AN EXTENSION TO THE VARIATIONAL ITERATION METHOD FOR SYSTEMS AND HIGHER-ORDER DIFFERENTIAL EQUATIONS

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submitted by **DERYA ALTINTAN** in partial fulfillment of the requirements for the degree of **Philosophy of Doctorate in Department of Scientific Computing, Middle East Technical University** by,

Prof. Dr. Ersan Akyıldız _____
Director, Graduate School of **Applied Mathematics**

Prof. Dr. Bülent Karasözen _____
Head of Department, **Scientific Computing**

Assoc. Prof. Dr. Ömür Uğur _____
Supervisor, **Scientific Computing**

Examining Committee Members:

Prof. Dr. Bülent Karasözen _____
Institute of Applied Mathematics, METU

Prof. Dr. Münevver Tezer _____
Department of Mathematics, METU

Prof. Dr. Gerhard Wilhelm Weber _____
Institute of Applied Mathematics, METU

Assoc. Prof. Dr. Galip Oturanç _____
Department of Mathematics, Selçuk University

Assoc. Prof. Dr. Ömür Uğur _____
Institute of Applied Mathematics, METU

Date: _____

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: DERYA ALTINTAN

Signature :

ABSTRACT

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Altıntan, Derya
Ph.D., Department of Scientific Computing
Supervisor : Assoc. Prof. Dr. Ömür Uğur

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It is obvious that differential equations can be used to model real-life problems. Although it is possible to obtain analytical solutions of some of them, it is in general difficult to find closed form solutions of differential equations. Finding thus approximate solutions has been the subject of many researchers from different areas.

In this thesis, we propose a new approach to Variational Iteration Method (VIM) to obtain the solutions of systems of first-order differential equations. The main contribution of the thesis to VIM is that proposed approach uses restricted variations only for the nonlinear terms and builds up a matrix-valued Lagrange multiplier that leads to the extension of the method (EVIM).

Close relation between the matrix-valued Lagrange multipliers and fundamental solutions of the differential equations highlights the relation between the extended version of the variational iteration method and the classical variation of parameters formula.

It has been proved that the exact solution of the initial value problems for (nonho-

mogenous) linear differential equations can be obtained by such a generalisation using only a single variational step.

Since higher-order equations can be reduced to first-order systems, the proposed approach is capable of solving such equations too; indeed, without such a reduction, variational iteration method is also extended to higher-order scalar equations. Further, the close connection with the associated first-order systems is presented.

Such extension of the method to higher-order equations is then applied to solve boundary value problems: linear and nonlinear ones. Although the corresponding Lagrange multiplier resembles the Green's function, without the need of the latter, the extended approach to the variational iteration method is systematically applied to solve boundary value problems, surely in the nonlinear case as well.

In order to show the applicability of the method, we have applied the EVIM to various real-life problems: the classical Sturm-Liouville eigenvalue problems, Brusselator reaction-diffusion, and chemical master equations. Results show that the method is simple, but powerful and effective.

Keywords: Variational Iteration Method, Lagrange Multipliers, Restricted Variations, Fundamental Matrix

ÖZ

VARYASYONAL İTERASYON METODUNUN SİSTEMLER VE YÜKSEK DERECELİ DİFERANSİYEL DENKLEMLER İÇİN GENİŞLETİLMESİ

Altıntan, Derya
Doktora, Bilimsel Hesaplama Bölümü
Tez Yöneticisi : Doç. Dr. Ömür Uğur

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Günlük hayatta karşılaşılan birçok problemin modellenmesinde diferansiyel denklemler kullanılmaktadır. Bu denklemlerinin bazılarının analitik çözümleri bilinmesine karşın diferansiyel denklemlerin kapalı formda çözümlerinin bulunması genellikle zordur. Dolayısıyla bu tip denklemlerin yaklaşık çözümlerinin bulunması farklı alanlardan birçok araştırmacının çalışma alanını oluşturmaktadır.

Bu tezde birinci derece diferansiyel denklem sistemlerinin çözümlerini elde etmek için Varyasyonal İterasyon Metoduna (VIM) yeni bir yaklaşım önerilmektedir. Tezin Varyasyonal İterasyon Metoduna ana katkısı önerilen metodun sınırlı varyasyonları yalnızca lineer olmayan kısımlarda kullanması ve matris değerli Lagrange çarpanları elde ederek metodun genişlemesini sağlamasıdır (EVIM).

Matris değerli Lagrange çarpanları ve diferansiyel denklemlerin temel çözümleri arasındaki bağlantı varyasyonal iterasyon metodunun genişlemiş versiyonu ile klasik parametrelerin değişimi formülü arasındaki bağlantının vurgulanmasını sağlamaktadır.

Ayrıca, böyle bir genelleştirme ile homojen olmayan lineer diferansiyel denklemler içeren başlangıç değer problemlerinin çözümlerinin sadece bir iterasyon ile bulunabileceğini ispatlanmaktır.

Yüksek dereceli diferansiyel denklemler birinci derece diferansiyel denklem sistemlerine indirgenebildiği için önerilen metod yüksek dereceli diferansiyel denklemlere de uygulanabilmektedir.

Çalışmamızda böyle bir indirgeme olmadan da varyasyonal iterasyon metodunun yüksek dereceli diferansiyel denklemler için genelleştirilebileceği ve karşılık gelen birinci derece sistemler ile bağlantısı sunulmaktadır.

Metodun yüksek dereceli diferansiyel denklemler için elde edilen bu genişlemesi lineer ve lineer olmayan sınır değer problemlerini çözmek için kullanılmaktadır. Elde edilen Lagrange çarpanı Green's fonksiyonuna benzemesine rağmen bu fonksiyona ihtiyaç duyulmadan genişletilmiş varyasyonal iterasyon metodu lineer ve lineer olmayan sınır değer problemlerinin çözümlerinin elde edilmesi için sistemli olarak uygulanmaktadır.

Metodun uygulanabilirliğini göstermek için EVIM, klasik Sturm-Liouville özdeğer problemleri, Brusselator denklemi ve Master denkleminden oluşan farklı problemlerin yaklaşık çözümlerinin bulunması için kullanılmaktadır. Elde edlen sonuçlar metodun oldukça kolay ve güçlü bir metod olduğunu göstermektedir.

Anahtar Kelimeler: Varyasyonal İterasyon Metodu, Lagrange Çarpanı, Sınırlı Varyasyonlar

To my Family...

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CHAPTER 1

INTRODUCTION

Many problems in different disciplines, for instance, biology, physics, chemistry, are modelled by differential equations. Solutions of these problems are used to make predictions about the future behaviour of the physical systems. Although it is possible to solve some simple models analytically, finding approximate if possible closed form solutions of complex models can be very difficult. Different methods have been proposed to obtain approximate solutions of differential equations. Apart from the classical discrete Runge-Kutta methods, there are others such as Adomian decomposition method [4] and homotopy perturbation method [29].

The Variational Iteration Method (VIM) [24, 25, 27] which was introduced by Chinese mathematician J.H. He in 1997 is one of the methods that obtains approximate solutions of differential equations. This method is a modification of the general Lagrange multiplier method which was proposed by Inokuti et al. in 1978 [30]. The key element of VIM is to construct a correction functional using Lagrange multiplier which can be identified via *variational theory* [26] for the corresponding differential equation. By using an initial function a better approximate function within the domain of the problem is obtained by the method. The method, in general, does not use any discretisation, linearisation and perturbation techniques [50].

The VIM has been successfully applied to a large class of problems from different areas. For example, He used the method to solve autonomous differential equations [27]. In [40], Momani, Abuasad and Odibat implemented the method to obtain the solution of nonlinear boundary value problems and in [37], they used the method to obtain the solution of two point boundary value problems. The method has also been applied

to integral equations [60], nonlinear singular boundary value problems [34], prey and predator problems with variable coefficients [62]. Moreover, the method is successfully applied to find eigenvalues of Sturm-Liouville type differential operators [5].

Over the years, modifications of the variational iteration method have been proposed: in [7], Batiha et al. proposed the Multistage Variational Iteration Method (MVIM). In [50], Soltani, Shirzadi proposed a new modification of VIM which aims to get the Lagrange multiplier more efficiently. In [14], piecewise variational iteration method was introduced for Riccati differential equations. In [15], an effective modification of the method which does not use any unknown parameters in the initial function was proposed. In [2], Abassy et al. proposed a new modification of the VIM which tries to reduce the computational work. In [45], Odibat developed modifications of VIM to approximate the solutions of nonlinear problems; in [56], Turkyilmazoglu proposed an optimal variational iteration method; in [49], Salkuyeh applied the method to linear systems of ordinary differential equations with constant coefficients; another modification of VIM was proposed in [1].

The aim of the present work is to introduce the extension of variational iteration method (EVIM) for first-order systems and higher-order initial as well as boundary value problems; and then, to apply the method to different types of problems in order to show advantages of the new approach.

In this chapter, we will investigate the basic principles of VIM and its multistage version, MVIM. Also, we will summarise some properties of calculus of variations. An illustrative example will be given to make a comparison between the VIM and MVIM.

1.1 Calculus of Variations

Calculus of variations is a branch of mathematics that analyses the extreme values of functionals that use functions as variables. Since VIM is based on calculus of variations, it will be useful to summarise some of the properties of it.

In this section, we will state some basic theory of calculus of variations; for more details we refer to [11, 46].

Let $F(t, x, x')$ be a given three times differentiable function with respect to all its variables and $x = x(t)$, $x' = x'(t)$ are continuous in the interval $a \leq t \leq b$. Our aim is to find $x = x(t)$, where the following integral takes its minimum (maximum):

$$J = \int_a^b F(t, x, x')dt. \tag{1.1}$$

To find the function where (1.1) takes its minimum (maximum) value, we must know the basics of variations of functions. The variation of any function $x(t)$ is denoted by δx and

$$\delta x = x(t) - \bar{x}(t),$$

where $\bar{x}(t)$ is any function whose properties depends on the given problem. The derivatives of variation δx is defined as follows

$$\begin{aligned} (\delta x)' &= x'(t) - \bar{x}'(t) = \delta x', \\ (\delta x)'' &= x''(t) - \bar{x}''(t) = \delta x'', \\ &\vdots \\ (\delta x)^{(k)} &= x^{(k)}(t) - \bar{x}^{(k)}(t) = \delta x^{(k)}, \end{aligned} \tag{1.2}$$

for all $k \in \mathbb{N}$.

After these definitions, let us investigate the integral (1.1). Suppose that this integral has its extreme value at $x = x(t)$ and define $\bar{x}(t) \in C^1([a, b], \mathbb{R})$ which is different from $x(t)$. The variation of $x(t)$ will then be $\delta x = x(t) - \bar{x}(t)$ and we let

$$x(t; \alpha) = x(t) + \alpha \delta x. \tag{1.3}$$

If we redefine the integral (1.1) as

$$\phi(\alpha) = \int_a^b F(t, x(t; \alpha), x'(t; \alpha))dt,$$

it is obvious that $\phi = \phi(\alpha)$, as a function of α, takes its extreme value when $\alpha = 0$. Therefore,

$$\phi'(0) = \frac{d\phi}{d\alpha}\Big|_{\alpha=0} = 0.$$

Note that we also use ϕ' to denote the derivative of $\phi(\alpha)$ with respect to α to avoid the abuse of notation, for simplicity. Hence,

$$\phi'(\alpha) = \frac{d}{d\alpha} \int_a^b F(t, x(t; \alpha), x'(t; \alpha))dt. \tag{1.4}$$

Since the function F has continuous derivatives, we get

$$\phi'(\alpha) = \int_a^b \frac{\partial}{\partial \alpha} F(t, x(t;\alpha), x'(t;\alpha))dt. \tag{1.5}$$

Hence, this yields

$$\phi'(\alpha) = \int_a^b \left(F_x \frac{\partial}{\partial \alpha} x(t;\alpha) + F_{x'} \frac{\partial}{\partial \alpha} x'(t;\alpha) \right) dt,$$

where

$$\begin{aligned} F_x &= \frac{\partial}{\partial x} F(t, x(t;\alpha), x'(t;\alpha)), \\ F_{x'} &= \frac{\partial}{\partial x'} F(t, x(t;\alpha), x'(t;\alpha)). \end{aligned} \tag{1.6}$$

By using the definition

$$x(t;\alpha) = x(t) + \alpha \delta x,$$

we get

$$\begin{aligned} \frac{\partial}{\partial \alpha} x(t;\alpha) &= \frac{\partial}{\partial \alpha}(x(t) + \alpha \delta x) = \delta x, \\ \frac{\partial}{\partial \alpha} x'(t;\alpha) &= \frac{\partial}{\partial \alpha}(x'(t) + \alpha \delta x') = \delta x'. \end{aligned} \tag{1.7}$$

Now, (1.5) takes the form

$$\phi'(\alpha) = \int_a^b \left(F_x \delta x + F_{x'} \delta x' \right) dt,$$

so that the integration by parts yields

$$\phi'(\alpha) = \int_a^b \left(F_x - \frac{\partial}{\partial t} \delta x F_{x'} \right) dt + \left(F_{x'} \delta x \right) \Big|_a^b. \tag{1.8}$$

Then, $\phi'(0) = 0$ implies

$$\int_a^b \left(F_x - \frac{\partial}{\partial t} F_{x'} \right) \delta x dt + \left(F_{x'} \delta x \right) \Big|_a^b = 0. \tag{1.9}$$

If we impose the conditions $\bar{x}(a) = x(a)$, $\bar{x}(b) = x(b)$, then the second term on the left hand side of the equation (1.9) will vanish, namely $\left(F_{x'} \delta x \right) \Big|_a^b = 0$. Furthermore, we have

$$F_x - \frac{d}{dt} F_{x'} = 0, \tag{1.10}$$

which is the so-called *Euler equation*.

In previous equations we assume that $\bar{x}(a) = x(a)$, $\bar{x}(b) = x(b)$, that is, $\delta x(a) = \delta x(b) = 0$, so that the boundary term $\left(F_{x'} \delta x \right) \Big|_a^b$ vanishes. On the other hand, in the case of $\bar{x}(a) \neq x(a)$ and $\bar{x}(b) \neq x(b)$, or $\bar{x}(a) \neq x(a)$ and $\bar{x}(b) = x(b)$, or $\bar{x}(a) = x(a)$

and $\bar{x}(b) \neq x(b)$, in order to obtain the equality in (1.9) one should impose the conditions,

$$F_x - \frac{d}{dt}F_{x'} = 0, \quad (F_{x'}\delta x)\Big|_a^b = 0.$$

See [11] for details.

In general we investigate the extreme values of the integral

$$J = \int_a^b F(t, x, x', x'', \ldots, x^{(n)})dt, \tag{1.11}$$

subject to the boundary conditions

$$\begin{aligned} &x(a) = x_a, \quad x'(a) = x'_a, \quad \ldots, \quad x^{(n-1)}(a) = x_a^{(n-1)}, \\ &x(b) = x_b, \quad x'(b) = x'_b, \quad \ldots, \quad x^{(n-1)}(b) = x_b^{(n-1)}, \end{aligned} \tag{1.12}$$

and the function F being $(n+2)$ times differentiable with respect to all of its variables. The argument in the preceding paragraphs will henceforth yield the so-called *Euler-Poisson equation*:

$$F_x - \frac{d}{dt}F_{x'} + \frac{d^2}{dt^2}F_{x''} + \cdots + (-1)^n\frac{d^n}{dt^n}F_{x^{(n)}} = 0. \tag{1.13}$$

The general solution of equation (1.13) includes $2n$ arbitrary constants to be identified by imposing the boundary conditions (1.12).

1.2 He's Variational Iteration Method

In the present section, we will describe the basic concepts of variational iteration method. The results in this section can also be found in [26] and the references therein.

Now, let us consider the following system

$$Tx(t) = g(t), \quad t \in I, \tag{1.14}$$

where T is a differential operator, x is a continuous function for $t \in I$ and $g(t)$ is a given function. The key factor of VIM is to split the differential operator T into its linear and nonlinear parts:

$$Lx(t) + Nx(t) = g(t). \tag{1.15}$$

where L and N denote the linear and nonlinear operators, respectively.

The VIM is a modification of the Lagrange multiplier method [30]. In the following, we will give a short description of the Lagrange multiplier method and explain the relation with the VIM. This part is taken from [26].

The Lagrange multiplier method uses x^0 as an initial function that satisfies $Lx^0 = 0$. Then, by using the functional

$$x(t_1) = x^0(t_1) + \int_{t_0}^{t_1} \lambda\Big\{Lx^0(s) + Nx^0(s) - g(s)\Big\}ds, \tag{1.16}$$

an approximation at a special point t_1 is obtained. Here, λ is called the Lagrange multiplier.

J. H. He constructs the correction functional as follows:

$$x^{n+1}(t) = x^n(t) + \int_{t_0}^{t} \lambda\Big\{Lx^n(s) + N\widetilde{x}^n(s) - g(s)\Big\}ds, \tag{1.17}$$

where $\lambda = \lambda(s;t)$ is referred to as the Lagrange multiplier which can be identified via the variational theory [25,26]. The iterates $x^n(t)$ represent the nth order approximate solution and the $\widetilde{x}^n(s)$'s denote the restricted variations, that is, $\delta\widetilde{x}^n(s) = 0$ for all $n \in \mathbb{N}$, see [12].

The intuitive idea of the method (see [28]) is to define the Lagrange multiplier which satisfies the following equation

$$\delta x^{n+1}(t) = \delta x^n(t) + \delta \int_{t_0}^{t} \lambda\Big\{Lx^n(s) + N\widetilde{x}^n(s) - g(s)\Big\}ds = 0. \tag{1.18}$$

For nonlinear differential equations, in order to obtain the Lagrange multipliers restricted variations are used. The less usage of restricted variations leads to more accurate Lagrange multiplier which causes *faster* approximations.

Although VIM has gained much interest, there has not been sufficient improvements of the method to systems of differential equations, especially the ODEs. Many papers in literature use the method as if the systems are uncoupled, or made uncoupled by forcing restricted variations. In this study we tried to improve the applicability of the method to systems without the need for unnecessary restricted variations so that the coupled systems can also be easily solved by the variational iterations.

1.3 Multistage Variational Iteration Method

In order to extend the validity of VIM for larger time intervals Batiha et al. proposed the MVIM [7]. According to MVIM, the solution of equation (1.15) in $[t_0, T)$ is obtained by dividing the interval into subintervals $[t_0, t_1), [t_1, t_2), \ldots, [t_n, T)$ and applying the following correction functional in each subinterval as

$$x^{n+1}(t) = x^n(t) + \int_{t^*}^{t} \lambda\Big\{ Lx^n(s) + N\widetilde{x}^n(s) - g(s)\Big\} ds, \tag{1.19}$$

where t^* takes the values $t_0, t_1, t_2, \ldots, t_n$ successively. Here, the initial function in $[t^*, t_n)$ is the approximate solution of the previous interval $[t_{n-1}, t^*)$ at the point t^*, namely, $x^0(t) = x^n(t^*)$. In the sequel, it will be observed that the Lagrange multipliers of both VIM and MVIM are the same. See [7, 12, 22, 23] for more details on the multistage version of the method.

In the following example, we will apply the VIM and MVIM to the Lorenz system.

1.4 An Example: the Lorenz System

The first chaotic system was proposed by Lorenz [36] in 1963. Equations in Lorenz system are

$$\dot{x}_1 = \sigma(x_2 - x_1), \tag{1.20a}$$

$$\dot{x}_2 = rx_1 - x_2 - x_1x_3, \tag{1.20b}$$

$$\dot{x}_3 = x_1x_2 - bx_3, \tag{1.20c}$$

where σ, r, b are positive real constants and $\dot{x}_i$ denote the time derivative dx_i/dt for $i = 1, 2, 3$.

In our application, we choose $\sigma = 2.4$, $r = 0.1$, $b = 5$ and start with an initial condition

$$(x_1(0), x_2(0), x_3(0))^T = (-1.6, -2, 3)^T.$$

According to the classical VIM, that is commonly used in literature, the following

correction functionals are constructed:

$$\begin{aligned} x_1^{n+1}(t) &= x_1^n(t) + \int_0^t \lambda_1\Big\{(x_1^n)'(s) + \sigma x_1^n(s) - \sigma\widetilde{x}_2^n(s)\Big\}ds, \\ x_2^{n+1}(t) &= x_2^n(t) + \int_0^t \lambda_2\Big\{(x_2^n)'(s) - r\widetilde{x}_1^n(s) + x_2^n(s) + \widetilde{x}_1^n(s)\widetilde{x}_3^n(s)\Big\}ds, \\ x_3^{n+1}(t) &= x_3^n(t) + \int_0^t \lambda_3\Big\{(x_3^n)'(s) - \widetilde{x}_1^n(s)\widetilde{x}_2^n(s) + bx_3^n(s)\Big\}ds, \end{aligned} \tag{1.21}$$

where $(x_i^n)'$ denotes the derivative dx_i^n/ds for $i = 1, 2, 3$. There, $\lambda_i = \lambda_i(s;t)$ are the Lagrange multipliers and $\widetilde{x}_i^n(s)$ are the restricted variations, that is, $\delta\widetilde{x}_i^n(s) = 0$ for $i = 1, 2, 3$ and for all $n \in \mathbb{N}$. It must be noted that $\delta x_1^n(0) = \delta x_2^n(0) = \delta x_3^n(0) = 0$, for all $n \in \mathbb{N}$. However, it is important to observe that there are many linear terms in (1.21) that are used as restricted variations: this makes the equations easier in order to solve for each of the Lagrange multipliers.

Indeed, to obtain the Lagrange multipliers we take the variation of correction functionals as follows:

$$\begin{aligned} \delta x_1^{n+1}(t) &= \delta x_1^n(t) + \delta\int_0^t \lambda_1\Big\{(x_1^n)'(s) + \sigma x_1^n(s) - \sigma\widetilde{x}_2^n(s)\Big\}ds, \\ \delta x_2^{n+1}(t) &= \delta x_2^n(t) + \delta\int_0^t \lambda_2\Big\{(x_2^n)'(s) - r\widetilde{x}_1^n(s) + x_2^n(s) + \widetilde{x}_1^n(s)\widetilde{x}_3^n(s)\Big\}ds, \\ \delta x_3^{n+1}(t) &= \delta x_3^n(t) + \delta\int_0^t \lambda_3\Big\{(x_3^n)'(s) - \widetilde{x}_1^n(s)\widetilde{x}_2^n(s) + bx_3^n(s)\Big\}ds. \end{aligned}$$

Having used the integration by parts and the calculus of variations, the Lagrange multipliers are thus obtained as

$$\lambda_1(s;t) = -e^{\sigma(s-t)}, \quad \lambda_2(s;t) = -e^{(s-t)}, \quad \lambda_3(s;t) = -e^{b(s-t)}. \tag{1.22}$$

Hence, the correction functionals of VIM are given by

$$\begin{aligned} x_1^{n+1}(t) &= x_1^n(t) + \int_0^t -e^{\sigma(s-t)}\Big\{(x_1^n)'(s) + \sigma x_1^n(s) - \sigma x_2^n(s)\Big\}ds, \\ x_2^{n+1}(t) &= x_2^n(t) + \int_0^t -e^{(s-t)}\Big\{(x_2^n)'(s) - rx_1^n(s) + x_2^n(s) + x_1^n(s)x_3^n(s)\Big\}ds, \\ x_3^{n+1}(t) &= x_3^n(t) + \int_0^t -e^{b(s-t)}\Big\{(x_3^n)'(s) - x_1^n(s)x_2^n(s) + bx_3^n(s)\Big\}ds. \end{aligned}$$

Having obtained $(n+1)$st approximation for the component x_1, one can use this to get $(n+1)$st approximation for x_2 and x_3; likewise, once the $(n+1)$st approximation for x_2 is obtained, it can be used in $(n+1)$st approximation for x_3. More precisely,

we consider, for instance the following recursive correction functionals:

$$\begin{aligned}
x_1^{n+1}(t) &= x_1^n(t) + \int_0^t -e^{\sigma(s-t)}\Big\{(x_1^n)'(s) + \sigma x_1^n(s) - \sigma x_2^n(s)\Big\}ds,\\
x_2^{n+1}(t) &= x_2^n(t) + \int_0^t -e^{(s-t)}\Big\{(x_2^n)'(s) - r x_1^{n+1}(s) + x_2^n(s) + x_1^{n+1}(s)x_3^n(s)\Big\}ds,\\
x_3^{n+1}(t) &= x_3^n(t) + \int_0^t -e^{b(s-t)}\Big\{(x_3^n)'(s) - x_1^{n+1}(s)x_2^{n+1}(s) + b x_3^n(s)\Big\}ds.
\end{aligned}$$

Such a formulation of VIM may be referred to as recursive VIM (rVIM). Clearly, approximate solution in rVIM will depend on the order of equations written in the system. Although this is out of the scope of the thesis, herewith, we prefer to give Table 1.1 to compare the approximate solutions obtained by VIM and rVIM. We use the following notations:

$$\varepsilon_i^{VIM}(t) = \left|x_i^E(t) - x_i^{VIM}(t)\right|, \quad \varepsilon_i^{rVIM}(t) = \left|x_i^E(t) - x_i^{rVIM}(t)\right|$$

for $i = 1, 2, 3$, where $x_i^E(t)$ denotes Runge-Kutta solution of x_i; and $x_i^{VIM}(t)$, and $x_i^{rVIM}(t)$ denote the approximate solutions of x_i at the point t obtained by VIM, and rVIM, respectively.

Table 1.1: Comparison of VIM and rVIM for Lorenz equation for nth-order approximation with $x_1^E(1) = -0.5938$, $x_2^E(1) = -0.2906$ and $x_3^E(1) = 0.0848$.

n	$\varepsilon_1^{VIM}(1)$	$\varepsilon_1^{rVIM}(1)$	$\varepsilon_2^{VIM}(1)$	$\varepsilon_2^{rVIM}(1)$	$\varepsilon_3^{VIM}(1)$	$\varepsilon_3^{rVIM}(1)$
0	1.0062	1.0062	1.7094	1.7094	2.9152	2.9152
1	1.3716	1.3716	2.4914	2.9976	0.5224	0.9361
2	1.5399	1.8353	0.5148	0.0538	0.7260	0.0547
3	0.2956	0.0635	0.0025	0.0052	0.0050	0.0114
4	0.0505	0.0009	0.0200	0.0011	0.0040	0.0039
5	0.0137	0.0001	0.0024	0.0035	0.0112	0.0046

Now it is time to go back to our original problem which has the correction functionals presented in (1.21). By inserting t^* instead of the lower limits of integrations in the correction functionals, we get the correction functionals for multistage version of the method as follows:

$$\begin{aligned}
x_1^{n+1}(t) &= x_1^n(t) + \int_{t^*}^t -e^{\sigma(s-t)}\Big\{(x_1^n)'(s) + \sigma x_1^n(s) - \sigma x_2^n(s)\Big\}ds,\\
x_2^{n+1}(t) &= x_2^n(t) + \int_{t^*}^t -e^{(s-t)}\Big\{(x_2^n)' - r x_1^n(s) + x_2^n(s) + x_1^n(s)x_3^n(s)\Big\}ds,\\
x_3^{n+1}(t) &= x_3^n(t) + \int_{t^*}^t -e^{b(s-t)}\Big\{(x_3^n)'(s) - x_1^n(s)x_2^n(s) + b x_3^n(s)\Big\}ds.
\end{aligned}$$

It must be noted that, unlike the case in VIM, we have $\delta x_1^n(t^*) = \delta x_2^n(t^*) = \delta x_3^n(t^*) = 0$ for all $n \in \mathbb{N}$ in the case of the multistage variational iteration method. Here, $t^* \in$

$\{0, t_1, t_2, \ldots, t_n\}$, and the interval $[0, T)$ is divided into subintervals $[0, t_1)$, $[t_1, t_2)$, ..., $[t_n, T)$.

Numerical comparison between the Runge-Kutta solution, VIM and MVIM for the fifth order approximate solutions for the Lorenz system is depicted in Figure 1.1.

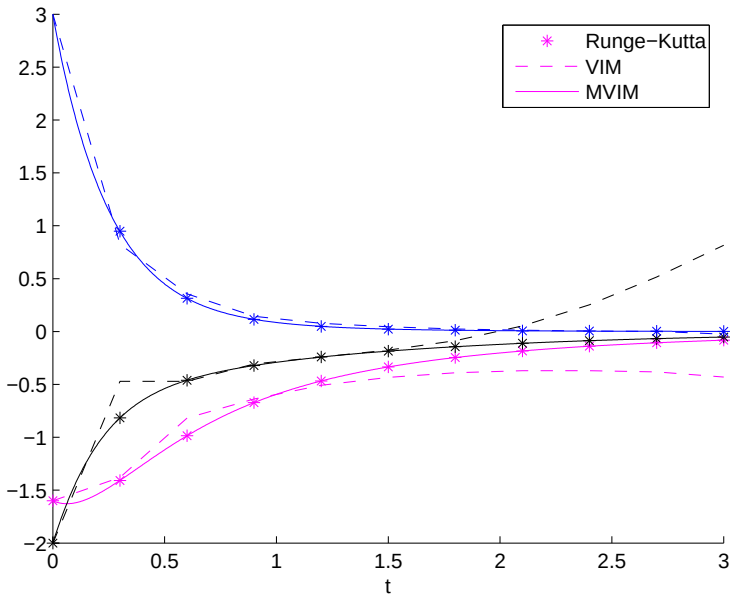

Figure 1.1: Comparison of VIM, MVIM and Runge-Kutta solution for the fifth-order approximation for the chaotic Lorenz system.

To be more specific, in Table 1.2 some numerical results are presented to show the advantage of using MVIM in practice when compared to the standard VIM. Here,

$$\varepsilon_i^{VIM}(t) = \left|x_i^E(t) - x_i^{VIM}(t)\right|, \quad \varepsilon_i^{MVIM}(t) = \left|x_i^E(t) - x_i^{MVIM}(t)\right|,$$

for $i = 1, 2, 3$ where $x_i^E(t)$ is the solution of x_i obtained by Runge-Kutta method, $x_i^{VIM}(t)$, $x_i^{MVIM}(t)$, denote the approximate solutions of x_i obtained by VIM, MVIM for the fifth-order approximations, respectively.

Table 1.2: Comparison of the VIM and MVIM for the fifth-order approximation for (1.20).

t	ε_1^{VIM}	ε_1^{MVIM}	ε_2^{VIM}	ε_2^{MVIM}	ε_3^{VIM}	ε_3^{MVIM}
0	0	0	0	0	0	0
0.3	0.0285	0.0000	0.3463	0.0003	0.1235	0.0002
0.6	0.1683	0.0003	0.0106	0.0005	0.0421	0.0004
0.9	0.0346	0.0001	0.0136	0.0004	0.0290	0.0002
1.2	0.0411	0.0002	0.0007	0.0002	0.0298	0.0001
1.5	0.0985	0.0002	0.0102	0.0002	0.0214	0.0000
1.8	0.1440	0.0002	0.0572	0.0002	0.0126	0.0000
2.1	0.1865	0.0001	0.1639	0.0001	0.0055	0.0000
2.4	0.2320	0.0001	0.3385	0.0001	0.0002	0.0000
2.7	0.2752	0.0001	0.5832	0.0001	0.0003	0.0000
3	0.3482	0.0001	0.8668	0.0001	0.0262	0.0000

CHAPTER 2

EXTENDED VARIATIONAL ITERATION METHOD

In the previous chapter, we have seen that variational iteration method is based on splitting the differential operator into linear and nonlinear parts. Although this method is applicable for many problems, when a system of differential equations is considered it can be difficult to split the linear and nonlinear parts in order to find the Lagrange multipliers.

Let us consider the following system of m first-order nonlinear differential equations

$$\begin{aligned}
\frac{dx_1}{dt} &= a_{11}x_1 + a_{12}x_2 + \cdots + a_{1m}x_m + f_1(t, x_1, x_2, \ldots, x_m), \\
\frac{dx_2}{dt} &= a_{21}x_1 + a_{22}x_2 + \cdots + a_{2m}x_m + f_2(t, x_1, x_2, \ldots, x_m), \\
&\vdots \\
\frac{dx_m}{dt} &= a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mm}x_m + f_m(t, x_1, x_2, \ldots, x_m),
\end{aligned} \tag{2.1}$$

with initial conditions

$$x_1(t_0) = \alpha_1, x_2(t_0) = \alpha_2, \ldots, x_m(t_0) = \alpha_m. \tag{2.2}$$

Here, $A(t) = (a_{ij})(t)$ is an $m \times m$ matrix and $f_j : I \times \mathbb{R}^m \to \mathbb{R}$ are given nonlinear functions for all $1 \leq i, j \leq m$. The correction functionals of the system in the classical approach of the variational iteration technique, however, are given separately by

$$\begin{aligned}
x_k^{n+1}(t) &= x_k^n(t) + \int_{t_0}^{t} \mu_k \Big\{ (x_k^n)'(s) - a_{k1}(s)\widetilde{x}_1^n(s) - a_{k2}(s)\widetilde{x}_2^n(s) - \cdots \\
&\quad - a_{k,k-1}(s)\widetilde{x}_{k-1}^n(s) - a_{kk}(s)x_k^n(s) - a_{k,k+1}(s)\widetilde{x}_{k+1}^n(s) - \cdots \\
&\quad - a_{km}(s)\widetilde{x}_m^n(s) - f_k(s, \widetilde{x}_1^n(s), \widetilde{x}_2^n(s), \ldots, \widetilde{x}_m^n(s)) \Big\} ds,
\end{aligned}$$

subject to the initial condition

$$x_k^0(t) = \alpha_k,$$

where $\mu_k = \mu_k(s;t)$ denote the Lagrange multipliers for $k = 1, 2, \ldots, m$, $\widetilde{x}_i^n(s)$ represent the restricted variations for all $i = 1, 2, \ldots, k-1, k+1, \ldots, m$ and $(x_k^n)'(s)$ is the derivative $dx_k^n(s)/ds$. See the example given in Section 1.4.

It must be noted that the classical approach employs the restricted variations *not only to the nonlinear terms, but also to the linear ones.* Accuracy of such an approach clearly depends on the order of the equations placed in the system. In order to overcome such an inconsistency and apply the method correctly, we present a new approach to VIM, and consider the system (2.1) as a whole. Such an investigation yields theoretically interesting results, and generalises the Lagrange multipliers.

2.1 Generalisation of the Lagrange Multipliers

It is possible to write system (2.1) and (2.2) as follows:

$$\dot{\mathbf{x}} = A(t)\mathbf{x} + \mathbf{f}(t, \mathbf{x}), \quad \mathbf{x}(t_0) = \alpha_0, \tag{2.3}$$

where

$$A(t) = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mm} \end{pmatrix}, \quad \mathbf{f}(t, \mathbf{x}) = \begin{pmatrix} f_1(t, x_1, x_2, \ldots, x_m) \\ f_2(t, x_1, x_2, \ldots, x_m) \\ \vdots \\ f_m(t, x_1, x_2, \ldots, x_m) \end{pmatrix},$$

$$\mathbf{x} = (x_1, x_2, \ldots, x_m)^T, \quad \mathbf{x}(t_0) = \alpha_0 = (\alpha_1, \alpha_2, \ldots, \alpha_m)^T,$$

and $\dot{\mathbf{x}}$ represents the derivative $d\mathbf{x}/dt$ of the state vector $\mathbf{x}$.

The correction functional of system (2.3) is written in the form

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) + \int_{t_0}^{t} \Lambda_A(s;t)\Big\{L\mathbf{x}^n(s) + N\widetilde{\mathbf{x}}^n(s)\Big\}ds. \tag{2.4}$$

Here, $\Lambda_A(s;t)$ denotes the Lagrange multiplier. Since the new system (2.3) is constructed by vectors and matrices, it is trivial that $\Lambda_A(s;t)$ is an $m \times m$ matrix-valued function. L and N are the linear and nonlinear operators, respectively. Finally, $\widetilde{\mathbf{x}}^n(s)$ is the restricted variation.

Linear and nonlinear terms in (2.3) can be written as follows:

$$L\mathbf{x} = \frac{d\mathbf{x}}{dt} - A(t)\mathbf{x}, \quad N\mathbf{x} = -\mathbf{f}(t, \mathbf{x}).$$

By using the calculus of variations and the integration by parts, we find that the Lagrange multiplier must satisfy the system

$$\begin{aligned} \Lambda'_A(s;t) &= -\Lambda_A(s;t)A(s), \\ \Lambda_A(t;t) &= -E, \end{aligned} \tag{2.5}$$

where E is the $m \times m$ identity matrix and $\Lambda'_A(s;t) = \dfrac{\partial \Lambda_A}{\partial s}$.

Before solving system (2.5), we consider the following differential equation

$$\dot{X} = A(t)X, \tag{2.6}$$

subject to the initial condition

$$X(s) = E.$$

It is known that the solution of system (2.6) satisfies the equation

$$X(t) = \Phi(t;s) := \Phi(t)\Phi^{-1}(s),$$

where $\Phi(t)$ is the fundamental matrix of the corresponding homogeneous system

$$\dot{\mathbf{x}} = A(t)\mathbf{x}. \tag{2.7}$$

From the theory of ordinary differential equations, the adjoint of (2.6) is of the form

$$\dot{Y} = -A^T(t)Y, \tag{2.8}$$

and we impose the following initial condition to the adjoint system (2.8):

$$Y(s) = -E.$$

Hence, the unique solution of the adjoint system satisfying the initial condition is given by

$$Y(t) = -\Psi(t;s) = -\Psi(t)\Psi^{-1}(s),$$

where $\Psi(t)$ denotes a fundamental matrix for the adjoint system

$$\dot{\mathbf{y}} = -A^T(t)\mathbf{y}$$

for (2.7). It is not difficult to prove $\Psi^T(t;s) = \Phi^{-1}(t;s)$. Furthermore, if we use the transpose of the system given in (2.8), we obtain

$$\dot{Y}^T = -Y^T A(t), \quad Y^T(s) = -E.$$

This, however, coincides with (2.5); therefore, the Lagrange multiplier can be written as follows:

$$Y^T(t) = \Lambda_A(t;s) = -\Psi^T(t;s) = -\Phi^{-1}(t;s).$$

Since $\Phi^{-1}(t;s) = \Phi(s;t)$, we thence prove the following theorem.

Theorem 2.1. *Let $\Lambda_A(s;t)$ be the Lagrange multiplier associated with the correction functional form (2.4) for the differential equation in (2.3). Then,*

$$\Lambda_A(s;t) = -\Phi(t)\Phi^{-1}(s) = -\Phi(t;s), \tag{2.9}$$

is true for any fundamental matrix $\Phi(t)$ of the corresponding linear homogeneous equation (2.7).

Corollary 2.1. *Let $A(t) = A$ be a constant $m \times m$ matrix in (2.3). Then, the corresponding Lagrange multiplier in (2.4) is given by*

$$\Lambda_A(s;t) = -e^{-A(s-t)}.$$

Proof. Since $\Phi(t) = e^{At}$ is a fundamental matrix, it follows from Theorem 2.1 that

$$\Lambda_A(s;t) = -\Phi(t;s) = -e^{At}e^{-As} = -e^{-A(s-t)}.$$

This completes the proof. ■

The corollary above gives us the opportunity to use linearisation of the systems considered in certain cases, for instance, about (hyperbolic) equilibrium points. Not only due to such applications, but also due to its theoretical importance, we will investigate first, in the next section, the case when the linear operators have constant coefficients.

2.2 Lagrange Multipliers associated with the Jordan Forms

In this section, we illustrate the alternative approach to VIM in order to solve systems of the form

$$\dot{\mathbf{x}} = A\mathbf{x} + \mathbf{f}(t,\mathbf{x}), \quad \mathbf{x}(t_0) = \alpha_0, \tag{2.10}$$

where A is $m \times m$ constant matrix and $\mathbf{f} : I \times \mathbb{R}^m \to \mathbb{R}^m$ are known nonlinear functions. Moreover, we wish the new approach should solve the system (2.10) by avoiding the

restricted variations in the linear terms. In fact, such systems as in (2.10) are of great importance in applied nonlinear dynamics when it is linearised about a hyperbolic fixed point.

In the previous section we have seen that by using Corollary 2.1 it is possible to obtain Lagrange multiplier of the system (2.10) directly. In this section, however, we will try to obtain Lagrange multiplier of system (2.10) by using Jordan canonical form of the matrix A.

Let us introduce the transformation $\mathbf{x} = P\mathbf{y}$ where P is $m \times m$ nonsingular matrix which satisfies $P^{-1}AP = J$. Substitution of the transformation into (2.10) gives us

$$P\dot{\mathbf{y}} = AP\mathbf{y} + \mathbf{f}(t, P\mathbf{y}),$$

and we obtain

$$\dot{\mathbf{y}} = J\mathbf{y} + \mathbf{F}(t, \mathbf{y}) \quad \mathbf{y}(t_0) = P^{-1}\alpha_0 = \beta_0 = (\beta_1, \beta_2, \ldots, \beta_m)^T, \tag{2.11}$$

where $\mathbf{F}(t, \mathbf{y}) = P^{-1}\mathbf{f}(t, P\mathbf{y})$. Then, the correction functional of the system (2.11) can be written in the following form

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_{t_0}^{t} \Lambda_J(s;t)\Big\{\mathcal{L}\mathbf{y}^n(s) + \mathcal{N}\widetilde{\mathbf{y}}^n(s)\Big\}ds, \tag{2.12}$$

where $\Lambda_J(s;t)$ is the Lagrange multiplier and $\widetilde{\mathbf{y}}^n(s)$ is the restricted variation. Linear and nonlinear terms are respectively defined by

$$\mathcal{L}\mathbf{y} = \frac{d\mathbf{y}}{dt} - J\mathbf{y}, \quad \mathcal{N}\mathbf{y} = -\mathbf{F}(t, \mathbf{y}).$$

Similar to $\Lambda_A(s;t)$, $\Lambda_J(s;t)$ is $m \times m$ matrix-valued function. By using the results of the previous section, we can obtain $\Lambda_J(s;t)$ in the following form

$$\Lambda_J(s;t) = -e^{-J(s-t)}. \tag{2.13}$$

On the other hand, if we did not use the transformation $\mathbf{x} = P\mathbf{y}$, we would obtain the Lagrange multiplier of the system (2.10) as follows:

$$\Lambda_A(s;t) = -e^{-A(s-t)}.$$

We can see the following relation between the Lagrange multiplier of the new system $\Lambda_J(s;t) = -e^{-J(s-t)}$ and the Lagrange multiplier of the original system $\Lambda_A(s;t) =$

$-e^{-A(s-t)}$:

$$\Lambda_J(s;t) = -e^{-J(s-t)} = -e^{-P^{-1}AP(s-t)} = -P^{-1}e^{-A(s-t)}P = P^{-1}\Lambda_A(s;t)P.$$

Hence, the relations between the linear and nonlinear terms of systems (2.4) and (2.12) can easily be obtained as

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_{t_0}^{t} \Lambda_J(s;t)\Big\{\mathcal{L}\mathbf{y}^n(s) + \mathcal{N}\widetilde{\mathbf{y}}^n(s)\Big\}ds,$$

so that the transformation $\mathbf{x} = P\mathbf{y}$ yields

$$P^{-1}\mathbf{x}^{n+1}(t) = P^{-1}\mathbf{x}^n(t) + \int_{t_0}^{t} P^{-1}\Lambda_A(s;t)P\Big\{\mathcal{L}(P^{-1}\mathbf{x}^n(s)) + \mathcal{N}(P^{-1}\widetilde{\mathbf{x}}^n(s))\Big\}ds,$$

and, hence,

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) + \int_{t_0}^{t} \Lambda_A(s;t)\Big\{P(\mathcal{L}\circ P^{-1})\mathbf{x}^n(s) + P(\mathcal{N}\circ P^{-1})\widetilde{\mathbf{x}}^n(s)\Big\}ds,$$

where $\circ$ denotes the compositions

$$(\mathcal{L}\circ P^{-1})\mathbf{x} = \mathcal{L}(P^{-1}\mathbf{x}) \quad \text{and} \quad (\mathcal{N}\circ P^{-1})\mathbf{x} = \mathcal{N}(P^{-1}\mathbf{x}).$$

Then, we get

$$L = P(\mathcal{L}\circ P^{-1}) \quad \text{and} \quad N = P(\mathcal{N}\circ P^{-1}).$$

Nevertheless, the following proposition is a consequence of (2.13).

Proposition 2.2. *Let $m = 2$, then the followings are true.*

Case I. if $J = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$, *then*

$$\Lambda_J(s;t) = -\begin{pmatrix} e^{-\lambda_1(s-t)} & 0 \\ 0 & e^{-\lambda_2(s-t)} \end{pmatrix},$$

Case II. if $J = \begin{pmatrix} \xi & \eta \\ -\eta & \xi \end{pmatrix}$, *then*

$$\Lambda_J(s;t) = -e^{-\xi(s-t)}\begin{pmatrix} \cos\eta(s-t) & -\sin\eta(s-t) \\ \sin\eta(s-t) & \cos\eta(s-t) \end{pmatrix},$$

Case III. if $J = \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$, *then*

$$\Lambda_J(s;t) = -e^{-\lambda(s-t)} \begin{pmatrix} 1 & -(s-t) \\ 0 & 1 \end{pmatrix}.$$

where $\lambda, \lambda_1, \lambda_2, \xi, \eta$ *are real constants depending on the eigenvalues of* A.

The proof of the above proposition is straightforward from Corollary 2.1 and the use of (2.13) with the definition of the exponential of a matrix. *It is important to note that the use of the restricted variations is only in the nonlinear term* $\mathcal{N}\mathbf{y} = -\mathbf{f}(t, \mathbf{y})$, *but not in the linear one* $\mathcal{L}\mathbf{y} = \left(\frac{d}{dt} - J\right)\mathbf{y}$. Finally, using the transformation, $\mathbf{x} = P\mathbf{y}$, we can obtain the solution of the original system (2.10).

Meanwhile, direct extension of the proposition to higher dimensions is trivial since the blocks of the Jordan form for an $m \times m$ matrix consist of the ones in Proposition 2.2.

Computationally, in order to obtain the Jordan form J of the coefficient matrix A of the system in its linear part, one may use standard algorithms for computing eigenvalues: by-products of such algorithms are the eigenvectors that form the columns of the transformation matrix P. Practically, this is not a big problem. Nevertheless, the variational iteration method assumes that the solution of the linear system is known *a priori*. Without loss of generality, one may introduce an arbitrary linear differential operator whose null-space is known, such as $L\mathbf{x} \equiv \dot{\mathbf{x}}$, as is commonly used in related literature. Unfortunately, however, this causes inaccurate results in computational applications.

Following examples illustrate how important to consider the linear parts for each case presented in Proposition 2.2.

Example 2.3 (Case I)**.** Consider the following system

$$\dot{\mathbf{x}} = A\mathbf{x} = \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix} \mathbf{x}, \quad \mathbf{x}(0) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{2.14}$$

the solution of system (2.14) has the following form

$$\mathbf{x}(t) = \Phi(t;0)\mathbf{x}(0) = \Phi(t)\Phi^{-1}(0)\mathbf{x}(0),$$

where the fundamental matrix $\Phi(t)$ is given by

$$\Phi(t) = \begin{pmatrix} 2e^t & 0 \\ e^t & e^{-t} \end{pmatrix}.$$

Therefore, this leads to the solution

$$\begin{aligned} \mathbf{x}(t) &= \begin{pmatrix} e^t & 0 \\ \frac{1}{2}\left(e^t + e^{-t}\right) & e^{-t} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= (e^t, \tfrac{1}{2}\left(e^t + e^{-t}\right))^T. \end{aligned} \tag{2.15}$$

Classical: According to the classical VIM, we obtain the following correction functionals of (2.14) separately as follows:

$$x_1^{n+1}(t) = x_1^n(t) + \int_0^t \mu_1 \Big\{ (x_1^n)'(s) - x_1^n(s) \Big\} ds, \tag{2.16a}$$

$$x_2^{n+1}(t) = x_2^n(t) + \int_0^t \mu_2 \Big\{ (x_2^n)'(s) - \widetilde{x}_1^n(s) + x_2^n(s) \Big\} ds, \tag{2.16b}$$

where $\mu_1 = \mu_1(s;t)$ and $\mu_2 = \mu_2(s;t)$ denote the Lagrange multipliers, and $\widetilde{x}_1^n(s)$ in (2.16b) is the restricted variation. It must be noted that $\delta x_1^n(0) = \delta x_2^n(0) = 0$. It is not difficult to observe that although $x_1^n(s)$ is a linear term, it is used as restricted variation in (2.16b).

The Lagrange multipliers in the classical sense, can be identified by

$$\mu_1(s;t) = -e^{-(s-t)}, \quad \mu_2(s;t) = -e^{(s-t)}.$$

Substituting the Lagrange multipliers into the correction functionals yields

$$\begin{aligned} x_1^{n+1}(t) &= x_1^n(t) + \int_0^t -e^{-(s-t)} \Big\{ (x_1^n)'(s) - x_1^n(s) \Big\} ds, \\ x_2^{n+1}(t) &= x_2^n(t) + \int_0^t -e^{(s-t)} \Big\{ (x_2^n)'(s) - x_1^n(s) + x_2^n(s) \Big\} ds, \end{aligned}$$

with $x_1^0(t) = 1$ and $x_2^0(t) = 1$, as the initial approximations.

Extended: The eigenvalues of A are $\lambda_1 = 1$, $\lambda_2 = -1$. Therefore, it is possible to find the nonsingular matrix P as

$$P = \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}, \quad P^{-1} = \begin{pmatrix} 1/2 & 0 \\ -1/2 & 1 \end{pmatrix}.$$

Then, by using the transformation $\mathbf{x} = P\mathbf{y}$ we obtain

$$\dot{\mathbf{y}} = P^{-1}AP\mathbf{y} = J\mathbf{y}, \quad \mathbf{y}(0) = P^{-1}\mathbf{x}(0), \tag{2.17}$$

where

$$J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad y(0) = (1/2, 1/2)^T.$$

According to the Extended Variational Iteration Method (EVIM), correction functional of system (2.17) is constructed to give

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_0^t \Lambda_J(s;t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s)\Big\}ds, \tag{2.18}$$

where we do not use any restricted variations at all. The Lagrange multiplier $\Lambda_J(s;t)$ is

$$\Lambda_J(s;t) = -e^{-J(s-t)} = -\begin{pmatrix} e^{-(s-t)} & 0 \\ 0 & e^{(s-t)} \end{pmatrix}.$$

Meanwhile, by using the relation $\Lambda_A(s;t) = P\Lambda_J(s;t)P^{-1}$, we have

$$\Lambda_A(s;t) = -\begin{pmatrix} -e^{-(s-t)} & 0 \\ \frac{1}{2}(e^{(s-t)} - e^{-(s-t)}) & -e^{(s-t)} \end{pmatrix}.$$

If we take $\mathbf{y}^0(t) = \mathbf{y}(0)$, we obtain $\mathbf{y}^1(t)$ in the following form

$$\begin{aligned} \mathbf{y}^1(t) &= \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} + \int_0^t \begin{pmatrix} e^{-(s-t)} & 0 \\ 0 & e^{(s-t)} \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} ds \\ &= \left(\frac{e^t}{2}, \frac{e^{-t}}{2}\right)^T, \end{aligned}$$

Hence, by using the transformation $\mathbf{x} = P\mathbf{y}$, we obtain $\mathbf{x}^1(t) = \left(e^t, \frac{1}{2}(e^t + e^{-t})\right)^T$ which is the exact solution of (2.14).

Example 2.4 (Case II)**.** Now, let us consider the system of the following form

$$\dot{\mathbf{x}} = A\mathbf{x} = \begin{pmatrix} -1 & 5 \\ -1 & 3 \end{pmatrix}\mathbf{x}, \quad \mathbf{x}(0) = \begin{pmatrix} 2 \\ 3 \end{pmatrix}. \tag{2.19}$$

The matrix A has complex eigenvalues $1 \mp i$. The transformation $\mathbf{x} = P\mathbf{y}$ yields to the reduced system

$$\dot{\mathbf{y}} = P^{-1}AP\mathbf{y} = J\mathbf{y}, \quad \mathbf{y}(0) = P^{-1}\mathbf{x}(0), \tag{2.20}$$

where

$$P = \begin{pmatrix} 1/2 & 1 \\ 0 & 1/2 \end{pmatrix}, \quad P^{-1} = \begin{pmatrix} 2 & -4 \\ 0 & 2 \end{pmatrix}, \quad J = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

In other words, we obtain

$$\dot{\mathbf{y}} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \mathbf{y}, \tag{2.21}$$

subject to the initial condition

$$\mathbf{y}(0) = (-8, 6)^T.$$

The correction functional of the reduced system (2.21) is given by

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_0^t \Lambda_J(s;t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s)\Big\}ds, \tag{2.22}$$

with $y^0(t) = (-8, 6)^T$, where the Lagrange multiplier $\Lambda_J(s;t)$ has the form

$$\Lambda_J(s;t) = -e^{-(s-t)} \begin{pmatrix} \cos(s-t) & -\sin(s-t) \\ \sin(s-t) & \cos(s-t) \end{pmatrix}.$$

By using the correction functional (2.22), we get

$$y^1(t) = (-8e^t\cos(t) + 6e^t\sin(t), 6e^t\cos(t) + 8e^t\sin(t))^T.$$

Hence,

$$x^1(t) = \big(2e^t\cos(t) + 11e^t\sin(t), 3e^t\cos(t) + 4e^t\sin(t)\big)^T,$$

which is the exact solution of (2.19).

Example 2.5 (Case III)**.** Finally, we consider the following system

$$\dot{\mathbf{x}} = A\mathbf{x} = \begin{pmatrix} 8 & -3 \\ 12 & -4 \end{pmatrix} \mathbf{x}, \quad \mathbf{x}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2.23}$$

Since the matrix A has repeated eigenvalues $\lambda_{1,2} = 2$, it has the Jordan canonical form $J = P^{-1}AP$, where

$$J = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} 6 & 1 \\ 12 & 0 \end{pmatrix}, \quad P^{-1} = \begin{pmatrix} 0 & 1/12 \\ 1 & -1/2 \end{pmatrix}.$$

The transformation $\mathbf{x} = P\mathbf{y}$ gives the following differential equation

$$\dot{\mathbf{y}} = J\mathbf{y} = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix} \mathbf{y}, \tag{2.24}$$

with initial condition

$$y(0) = (0, 1)^T.$$

Hence, the corresponding correction functional is of the form

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_0^t \Lambda_J(s;t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s)\Big\}ds,$$

where

$$\Lambda_J(s;t) = -e^{-2(s-t)} \begin{pmatrix} 1 & -(s-t) \\ 0 & 1 \end{pmatrix}.$$

Then, the first approximation is obtained as $y^1(t) = (e^{2t}t, e^{2t})^T$. This result yields $x^1(t) = (6e^{2t}t + e^{2t}, 12e^{2t}t)^T$, the exact solution of (2.23).

In the next section, illustrations and verifications of the results will be presented. Firstly, we will apply EVIM to an equation with constant coefficients, namely Lorenz equation. Secondly, the method will be used to obtain the solution of Cauchy-Euler equation which has variable coefficients. It is shown that unlike the classical VIM, EVIM obtains the solution with a single iteration. Finally, we will approximate the solution of a (nonlinear) Bernoulli equation and compare it with the modified variational iteration method for solving Riccati differential equations proposed by Geng [13].

2.3 Illustrative Examples for the Extended Variational Iterations

2.3.1 Lorenz System — revisited

In this section of the thesis, we will apply EVIM to autonomous systems, but of the form

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t)), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0, \tag{2.25}$$

where $\mathbf{x}$ is an m vector, A is an $m \times m$ constant matrix, and $\mathbf{f} : \mathbb{R}^m \longrightarrow \mathbb{R}^m$ is a function that is generally nonlinear in the components of $\mathbf{x}$.

The Lorenz system is described by the following differential system

$$\begin{aligned} \dot{x}_1 &= \sigma(x_2 - x_1), \\ \dot{x}_2 &= rx_1 - x_2 - x_1x_3, \\ \dot{x}_3 &= x_1x_2 - bx_3, \end{aligned} \tag{2.26}$$

where σ, r, b are positive real numbers.

In our example, we will use the same values for the parameters and initial conditions that were used in Section 1.4, namely, $\sigma = 2.4$, $r = 0.1$, $b = 5$ and

$$(x_1(0), x_2(0), x_3(0))^T = (-1.6, -2, 3)^T.$$

Equation (2.26) can be written as follows:

$$\dot{\mathbf{x}} = A\mathbf{x} + \mathbf{f}(\mathbf{x}), \quad \mathbf{x}(0) = (-1.6, -2, 3)^T, \tag{2.27}$$

where

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad A = \begin{pmatrix} -2.4 & 2.4 & 0 \\ 0.1 & -1 & 0 \\ 0 & 0 & -5 \end{pmatrix}, \quad \mathbf{f}(\mathbf{x}) = \begin{pmatrix} 0 \\ -x_1 x_3 \\ x_1 x_2 \end{pmatrix}.$$

Introducing $\mathbf{x} = P\mathbf{y}$ for $\mathbf{y} = (y_1, y_2, y_3)^T$, the system (2.27) can be transformed to the following equation

$$\begin{aligned} \dot{\mathbf{y}} &= J\mathbf{y} + \mathbf{F}(\mathbf{y}) = \begin{pmatrix} -2.5544 & 0 & 0 \\ 0 & -0.8456 & 0 \\ 0 & 0 & -5 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \\ &\quad + \begin{pmatrix} 1.4045 y_1 y_3 + 1.1813 y_2 y_3 \\ -1.6699 y_1 y_3 - 1.4045 y_2 y_3 \\ -0.0641 y_1^2 + 0.4886 y_1 y_2 + 0.4563 y_2^2 \end{pmatrix}, \end{aligned} \tag{2.28}$$

and the initial state of the system (2.28) is given

$$\mathbf{y}(0) = (-1.3564, 3.5189, 3.0000)^T.$$

Here, the transformation matrix P has the form

$$P = \begin{pmatrix} -0.9979 & -0.8393 & 0 \\ 0.0642 & -0.5436 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Hence, we can construct the following correction functional

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_0^t \Lambda_J(s;t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s) - \mathbf{F}(\widetilde{\mathbf{y}}^n(s))\Big\} ds, \tag{2.29}$$

with $\mathbf{y}^0(t) = \mathbf{y}(0)$, and $\widetilde{\mathbf{y}}^n(s)$ is the restricted variation vector. The Lagrange multiplier $\Lambda_J(s;t)$ is as follows

$$\Lambda_J(s;t) = \operatorname{diag}\left(-e^{2.5544(s-t)},\ -e^{0.8456(s-t)},\ -e^{5(s-t)}\right).$$

It must be noted that there are differences between $\Lambda_J(s;t)$ and the Lagrange multipliers $\lambda_1(s,t)$, $\lambda_2(s,t)$, $\lambda_3(s,t)$ obtained in Section 1.4: see (1.22) on page 8.

Furthermore, using the multistage version of the VIM, we divide the interval $[0,T)$ into subintervals $[0,t_1), [t_1,t_2), \ldots, [t_n,T)$ and rewrite the correction functional (2.29) as

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_{t^\star}^{t} \Lambda_J(s;t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s) - \mathbf{F}(\widetilde{\mathbf{y}}^n(s))\Big\}ds, \tag{2.30}$$

where $t^\star \in \{0, t_1, t_2, \ldots, t_n\}$.

Figure 2.1 illustrates the results of Runge Kutta solution, EVIM, MEVIM for the fifth order approximate solution. Further, we use the following notations in Table 2.1

$$\varepsilon_i^{EVIM}(t) = \left|x_i^E(t) - x_i^{EVIM}(t)\right|, \quad \varepsilon_i^{MEVIM}(t) = \left|x_i^E(t) - x_i^{MEVIM}(t)\right|,$$

for $i = 1, 2, 3$, where $x_i^E(t)$ denotes Runge-Kutta solution of x_i and $x_i^{EVIM}(t)$, $x_i^{MEVIM}(t)$, denote the fifth-order approximate solutions of x_i obtained by EVIM, MEVIM, respectively.

Table 2.1: Comparison of the EVIM and MEVIM for the fifth-order approximation for (2.26).

t	ε_1^{EVIM}	ε_1^{MEVIM}	ε_2^{EVIM}	ε_2^{MEVIM}	ε_3^{EVIM}	ε_3^{MEVIM}
0	0	0	0	0	0	0
0.3	0.1882	0.0005	0.3152	0.0004	0.1382	0.0001
0.6	0.1064	0.0001	0.0494	0.0003	0.0229	0.0004
0.9	0.0342	0.0001	0.0061	0.0002	0.0003	0.0002
1.2	0.0178	0.0001	0.0110	0.0001	0.0060	0.0000
1.5	0.0092	0.0001	0.0161	0.0001	0.0125	0.0000
1.8	0.0075	0.0001	0.0181	0.0001	0.0160	0.0000
2.1	0.0095	0.0001	0.0185	0.0001	0.0215	0.0000
2.4	0.0122	0.0001	0.0172	0.0001	0.0344	0.0000
2.7	0.0143	0.0001	0.0099	0.0000	0.0574	0.0000
3	0.0333	0.0001	0.0208	0.0000	0.0762	0.0000

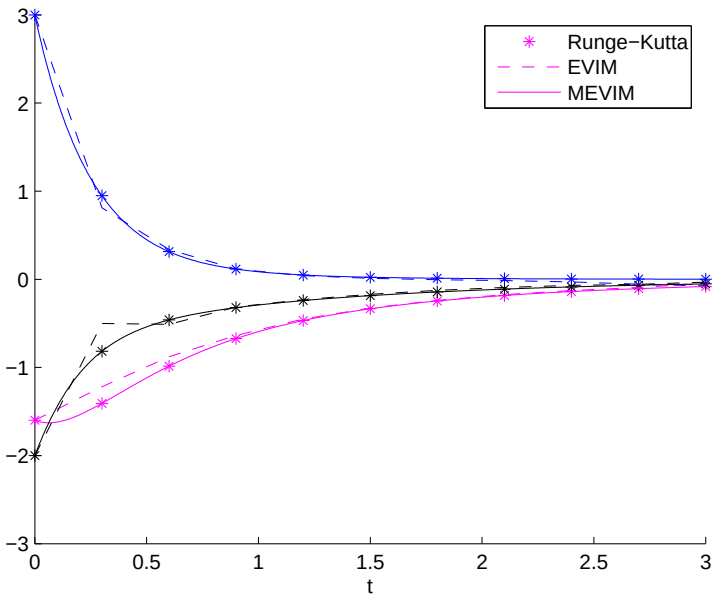

Figure 2.1: Comparison of EVIM, MEVIM and Runge-Kutta solution for the Lorenz system.

2.3.2 Cauchy-Euler Equations

Example in Section 2.3 demonstrates that EVIM can be applied to first-order differential equations of the form

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t)), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0. \tag{2.31}$$

Here, $\mathbf{x}$ is an $m-$vector, A is an $m \times m$ constant matrix and $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ is given nonlinear function.

We must recall that approximate solutions of (2.31) are obtained via the following correction functional

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) + \int_0^t -\Phi(t;s)\Big\{(\mathbf{x}^n)'(s) - A\mathbf{x}^n(s) - \mathbf{f}(\mathbf{x}^n(s))\Big\}ds,$$

where $\Phi(t;s) = \Phi(t)\Phi^{-1}(s)$, and $\Phi(t)$ is the fundamental solution of the linear homogeneous equation, $\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t)$.

The EVIM is surely applicable to the systems of the form

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{f}(t), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0, \tag{2.32}$$

in particular. The difference between (2.31) and (2.32) is that in the former A is a constant matrix while in the latter it is an $m \times m$ matrix of functions defined on I. However, (2.32) is linear, but (2.31) is in general nonlinear.

In Chapter 2, it is seen that EVIM obtains the exact solution of $\dot{\mathbf{x}}(t) = A\mathbf{x}(t)$ with only a single iteration. This example shows that when the initial approximation satisfies the initial condition then the first approximation obtained via EVIM is the exact solution of (2.32). This fact will be proved in Theorem 2.6.

Consider the following Cauchy-Euler equation,

$$t^2\ddot{x} - 3t\dot{x} + 4x = t, \quad t \in [1, \infty), \tag{2.33}$$

subject to the initial condition $x(1) = 2$, $\dot{x}(1) = 2$. By using the transformation $x_1 = x$, $x_2 = \dot{x}$, equation (2.33) and the initial conditions can be rewritten as

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{f}(t), \quad \mathbf{x}(1) = (2, 2)^T, \tag{2.34}$$

where

$$A(t) = \begin{pmatrix} 0 & 1 \\ -4/t^2 & 3/t \end{pmatrix}, \quad \mathbf{f}(t) = \begin{pmatrix} 0 \\ 1/t \end{pmatrix}.$$

The fundamental matrix $\Phi(t)$ of the homogeneous system $\dot{\mathbf{x}} = A(t)\mathbf{x}(t)$ is

$$\Phi(t) = \begin{pmatrix} t^2 & t^2\ln(t) \\ 2t & 2t\ln(t) + t \end{pmatrix},$$

and hence, the solution of (2.34) is found to be

$$\mathbf{x}(t) = \big(t^2 - t^2\ln(t) + t,\ t - 2t\ln(t) + 1\big)^T.$$

Classical: For an approximate solution using VIM in literature so far, the following correction functionals are used:

$$\begin{aligned} x_1^{n+1}(t) &= x_1^n(t) + \int_1^t \lambda_1\Big\{(x_1^n)'(s) - \widetilde{x}_2^n(s)\Big\}ds, \\ x_2^{n+1}(t) &= x_2^n(t) + \int_1^t \lambda_2\Big\{(x_2^n)'(s) + \frac{4\widetilde{x}_1^n(s)}{s^2} - \frac{3\widetilde{x}_2^n(s)}{s} + \frac{1}{\widetilde{s}}\Big\}ds. \end{aligned} \tag{2.35}$$

Here, $\lambda_1 = \lambda_1(s;t), \lambda_2 = \lambda_2(s;t)$ are the Lagrange multipliers and $\widetilde{x}_1^n(s)$, $\widetilde{x}_2^n(s)$ are the restricted variations and that $\delta x_1^n(1) = \delta x_2^n(1) = 0$ holds for all $n \in \mathbb{N}$.

The Lagrange multipliers considered in the classical approach are in general

$$\lambda_1(s;t) = -1, \quad \lambda_2(s;t) = -1,$$

and the initial approximations for (2.35) are in general $x_1^0(t) = 2$, $x_2^0(t) = 2$.

Extended: Having generalised the Lagrange multipliers, the new approach used in this thesis gives the following correction functional:

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) + \int_1^t \Lambda_A(s;t)\Big\{(\mathbf{x}^n)'(s) - A(s)\mathbf{x}^n(s) - \widetilde{\mathbf{f}}(s)ds\Big\},$$

where $\widetilde{\mathbf{f}}(s)$ denotes the restricted variation, and the Lagrange multiplier, in this setting, is given by

$$\Lambda_A(s;t) = -\begin{pmatrix} \frac{t^2}{s^2}\left(1 - 2\ln\left(\frac{t}{s}\right)\right) & \frac{t^2}{s}\ln\left(\frac{t}{s}\right) \\ -\frac{4t}{s^2}\ln\left(\frac{t}{s}\right) & \frac{t}{s}\left(1 + 2\ln\left(\frac{t}{s}\right)\right) \end{pmatrix}.$$

Starting with the initial approximation $x^0(t) = (2,2)^T$ we immediately obtain the exact solution

$$x^1(t) = \left(t^2 - t^2\ln(t) + t,\ t - 2t\ln(t) + 1\right)^T$$

of (2.34). Consequently, the solution $x(t)$ of (2.33) is the first component of $x^1(t)$; namely,

$$x(t) = t^2 - t^2\ln(t) + t.$$

Table 2.2 shows the absolute error of the fifth-order iteration obtained by the VIM for $t \in [1,4]$:

$$\varepsilon_i^{VIM}(t) = \left|x_i^E(t) - x_i^{VIM}(t)\right|,$$

for $i = 1,2$, where $x_i^{VIM}(t)$ denotes the approximate solutions obtained by VIM for the fifth-order iteration and $x_i^E(t)$ denotes the exact solution obtained by EVIM at the point t for $i = 1,2$.

Furthermore, by

$$\varepsilon^{VIM}(t) = \left\|x^E(t) - x^{VIM}(t)\right\|_2,$$

we define the errors in the two-norm.

It must be noted that while EVIM obtains the exact solution at the single step, however, error in VIM is accumulated when t gets relatively large.

Table 2.2: Comparison of the classical VIM and EVIM for the fifth-order approximation for (2.34).

t	ε_1^{VIM}	ε_2^{VIM}	ε^{VIM}
1	0	0	0
1.5	0.0002	0.0005	0.0006
2	0.0084	0.0105	0.0134
2.5	0.0626	0.0417	0.0752
3	0.2399	0.0914	0.2567
3.5	0.6468	0.1445	0.6628
4	1.4081	0.1802	1.4195

2.3.3 Bernoulli Equations

In Cauchy-Euler equation, we apply the method to the system of the form

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{f}(t), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0. \tag{2.36}$$

In general, the method is also applicable to the systems of the form

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{f}(t, \mathbf{x}(t)), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0. \tag{2.37}$$

where $\mathbf{f} : I \times \mathbb{R}^m \longrightarrow \mathbb{R}^m$ is a given function, A is $m \times m$ matrix and $\mathbf{x}$ is an m-vector.

In this part, extended multistage variational iteration method is used for solving a Bernoulli differential equation. The results are compared with the modified variational iteration method for solving Riccati differential equations proposed by Geng [13].

Bernoulli equation is a first-order nonlinear differential equation of the form

$$\dot{x}(t) + P(t)x(t) = Q(t)x^q(t), \quad x(0) = \alpha_0, \tag{2.38}$$

where P and Q are continuous functions on $I = [0, T]$ and $q \notin \{0, 1\}$. For this specific example we let $P(t) = Q(t) = t$ and $q = 2$ so that (2.38) takes the following form

$$\dot{x}(t) + tx(t) = tx^2(t), \quad x(0) = \alpha_0 \tag{2.39}$$

and the exact solution of which is easily found to be

$$x(t) = \frac{1}{1 - e^{t^2/2}(1 - 1/\alpha_0)}.$$

According to the extended multistage variational iteration method, we construct the following correction functional

$$x^{n+1}(t) = x^n(t) + \int_{t^*}^{t} \lambda \Big\{ (x^n)'(s) + sx^n(s) - s(\widetilde{x}^n)^2(s) \Big\} ds, \tag{2.40}$$

where $\lambda = \lambda(s;t)$ is the Lagrange multiplier, $\widetilde{x}^n(s)$ is the restricted variation. The initial approximation is $x^0(t) = \alpha_0$. Here, the interval $[0,T]$ is divided into $m+1$ subintervals, $[t_0,t_1),[t_1,t_2),\ldots,[t_m,t_{m+1})$, with the convention that $t_0 = 0$ and $t_{m+1} = T$. In (2.40), t^* is chosen to be the left boundary points of the subintervals, and within each subinterval $[t^*,t_k)$ with $1 \le k \le m+1$, the initial approximate solution is $x^n(t^*)$ which is obtained from the preceding subinterval or the initial condition $x(0) = \alpha_0$.

Either by using calculus of variations, but including all linear terms and that $\delta x^n(t^*) = 0$, or directly from Theorem 2.1, we obtain

$$\lambda(s;t) = -e^{(s^2-t^2)/2}.$$

Then, the Lagrange multiplier yields the following correction functional

$$x^{n+1}(t) = x^n(t) + \int_{t^*}^{t} -e^{(s^2-t^2)/2}\Big\{(x^n)'(s) + sx^n(s) - s(x^n)^2(s)\Big\}ds,$$

with the initial approximation $x^0(t) = \alpha_0$.

In [13], Geng proposed a modification of VIM for equations of the type

$$\begin{aligned} \dot{x}(t) &= R(t) + P(t)x(t) + Q(t)x^2(t), \quad 0 \le t \le T, \\ x(0) &= \alpha \end{aligned} \tag{2.41}$$

where $R(t), P(t), Q(t)$ are continuous functions in $[0,T]$. Geng defined the following iteration formula to solve the system (2.41)

$$x^{n+1}(t) = x^n(t) - \gamma \int_0^t \Big\{(x^n)'(s) - R(s) - P(s)x^n(s) - Q(s)(x^n)^2(s)\Big\}ds,$$

for $0 \le t \le T$, where $x^0(t) = \alpha$ and $|\gamma|$ is chosen to be relatively "small", generally less than unity [13].

In Table 2.3, we compare both methods for the system (2.41) for the fifth and the tenth iterations with $\alpha_0 = 1/2$, $T = 4$ and $\gamma = 0.001$. It can be seen that the multistage version of the new approach (MEVIM) is more effective than the method proposed in [13], without the need for searching a (best) value for the artificial parameter γ.

One might have observed that the extended VIM can solve certain problems exactly in one step. In fact, this is not a coincidence: the newly extended version of the method solves linear equations in just a single step as long as the initial approximation satisfies the initial condition. Of course, it cannot solve nonlinear ones within a single iteration.

Table 2.3: Comparison of the extended multistage variational iteration method and the proposed approach in [13] for $\gamma = 0.001$ for the fifth- and tenth-order approximations.

		5TH-ORDER		10TH-ORDER	
t	Exact	Error MEVIM	Error VIM [13]	Error MEVIM	Error VIM [13]
0	0.5000	0	0	0	0
0.5	0.4688	0.0000	0.0310	0.0000	0.0309
1	0.3775	0.0017	0.1218	0.0000	0.1212
1.5	0.2451	0.0267	0.2535	0.0043	0.2520
2	0.1192	0.0890	0.3782	0.0375	0.3757
2.5	0.0421	0.1431	0.4539	0.0811	0.4500
3	0.0110	0.1680	0.4833	0.1036	0.4776
3.5	0.0022	0.1756	0.4901	0.1106	0.4824
4	0.0003	0.1772	0.4896	0.1122	0.4795

Thus, before the convergence analysis of such a functional iteration scheme, we close this section by stating and proving the theorem on that solution to linear systems can be solved by a single step of the extended version of VIM.

Theorem 2.6. *Consider the following linear initial value problem*

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{f}(t), \quad \mathbf{x}(0) = \alpha_0, \quad t \in I := [0, \ell], \tag{2.42}$$

where $\mathbf{x}$ *is an* m*-vector,* $A(t) = (a_{ij}(t))$*,* $a_{ij} \in \mathcal{C}(I)$ *is an* $m \times m$ *matrix. Let* $\mathbf{x}^0(t) \in \mathcal{C}^1(I)$ *such that* $\mathbf{x}^0(0) = \alpha_0$ *be a given initial approximation. Then,* $x^1(t)$ *defined by the correction functional*

$$\mathbf{x}^1(t) = \mathbf{x}^0(t) - \int_0^t \Phi(t;s)\Big\{(\mathbf{x}^0)'(s) - A(s)\mathbf{x}^0(s) - \mathbf{f}(s)\Big\}ds. \tag{2.43}$$

is the exact solution of (2.42).

Proof. It is obvious that using the correction functional (2.43) we have

$$\mathbf{x}^1(0) = \mathbf{x}^0(0) = \alpha_0.$$

Upon calculating the derivative $\dot{\mathbf{x}}^1$ as

$$\begin{aligned} \dot{\mathbf{x}}^1(t) &= \dot{\mathbf{x}}^0(t) - \Phi(t;t)\Big\{(\dot{\mathbf{x}}^0)(t) - A(t)\mathbf{x}^0(t) - \mathbf{f}(t)\Big\} \\ &- \int_0^t \frac{\partial}{\partial t}\Phi(t;s)\Big\{(\mathbf{x}^n)'(s) - A(s)\mathbf{x}^n(s) - \mathbf{f}(s)\Big\}ds \end{aligned}$$

and using the fact that

$$\begin{aligned} \frac{\partial \Phi(t;s)}{\partial t} &= A(t)\Phi(t;s), \\ \Phi(t;t) &= E, \end{aligned}$$

we obtain

$$\dot{\mathbf{x}}^1(t) = A(t)\mathbf{x}^0(t) + \mathbf{f}(t) - A(t)\int_0^t \Phi(t;s)\Big\{(\mathbf{x}^0)'(s) - A(s)\mathbf{x}^0(s) - \mathbf{f}(s)\Big\}ds.$$

Hence,

$$\dot{\mathbf{x}}^1(t) = A(t)\mathbf{x}^1(t) + \mathbf{f}(t)$$

completes the proof. ■

2.4 Convergence Analysis of EVIM

Variational iteration method has been used to approximate the solutions of different problems. The method gives convergent successive approximations without using neither linearisation nor perturbation techniques; and hence, the method reduces the computational time in many applications.

The convergence of the method have been studied by researchers from different areas and for different problems. For example; Torvattanabun and Koonprasert [55] studied the convergence of the method for solving a first-order linear system of PDEs with constant coefficients. Salkuyeh proposed a theorem for the convergence of the method in solving linear system of ODEs with constant coefficients in [49]. Tatari and Dehghan [54] investigated the sufficient conditions to prove the convergence of the method. In [48], Ramos considered the first and second order time differentials and proved that the iterative process of VIM can be obtained by using adjoint operators, Green's function, integration by parts and the method of weighted residuals. Ramos also claimed that VIM is a specialised version of the Picard-Lindelof iterative process for initial-value problems in ODE; the use of the Banach's fixed point theory for initial-value problems in PDE ensures the convergence of the method when the mapping is Lipschitz continuous and contractive.

In this section of the present work we will investigate the conditions which guarantees the convergence of EVIM and see the close relationship between the iterative process obtained by EVIM and variations of parameters formula.

Now, let us consider the following system:

$$\dot{\mathbf{x}} = A(t)\mathbf{x}(t) + \mathbf{f}(t,\mathbf{x}), \quad t \in I := [0,\ell] \tag{2.44}$$

subject to the initial condition

$$\mathbf{x}(0) = \alpha_0,$$

where $\mathbf{x}$ is an $m-$vector, $A(t) = (a_{ij}(t))$, $a_{ij} \in \mathcal{C}(I)$ is an $m \times m$ matrix and $\mathbf{f} : I \times \mathbb{R}^m \to \mathbb{R}^m$ for $m \in \mathbb{N}$.

Applying EVIM gives us the following iterative process:

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) + \int_0^t \Lambda_A(s;t)\Big\{(\mathbf{x}^n)'(s) - A(s)\mathbf{x}^n(s) - \mathbf{f}(s, \widetilde{\mathbf{x}}^n(s))\Big\}ds, \tag{2.45}$$

where $\mathbf{x}^n(t)$ denotes the nth-order approximate solution and $\Lambda_A(s;t)$ is the $m \times m$ matrix valued Lagrange multiplier. In Section 2.1, we have proved that

$$\Lambda_A(s;t) = -\Phi(t)\Phi^{-1}(s) = -\Phi(t;s),$$

where $\Phi(t)$ denotes the fundamental matrix of the corresponding homogeneous differential equation $\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t)$.

Then, the correction functional (2.45) can be rewritten as follows

$$\mathbf{x}^{n+1}(t) = \mathbf{x}^n(t) - \int_0^t \Phi(t;s)\Big\{(\mathbf{x}^n)'(s) - A(s)\mathbf{x}^n(s) - \mathbf{f}(s, \mathbf{x}^n(s))\Big\}ds \tag{2.46}$$

and the integration by parts yields

$$\mathbf{x}^{n+1}(t) = \Phi(t;0)\mathbf{x}^n(0) + \int_0^t \Big\{\Phi'(t;s)\mathbf{x}^n(s) + \Phi(t;s)A(s)\mathbf{x}^n(s) + \Phi(t;s)\mathbf{f}(s, \mathbf{x}^n(s))\Big\}ds.$$

Hence, by using the fact that $\Phi'(t;s) = -\Phi(t;s)\, A(s)$, we obtain

$$\mathbf{x}^{n+1}(t) = \Phi(t;0)\mathbf{x}^n(0) + \int_0^t \Big\{\Phi(t;s)\mathbf{f}(s, \mathbf{x}^n(s))\Big\}ds. \tag{2.47}$$

This formula is nothing else but the fixed point iteration for the variation of parameters formula. However, $\mathbf{f}$, in general, is a nonlinear function of the components of $\mathbf{x}$. Meanwhile, in the case when $\mathbf{f}$ is independent of $\mathbf{x}$, but depends only on t, then Theorem 2.6 becomes an obvious fact of (2.47).

To prove that the sequence $\{\mathbf{x}^n\}_{n=1}^{\infty}$ converges to the exact solution of (2.44), we state the following theorem.

Theorem 2.7. *Let $\mathbf{x}(t) \in \mathcal{C}^1(I)$ for $t \in I = [0, \ell]$ be the exact solution of (2.44) and $\mathbf{x}^n(t) \in \mathcal{C}^1(I)$ be the nth order approximate solution obtained by the correction functional (2.47) with $\mathbf{x}^0(t) = \alpha_0$, $\mathbf{x}^n(0) = \alpha_0$ for all $n \in \mathbb{N}$. Let $\mathbf{f} \in (\mathcal{C}(I), Lip)$; that*

is $\mathbf{f}$ *is a continuous function and it satisfies Lipschitz condition (with respect to* $\mathbf{x}$*) in* I*, with Lipschitz constant* $k > 0$*. Furthermore,* $\|\Phi(t;s)\| \leq F$*, and* $\|\mathbf{f}(s,\mathbf{x}(s))\| \leq M$ *for all* $s \in I$*. Then, the sequence* $\{\mathbf{x}^n\}_{n=1}^{\infty} \in \mathcal{C}^1(I)$ *converges uniformly to* $\mathbf{x}$*.*

Proof. It is a known fact that the unique solution of (2.44) has the following form

$$\mathbf{x}(t) = \Phi(t;0)\mathbf{x}(0) + \int_0^t \Phi(t;s)\mathbf{f}(s,\mathbf{x}(s))ds. \tag{2.48}$$

The proof of the theorem is based on three steps. Firstly, we will find an error bound for $\left\|\mathbf{x}^{n+1}(t) - \mathbf{x}^n(t)\right\|$. Secondly, we will prove that $\mathbf{x}^n(t)$ is a Cauchy sequence via error bound obtained in the first step. Thirdly, we will show that $\mathbf{x}^n(t)$ converges to $\mathbf{x}(t)$.

Let $n = 0$, then the subtraction of first and zeroth approximation is

$$\left\|\mathbf{x}^1(t) - \mathbf{x}^0(t)\right\| \leq \|(\Phi(t;0) - E)\alpha_0\| + \left\|\int_0^t \Phi(t;s)\mathbf{f}(s,\mathbf{x}^0(s))ds\right\|,$$

where E denotes the $m \times m$ identity matrix. Since we have $\Phi(t;s)$ is bounded, the $(\Phi(t;0) - E)$ is also bounded, that is, $\|\Phi(t;0) - E\| \leq C$. As a result, we obtain

$$\left\|\mathbf{x}^1(t) - \mathbf{x}^0(t)\right\| \leq C\|\alpha_0\| + FMt.$$

For $n \geq 0$,

$$\begin{aligned} \mathbf{x}^{n+1}(t) - \mathbf{x}^n(t) &= \Phi(t;0)\mathbf{x}^n(0) + \int_0^t \Phi(t;s)\mathbf{f}(s,\mathbf{x}^n(s))ds \\ &- \Phi(t;0)\mathbf{x}^{n-1}(0) - \int_0^t \Phi(t;s)\mathbf{f}(s,\mathbf{x}^{n-1}(s))ds \end{aligned} \tag{2.49}$$

By using the fact that $\mathbf{x}^n(0) = \mathbf{x}^{n-1}(0)$, we get

$$\begin{aligned} \left\|\mathbf{x}^{n+1}(t) - \mathbf{x}^n(t)\right\| &= \left\|\int_0^t \Phi(t;s)\left(\mathbf{f}(s,\mathbf{x}^n(s)) - \mathbf{f}(s,\mathbf{x}^{n-1}(s))\right)ds\right\| \\ &\leq Fk\int_0^t \left\|\mathbf{x}^n(s) - \mathbf{x}^{n-1}(s)\right\| ds. \end{aligned} \tag{2.50}$$

Now, iteratively we obtain

$$\begin{aligned} \left\|\mathbf{x}^2(t) - \mathbf{x}^1(t)\right\| &\leq Fk\int_0^t \left\|\mathbf{x}^1(s) - \mathbf{x}^0(s)\right\| ds \leq Fk\left(C\|\alpha_0\|\, t + FM\frac{t^2}{2!}\right) \\ \left\|\mathbf{x}^3(t) - \mathbf{x}^2(t)\right\| &\leq Fk\int_0^t \left\|\mathbf{x}^2(s) - \mathbf{x}^1(s)\right\| ds \leq (Fk)^2\left(C\|\alpha_0\|\frac{t^2}{2!} + FM\frac{t^3}{3!}\right) \\ \left\|\mathbf{x}^4(t) - \mathbf{x}^3(t)\right\| &\leq Fk\int_0^t \left\|\mathbf{x}^3(s) - \mathbf{x}^2(s)\right\| ds \leq (Fk)^3\left(C\|\alpha_0\|\frac{t^3}{3!} + FM\frac{t^4}{4!}\right) \\ &\vdots \\ \left\|\mathbf{x}^{n+1}(t) - \mathbf{x}^n(t)\right\| &\leq Fk\int_0^t \left\|\mathbf{x}^n(s) - \mathbf{x}^{n-1}(s)\right\| ds \leq (Fk)^n\left(C\|\alpha_0\|\frac{t^n}{n!} + FM\frac{t^{n+1}}{(n+1)!}\right). \end{aligned} \tag{2.51}$$

Now, we obtain an error bound for $\left\|\mathbf{x}^{n+1}(t)-\mathbf{x}^{n}(t)\right\|$, completing step one.

The second step is to show that $\mathbf{x}^n(t)$ is a Cauchy sequence. Suppose that $m<n$,

$$\begin{aligned}
\|\mathbf{x}^n(t)-\mathbf{x}^m(t)\| &= \left\|\left(\mathbf{x}^n(t)-\mathbf{x}^{n-1}(t)\right)+\left(\mathbf{x}^{n-1}(t)-\mathbf{x}^{n-2}(t)\right)+\ldots+\left(\mathbf{x}^{m+1}(t)-\mathbf{x}^{m}(t)\right)\right\| \\
&\leq \sum_{j=m}^{n-1}\left\|\mathbf{x}^{j+1}(s)-\mathbf{x}^{j}(s)\right\|ds \\
&\leq \sum_{j=m}^{n-1}(Fk)^j\left(C\left\|\alpha_0\right\|\frac{t^j}{j!}+FM\frac{t^{j+1}}{(j+1)!}\right) \\
&= \sum_{j=m}^{n-1}(Fk)^j\left(C\left\|\alpha_0\right\|\frac{t^j}{j!}\right)+\sum_{j=m}^{n-1}(Fk)^j\left(FM\frac{t^{j+1}}{(j+1)!}\right)
\end{aligned}$$

These sums are parts of Taylor series for e^{Fkt}. By taking m sufficiently large it is possible to make $\|\mathbf{x}^n(t)-\mathbf{x}^m(t)\|$ less than any $\epsilon>0$. This shows that the sequence $\mathbf{x}^n(t)$ is Cauchy sequence.

Since $\mathbf{x}^n(t)$ is a Cauchy sequence of continuous functions and $I=[0,\ell]$ is a compact interval, then $\mathbf{x}^n(t)$ converges uniformly to a continuous function $\mathbf{x}(t)$, that is

$$\begin{aligned}
\mathbf{x}(t) &= \lim_{n\to\infty}\mathbf{x}^{n+1}(t) \\
&= \lim_{n\to\infty}\Phi(t;0)\mathbf{x}^n(0)+\int_0^t\Phi(t;s)\mathbf{f}(s,\mathbf{x}^n(s))ds \\
&= \Phi(t;0)\alpha_0+\lim_{n\to\infty}\int_0^t\Phi(t;s)\mathbf{f}(s,\mathbf{x}^n(s))ds
\end{aligned} \tag{2.52}$$

Now,

$$\begin{aligned}
\lim_{n\to\infty}\int_0^t\Phi(t;s)\mathbf{f}(s,\mathbf{x}^n(s))ds &= \int_0^t\Phi(t;s)\mathbf{f}(s,\mathbf{x}(s))ds \\
&+ \int_0^t\Phi(t;s)\left(\mathbf{f}(s,\mathbf{x}^n(s))-\mathbf{f}(s,\mathbf{x}(s))\right)ds.
\end{aligned} \tag{2.53}$$

Since $\mathbf{x}^n(t)-\mathbf{x}(t)$ converges uniformly to 0, then

$$\left\|\int_0^t\Phi(t;s)\left(\mathbf{f}(s,\mathbf{x}^n(s))-\mathbf{f}(s,\mathbf{x}(s))\right)ds\right\|\leq F\ell k\left\|\mathbf{x}^n(s)-\mathbf{x}(s)\right\|\longrightarrow 0.$$

Finally,

$$\lim_{n\to\infty}\mathbf{x}^{n+1}(t)=\Phi(t;0)\alpha_0+\int_0^t\Phi(t;s)\mathbf{f}(s,\mathbf{x}(s))ds.$$

which is the exact solution of (2.44). ■

For more details of the convergence properties of successive approximations, we refer [8].

CHAPTER 3

SOLUTION OF INITIAL VALUE AND BOUNDARY VALUE PROBLEMS BY THE VARIATIONAL ITERATION METHOD

In this chapter of the present work, we will consider the mth order linear nonhomogeneous ordinary differential equations as well as nonlinear ones. We will mainly show the existence of a close relation between the Lagrange multipliers and the adjoint equations.

By using these relations, we will prove the basic properties of Lagrange multipliers and show that it is also possible to obtain the solution of linear equations with only a single variational iteration.

In the sequel, VIM represents the variational iteration method which does not use any restricted variation while obtaining the scalar-valued Lagrange multiplier for an mth order differential equations and EVIM represents the extended variational iteration method which obtains the matrix-valued Lagrange multiplier for the corresponding first-order differential equation.

3.1 Solution of Initial Value Problems

Let us consider the following higher order differential equation:

$$p_0(t)\dot{x}^{(m)}(t) + p_1(t)\dot{x}^{(m-1)}(t) + p_2(t)\dot{x}^{(m-2)}(t) + \cdots + p_m(t)x(t) = 0, \qquad (3.1)$$

for $t \in I = [a, b]$ and subject to the initial conditions

$$x(a) = x_a,\ \dot{x}(a) = \dot{x}_a,\ \dot{x}^{(2)}(a) = \dot{x}_a^{(2)},\ \ldots,\ \dot{x}^{(m-1)}(a) = \dot{x}_a^{(m-1)},$$

where $p_i \in C^{m-i}(I, R)$, $p_0(t) > 0$ for all $t \in I$, and $\dot{x}^{(i)}$ represents the ith derivative $d^i x(t)/dt^i$ for all $i = 1, 2, \ldots, m$.

Let $L_{m,t}$ denotes the following differential operator:

$$L_{m,t} = p_0(t)\frac{d^m}{dt^m} + p_1(t)\frac{d^{m-1}}{dt^{m-1}} + p_2(t)\frac{d^{m-2}}{dt^{m-2}} + \cdots + p_m(t). \tag{3.2}$$

By using the VIM, we can construct the following correction functional for equation (3.1)

$$\begin{aligned} x_{n+1}(t) &= x_n(t) + \int_a^t \lambda\Big\{p_0(s)x_n^{(m)}(s) + p_1(s)x_n^{(m-1)}(s) \\ &\quad + p_2(s)x_n^{(m-2)}(s) + \cdots + p_m(s)x_n(s)\Big\}ds. \end{aligned} \tag{3.3}$$

Here, $\lambda = \lambda(s; t)$ is the Lagrange multiplier, $x_n(t)$ represents the nth order approximate solution, and $x_n^{(j)}(s)$ is the derivative $d^j x_n(s)/ds^j$ for $j = 1, 2, \ldots, m$.

By using integration by parts, it is easy to obtain the following equality [42]

$$\begin{aligned} \int_a^t \lambda p_{m-r}(s)x_n^{(r)}(s)ds &= \lambda p_{m-r}(s)x_n^{(r-1)}(s) \mid_{s=a}^{s=t} \\ &\quad -(\lambda p_{m-r}(s))' x_n^{(r-2)}(s) \mid_{s=a}^{s=t} + \ldots \\ &\quad +(-1)^{r-1}(\lambda p_{m-r}(s))^{(r-1)} x_n(s) \mid_{s=a}^{s=t} \\ &\quad +(-1)^r \int_a^t x(s)(\lambda p_{m-r}(s))^{(r)} ds, \end{aligned} \tag{3.4}$$

for all $r = 1, 2, \ldots, m$. Taking the variation of both parts of the correction functional yields

$$\begin{aligned} \delta x_{n+1}(t) &= \delta x_n(t) + \delta \int_a^t \lambda L_{m,s} x_n(s) ds \\ &= \delta x_n(t) + \int_a^t \lambda L_{m,s} \delta x_n(s) ds. \end{aligned} \tag{3.5}$$

Using the equality in (3.4) and $\delta x_n(a) = 0$, we obtain

$$\begin{aligned}
\delta x_{n+1}(t) &= \Big\{(-1)^{m-1}(\lambda p_0)^{(m-1)} + (-1)^{m-2}(\lambda p_1)^{(m-2)} \\
&\quad + \cdots + \lambda p_{m-1} + 1\Big\}\delta x_n(s)\Big|_{s=t} \\
&+\Big\{(-1)^{m-2}(\lambda p_0)^{(m-2)} + (-1)^{m-3}(\lambda p_1)^{(m-3)} \\
&\quad + \cdots + \lambda p_{m-2}\Big\}\delta(x_n)'(s)\Big|_{s=t} \\
&+\Big\{(-1)^{m-3}(\lambda p_0)^{(m-3)} + (-1)^{m-4}(\lambda p_1)^{(m-4)} \\
&\quad + \cdots + \lambda p_{m-3}\Big\}\delta(x_n)''(s)\Big|_{s=t} \\
&\vdots \\
&+p_0\lambda\delta(x_n)^{(m-1)}\Big|_{s=t} + \int_a^t \delta x_n(s) L^\dagger_{m,s}\lambda ds
\end{aligned}$$

where we have used $\lambda = \lambda(s;t)$ and $p_i = p_i(s)$ for all $i = 0, 1, \ldots, m-1$. Here, $L^\dagger_{m,s}$ is given by

$$\begin{aligned}
L^\dagger_{m,s}(\cdot) &= (-1)^m \frac{d^m}{ds^m}(p_0(s)\cdot) + (-1)^{m-1}\frac{d^{m-1}}{ds^{m-1}}(p_1(s)\cdot) + (-1)^{m-2}\frac{d^{m-2}}{ds^{m-2}}(p_2(s)\cdot) \\
&\quad + \cdots + (p_m(s)\cdot),
\end{aligned}$$

and hence,

$$\begin{aligned}
L^\dagger_{m,s}\lambda(s;t) &= (-1)^m(p_0(s)\lambda(s;t))^{(m)} + (-1)^{m-1}(p_1(s)\lambda(s;t))^{(m-1)} \\
&\quad + (-1)^{m-2}(p_2(s)\lambda(s;t))^{(m-2)} + \cdots + p_m(s)\lambda(s;t),
\end{aligned}$$

The operator $L^\dagger_{m,s}$ is called the *adjoint* of $L_{m,s}$ in (3.2). Thus, the following conditions makes the correction functionals stationary:

$$\begin{aligned}
0 &= \Big\{(-1)^{m-1}(\lambda(s;t)p_0(s))^{(m-1)} + (-1)^{m-2}(\lambda(s;t)p_1(s))^{(m-2)} \\
&\quad + \cdots + \lambda(s;t)p_{m-1}(s) + 1\Big\}\Big|_{s=t}, \\
0 &= \Big\{(-1)^{m-2}(\lambda(s;t)p_0(s))^{(m-2)} + (-1)^{m-3}(\lambda(s;t)p_1(s))^{(m-3)} \\
&\quad + \cdots + \lambda(s;t)p_{m-2}(s)\Big\}\Big|_{s=t}, \\
0 &= \Big\{(-1)^{m-3}(\lambda(s;t)p_0(s))^{(m-3)} + (-1)^{m-4}(\lambda(s;t)p_1(s))^{(m-4)} \\
&\quad + \cdots + \lambda(s;t)p_{m-3}(s)\Big\}\Big|_{s=t}, \\
&\vdots \\
0 &= p_0(s)\lambda(s;t)\Big|_{s=t},
\end{aligned} \tag{3.6}$$

Consequently, we have

$$L^\dagger_{m,s}\lambda(s;t) = 0, \tag{3.7}$$

and using the fact that $\lambda(t,t)=0$, by backward substitution in (3.6), we obtain

$$\begin{array}{rcl} \left.\dfrac{\partial^j \lambda(s;t)}{\partial s^j}\right|_{s=t} & = & 0, \quad \text{for} j=0,1,2,\ldots,m-1, \\ \left.\dfrac{\partial^{m-1} \lambda(s;t)}{\partial s^{m-1}}\right|_{s=t} & = & \dfrac{(-1)^m}{p_0(t)} \end{array} \tag{3.8}$$

Without loss of generality we assume $p_0(t)=1$ and write

$$L_{m,t}x = \frac{d^m x}{dt^m} + p_1(t)\frac{d^{m-1}x}{dt^{m-1}} + p_2(t)\frac{d^{m-2}x}{dt^{m-2}} + \ldots + p_m(t)x = 0, \tag{3.9}$$

for which the associated system of first order equations is

$$\dot{\mathbf{x}} = A(t)\mathbf{x}, \tag{3.10}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_m)^T = (\dot{x}, \dot{x}^{(2)}, \ldots, \dot{x}^{(m-1)})^T$ and $A(t)$ is the companion matrix with the following form:

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ -p_m & -p_{m-1} & -p_{m-2} & \cdots & -p_1 \end{pmatrix}. \tag{3.11}$$

Initial conditions turn out to be

$$\mathbf{x}(a) = (x_a, \dot{x}_a, \dot{x}_a^{(2)}, \ldots, \dot{x}_a^{(m-1)})^T.$$

If we apply EVIM to system (3.10), we obtain the following functional

$$\mathbf{x}_{n+1}(t) = \mathbf{x}_n(t) + \int_a^t \Lambda\Big\{(\mathbf{x}_n(s))' - A(s)\mathbf{x}_n(s)\Big\}ds, \tag{3.12}$$

where the Lagrange multiplier $\Lambda = \Lambda(s;t)$ satisfies the following matrix differential equation:

$$\begin{array}{rcl} \Lambda'(s;t) & = & -\Lambda(s;t)A(s), \\ \Lambda(t;t) & = & -E. \end{array} \tag{3.13}$$

Here, we recall that $'$ denotes the derivative with respect to s and $\dot{}$ denotes the derivative with respect to t.

In Section 2.1, it is proven that the solution of (3.12) satisfies $\Lambda(t;s) = -\Psi^T(t;s)$ where $\Psi(t)$ denotes the fundamental matrix of the adjoint equation

$$\dot{\mathbf{y}} = -A^T(t)\mathbf{y}, \tag{3.14}$$

with

$$-A^T = \begin{pmatrix} 0 & 0 & \cdots & 0 & p_m \\ -1 & 0 & \cdots & 0 & p_{m-1} \\ 0 & -1 & \cdots & 0 & p_{m-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & p_1 \end{pmatrix}. \tag{3.15}$$

The components of (3.14) give

$$\dot{y}_1 = p_m y_m, \quad \dot{y}_k = -y_{k-1} + p_{m-k+1} y_m, \quad k = 2, 3, \ldots, m,$$

by using (3.15). By differentiating the kth relation $(k-1)$ times we observe that y_m satisfies the adjoint differential equation

$$\begin{aligned} L^{\dagger}_{m,t} y_m &= (-1)^m \frac{d^m}{dt^m} y_m + (-1)^{m-1} \frac{d^{m-1}}{dt^{m-1}} (p_1 y_m) \\ &\quad + (-1)^{m-2} \frac{d^{m-2}}{dt^{m-2}} (p_2 y_m) + \cdots + p_m y_m \\ &= 0. \end{aligned}$$

Since the Lagrange multiplier $\lambda(s;t)$ of (3.3) will also satisfy $L^{\dagger}_{m,s}\lambda(s;t) = 0$, it is obvious that $\lambda(s;t)$ and $y_m(t)$ solve the same differential equation but written with respect to different variables: s and t, respectively.

If the fundamental solution of (3.14) is $\Psi(t)$ then the components of the last row of this matrix will be the linearly independent solutions of $y_m(t)$. By using this fact, we can write

$$\lambda(t;s) = e_m^T \Psi(t;s) c, \tag{3.16}$$

where $e_m = (0, 0, \ldots, 1)^T_{1\times m}$ and $c = (c_1, c_2, \ldots, c_m)^T$ where $c_i \in \mathbb{R}$ for $i = 1, 2, \ldots, m$. By changing the roles of s and t we get

$$\lambda(s;t) = e_m^T \Psi(s;t) c. \tag{3.17}$$

Using the relation $\Psi(s;t) = \Lambda^T(s;t)$, we obtain the following relation for the Lagrange multiplier of the VIM and that of the EVIM

$$\lambda(s;t) = e_m^T \Lambda^T(s;t) c. \tag{3.18}$$

This result can be reduced to the following summation:

$$\lambda(s;t) = \sum_{i=1}^{m} c_i \Lambda_{im}(s;t), \tag{3.19}$$

with $\Lambda = (\Lambda im)\,, \quad 1 \leq i \leq m$ as the Lagrange multiplier. Using (3.13) we can write

$$\Lambda'_{ij}(s;t) = -(\Lambda_{i(j-1)}(s;t) - p_{m-j+1}\Lambda_{im}(s;t)), \quad i,j = 1,2,\ldots,m, \tag{3.20}$$

with $\Lambda_{i0} = 0$. Equations (3.8) and (3.20) show that

$$c_1 = 1,\ c_i = 0, \quad i = 2,3,\ldots,m.$$

Hence,

$$\lambda(s;t) = \Lambda_{1m}(s;t).$$

Now, it is easy to find the derivatives of $\lambda(s;t)$ with respect to t. Firstly, we remember $\Lambda(s;t) = -\Phi(t;s)$ so that

$$\begin{aligned} \dot{\Lambda}(s;t) &= A(t)\Lambda(s;t), \\ \Lambda(s;s) &= -E. \end{aligned} \tag{3.21}$$

This yields immediately that

$$L_{m,t}\lambda(s;t) = 0 \tag{3.22}$$

holds. In fact, equation (3.20) gives the derivative of the components $\Lambda(s;t)$ as follows

$$\dot{\Lambda}_{ij}(s;t) = \Lambda_{(i+1)j}(s;t), \quad \dot{\Lambda}_{mj}(s;t) = -\sum_{i=1}^{m} p_i \Lambda_{(m+1-i)j}(s;t), \quad \Lambda_{jj}(s;s) = -1.$$

By using the result $\lambda(s;t) = \Lambda_{1m}(s;t)$ and the derivative components of $\Lambda(s;t)$, we get

$$L_{m,t}\lambda(s;t) = 0,$$

subject to the initial conditions

$$\frac{\partial^j \lambda(s;t)}{\partial t^j}\Big|_{t=s} = 0, \quad \frac{\partial^{m-1} \lambda(s;t)}{\partial t^{m-1}}\Big|_{t=s} = -1, \quad j = 0,1,\ldots,m-2.$$

Recall that we have obtained that Lagrange multiplier $\lambda(s;t)$ satisfies adjoint equation with respect to variable s; that is, $L^{\dagger}_{m,s}\lambda(s;t) = 0$, and the values of the derivatives of $\lambda(s;t)$ with respect to s when $s = t$ were given in (3.8).

By using the previous discussions, we can prove the following theorem which states that if the initial approximation satisfies the initial condition then the solution of mth order linear nonhomogenous ordinary differential equation can be obtained by a single step of VIM. A similar result for EVIM was presented in Theorem 2.6.

Theorem 3.1. *Let*

$$L_{m,t}x = \frac{d^m x}{dt^m} + p_1(t)\frac{d^{m-1}x}{dt^{m-1}} + p_2(t)\frac{d^{m-2}x}{dt^{m-2}} + \cdots + p_m(t)x = f(t) \tag{3.23}$$

subject to the initial conditions

$$x(a) = x_a, \dot{x}(a) = \dot{x}_a, \dot{x}^{(2)}(a) = \dot{x}_a^{(2)}, \ldots, \dot{x}^{(m-1)}(a) = \dot{x}_a^{(m-1)},$$

where $t \in I = [a, b]$, $p_i \in C^{m-i}(I, R)$, *for all* $t \in I$, *and* $\dot{x}^{(i)}$ *represents the derivative* $d^i x(t)/dt^i$ *for all* $i = 1, 2, \ldots, m$. *Construct* $x_0 \in C(I, \mathbb{R})$ *which satisfies the initial conditions. Then,*

$$x_1(t) = x_0(t) + \int_a^t \lambda(s;t)\Big\{L_{m,s}x_0(s) - f(s)\Big\}ds$$

is the solution of (3.23).

Proof. By using the previous discussions, it is easy to prove that

$$\dot{x}_1^{(j)}(t) = \dot{x}_0^{(j)}(t) + \int_a^t \frac{\partial^j \lambda(s;t)}{\partial t^j}\Big\{L_{m,s}x_0(s) - f(s)\Big\}ds, \quad j = 1, 2, \ldots, m-1,$$

and

$$\begin{aligned}\dot{x}_1^{(m)}(t) &= \dot{x}_0^{(m)}(t) + \frac{\partial^{m-1}\lambda(s;t)}{\partial t^{m-1}}\Big|_{s=t}\Big\{L_{m,t}x_0(t) - f(t)\Big\} \\ &\quad + \int_a^t \frac{\partial^{m-1}\lambda(s;t)}{\partial t^{m-1}}\Big\{L_{m,s}x_0(s) - f(s)\Big\}ds.\end{aligned}$$

Hence,

$$L_{m,t}x_1(t) = L_{m,t}x_0(t) - \Big\{L_{m,t}x_0(t) - f(t)\Big\} + \int_a^t L_{m,t}\lambda(s;t)\Big\{L_{m,s}x_0(s) - f(s)\Big\}ds.$$

Since $L_{m,t}\lambda(s;t) = 0$ from (3.22), then we obtain

$$L_{m,t}x_1(t) = f(t)$$

and also $\dot{x}_1^{(j)}(a) = \dot{x}_0^{(j)}(a)$ for $j = 0, 1, \ldots, m-1$. This completes the proof. ■

In order to illustrate the results of Theorem 3.1, we will consider the following example.

Example 3.2. Let us reconsider the following Cauchy-Euler differential equation

$$t^2\ddot{x} - 3t\dot{x} + 4x = t, \text{ with } x(1) = 2, \quad \dot{x}(1) = 2. \tag{3.24}$$

By dividing t^2, equation (3.24) can be reduced to

$$\ddot{x} - \frac{3}{t}\dot{x} + \frac{4}{t^2}x = \frac{1}{t}. \tag{3.25}$$

In Section 2.3.2, this system is solved by EVIM and the Lagrange multiplier of the extended version of the method is obtained as

$$\Lambda_A(s;t) = -\begin{pmatrix} \frac{t^2}{s^2}\left(1-2\ln\left(\frac{t}{s}\right)\right) & \frac{t^2}{s}\ln\left(\frac{t}{s}\right) \\ -\frac{4t}{s^2}\ln\left(\frac{t}{s}\right) & \frac{t}{s}\left(1+2\ln\left(\frac{t}{s}\right)\right) \end{pmatrix}.$$

Classical VIM constructs the following recursive functional

$$x_{n+1}(t) = x_n(t) + \int_1^t \lambda(s;t)\Big\{(x_n)''(s) - \frac{3}{s}(x_n)'(s) + \frac{4}{s^2}x_n(s) - \frac{1}{s}\Big\}ds.$$

By using the previous discussions, we obtain

$$\lambda(s;t) = \Lambda_{12}(s;t) = -\frac{t^2}{s}\ln\left(\frac{t}{s}\right).$$

It is also possible to obtain $\lambda(s;t)$ via (3.7) and (3.8), that is

$$\begin{array}{rcl} \lambda''(s;t) & + & \left(\frac{3\lambda(s;t)}{s}\right)' + \frac{4\lambda(s;t)}{s^2} = 0, \\ \lambda(t;t) & = & 0, \quad \frac{\partial\lambda(s;t)}{\partial s}\Big|_{s=t} = 1, \end{array} \tag{3.26}$$

which has the solution

$$\lambda(s;t) = \frac{-t^2}{s}\ln\left(\frac{t}{s}\right).$$

Let $x_0(t) = 2t$ that satisfies $x_0(1) = 2$, $\dot{x_0}(1) = 2$. Then,

$$x(t) = x_1(t) = t - t^2\ln t + t^2$$

is the exact solution of (3.24).

3.2 Solutions of Linear Boundary Value Problems

In Section 3.1, the following type of problems are considered

$$L_{m,t}x = f(t), \tag{3.27}$$

subject to the initial conditions

$$x(a) = x_a,\ \dot{x}(a) = \dot{x}_a,\ \dot{x}^{(2)}(a) = \dot{x}_a^{(2)},\ \ldots,\ \dot{x}^{(m-1)}(a) = \dot{x}_a^{(m-1)}. \tag{3.28}$$

It is proved that if the zeroth approximation of VIM satisfies the initial conditions (3.28), then the first approximation of the VIM will be the (exact) solution of initial value problem.

In this section, we will propose an algorithm for the following type of systems

$$Sx = f(t) \tag{3.29}$$

where S is a differential operator generated by

$$L_{m,t}x = p_0(t)\dot{x}^{(m)}(t) + p_1(t)\dot{x}^{(m-1)}(t) + p_2(t)\dot{x}^{(m-2)}(t) + \ldots + p_m(t)x(t) \tag{3.30}$$

and the boundary conditions

$$U_v(x) = \sum_{j=1}^{m} M_{vj}x^{(j-1)}(a) + N_{vj}x^{(j-1)}(b) = 0, \quad v = 1, 2, \ldots, m, \tag{3.31}$$

where $I = [a, b], \quad a, b \in \mathbb{R}$, $p_j : I \to \mathbb{R}$, and $p_j \in C^{m-j}(I, \mathbb{R})$ and $f : I \to \mathbb{R}$ is a continuous function.

Before launching into the new algorithm, we will state some basic theory of nonhomogenous boundary value problems of type (3.29). For the definitions and theorems given in the section, we refer [8, 9, 42].

Using matrices and column vectors to analyse the system (3.31) will simplify the discussions throughout the section. Let $\hat{x}$ denotes the column vector with components, $x, \dot{x}, \dot{x}^{(2)}, \ldots, \dot{x}^{(m-1)}$. Namely,

$$\hat{x}(t) = (x(t), \dot{x}(t), \dot{x}^{(2)}(t), \ldots, \dot{x}^{(m-1)}(t))^T \quad \text{for} \quad t \in [a, b].$$

Then, the boundary conditions

$$U_v(x) = \sum_{j=1}^{m} M_{vj}x^{(j-1)}(a) + N_{vj}x^{(j-1)}(b) = 0, \quad v = 1, 2, \ldots, m, \tag{3.32}$$

form the following system

$$U(x) = M\hat{x}(a) + N\hat{x}(b),$$

where $U = (U_1, U_2, \ldots, U_m)^T$ and M, N are $m \times m$ matrices with components M_{vj}, N_{vj}, respectively.

Unless stated otherwise, we assume that M, N forms a matrix with property that

$$\text{rank}(M : N) = m,$$

where $(M : N)$ is defined by the matrix

$$(M : N) = \begin{pmatrix} M_{11} & \cdots & M_{1m} & N_{11} & \cdots & N_{1m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ M_{m1} & \cdots & M_{mm} & N_{m1} & \cdots & N_{mm} \end{pmatrix}.$$

The former condition, $\text{rank}(M : N) = m$, implies that the homogeneous boundary value problem

$$L_{m,t}x = 0, \quad U(x) = 0,$$

has m linearly independent boundary conditions and hence, the problem has only the trivial solution. In that case, the solution of nonhomogenous boundary value problem (3.29) is determined by means of the Green's function:

The Green's function of the operator S is the function which has the following properties:

- $G(t, s)$ is continuous and has continuous derivatives with respect to t up to order $(m - 2)$ inclusive for all values of t and s in the interval $[a, b]$,

- For any fixed value of s in the interval (a, b) the function $G(t, s)$ has continuous derivatives of orders $(m - 1)$ and m with respect to t in each of the intervals $[a, s)$ and $(s, b]$; the $(m - 1)$th derivative is discontinuous at $t = s$ with a jump of $\dfrac{1}{p_0(s)}$,
$$\frac{\partial^{m-1}G}{\partial t^{m-1}}(s + 0, s) - \frac{\partial^{m-1}G}{\partial t^{m-1}}(s - 0, s) = \frac{1}{p_0(s)}.$$

- In each of the intervals $[a, s)$ and $(s, b]$, $G(t, s)$, considered as a function of t, satisfies the function $\ell(G) = 0$ and the boundary conditions $U_v(G) = 0$ for $v = 1, 2, \ldots, m$.

Theorem 3.3. *If the boundary value problem $Sx = 0$ has only the trivial solution, then the operator S has one and only one Green's function.*

Then, the solutions of systems (3.29) for any continuous function $f(t)$, $t \in I$ can be obtained via following theorem.

Theorem 3.4. *If the equation $Sx = 0$ has only the trivial solution, namely, $x(t) = 0$ for all $t \in I$, then for any function $f(t)$ which is continuous in the interval I, then there exists a solution of the equation $Sx = f$; this solution is expressed by the formula*

$$x(t) = \int_a^b G(t,s)f(s)ds,$$

where $G(t,s)$ denotes the Green's function for the operator S.

We have seen that the solution of nonhomogenous boundary value problems (3.29) can be obtained with Green's function.

Now, using the results of Section 3.1, we will prove the following theorem for boundary value problems (3.29). Following the theorem, we will propose an algorithm to obtain the solution of boundary value problem (3.29) without any need of Green's function, by an example.

Theorem 3.5. *Let*

$$Sx = f(t) \tag{3.33}$$

that is

$$L_{m,t}x = \frac{d^m x}{dt^m} + p_1(t)\frac{d^{m-1}x}{dt^{m-1}} + p_2(t)\frac{d^{m-2}x}{dt^{m-2}} + \ldots + p_m(t)x = f(t),$$

subject to the boundary conditions

$$U(x) = 0,$$

where $t \in I = [a,b]$, $\quad a,b \in \mathbb{R}$, $f : I \to \mathbb{R}$ is a continuous function. Let $x_0 \in C(I,\mathbb{R})$ which satisfies the boundary conditions. Then,

$$x_1(t) = \widetilde{x}_1(t) - y_1(t), \tag{3.34}$$

will be the solution of (3.33). Here, $\widetilde{x}_1(t)$ is the approximation obtained by the following correction functional of VIM

$$\widetilde{x}_1(t) = x_0(t) + \int_a^t \lambda(s;t)\Big\{L_{m,s}x_0(s) - f(s)\Big\}ds.$$

Moreover, $y_1 : I \longrightarrow \mathbb{R}$ is a function satisfies the following equations

$$\begin{aligned} L_{m,t}y_1 &= 0, \\ U(y_1) &= U(\widetilde{x}_1). \end{aligned} \tag{3.35}$$

Proof. In previous section, it was shown that

$$L_{m,t}\widetilde{x}_1(t) = f(t).$$

Therefore,

$$L_{m,t}\left(\widetilde{x}_1 - y_1\right) = L_{m,t}(\widetilde{x}_1) - L_{m,t}(y_1) = f(t),$$

and

$$U\left(\widetilde{x}_1(t) - y_1(t)\right) = U\left(\widetilde{x}_1(t)\right) - U\left(y_1(t)\right) = 0.$$

Hence, the proof is completed. ■

This theorem shows that for systems of the type (3.33), it is possible to obtain the solution of boundary value problem via a modified algorithm for the VIM. Moreover, the proposed method does not need Green's function [42].

In order to illustrate the results of the theorem and to forecast the basics of the modified algorithm in the next section, we consider the following boundary value problem

$$\ddot{x} + x = t^2, \quad \text{with} \quad x(0) = 0,\ \dot{x}(\pi) = 0 \tag{3.36}$$

Let

$$x_0(t) = \cos(t) - 1$$

be the initial approximation that satisfies boundary conditions, namely $x_0(0) = 0$, $\dot{x}_0(\pi) = 0$. The VIM constructs the following approximation

$$\widetilde{x}_1(t) = x_0(t) + \int_0^t \lambda(s;t)\Big\{(x_0)''(s) + x_0(s) - s^2\Big\}ds.$$

By using the previous discussions, we obtain the following equations for Lagrange multiplier $\lambda(s;t)$:

$$\begin{aligned} &\lambda''(s;t) + \lambda(s;t) = 0, \\ &\lambda(t;t) = 0, \quad \lambda'(s;t)\mid_{s=t} = 1. \end{aligned} \tag{3.37}$$

Solving this gives

$$\lambda(s;t) = \sin(s-t)$$

so that

$$\widetilde{x}_1(t) = \cos(t) - 1 + \int_0^t \sin(s-t)\Big\{-1 - s^2\Big\}ds = 2\cos(t) + t^2 - 2.$$

However,

$$\widetilde{x}_1(0) = 0, \quad \dot{\widetilde{x}}_1(\pi) = 2\pi.$$

Thus, our aim is to find a function y_1 that satisfies

$$\ddot{y}_1 + y_1 = 0, \quad y_1(0) = 0 \text{ and } \dot{y}_1(\pi) = 2\pi.$$

This is an easy task, and

$$y_1(t) = -2\pi \sin(t)$$

will suffice. Consequently,

$$x_1(t) = \widetilde{x}(t) - y_1(t) = 2\cos(t) + t^2 - 2 + 2\pi \sin(t)$$

is the exact solution of the boundary value problem in (3.36).

3.3 A New Algorithm for Boundary Value Problems

In the previous section, we analysed the nonhomogenous boundary value problems of the type

$$L_{m,t}x = f(t), \quad U(x) = 0, \tag{3.38}$$

where $t \in I = [a, b], \quad a, b \in \mathbb{R}$, $f : I \to \mathbb{R}$ is a continuous function. It is proved that the solution of such systems can be expressed by an approximate solution of VIM and a function determined by the boundary conditions.

In this section of the current work, we will propose an algorithm for the systems of the following form

$$L_{m,t}x = f(t, x(t), \dot{x}(t), \dot{x}^{(2)}(t), \ldots, \dot{x}^{(m-1)}(t)), \quad U(x) = 0, \tag{3.39}$$

where $t \in I$ and f is a continuous function with respect to all its components. Although the theory of (linear) boundary value problems of the type (3.38) is widely known, the corresponding theory of nonlinear systems, such as (3.39), has not been studied as much. Herewith, we shall introduce a new approach for solving such nonlinear boundary value problems.

Now, let's consider the following boundary value problem

$$L_{m,t}y = 0, \quad U(y) = u \tag{3.40}$$

where u is a given m-vector. Let $\phi_1, \phi_2, \ldots, \phi_m$ be linearly independent solutions of differential equation $L_{m,t}y = 0$ and $\hat{\Phi}$ is the fundamental matrix for $L_{m,t}y = 0$ in the following:

$$\hat{\Phi} = [\hat{\phi}_1, \hat{\phi}_2, \ldots, \hat{\phi}_m] = \begin{pmatrix} \phi_1 & \phi_2 & \cdots & \phi_m \\ \dot{\phi}_1 & \dot{\phi}_2 & \cdots & \dot{\phi}_m \\ \vdots & \vdots & \ddots & \vdots \\ \dot{\phi}_1^{(m-1)} & \dot{\phi}_2^{(m-1)} & \cdots & \dot{\phi}_m^{(m-1)} \end{pmatrix}.$$

Further, the boundary conditions of (3.39) can be extended as follows [9]:

$$U\hat{\Phi} = M\hat{\Phi}(a) + N\hat{\Phi}(b).$$

Before going back to the problem, finally, let us consider the solution of $L_{m,t}y = 0$ in the form

$$y = c_1\phi_1 + c_2\phi_2 + \cdots + c_m\phi_m,$$

where $c_1, c_2, \ldots, c_m$ are parameters identified by boundary conditions $U(y) = u$.

By using the fundamental matrix, it is possible to write

$$U(y) = U\hat{\Phi}c = u$$

where c is the column vector $c = (c_1, c_2, \ldots, c_m)^T$. We must recall that we have m linearly independent boundary conditions, that is, the nonsingularity of $U\hat{\Phi}$. Hence, the unknown parameter c can be determined uniquely as

$$c = (U\hat{\Phi})^{-1}u.$$

Now, it is time to go back to our original problem (3.39). We will propose the new algorithm to approximate the solutions of the (nonlinear) boundary value problems in (3.39).

For systems (3.39), the VIM constructs the following correction functional

$$x_{n+1}(t) = x_n(t) + \int_a^t \lambda\Big\{L_{m,s}(x_n(s)) - f\Big\}ds, \tag{3.41}$$

where $\lambda = \lambda(s;t)$ is the Lagrange multiplier and

$$f = f(s, x_n(s), (x_n)'(s), (x_n)'^{(2)}(s), \ldots, (x_n)'^{(m-1)}(s))$$

with $x'^{(i)} = d^i x/ds^i$ for $i = 1, 2, \ldots, (m-1)$. In our algorithm, we will modify correction functional (3.41) as follows

$$\widetilde{x}_{n+1}(t) = x_n(t) + \int_a^t \lambda\big\{L_{m,s}(x_n(s)) - f\big\}ds. \tag{3.42}$$

Here, x_n shows the nth approximate solution that satisfies the boundary conditions and $\widetilde{x}_{n+1}$ is the solution that does not necessarily satisfy the boundary conditions $U(x) = 0$. So without loss of generality we assume

$$U(\widetilde{x}_{n+1}) = u_{n+1}.$$

By the preceding discussions it is possible to construct a function y_{n+1} so that

$$L_{m,t}y_{n+1} = 0, \quad U(y_{n+1}) = u_{n+1}.$$

Then, our proposed algorithm gives the $(n+1)$th approximate solution as follows

$$x_{n+1}(t) = \widetilde{x}_{n+1}(t) - y_{n+1}(t).$$

It must be noted that

$$\begin{aligned} L_{m,t}x_{n+1} &= L_{m,t}\widetilde{x}_{n+1} - L_{m,t}y_{n+1} = \widetilde{f}, \\ U(x_{n+1}) &= U(\widetilde{x}_{n+1}) - U(y_{n+1}) = 0. \end{aligned}$$

where $\widetilde{f} = L_{m,t}\widetilde{x}_{n+1}$. Recursive application of the procedure for $n = 0, 1, 2, \ldots$ will yield the result.

As an illustrative example of the algorithm, consider the following system

$$\ddot{x} = -(\dot{x})^2 - 1 \tag{3.43}$$

subject to the boundary conditions

$$x(0) = 0, \quad \dot{x}(1) = 0.$$

The exact solution of (3.43) subject to the boundary conditions is

$$x(t) = \ln(\cos(t) + \tan(1)\sin(t)).$$

Let $x_0 = 0$ where $x_0(0) = 0$, $\dot{x}_0(1) = 0$. The modified correction functional will give $\widetilde{x}_1$ as follows:

$$\begin{aligned} \widetilde{x}_1(t) &= x_0(t) + \int_0^t (s-t)\big\{1\big\}ds, \\ &= -t^2/2 \end{aligned} \tag{3.44}$$

with $\widetilde{x}_1(0) = 0$, $\dot{\widetilde{x}}_1(1) = -1$. Clearly, $\hat{\phi}_1 = 1$ and $\hat{\phi}_2 = t$ are the fundamental solutions of $\ddot{y} = 0$. Therefore,

$$y_1(t) = c_0 + c_1 t$$

is also a solution of the homogeneous system $\ddot{y} = 0$ where c_0, c_1 are constants to be determined from the relations $y_1(0) = 0$ and $\dot{y}_1(1) = -1$. Hence, we obtain $c_0 = 0$, $c_1 = -1$ and thus $y_1(t) = -t$. So, the first variational iterate x_1 turns to be

$$x_1(t) = \widetilde{x}_1(t) - y_1(t) = -\frac{t^2}{2} + t$$

that also satisfies the boundary conditions. Carrying out this recursive algorithm, we approximate the solution to the boundary value problem.

Table 3.1 and Figure 3.1 show the approximate solutions $x_i(t)$ for $i = 1, 3, 5, 7$. There, $x^E(t)$ denotes the exact solution at t. Namely, $x^E(t) = \ln(\cos(t) + \tan(1)\sin(t))$. One can see that the proposed method gets very close results to the exact solution at the 7th variational iterate.

Table 3.1: The results of the proposed algorithm for (3.43).

t	$x_1(t)$	$x_3(t)$	$x_5(t)$	$x_7(t)$	$x_E(t)$
0	0	0	0	0	0
0.1	0.0950	0.1352	0.1399	0.1402	0.1402
0.2	0.1800	0.2472	0.2539	0.2542	0.2542
0.3	0.2550	0.3398	0.3472	0.3475	0.3475
0.4	0.3200	0.4156	0.4233	0.4236	0.4237
0.5	0.3750	0.4769	0.4847	0.4850	0.4850
0.6	0.4200	0.5253	0.5330	0.5333	0.5334
0.7	0.4550	0.5618	0.5695	0.5699	0.5699
0.8	0.4800	0.5873	0.5951	0.5954	0.5955
0.9	0.4950	0.6025	0.6102	0.6105	0.6106
1	0.5000	0.6075	0.6152	0.6155	0.6156

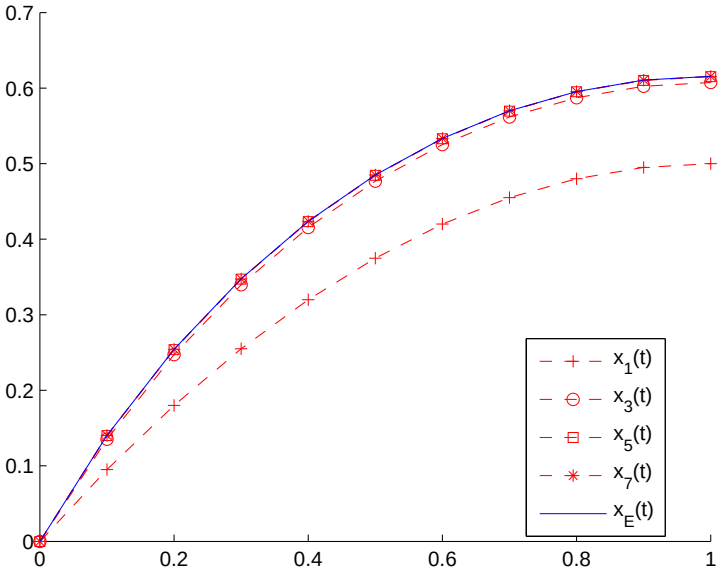

Figure 3.1: Comparison of the approximate solutions obtained by the proposed algorithm and the exact solution of (3.43).

CHAPTER 4

APPLICATIONS

In this chapter, we implement the variational iteration method to solve various types of problems. In the first section, we will apply the method to linear Sturm-Liouville eigenvalue problems. In the second section, we will apply the method to Brusselator model, and in the third one, we will use the method to solve the Chemical Master Equation (CME).

4.1 Variational Iteration Method for Sturm-Liouville Differential Equations

A linear Sturm-Liouville operator has the form,

$$Tx(t) := Lx(t) = \lambda r(t)x(t), \tag{4.1}$$

where $L = -\dfrac{d}{dt}\left[p(t)\dfrac{d}{dt}\right] + q(t), \quad t \in I := [a, b]$. Associated with the differential equation (4.1) are the separated homogeneous boundary conditions

$$\begin{aligned} \alpha_1 x(a) + \beta_1 \dot{x}(a) &= 0, \\ \alpha_2 x(b) + \beta_2 \dot{x}(b) &= 0, \end{aligned}$$

where α_1, α_2, β_1 and β_2 are arbitrary constants provided that $\alpha_i^2 + \beta_i^2 \neq 0$ for $i = 1, 2$. The values of λ for which the boundary value problem has a nontrivial solution are called eigenvalues of L. A nontrivial solution corresponding to an eigenvalue is called an eigenfunction. We will assume that $p(t)$, $\dot{p}(t)$, $q(t)$ and $r(t)$ are continuous functions such that $p(t) > 0$ and $r(t) > 0$ for all $t \in I$ [8, 53], for simplicity.

The main objective of this section is to implement VIM for computing eigenvalues of Sturm-Liouville problems.

Example 4.1. Consider the Sturm-Liouville system

$$-\ddot{x}(t) - \lambda x(t) = 0, \quad t \in I = (-\ell, \ell), \quad \ell > 0, \tag{4.2}$$

with homogeneous boundary conditions

$$x(-\ell) = 0, \quad x(\ell) = 0. \tag{4.3}$$

The correction functional of differential equation (4.2) has the following form:

$$x_{n+1}(t,\lambda) = x_n(t,\lambda) + \int_{-\ell}^{t} \mu\Big\{ - x_n''(s,\lambda) - \lambda x_n(s,\lambda)\Big\} ds, \tag{4.4}$$

where $\mu = \mu(s;t,\lambda)$ is the Lagrange multiplier [26, 30]. Then, we have

$$\delta x_{n+1}(t,\lambda) = \delta x_n(t,\lambda) + \delta \int_{-\ell}^{t} \mu\,(s;t,\lambda)\Big\{ - x_n''(s,\lambda) - \lambda x_n(s,\lambda)\Big\} ds.$$

Note that $\delta x_n(-\ell,\lambda) = 0$. Calculus of variations and integration by parts give the stationary conditions

$$\begin{aligned} \mu''(s;t,\lambda) + \lambda\mu(s;t,\lambda) &= 0, \\ 1 + \mu'(s;t,\lambda)\,|_{s=t} &= 0, \\ \mu\,(s;t,\lambda)\,|_{s=t} &= 0, \end{aligned}$$

for which the Lagrange multiplier μ should satisfy. Solving this system of equations for μ yields

$$\mu(s;t,\lambda) = -\frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda}(s-t)).$$

Thus, by inserting the Lagrange multiplier into (4.4) we obtain

$$\begin{aligned} x_{n+1}(t,\lambda) &= x_n(t,\lambda) \\ &+ \int_{-\ell}^{t} -\frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda}(s-t))\Big\{ - x_n''(s,\lambda) - \lambda x_n(s,\lambda)\Big\} ds. \end{aligned} \tag{4.5}$$

As an initial approximating solution, let us choose

$$x_0(t,\lambda) = A + Bt,$$

where A and B are constants that are going to be defined by imposing the boundary conditions (4.3) on the iterates and normalisation of the corresponding eigenfunctions. Substituting $x_0(t,\lambda)$ in (4.5) gives

$$x_1(t,\lambda) = A\cos(\sqrt{\lambda}t) + \frac{B}{\sqrt{\lambda}} \sin(\sqrt{\lambda}t).$$

If the function $x_1(t,\lambda)$ is now forced to satisfy the boundary conditions at $t=-\ell$ and $t=\ell$, then we get

$$\begin{aligned} x_1(-\ell,\lambda) &= A\cos(\sqrt{\lambda}\ell) - \frac{B}{\sqrt{\lambda}}\sin(\sqrt{\lambda}\ell) = 0, \\ x_1(\ell,\lambda) &= A\cos(\sqrt{\lambda}\ell) + \frac{B}{\sqrt{\lambda}}\sin(\sqrt{\lambda}\ell) = 0. \end{aligned}$$

In order to have a nontrivial solution $x_1(t,\lambda)$, the system yields two infinite sequences of eigenvalues λ_n,

$$\begin{aligned} \lambda_n &= \left(\frac{(2n+1)\pi}{2\ell}\right)^2, \quad n=0,1,2,\ldots, \\ \lambda_n &= \left(\frac{n\pi}{\ell}\right)^2, \quad n=1,2,\ldots. \end{aligned}$$

The corresponding linearly independent eigenfunctions u_n and v_n are

$$\begin{aligned} u_n(t) &= A\cos\left(\frac{(2n+1)\pi}{2\ell}t\right), \quad n=0,1,2,\ldots, \\ v_n(t) &= B\frac{\ell}{n\pi}\sin\left(\frac{n\pi}{\ell}t\right), \quad n=1,2,\ldots. \end{aligned}$$

Here $u_n(t), v_n(t) \in \mathcal{C}(I,\mathbb{R})$; that is $u_n(t)$ and $v_n(t)$ are continuous real valued functions on $I=(-\ell,\ell)$. The usual inner product on $\mathcal{C}(I,\mathbb{R})$ is defined by

$$\langle u_n, v_n\rangle = \int_{-\ell}^{\ell} u_n(s)v_n(s)ds, \quad u_n, v_n \in \mathcal{C}(I,\mathbb{R}),$$

and the norm induced by the inner product is

$$\|u_n\|_2 = \langle u_n, u_n\rangle^{\frac{1}{2}} = \left(\int_{-\ell}^{\ell} |u_n(s)|^2 ds\right)^{\frac{1}{2}}.$$

Consequently, we obtain

$$A = \frac{1}{\sqrt{\ell}}, \quad B = \frac{n\pi}{\ell^{\frac{3}{2}}}.$$

Therefore, the normalised eigenfunctions $t_n(t) = \dfrac{u_n(t)}{\|u_n\|_2}$ and $z_n(t) = \dfrac{v_n(t)}{\|v_n\|_2}$ have the forms

$$\begin{aligned} t_n(t) &= \frac{1}{\sqrt{\ell}}\cos\left(\sqrt{\lambda_n}t\right) \quad \text{with} \quad \lambda_n = \left(\frac{(2n+1)\pi}{2\ell}\right)^2, \quad n=0,1,2,\ldots, \\ z_n(t) &= \frac{1}{\sqrt{\ell}}\sin\left(\sqrt{\lambda_n}t\right) \quad \text{with} \quad \lambda_n = \left(\frac{n\pi}{\ell}\right)^2, \quad n=1,2,\ldots. \end{aligned}$$

These eigenvalues and eigenfunctions are the exact eigen-pairs of the Sturm-Liouville system in (4.2).

Example 4.2. As another example consider the eigenvalue problem

$$-\ddot{x}(t) - \lambda x(t) = 0, \quad t \in I = (-\ell, \ell), \quad \ell > 0, \tag{4.6}$$

with Neumann boundary conditions,

$$\dot{x}(-\ell) = 0, \quad \dot{x}(\ell) = 0. \tag{4.7}$$

Using variational iteration method, we can construct the correction functional of (4.6) as follows:

$$\begin{aligned} x_{n+1}(t,\lambda) &= x_n(t,\lambda) \\ &+ \int_{-\ell}^{t} \mu\Big\{ - x_n''(s,\lambda) - \lambda x_n(s,\lambda)\Big\} ds, \end{aligned} \tag{4.8}$$

where $\mu = \mu\,(s;t,\lambda)$ is the Lagrange multiplier. Note that $\delta x_n(-\ell,\lambda) = 0$.

The Lagrange multiplier can be identified as

$$\mu(s;t,\lambda) = -\frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda}(s-t)),$$

so that the iterations in (4.8) can be written as follows:

$$\begin{aligned} x_{n+1}(t,\lambda) &= x_n(t,\lambda) \\ &+ \int_{-\ell}^{t} -\frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda}(s-t))\Big\{ - x_n''(s,\lambda) - \lambda x_n(s,\lambda)\Big\} ds. \end{aligned} \tag{4.9}$$

We begin with an initial approximation $x_0(t,\lambda) = A + Bt$ where A and B are constants to be determined as before. By the correction functional (4.9), we get

$$x_1(t,\lambda) = A\cos(\sqrt{\lambda}t) + \frac{B}{\sqrt{\lambda}} \sin(\sqrt{\lambda}t). \tag{4.10}$$

Then,

$$\begin{aligned} x_1'(-\ell,\lambda) &= A\sqrt{\lambda}\sin(\sqrt{\lambda}\ell) + B\cos(\sqrt{\lambda}\ell) = 0, \\ x_1'(\ell,\lambda) &= -A\sqrt{\lambda}\sin(\sqrt{\lambda}\ell) + B\cos(\sqrt{\lambda}\ell) = 0. \end{aligned}$$

Thus, the eigenvalues of this system have the form

$$\begin{aligned} \lambda_n &= \left(\frac{(2n+1)\pi}{2\ell}\right)^2, \quad n = 0, 1, 2, \ldots \\ \lambda_n &= \left(\frac{n\pi}{\ell}\right)^2, \quad n = 1, 2, \ldots. \end{aligned}$$

Corresponding linearly independent nontrivial solutions are

$$\begin{aligned} u_n(t) &= B\frac{2\ell}{(2n+1)\pi}\sin\left(\sqrt{\lambda_n}t\right) \text{ with } \lambda_n = \left(\frac{(2n+1)\pi}{2\ell}\right)^2, \quad n = 0, 1, 2, \ldots, \\ v_n(t) &= A\cos\left(\sqrt{\lambda_n}t\right) \text{ with } \lambda_n = \left(\frac{n\pi}{\ell}\right)^2, \quad n = 1, 2, \ldots. \end{aligned}$$

So, the normalisation constants are

$$A = \frac{1}{\sqrt{\ell}}, \quad B = \frac{(2n+1)\pi}{2\ell^{\frac{3}{2}}}.$$

Let $t_n(t) = \dfrac{u_n(t)}{\|u_n\|_2}$ and $z_n(t) = \dfrac{v_n(t)}{\|v_n\|_2}$, then

$$\begin{aligned} t_n(t) &= \frac{1}{\sqrt{\ell}}\sin\left(\frac{(2n+1)\pi}{2\ell}t\right) \quad n = 0, 1, 2, \ldots, \\ z_n(t) &= \frac{1}{\sqrt{\ell}}\cos\left(\frac{n\pi}{\ell}t\right), \quad n = 1, 2, \ldots. \end{aligned}$$

Example 4.3. Now consider the following equation [53],

$$-\ddot{x}(t) + (t^2 - \lambda)x(t) = 0, \quad t \in I = (-\infty, \infty). \tag{4.11}$$

The solutions of the system (4.11) are in the following form

$$x_n^{\infty} = A_n e^{-t^2/2} H_n(t), \quad \lambda_n^{\infty} = 2n + 1, \quad n = 0, 1 \ldots.$$

where $H_n(x)$ denotes the Hermite polynomials and A_n are normalisation constants [53].

Let us consider system (4.11) in a truncated domain, $-\ell \leq t \leq \ell$ for all $\ell > 0$. The new system is,

$$-\ddot{x} + (t^2 - \lambda)x(t) = 0, \tag{4.12}$$

with Dirichlet boundary conditions $x(-\ell) = 0$, $x(\ell) = 0$. To find the approximate solution of equation (4.12) by means of variational method, the following correction functional can be constructed as

$$\begin{aligned} x_{n+1}(t, \lambda) &= x_n(t, \lambda) \\ &+ \int_{-\ell}^{t} \mu\Big\{ - x_n''(s, \lambda) + s^2\widetilde{x}_n(s, \lambda) - \lambda x_n(s, \lambda)\Big\} ds, \end{aligned}$$

where $\mu = \mu(s; t, \lambda)$ is the Lagrange multiplier and $\widetilde{x}_n$ denotes restricted variation that is $\delta\widetilde{x}_n = 0$. Following the discussions presented in the previous examples, we obtain

the iteration formula

$$\begin{aligned} x_{n+1}(t,\lambda) &= x_n(t,\lambda) \\ &+ \int_{-\ell}^{t} -\frac{1}{\sqrt{\lambda}}\sin(\sqrt{\lambda}(s-t))\Big\{ -x_n''(s,\lambda) + s^2 x_n(s,\lambda) - \lambda y_n(s,\lambda)\Big\}ds. \end{aligned}$$

Let us start again with an initial approximation $x_0(t,\lambda) = A + Bt$, where A and B are real unknown constants. Then,

$$\begin{aligned} x_1(t,\lambda) &= A + Bt \\ &+ \int_{-\ell}^{t} -\frac{1}{\sqrt{\lambda}}\sin(\sqrt{\lambda}(s-t))\Big\{s^2(A+Bs) - \lambda(A+Bs)\Big\}ds. \end{aligned}$$

In Table 4.1, we present the eigenvalues of system (4.12) for different values of ℓ and they are compared with the exact values $\lambda_n^\infty = 2n+1$ for $n = 0, 1\ldots$.

Table 4.1: Eigenvalues of equation (4.12) obtained by the variational iteration method for $\ell = 2, \pi$ and 4.5.

n	ℓ	Number of iterations	λ	$\lvert\lambda - \lambda_n^\infty\rvert$	λ_n^∞
0	2	3	1.0823	0.0823	1
		5	1.0749	0.0750	
		6	1.0749	0.0749	
		7	1.0749	0.0749	
	π	3	1.3952	0.3952	1
		5	1.0177	0.0177	
		6	1.0030	0.0030	
		7	1.0006	0.0006	
	4.5	3	NaN		1
		5	NaN		
		6	1.2771	0.2771	
		7	1.1007	0.1007	
1	2	3	1.0823	1.9177	3
		5	1.9177	1.9251	
		6	1.0749	1.9251	
		7	1.0749	1.9251	
	π	3	3.1665	0.1665	3
		5	4.8576	1.8576	
		6	1.0030	1.9970	
		7	1.0030	1.9970	
	4.5	3	NaN		3
		5	NaN		
		6	3.2916	0.2916	
		7	4.0764	1.0764	

4.2 Variational Iteration Method for Brusselator Reaction-Diffusion System

In this section of the present work, we will investigate the dynamical behaviour of Brusselator reaction system which was proposed by Prigogine and Lefever as a model for chemical dynamics [47]. The mechanism of Brusselator system is as follows [3, 35, 44, 47, 58, 61]

$$A \longrightarrow X, \tag{4.13a}$$

$$B + X \longrightarrow Y + D, \tag{4.13b}$$

$$2X + Y \longrightarrow 3X, \tag{4.13c}$$

$$X \longrightarrow E. \tag{4.13d}$$

Here, A and B denote the input chemicals, D and E are output chemicals and X, Y are intermediates. It is a known fact that the reaction step (4.13c) can be observed in the formation of ozone by atomic oxygen, inenzymatic reactions, in plasma and laser physics [3, 57, 61]. The differential equations associated with (4.13) are given [47]:

$$\begin{aligned} \frac{\partial X}{\partial t} &= c_1 A - c_2 B X + c_3 X^2 Y - c_4 D_x \nabla^2 X \\ \frac{\partial Y}{\partial t} &= c_2 B X - c_3 X^2 Y D_y \nabla^2 Y, \end{aligned} \tag{4.14}$$

where c_1, c_2, c_3, c_4 denote the reaction constants of (4.13a), (4.13b), (4.13c), (4.13d), respectively.

Let $u = u(x, y, t)$ and $v = v(x, y, t)$ denote the concentration of products at time t, A, B are the constant concentrations of two input chemicals and α is a constant represents D_x, D_y and L is the reactor length.

Then, the partial differential equations that represents the Brusselator model is as follows [3, 57]:

$$\begin{aligned} \frac{\partial u}{\partial t} &= A + u^2 v - (B+1)u + \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ \frac{\partial v}{\partial t} &= Bu - u^2 v + \alpha \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \end{aligned} \tag{4.15}$$

for $0 < x, y < L$, $0 < t < T$. Then, we impose the Dirichlet boundary conditions of

the following type:

$$\begin{aligned} u(t,x,0) &= 0, \quad v(t,x,0)=0, \quad \text{for} \quad 0<x<L, \quad 0<t<T, \\ u(t,x,1) &= 0, \quad v(t,x,1)=0, \quad \text{for} \quad 0<x<L, \quad 0<t<T, \\ u(t,0,y) &= 0, \quad v(t,0,y)=0, \quad \text{for} \quad 0<y<L, \quad 0<t<T, \\ u(t,1,y) &= 0, \quad v(t,1,y)=0, \quad \text{for} \quad 0<y<L, \quad 0<t<T, \end{aligned} \tag{4.16}$$

and initial conditions

$$u(0,x,y)=x, \quad v(0,x,y)=xy^2 \quad 0<x,y<L. \tag{4.17}$$

Semi-discrete methods which discretise in space and leave time variable continuous is a way to approximate solutions of system (4.15).

Let the discretisation of the domain be such that $x_i = i\Delta_x$, $y_j = j\Delta_y$, $i = 0, 1, \ldots, n+1$, $j = 0, 1, \ldots, m+1$ with $\Delta_x = \dfrac{1}{n+1}$, $\Delta_y = \dfrac{1}{m+1}$. Then, the second derivatives u_{xx}, u_{yy} and v_{xx}, v_{yy} can be replaced, respectively, with the following differences:

$$\begin{aligned} u_{xx}(t,x_i,y_j) &\approx \frac{u(t,x_{i+1},y_j)-2u(t,x_i,y_j)+u(t,x_{i-1},y_j)}{(\Delta x)^2}, \\ v_{xx}(t,x_i,y_j) &\approx \frac{v(t,x_{i+1},y_j)-2v(t,x_i,y_j)+v(t,x_{i-1},y_j)}{(\Delta x)^2}, \end{aligned}$$

and

$$\begin{aligned} u_{yy}(t,x_i,y_j) &\approx \frac{u(t,x_i,y_{j+1})-2u(t,x_i,y_j)+u(t,x_i,y_{j-1})}{(\Delta y)^2}, \\ v_{yy}(t,x_i,y_j) &\approx \frac{v(t,x_i,y_{j+1})-2v(t,x_i,y_j)+v(t,x_i,y_{j-1})}{(\Delta y)^2}, \end{aligned}$$

for $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, m$.

Let $u_{i,j}$ and $v_{i,j}$ denote the $u(t, x_i, y_j)$ and $v(t, x_i, y_j)$, respectively. It is possible to obtain a system of ODEs at mesh points x_i, y_j for $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, m$; such as,

$$\begin{aligned} \dot{u}_{i,j} &= A + u_{i,j}^2 v_{i,j} - (B+1)u_{i,j} \\ &+ \alpha\left(\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{(\Delta x)^2} + \frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{(\Delta y)^2}\right), \\ \dot{v}_{i,j} &= Bu_{i,j} - u_{i,j}^2 v_{i,j} \\ &+ \alpha\left(\frac{v_{i+1,j}-2v_{i,j}+v_{i-1,j}}{(\Delta x)^2} + \frac{v_{i,j+1}-2v_{i,j}+v_{i,j-1}}{(\Delta y)^2}\right). \end{aligned} \tag{4.18}$$

Here,$\dot{u}_{i,j}$, $\dot{v}_{i,j}$ denote $du_{i,j}/dt$, $dv_{i,j}/dt$. From boundary conditions we know that

$$\begin{aligned} u_{i,0} &= 0, \quad v_{i,0}=0, \quad i=0,1,\ldots,n+1, \\ u_{i,m+1} &= 0, \quad v_{i,m+1}=0, \quad i=0,1,\ldots,n+1, \\ u_{0,j} &= 0, \quad v_{0,j}=0, \quad j=0,1,\ldots,m+1, \\ u_{n+1,j} &= 0, \quad v_{n+1,j}=0, \quad j=0,1,\ldots,m+1. \end{aligned} \tag{4.19}$$

and the initial conditions

$$\begin{aligned} u(0,x_i,y_j) &= x_i, \quad i=1,2,\ldots,n, \quad j=1,2,\ldots,m, \\ v(0,x_i,y_j) &= x_i y_j^2, \quad i=1,2,\ldots,n, \quad j=1,2,\ldots,m. \end{aligned} \tag{4.20}$$

To simplify the notation, let us write the system (4.18) as follows:

$$\dot{\mathbf{z}} = S\mathbf{z} + f(\mathbf{z}), \tag{4.21}$$

where $\mathbf{z} = (u_{i,j}, v_{i,j})$,

$$S = \begin{pmatrix} -(B+1) - \dfrac{2\alpha}{(\Delta x)^2} - \dfrac{2\alpha}{(\Delta y)^2} & 0 \\ B & -\dfrac{2\alpha}{(\Delta x)^2} - \dfrac{2\alpha}{(\Delta y)^2} \end{pmatrix},$$

and

$$f(\mathbf{z}) = \begin{pmatrix} \alpha\left(\dfrac{u_{i+1,j}+u_{i-1,j}}{(\Delta x)^2} + \dfrac{u_{i,j+1}+u_{i,j-1}}{(\Delta y)^2}\right) + A + u_{i,j}^2 v_{i,j} \\ \alpha\left(\dfrac{v_{i+1,j}+v_{i-1,j}}{(\Delta x)^2} + \dfrac{v_{i,j+1}+v_{i,j-1}}{(\Delta y)^2}\right) - u_{i,j}^2 v_{i,j} \end{pmatrix}.$$

Let, now, $A = 0.5, B = 1, \alpha = 1/64,\ \Delta_x = 0.25,\ \Delta_y = 0.25,\ L = 1$ and $T = 1$ so that (4.21) can be rewritten as

$$\dot{\mathbf{z}} = \begin{pmatrix} -3 & 0 \\ 1 & -1 \end{pmatrix} \mathbf{z} + \begin{pmatrix} 0.25\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) + 0.5 + u_{i,j}^2 v_{i,j} \\ 0.25\left(v_{i+1,j} + v_{i-1,j} + v_{i,j+1} + v_{i,j-1}\right) - u_{i,j}^2 v_{i,j} \end{pmatrix}.$$

Transforming the variable $\mathbf{z}$ to $\mathbf{w}$ by setting $\mathbf{w} = P\mathbf{z}$, we obtain a diagonalised system in $\mathbf{w}$ as

$$\dot{\mathbf{w}} = J\mathbf{w} + P^{-1} f(P\mathbf{z}), \tag{4.22}$$

where

$$P = \begin{pmatrix} 0 & 0.89 \\ 1 & -0.45 \end{pmatrix}, \quad P^{-1} = \begin{pmatrix} 0.5 & 1 \\ 1.12 & 0 \end{pmatrix}, \text{ and } J = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix}.$$

Correction functional of the transformed system is

$$\mathbf{w}^{n+1}(t) = \mathbf{w}^n(s) + \int_0^t \Lambda_J(s,t)\Big\{(\mathbf{w}^n)'(s) - J\mathbf{w}^n(s) + P^{-1} f(\widetilde{\mathbf{w}}^n(s))\Big\}$$

for $t \in [0,1]$, and with $\widetilde{\mathbf{w}}^n(s)$ being the restricted variation. It must be noted that initial conditions (4.20) and boundary conditions (4.19) are transformed to the new

variable $\mathbf{w}$, and initial condition of new variable is used as the zeroth approximate solution. The Lagrange multiplier $\Lambda_J(s,t)$ is

$$\Lambda_J(s,t) = -e^{-J(s-t)} = \begin{pmatrix} -e^{(s-t)} & 0 \\ 0 & -e^{3(s-t)} \end{pmatrix}.$$

If we divide $[0,1]$ time interval into subintervals $[0,t_1), [t_1,t_2), \ldots, [t_9,1)$ where $t_i = i\Delta_\ell$ with $\Delta_\ell = 0.1$, for every $i = 1,2,\ldots,9$, then we can construct the following correction functional of MEVIM:

$$\mathbf{w}^{n+1}(t) = \mathbf{w}^n(s) + \int_{t^*}^{t} -e^{-J(s-t)}\Big\{(\mathbf{w}^n)'(s) - J\mathbf{w}^n(s) + P^{-1}f(\widetilde{\mathbf{w}}^n(s))\Big\},$$

where $t^* \in \{0, t_1, t_2, \ldots, t_9\}$ and

$$\mathbf{w}(t^*) = \mathbf{w}^n(t^*), \tag{4.23}$$

where $\mathbf{w}$ at the right hand-side of (4.23) denotes the nth order approximate solution in $[t_k, t^*)$ where $k \in \{0,1,\ldots,t_9\}$.

In Table 4.2, we compare the fifth order approximate solutions of MEVIM and EVIM with results obtained by Runge-Kutta methods for solving system (4.18). We use the notation

$$\varepsilon_{u_{i,j}}^{EVIM}(t) = \left|u_{i,j}^{EVIM}(t) - u_{i,j}^{E}(t)\right|, \quad \varepsilon_{u_{i,j}}^{MEVIM}(t) = \left|u_{i,j}^{MEVIM}(t) - u_{i,j}^{E}(t)\right|,$$

$$\varepsilon_{v_{i,j}}^{EVIM}(t) = \left|v_{i,j}^{EVIM}(t) - v_{i,j}^{E}(t)\right|, \quad \varepsilon_{v_{i,j}}^{MEVIM}(t) = \left|v_{i,j}^{MEVIM}(t) - v_{i,j}^{E}(t)\right|.$$

Here, $u_{i,j}^{EVIM}(t)$, $u_{i,j}^{MEVIM}(t)$, $u_{i,j}^{E}(t)$ denote the approximate solutions of u at points $x_i,\ y_j,\ t$ obtained by EVIM, MEVIM, and Runge-Kutta, respectively. Similarly, $v_{i,j}^{EVIM}(t)$, $v_{i,j}^{MEVIM}(t)$, and $v_{i,j}^{E}(t)$ denote the approximate solutions of v at points $x_i,\ y_j,\ t$ obtained by EVIM, MEVIM and Runge-Kutta, respectively.

Now, let us consider the Brusselator system (4.15) with $\alpha = 0$ so that we have an ODE case. Then, we get the following system

$$\begin{aligned} \dot{u} &= A - (B+1)u + u^2 v, \\ \dot{v} &= Bu - u^2 v, \end{aligned} \tag{4.24}$$

where u and v denote the concentrations of two reactants at time t and $a, b \in \mathbb{R}$ with $A, B > 0$. It is easy to observe that $(u^*, v^*) = (A, \frac{B}{A})$ is an equilibrium point of the

Table 4.2: Absolute errors for the fifth-order approximation of EVIM and MEVIM.

t	$\varepsilon_{u_{2,2}}^{EVIM}$	$\varepsilon_{u_{2,2}}^{MEVIM}$	$\varepsilon_{v_{4,4}}^{EVIM}$	$\varepsilon_{v_{4,4}}^{MEVIM}$
0	0	0	0	0
0.1	0.0198	0.0202	0.7727	0.8232
0.2	0.0320	0.0327	0.5856	0.2407
0.3	0.0379	0.0261	0.1699	0.1488
0.4	0.0392	0.0138	0.2272	0.0364
0.5	0.0370	0.0110	0.5621	0.1846
0.6	0.0325	0.0104	0.8188	0.0268
0.7	0.0266	0.0062	0.9857	0.1251
0.8	0.0200	0.0043	1.0656	0.1598
0.9	0.0132	0.0042	1.0731	0.1909
1	0.0065	0.0022	1.0228	0.1705

system. It is known that when $1 - B + A^2 \geq 0$, the equilibrium point is a stable one [57].

Classical: Let us suppose that $A = 3$ and $B = 1$, so that the equilibrium point is stable; and let $(u(0), v(0))^T = (1, 2)^T$ be the initial state of the system. To find the approximate solution of system (4.24) by means of variational iteration method, we can construct the following correction functionals

$$\begin{aligned} u^{n+1}(t) &= u^n(t) + \int_0^t \mu_1 \left\{ (u^n)'(s) + 2u(s) - (u^n(s))^2 \widetilde{v}^n(s) - 3 \right\} ds, \\ v^{n+1}(t) &= v^n(t) + \int_0^t \mu_2 \left\{ (v^n)'(s) - \widetilde{u}^n(s) + (\widetilde{u}^n(s))^2 v^n(s) \right\} ds, \end{aligned}$$

where $\mu_1 = \mu_1(s;t), \mu_2 = \mu_2(s;t)$ are the general Lagrange multipliers and $\widetilde{u}^n(s)$ and $\widetilde{v}^n(s)$ are restricted variations, i.e., $\delta\widetilde{u}^n(s) = \delta\widetilde{v}^n(s) = 0$. We therefore calculate the Lagrange multipliers as

$$\mu_1(s;t) = -e^{2(s-t)}, \quad \mu_2(s;t) = -1.$$

By substituting the multipliers into the correction functionals, we obtain the following formulae for the approximate solutions:

$$\begin{aligned} u^{n+1}(t) &= u^n(t) + \int_0^t (-e^{2(s-t)}) \left\{ (u^n)'(s) + 2u(s) - (u^n(s))^2 v^n(s) - 3 \right\} ds, \\ v^{n+1}(t) &= v^n(t) + \int_0^t (-1) \left\{ (v^n)'(s) - u^n(s) + (u^n(s))^2 v^n(s) \right\} ds, \end{aligned}$$

with initial approximations $u^0(t) = 1$ and $v^0(t) = 2$.

Extended: Using matrices and vectors, $\mathbf{x} = (u, v)^T$, system (4.24) can be rewritten

as follows

$$\dot{\mathbf{x}} = M\mathbf{x} + \mathbf{f}(t, \mathbf{x}), \quad \mathbf{x}(0) = (1, 2)^T, \tag{4.25}$$

where

$$M = \begin{pmatrix} -2 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{f}(t, \mathbf{x}) = \begin{pmatrix} 3 + x_1^2 x_2 \\ -x_1^2 x_2 \end{pmatrix}.$$

It must be noted that same as the classical VIM, we choose $a = 1$ and $b = 3$. Setting $\mathbf{x} = P\mathbf{y}$, the transformed equation turns to be

$$\dot{\mathbf{y}} = J\mathbf{y} + \mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 3/2 - 2y_2^2(y_1 - y_2) \\ 3/2 + 2y_2^2(y_1 - y_2) \end{pmatrix}, \tag{4.26}$$

together with the initial value

$$\mathbf{y}(0) = (5/2, 1/2)^T,$$

where $P = \begin{pmatrix} 0 & 2 \\ 1 & -1 \end{pmatrix}$ and $P^{-1} = \begin{pmatrix} 1/2 & 1 \\ 1/2 & 0 \end{pmatrix}$. The correction functional of system (4.26) can be written as

$$\mathbf{y}^{n+1}(t) = \mathbf{y}^n(t) + \int_0^t \Lambda_J(s; t)\Big\{(\mathbf{y}^n)'(s) - J\mathbf{y}^n(s) - \mathbf{f}(s, \widetilde{\mathbf{y}}^n(s))\Big\}ds,$$

with initial approximation $\mathbf{y}^0(t) = \mathbf{y}(0)$, where $\widetilde{\mathbf{y}}^n(s)$ denotes the restricted variation vector. Hence, we obtain the Lagrange multiplier $\Lambda_J(s; t)$ as

$$\Lambda_J(s, t) = -\begin{pmatrix} 1 & 0 \\ 0 & e^{2(s-t)} \end{pmatrix}.$$

Then, by using the transformation $\mathbf{x} = P\mathbf{y}$ one can construct an approximate solution of original system (4.25).

Table 4.3 shows the absolute errors of the nth order approximations obtained from the application of the classical and the extended approach. Henceforth, we define

$$\varepsilon_i^{VIM} = \left|x_i^{VIM} - x_i^E\right|, \quad \varepsilon_i^{EVIM} = \left|x_i^{EVIM} - x_i^E\right|, \quad i = 1, 2,$$

where x_i^E is the Runge-Kutta solution, and x_i^{VIM} and x_i^{EVIM} are the solutions obtained by VIM and EVIM at $t = 0.5$, respectively.

Figure 4.1 illustrates a comparison between the two approaches for the tenth-order approximation.

Table 4.3: Comparison of the classical and the proposed approach to VIM for the Brusselator system at point $t = 0.5$.

n	ε_1^{VIM}	ε_1^{EVIM}	ε_2^{VIM}	ε_2^{EVIM}
1	0.969744	0.969744	0.899420	1.175330
2	0.171587	0.045379	0.062814	0.078816
3	0.034040	0.046744	0.004173	0.046531
4	0.011708	0.008104	0.006337	0.008572
5	0.001194	0.001062	0.000142	0.001055
6	0.000402	0.000083	0.000199	0.000087
7	0.000042	0.000006	0.000004	0.000006
8	0.000008	0.000000	0.000003	0.000000
9	0.000001	0.000000	0.000000	0.000000
10	0.000000	0.000000	0.000000	0.000000

In the previous applications, we have applied EVIM to the differential systems of the form

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + \mathbf{f}(t, \mathbf{x}(t)), \quad t \in I, \quad \mathbf{x}(0) = \alpha_0.$$

where A is 2×2 matrix, $\mathbf{f} : I \times \mathbb{R}^2 \to \mathbb{R}^2$ is a given nonlinear function and $\mathbf{x}$ is 2-vector.

In the next example, we will illustrate that EVIM and MEVIM is more suitable than the classical VIM and MVIM for systems where A is an $n \times n$ matrix, where n is larger than 2.

To prove the efficiency of the method for such systems, we will use the Brusselator model which was proposed by Tyson [58] in 1972. This system is constructed by using two Brusselators. In this model the outputs of the first Brusselator model are used as the inputs of the second one. The reactions of the new models are given by [61]:

$$\begin{gathered} A \longrightarrow X, \quad B + X \longrightarrow Y + D, \quad 2X + Y \longrightarrow 3X, \quad X \longrightarrow E, \\ D + E \longrightarrow F + G, \quad 2E + F \longrightarrow 3H, \quad H \longrightarrow K. \end{gathered} \tag{4.27}$$

The differential equation associated by (4.27) are [58, 61]

$$\begin{aligned} \dot{z}_1 &= f_1(\mathbf{z}, A, B) = A - Bz_1 + (z_1)^2 z_2 - z_1, \\ \dot{z}_2 &= f_2(\mathbf{z}, A, B) = Bz_1 - (z_1)^2 z_2, \\ \dot{z}_3 &= f_3(\mathbf{z}, A, B) = z_1 - z_3 z_4, \\ \dot{z}_4 &= f_4(\mathbf{z}, A, B) = Bz_1 - z_3 z_4 + (z_4)^2 z_5 - z_4, \\ \dot{z}_5 &= f_5(\mathbf{z}, A, B) = z_3 z_4 - (z_4)^2 z_5, \end{aligned} \tag{4.28}$$

where $\mathbf{z} = (z_1, z_2, z_3, z_4, z_5)^T = (X, Y, D, H, F)^T$, A and B are real constants and

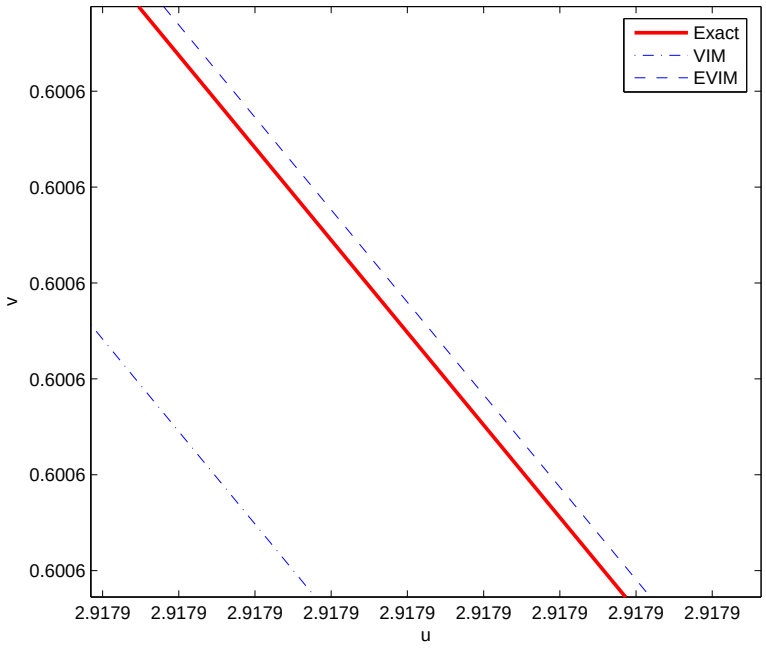

Figure 4.1: Comparison between the classical and the proposed approach to VIM for the tenth-order approximation.

$t \in [0, T], T > 0$. Let $A = 1$, $B = 0.5$. Then, (4.28) can be written

$$\dot{\mathbf{z}} = M\mathbf{z} + f(\mathbf{z}) \tag{4.29}$$

where

$$M = \begin{pmatrix} -1.5 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad f(\mathbf{z}) = \begin{pmatrix} (z_1)^2 z_2 + 1 \\ -(z_1)^2 z_2 \\ -(z_3) z_4 \\ -z_3 z_4 + (z_4)^2 z_5 \\ z_3 z_4 - (z_4)^2 z_5 \end{pmatrix}.$$

Let us impose the initial conditions to be

$$\mathbf{z}(0) = (0.8, 0.4, 1.8, 0.4, 3.75)^T.$$

Since the matrix A is a constant matrix, it is possible to introduce $\mathbf{w} = P\mathbf{z}$ transfor-

mation where

$$P = \begin{pmatrix} 0 & 0 & 0 & 0.6255 & 0 \\ 1 & 1 & 0 & -0.2085 & 0 \\ 0 & 0 & 1 & -0.4170 & 0 \\ 1 & 0 & 0 & -0.6255 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then, (4.29) is transformed to

$$\dot{\mathbf{w}} = J\mathbf{w} + f(\mathbf{w}), \tag{4.30}$$

with $\mathbf{w}(0) = (1.2000, 0.6667, 2.3333, 1.2789, 3.7500)^T$. To obtain the approximate solutions of system (4.30) by means of EVIM, the following correction functional will be constructed

$$\mathbf{w}^{n+1}(t) = \mathbf{w}^n(s) + \int_0^t -e^{-J(s-t)}\Big\{(\mathbf{w}^n)'(s) - J\mathbf{w}^n(s) + f(\widetilde{\mathbf{w}}^n(s))\Big\} \tag{4.31}$$

for $t \in [0,1]$. If we want to apply MEVIM, correction functional (4.31) takes the following form,

$$\mathbf{w}^{n+1}(t) = \mathbf{w}^n(s) + \int_{t^*}^t -e^{-J(s-t)}\Big\{(\mathbf{w}^n)'(s) - J\mathbf{w}^n(s) f(\widetilde{\mathbf{w}}^n(s))\Big\} \tag{4.32}$$

where $t^* \in \{t_1, t_2, \ldots, t_n\}$ where $[0,1) = [0,t_1) \cup [t_1,t_2) \ldots [t_n,1)$. It must be noted that for both cases $\mathbf{w}^0 = \mathbf{w}(0) = (1.2000, 0.6667, 2.3333, 1.2789, 3.7500)^T$ and the nth approximate solution of the original system (4.28) is obtained using the transformation $\mathbf{z}^n = P\mathbf{w}^n$. In our application we divide $[0,1]$ interval into subintervals with same width, $\Delta t = 1/10$.

In Table 4.2 one can see absolute errors of EVIM, VIM, MEVIM, MVIM for the fifth iteration for z_3, respectively. Here

$$\begin{aligned} \varepsilon^{VIM}(t) &= \left|z_3^{VIM}(t) - z_3^E(t)\right|, \quad \varepsilon^{EVIM}(t) = \left|z_3^{EVIM}(t) - z_3^E(t)\right|, \\ \varepsilon^{MVIM}(t) &= \left|z_3^{MVIM}(t) - z_3^E(t)\right|, \quad \varepsilon^{MEVIM}(t) = \left|z_3^{MEVIM}(t) - z_3^E(t)\right| \end{aligned} \tag{4.33}$$

where $z_3^{VIM}(t)$, $z_3^{EVIM}(t)$, $z_3^{MVIM}(t)$,$z_3^{MEVIM}(t)$ denotes the fifth approximate solution for VIM, EVIM, MVIM, MEVIM respectively and $z_3^E(t)$ denotes the solution obtained by Runge-Kutta methods at point t for z_3.

Table 4.4: Absolute errors for the fifth-order approximation by VIM, EVIM, MVIM, MEVIM.

t	ε^{VIM}	ε^{EVIM}	ε^{MVIM}	ε^{MEVIM}
0	0	0	0	0
0.1	0.010190	0.005771	0.012240	0.000067
0.2	0.038577	0.001077	0.044447	0.000079
0.3	0.081152	0.003066	0.090494	0.000074
0.4	0.136741	0.006963	0.146617	0.000062
0.5	0.204848	0.014039	0.210261	0.000049
0.6	0.285255	0.025837	0.279576	0.000037
0.7	0.377684	0.044410	0.353155	0.000027
0.8	0.482068	0.071853	0.429895	0.000019
0.9	0.595540	0.110339	0.508911	0.000013
1	0.722966	0.156493	0.589486	0.000008

4.3 Variational Iteration Method for the Chemical Master Equation

There are two popular approaches for modelling the biological and chemical processes: deterministic and stochastic. Deterministic approach assumes the dynamics of these processes are *continuous and deterministic* [18].

This traditional approach defines the dynamical behaviour of reactions by using system of ODEs called Reaction Rate Equations (RRE) [41]. A reaction system includes d active species and r reactions; deterministic approach obtains the following RREs:

$$\begin{aligned} dy_1/dt &= f_1(y_1, y_2, \ldots, y_d), \\ dy_2/dt &= f_2(y_1, y_2, \ldots, y_d), \\ &\vdots \\ dy_d/dt &= f_d(y_1, y_2, \ldots, y_d), \end{aligned}$$

with the initial conditions

$$y_1(0) = \xi_1,\ y_2(0) = \xi_2, \ldots,\ y_d(0) = \xi_d. \tag{4.34}$$

Here, y_j denotes the concentration of each species, f_i are given nonlinear functions constructed by the reaction rates c_i for $i = 1, 2, \ldots, r$, and concentrations of species are denoted by y_j for $j = 1, 2, \ldots, d$.

Although this approach is valid for many systems, it is not appropriate when the concentrations of some species are low and stochastic fluctuations may also effect the dynamical behaviour of the system, for instance, gene expression [6,10,39], separation of infectious [33,51].

Therefore, stochastic approach is proposed by Gillespie [17–19, 21]. This model assumes the dynamics of processes are *discrete and stochastic* [18]. Stochastic approach assumes a Markov process modelled by the Chemical Master Equation (CME) which is a single differential equation of probability function in which time and population of molecules are independent variables [17, 19]. For a system with d species and r reactions, stochastic approach produces the following CME

$$\frac{\partial}{\partial t}P(x,t|x_0,t_0) = \sum_{\mu=1}^{r}\left(\alpha_\mu(x-v_\mu)P(x-v_\mu,t|x_0,t_0) - \alpha_\mu(x)P(x,t|x_0,t_0)\right)$$

with initial condition

$$P(x,t=t_0|x_0,t_0) = \begin{cases} 1, & \text{if } x = x_0 \\ 0, & \text{if } x \neq x_0. \end{cases} \tag{4.35}$$

Here, $x = (x_1, x_2, \ldots, x_d)^T$ where the components x_j denotes the number of jth species, and $\alpha_\mu(x)$ is the propensity function which represents the probability that one R_μ reaction will occur in the infinitesimal time interval $[t, t+dt)$. The vector v_μ is the stoichiometric vector that $v_{\mu j}$ is the change in the number of jth species produced by one R_μ reaction for $\mu = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, d$.

Although the deterministic and stochastic approach are based on the different ideas. In certain special cases the time derivative of expected value of CME is as the same as the one in the RRE [59]. In this section of the present work, we will apply EVIM to Chemical Master Equation (CME). In our application, we consider the reactions in Table 4.3.

Table 4.5: Reactions, propensity functions and stoichiometric vectors.

Reactions	Propensity function	Stoichiometric vector
$R_1 : S_1 \xrightarrow{c_1} S_2$	$\alpha_1(x) = c_1 x_1$	$v_1 = (-1, 1)^T$
$R_2 : S_2 \xrightarrow{c_2} S_1$	$\alpha_2(x) = c_2 x_2$	$v_2 = (1, -1)^T$
$R_3 : * \xrightarrow{c_3} S_1$	$\alpha_3(x) = c_3$	$v_3 = (1, 0)^T$
$R_4 : S_2 \xrightarrow{c_4} *$	$\alpha_4(x) = c_4 x_2$	$v_1 = (0, -1)^T$

The stochastic approach obtains the following CME for reaction system in Table 4.3

$$\begin{aligned} \frac{\partial}{\partial t}P(t,x_1,x_2) &= c_1(x_1+1)P(t,x_1+1,x_2-1) - c_1x_1P(t,x_1,x_2) \\ &+ c_2(x_2+1)P(t,x_1-1,x_2+1) - c_2x_2P(t,x_1,x_2) \\ &+ c_3P(t,x_1-1,x_2) - c_3P(t,x_1,x_2) \\ &+ c_4(x_2+1)P(t,x_1,x_2+1) - c_4x_2P(t,x_1,x_2). \end{aligned} \tag{4.36}$$

In this part of the application, rather than using stochastic approaches [16,17,20], we will use EVIM to obtain the solution of CME in (4.36). Hence, we rewrite equation (4.36) as an equivalent matrix-vector form as follows [38]:

$$\dot{\mathbf{p}}(t) = \mathcal{A}\mathbf{p}(t), \tag{4.37}$$

subject to the initial condition

$$\mathbf{p}(0) = \mathbf{p}_0.$$

In this setting we assume that we have a restricted domain $\Omega_{m+1,n+1}$, meaning that there can be maximum m numbers of species S_1 and n numbers of species S_2. In (4.37), $\mathbf{p}(t)$ represents a column vector

$$\mathbf{p}(t) = (P(t,0,0), P(t,0,1), \ldots, P(t,0,n), \ldots, P(t,m,0), P(t,m,1), \ldots, P(t,m,n))^T.$$

The matrix $\mathcal{A} = (a_{ij})$ is called the *infinitesimal generator matrix* or the *transition rate matrix* for $i,j = 1,2,\ldots,mn$. If $i \neq j$ then, a_{ij} denotes the propensity where state of the system i is changing to j. In case when $i = j$, we have $a_{jj} = -\sum_{i \neq j} a_{ij}$. See, for instance, [43,52,59].

Hence, EVIM gives the following correction functional for system (4.37).

$$\mathbf{p}^{n+1}(t) = \mathbf{p}^n(t) + \int_0^t \Lambda_A(s;t)\Big\{\mathbf{p}^{n\prime}(s) - \mathcal{A}\mathbf{p}^n(s)\Big\}ds,$$

with

$$\mathbf{p}^0(t) = \mathbf{p}_0.$$

Let there be exactly one S_1 molecule and no S_2 molecule initially so that the initial state of the system is $x(0) = (1,0)^T$ and the initial probability function is

$$P(x,0) = \begin{cases} 1, & \text{if } x = (1,0)^T \\ 0, & \text{if } x \neq (1,0)^T. \end{cases} \tag{4.38}$$

Let our truncated domain be $\Omega_{10,10}$ and the reaction rates are given as $c_1 = 1$, $c_2 = 0.02$, $c_3 = 0.3$, and $c_4 = 0.4$.

It must be noted that system (4.36) is a linear system. Therefore, EVIM will yield the exact solution at the first step. In our specific example we have a very small domain, $\Omega_{10,10}$ and we have only monomolecular reactions which is the reason for

obtaining linear system. Although we construct such an example, in many cases domain can be very big and all reactions cannot be monomolecular. In order to cover such cases, many algorithms are proposed to obtain realisations of Chemical Master Equation [16, 17, 20, 31].

Figure 4.2 shows the expected number of species S_1 and S_2 obtained by EVIM and by the method in [31] with Strang splitting. One can easily see that the results are very close to each other, however, the proposed approach (EVIM) yields the exact solution at a single iterate without the need for a stochastic method.

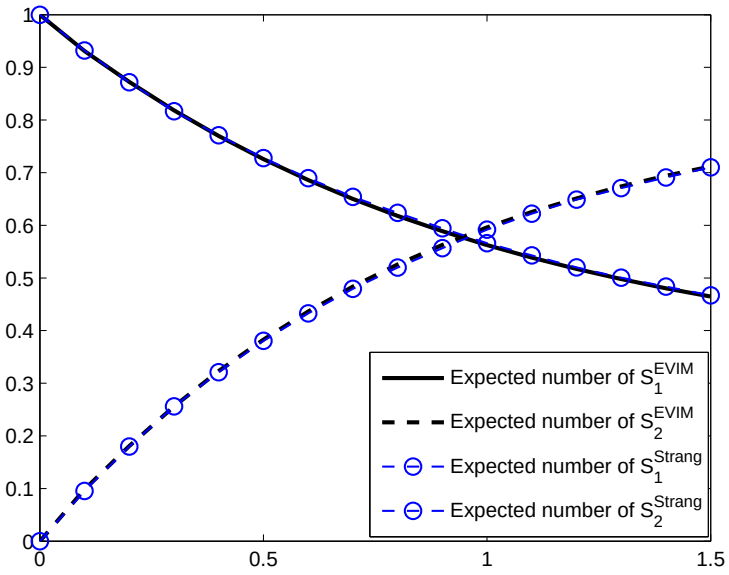

Figure 4.2: Expected number of species obtained by EVIM and the method in [31] with Strang splitting.

In [31], Jahnke and Altintan proposed an efficient simulation algorithm. The authors divide the system into subsystems. Since the reaction channels in some subsystems are monomolecular, their realisations are obtained by convolution of Multinomial and Poisson distributions [32]. If it is not possible to reduce the reactions into monomolecular ones, then SSA [17, 18] is used to obtain realisations of such subsystems. The state of the system is then updated by using Strang and Trotter Splitting.

CHAPTER 5

CONCLUSION

In this thesis, we introduced a new approach to Variational Iteration Method which generalises the Lagrange multipliers and computes approximate solutions of system of differential equations more rapidly when compared with the classical variational iteration method.

The Variational Iteration Method is a modification of the Lagrange multiplier method. It is based on the splitting differential operator into linear and nonlinear parts and constructing the correction functional. The key element of the correction functional is the Lagrange multiplier which is obtained via variational theory. If the system is coupled, restricted variations are used to make the system uncoupled, and unfortunately the accuracy of the approximate solution depends on these restricted variations. Less usage of restricted variations gives better approximate solutions which causes faster convergence.

In this study, we propose a new approach for the first order differential equations. Since higher order differential equations can be reduced to first order systems, the method is applicable to higher order differential equations, too. In the method, by using matrices and vectors we rewrite differential equations and construct correction functional for this new system. Restricted variations are only used for nonlinear terms. Also, the Lagrange multipliers are defined as matrix-valued functions. It has also been proved that there is a close relation between the Lagrange multipliers and fundamental matrices of homogeneous system. This relation leads to obtaining Lagrange multipliers rather easily.

There are two main advantages of the new approach to the classical one: The first is that the proposed approach defines the Lagrange multipliers as matrix-valued functions while the classical approach defines them as scalar-valued. The second, as a consequence of the first, is that the new approach uses restricted variations only for the nonlinear terms while the classical one uses also the linear terms, beside the nonlinear ones, as restricted variations.

Meanwhile, to speed up calculations, we showed that the Jordan canonical forms can also be used to obtain the Lagrange multipliers for systems with constant coefficients. Although the Lagrange multiplier of such systems are obtained via calculus of variations and side conditions, the proposed method presents an alternative, but easier way to compute them by using eigenvalues of the coefficient matrix.

Not only the case when the coefficient matrix is constant, but also the case when the system has variable coefficients is illustrated by several examples within the context. Particularly, the Cauchy-Euler and Bernoulli differential equations are easily solved via the proposed approach accurately.

The proposed method is shown to have a close relation with the variation of parameters formula. Hence, the convergence of the method is analysed via convergence of fixed point iteration for variation of parameters formula.

It is also proved that Lagrange multiplier of the classical VIM and extended approach are related to each other. Moreover, it is shown that for higher order differential equations, VIM obtains the solutions of initial value problems with a single iteration whenever the initial approximation satisfies the initial conditions. By realising this fact, VIM is modified to obtain the solutions of linear nonhomogeneous boundary value problems. Similar to the initial value problems, it is shown that when the initial approximation satisfies the boundary conditions the exact solution of the problem is obtained via the first approximation. The advantage here is that the proposed approach does not use the theory of Green's functions. Naturally, the algorithm is also extended to the nonlinear boundary value problems.

As a consequence of boundary value problems, the method is applied to Sturm-Liouville eigenvalue and boundary problems, including the harmonic oscillator. For

such type of problems, an initial approximation is constructed that includes parameters to be determined from the boundary conditions with just a single iteration corresponding eigenvalues and eigenfunctions of Sturm-Liouville problem can be found. However, due to unbounded domain of the harmonic oscillator, this is not the case.

In order to show the validity of the method for huge matrices, the method is applied to Brusselator equation that models the Brusselator reaction system and chemical master equation that models the real-life problems with stochastic approach. Numerical results show that the method is very powerful and easily applicable to different type of problems from different research areas.

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VITA

PERSONAL INFORMATION

Surname, Name	:	Altıntan, Derya
Nationality	:	Turkish (T.C.)
Date and Place of Birth	:	August 19, 1980, Ankara
Phone	:	+90 312 2105610
Fax	:	+90 312 2102985
e-mail	:	altintan@metu.edu.tr

ACADEMIC DEGREES

Ph.D. Department of Scientific Computing, 2011, June

Institute of Applied Mathematics

Middle East Technical University, Ankara

Supervisor: Assoc. Prof. Dr. Ömür Uğur

Thesis Title: An Extension to the Variational Iteration Method for Systems and Higher-Order Differential Equations

M.Sc. Department of Scientific Computing, 2006, July

Institute of Applied Mathematics

Middle East Technical University, Ankara

Supervisor: Prof. Dr. Marat Akhmet

Cosupervisor: Prof. Dr. Tanıl Ergenç

Thesis Title: Equations of the Logistic Equation with Piecewise Constant Argument

B.Sc. Department of Mathematics, 2003, June
Ankara University, Ankara

FOREIGN LANGUAGES

Turkish (native), English (High level)

WORKING EXPERIENCE & TRAINING

2004–Present Research Assistant, Institute of Applied Mathematics, Department of Scientific Computing, Middle East Technical University, Ankara

RESEARCH VISITS

20 April 2009– 20 March 2010: Karlsruhe Institute of Technology, Germany, Supervised by JProf.Dr. Tobias Jahnke

PUBLICATIONS

A. Papers published in International Journals:

A1. D. Altıntan, Ö. Uğur; Generalisation of the Lagrange multipliers for variational iterations applied to systems of differential equations, *Mathematical and Computer Modelling*, 54, pp. 2040-2050, 2011.

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B. Presentations in International Conferences:

B1. D. Altıntan, Ö. Uğur; Generalized Multistage Variational Iteration Method. *8th ENUMATH 2009*, 29 June–3 July 2009, Uppsala, Sweden.

B2. D. Altıntan, Ö. Uğur; How to solve boundary value problems by using Variational Iteration Method. *24th Biennial Conference on Numerical Analysis*, 28 June– 1 July 2011, Glasgow, United Kingdom.

C. Presentations in National Conferences:

C1. M. Akhmet, D. Altıntan, T. Ergenç; Parçalı sabit fonksiyonlar içeren Lojistik denklemlerin kaotik yapısı, *23. Ulusal Matematik Sempozyumu*, 04–07 Ağustos 2010, Kayseri.

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