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Extended Parker–Sochacki method for Michaelis–Menten enzymatic reaction model

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ABSTRACT

In this article, a new approach—namely, the extended Parker–Sochacki method (EPSM)—is presented for solving the Michaelis–Menten nonlinear enzymatic reaction model. The Parker–Sochacki method (PSM) is combined with a new resummation method called the Sumudu–Padé resummation method to obtain approximate analytical solutions for the model. The obtained solutions by the proposed approach are compared with the solutions of PSM and the Runge–Kutta numerical method (RKM). The comparison proves the practicality, efficiency, and correctness of the presented approach. It serves as a basis for solving other nonlinear biochemical reaction models in the future.

Consider the Michaelis–Menten enzymatic reaction model [1] for describing the enzyme processes:

$$E + A \rightleftharpoons Y \rightarrow E + X, \tag{1}$$

where E is the enzyme, A is the substrate, Y is the intermediate complex, and X is the product. The time evolution of Scheme (1) can be evaluated by solving the system of coupled nonlinear ordinary differential equations (ODEs) [2]:

$$\frac{dA}{dt} = -k_1 EA + k_{-1} Y \tag{2}$$

$$\frac{dE}{dt} = -k_1 EA + (k_{-1} + k_2) Y \tag{3}$$

$$\frac{dY}{dt} = k_1 EA - (k_{-1} + k_2) Y \tag{4}$$

$$\frac{dX}{dt} = k_2 Y \tag{5}$$

subject to the initial conditions

$$A(0) = A_0, \quad E(0) = E_0, \quad Y(0) = 0, \quad X(0) = 0, \tag{6}$$

where the parameters k_1, k_{-1}, and k_2 are positive rate constants for each reaction. Systems (2) to (5) can be reduced to only two equations for A and Y and in dimensionless form of concentrations of substrate, x, and intermediate complex between enzyme and substrate, y, are given by Ref. [2]:

$$\frac{dx}{dt} = -x + (\beta - \alpha) y + xy \tag{7}$$

$$\frac{dy}{dt} = \frac{1}{\varepsilon}(x - \beta y - xy) \tag{8}$$

subject to the initial conditions

$$x(0) = 1, \quad y(0) = 0, \tag{9}$$

where α, β and ε are dimensionless parameters.

The time evolution of the reaction can be found from numerical methods, but they are sensitive to the selection of the time step size [3]. In general, different approximate methods have been introduced for solving nonlinear ODEs such as the homotopy

Abbreviations: ODE, ordinary differential equation; PSM, Parker–Sochacki method; RKM, Runge–Kutta method; EPSM, extended Parker–Sochacki method.

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perturbation method (HPM) [4,5], the homotopy analysis method (HAM) [6,7], the variational iteration method (VIM) [8–10], and the differential transformation method (DTM) [11,12]. Nowadays, there is a need for more satisfactory methods.

In Refs. [13] and [14], approximate numeric–analytic solutions for the Michaelis–Menten enzymatic reaction model are obtained using the multistage homotopy perturbation method (MHPM) and the multistage variational iteration method (MVIM), respectively. The two mentioned methods divide the domain into small sub-intervals and evaluate the solution for each sub-interval, meaning that there is no global form for the solution for the entire domain.

The power series method, which gives a Taylor series solution, is a promising method. For a long time, this method has been used for linear problems. The power series method was extended to solve nonlinear ordinary differential equations by Parker and Sochacki [15]. However, power series solutions suffer from the problem of limited convergence intervals. Outside the intervals of convergence these solutions are not valid.

In this work, the Parker–Sochacki method (PSM) is used to obtain approximate analytical solutions, specifically power series solutions, for the system of coupled nonlinear ODEs (7) and (8). Hence, a new resummation method, called the Sumudu–Padé resummation method, is presented and applied to the obtained series solutions for extending the domain of validity and obtaining a good approximation to the exact solution. The obtained approximate solutions are compared with the Runge–Kutta method (RKM) solutions. In general, results show that the extended Parker–Sochacki method (EPSM) gives precise approximated solutions.

The next section presents a concise review for the Parker–Sochacki method. The Sumudu–Padé resummation method is discussed in the subsequent section. In the section following that, the system of coupled nonlinear ODEs (7) and (8) is solved using the proposed method, and the results are discussed. Finally, conclusions are given in the final section.

Basic idea of the Parker–Sochacki method

The Parker–Sochacki method [15–18] can be used for solving a system of first-order ODEs. If the model is not a system of first-order differential equations, auxiliary variables can be used to write it in that form. The solution of the original ODEs is a subset of the solution of the new system. The method produces Maclaurin series for each variable to any degree required, thereby allowing arbitrarily accurate solutions for the ODE system inside the regions of convergence. To apply the Parker–Sochacki method, we should begin by defining Maclaurin series for each variable:

$$z(t) = \sum_{n=0}^{\infty} z_n t^n \tag{10}$$

with $z_0 = z(0),\ z_1 = z'(0),\ z_2 = \frac{1}{2!}z''(0)$, and so on. Now, we can define a series for the first derivative in terms of the original series:

$$z'(t) = \sum_{n=0}^{\infty} z_n' t^n = \sum_{n=0}^{\infty} (n+1) z_{(n+1)} t^n. \tag{11}$$

Equating terms, we get $z_n' = (n+1)z_{(n+1)}$. Rearranging for coefficients of the original series, we get the relation

$$z_{(n+1)} = z_n' \big/ (n+1). \tag{12}$$

The core of the method is to use the system of ODEs to replace z_n' with an expression in terms of the system variables. Therefore, each coefficient of the Maclaurin series can be calculated using the previous coefficients, and solutions of arbitrary order can be obtained easily.

Sumudu–Padé resummation method

Sumudu transform

During the early 1990s, a new integral transform called the Sumudu transform was introduced by Watugala [19], who applied it for solving ordinary differential equations in control engineering problems. The Sumudu transform is defined over the set of functions

$$A = \left\{ f(t) \,|\, \exists M, \tau_1, \tau_2 > 0,\ |f(t)| < M e^{\frac{|t|}{\tau_j}},\ if\ t \in (-1)^j \times [0, \infty) \right\} \tag{13}$$

by the following formula:

$$F(u) = S[f(t)] = \frac{1}{u} \int_0^{\infty} e^{-\left(\frac{t}{u}\right)} f(t) dt,\ u \in (-\tau_1, \tau_2). \tag{14}$$

Some Sumudu transform properties were established by Asiru [20], and its fundamental properties were established by Belgacem and coworkers [21,22]. The Sumudu transform has very useful properties that can help to solve complex applications in science and engineering. One of the strong points of this transform is having units preserving properties that enable it to solve problems without resorting to the frequency domain. This point is very helpful, especially for problems with physical dimensions.

Padé approximant

The Padé approximant [23,24] is a type of rational approximation. It is suitable for approximating a divergent function. The approximant is derived by expanding a function as a ratio of two power series and determining both the numerator and denominator coefficients.

If we have a power series $\sum_{i=0}^{\infty} \boldsymbol{c_i z^i}$ representing a function $\boldsymbol{f(z)}$, such that

$$\boldsymbol{f(z)} = \sum_{i=0}^{\infty} \boldsymbol{c_i z^i} \tag{15}$$

a Padé approximant is a rational function:

$$[\boldsymbol{L/M}] = \frac{\boldsymbol{a_0 + a_1 z + \ldots + a_L z^L}}{\boldsymbol{b_0 + b_1 z + \ldots + b_M z^M}} \tag{16}$$

where $\boldsymbol{b_0}$ is chosen to be equal to 1. So, there are $\boldsymbol{L + M + 1}$ unknown coefficients. Normally, the $[\boldsymbol{L/M}]$ should fit the power series Eq. (15) through the orders $1, \boldsymbol{z}, \boldsymbol{z}^2, \ldots, \boldsymbol{z}^{\boldsymbol{L+M}}$. Hence,

$$\sum_{i=0}^{\infty} \boldsymbol{c_i z^i} = \frac{\boldsymbol{a_0 + a_1 z + \ldots + a_L z^L}}{\boldsymbol{b_0 + b_1 z + \ldots + b_M z^M}} + \boldsymbol{O}\left(\boldsymbol{z}^{\boldsymbol{L+M+1}}\right). \tag{17}$$

From Eq. (17), we have

$$\begin{aligned} &\left(\boldsymbol{b_0 + b_1 z + \ldots + b_M z^M}\right)(\boldsymbol{c_0 + c_1 z + \ldots}) \\ &= \boldsymbol{a_0 + a_1 z + \ldots + a_L z^L} + \boldsymbol{O}\left(\boldsymbol{z}^{\boldsymbol{L+M+1}}\right). \end{aligned} \tag{18}$$

Denominator coefficients $\boldsymbol{b_1, \ldots, b_M}$ can be found from Eq. (18) by equating the coefficients of $\boldsymbol{z}^{\boldsymbol{L+1}}, \boldsymbol{z}^{\boldsymbol{L+2}}, \ldots, \boldsymbol{z}^{\boldsymbol{L+M}}$. Numerator