, p)^T$ where $p = (g_L, I)$ and the other unknown parameters included in ϑ, gives that $\vartheta = (v_1, v_2, v_3, v_4, \varepsilon_0, g_{Ca}, g_K)$. Here the estimation of the parameter I is not the value of p but it comes from $I - 0.5E_L$ and the parameters v_1, v_2 are not directly estimated but it is simply considered the ratios $1/v_2$ and v_1/v_2 instead. The measured data of $y = x$ is numerically evaluated by the Runge-Kutta method at the real values of all the model's parameters with $t_i - t_{i-1} = 0.002$ for $i = 1, 2, \ldots, N$. The period of oscillations provided the integration interval $[t_0, t_T] = [10,\ 25.1692]$. Estimating the values of p and ϑ requires to satisfy that $\hat{Y}(\hat{\vartheta}, t) = Y(t)$ over the period of time $[t_0, t_T]$ according to Theorem 1, however, $Y(t)$ depends not only on $x(t)$ but also on $x(t - \tau)$. It practically needs to apply Remark 1 as the estimated values of parameters minimize the Least Square Eq. (13). The solution of Eq. (2) is defined as a period of time which satisfied $x(t_0) = x(t_T)$. Moreover, the fundamental solution matrices $\varphi(t, t_0)$ for all $t \in [t_0, t_T]$ should be essentially calculated to evaluate $\hat{Y}(\hat{\vartheta}, t)$. In this example, the linearly independent solutions of the linear system:

$$\dot{P} = \begin{pmatrix} \lambda & X_D(t) & 1 \\ -X_D(t) & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} P, \quad \lambda = -1$$

Table 2. First row and second rows show the true and estimated values of g_L and I and the initial value x_0, respectively. vector $p = (g_L, I)$.

g_L	I	x_0
−0.5	10	21.97
−0.485	10.639	21.9154

is numerically evaluated using the improved Euler method starting from the initial vectors $(1,0,0)^T,\ (0,1,0)^T,\ (0,0,1)^T$.

Results and discussion

To find the numerical solution of Eq. (13), Improved Nelder Mead method,[23] which is called the nonlinear simplex method. The method took around 2591 iterations and the estimated values of $(v_1, v_2, v_3, v_4, \varepsilon_0, g_{Ca}, g_K)$ are shown in Table 1 which includes the true values of the parameters compared with their estimated values. Table 2 shows the final solution of the integral representation including the estimated values of x_0 and $p = (g_L, I - 0.5E_L)$ and then the value of I. In Fig. 2, the results of the estimations of the parameters are represented in the blue curve at the iterations of applying the Nelder Mead method.

It spent approximately 1.5 hours on a standard PC in Matlab R2020. Most of the time was spent in the

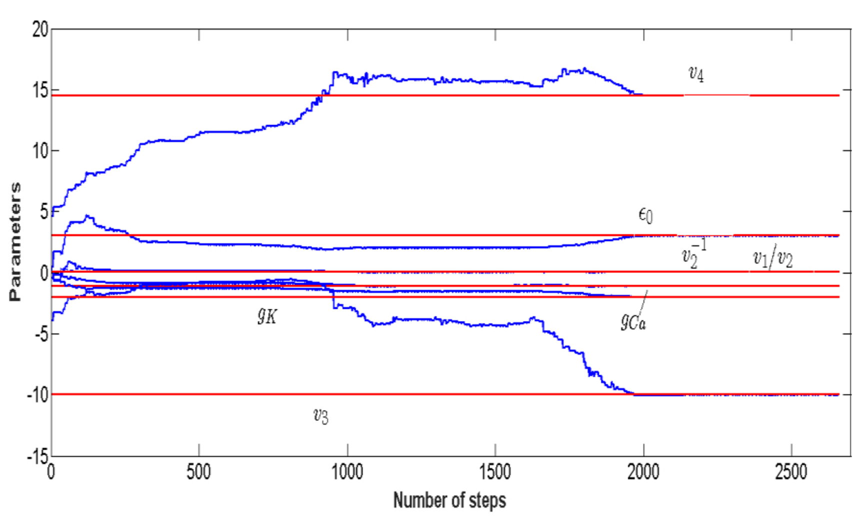

Fig. 2. Number of steps spent to estimate $v_1/v_2,\ 1/v_2,\ v_3,\ v_4,\ \varepsilon_0,\ g_{Ca},\ g_K$ by Nelder Mead's method. The estimated values at all the steps and the true values are shown in blue curves and red lines, respectively.

calculations of integrals of Eq. (9) was performed using the cumsum of data in Matlab containing the cumulative sum of elements of every vector.

This proposed technique returns the estimates of the initial condition and the unknown parameters which are nonlinearly included in the right-hand side of the system. In this regard, it would fairly compare the time spent calculating the integrals of the dynamical system DDEs of the explicit integral representation with other functions like, for example, sensitivity functions. This will be practically implemented in our future work for solving delay differential equations of both diabetic and tumor cell problems.

Conclusion

This paper proposed an improved inverse problem framework for especially solving a class of systems of delay differential equations. This formula represented the solutions of DDEs as sums of computable quantities which include the process of estimating parameters explicitly. The formal neural cells system of the Morris-Lecar model showed very high performance for the method. This technique introduced fast estimation for the state variable and the unknown parameters. The technique employed ideas of using adaptive observers design to express and represent measured trajectories as explicit functions of unknown parameters and initial conditions. The integral representation considered fast and efficient model evaluations by parallel computation techniques in Matlab, and introduced solution form to inverse problems that may match variables and parameters that are nonlinearly entering the right-hand side of the model to be explicitly estimated. This could reduce the dimensionality of the parametrized problem to have more accurate estimations and fast calculations using the estimator Nelder-Mead method. Moreover, the results of estimations in the example showed how the method is highly effective in solving systems of nonlinear equations with delay in time and estimating large numbers of unknown parameters without needing crucial conditions of other methods like Newton and Newton-Raphson.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images, that are not ours, have been included with the necessary permission for re-publication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at the University of Basrah, Iraq.

Authors' contribution statement

I.K. proposed the concept of the developed design of the method by proving the theory of the method and finding the final results. J.M. analyzed the final results starting with finding the experimental data and simulating the model of the example and applying the method, and contributed to writing, revising, and proofreading the manuscript.

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المسألة العكسية لنظام معادلات التأخير التفاضلية و تخمين سريع للمعاملات

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الخلاصة

هذا البحث يقترح صيغة تكاملية صريحة لمعادلات تفاضلية غير خطية ذات تأخير بالوقت كتطوير لطريقة ايفان واخرون لحل المعادلات التفاضلية الاعتيادية. التمثيلات التكاملية لمعادلات التأخير ذات المعاملات تعتمد على معلمات الأنظمة بصيغة صريحة كمعادلات ذات معاملات قابلة للحساب. تلك الانظمة تحتوي معادلات خطية وغير خطية وممكن استخدام تلك الطريقة لمناقشة كفائتها في تخمين المعاملات تلك الانظمة. حلول معادلات التاخير التفاضلية تمثل بواسطة عمليات جمع تراكمي لتكاملات قابلة للحساب والتي تعتمد بصورة صريحة على القيمة الابتدائية والمعاملات الغير معلومة القيمة. هذا يسمح باستخدام بعض عمليات الجمع المتوازية السريعه الحسابات في برنامج الماتلاب لزيادة سرعة التخمين. من جهة اخرى فان تقليص بُعد متجه المعلمات الغير معلومة القيمة تُظهر اكثر سرعة للحسابات وتعطي نتائج اكثر دقة في التطبيق. تخمين المعاملات يظهر في النموذج باستخدام طريقة التربيعات الصغرى. تلك الطريقة تعطي نظام استنتاجي لتحديد البيانات بقيم محددة للمعاملات وإيجاد أفضل نموذج مطابق. في مثال أنظمة الخلايا العصبية لموريس ليكار، تطابق معادلات التأخير التفاضلية مع المعادلات الاستنتاجية لنشاط الخلايا العصبية يظهر عن طريق مطابقة البيانات المستنتجة مع البيانات الحقيقة من خلال الدقة العالية في تخمين المعلمات.

الكلمات المفتاحية: معادلات التاخير التفاضلية، التمثيل التكاملي، طريقة التربيعات الصغرى، نموذج موريس ليكار للخلايا العصبية، تخمين المعاملات.