An Analytic Approximation to the Solution of Schrodinger Equation by VIM

Kh. Hosseinzadeh

Department of Mathematics
Shahrood University of Technology
P. O. Box 316, Shahrood, Iran

Abstract

In this article, variational iteration method has been employed to solve the non-linear Schrodinger equation with initial condition. The solutions obtained by the variational iteration method are infinite power series for appropriate initial condition which can in turn be expressed in a closed form, the exact solutions. To illustrate the ability and reliability of the method some example are provided. The results show that the variational iteration method is a powerful mathematical tool to solving Schrodinger equation it is also a promising method to solve other nonlinear equations.

Keywords: Schrodinger equation, Variational iteration method, Lagrange multiplier, Correction functional

1 Introduction

The variational iteration method was first introduced by He [1] since the beginning of the 1998’s. In recent years the applications of variational iteration method in mathematical and physical problems has been devoted by scientists, because this method continuously deforms a simple problem which is easy to solve into the difficult problem under study. Variational iteration method is a powerful device for solving functional equations. Numerical methods which are commonly used such as finite difference or characteristics method need large
size of computational works and usually affected of round-off error causes the loss accuracy in the results. Analytical methods commonly used for solving Schrodinger equation are very restricted and can be used in very special cases so they can not be used to solve equations of numerous realistic scenarios. The variational iteration method which is a modified general Lagrange multiplier method [2], has been shown to solve effectively, easily and accuracy, large class of nonlinear problems with approximations which convergence rapidly to accurate solution. To illustrate the method, consider the following nonlinear equation

\[ Lu(t) + N u(t) = g(t) \]  

(1)

Were \( L \) is a linear operator, \( N \) is a nonlinear operator and \( g(t) \) is a known analytical function. According to the variational iteration method, we can construct the following correction functional.

\[ u_{n+1}(t) = u_n(t) + \int_0^t \lambda(\xi)(Lu_n(\xi) + Nu_n(\xi) - g(\xi)) d\xi \]  

(2)

Where \( \lambda \) is general Lagrange multiplier which can be identified via variational theory, \( u_0(t) \) is an initial approximation with possible unknowns, and \( \tilde{u}_n \) is considered as restricted variation [3], i.e. \( \delta \tilde{u}_n = 0 \). Therefore, we first determine the Lagrange multiplier \( \lambda \) that will be identified optimally via integration by parts. The successive approximations \( u_{n+1}(t) \) of the solution \( u(t) \) will be readily obtained upon using the obtained Lagrange multiplier and by using any selective function \( u_0 \). Consequently, the exact solution may be obtained by using \( u = \lim_{n \to \infty} u_n \).

2 Method of solution

Consider the following Schrodinger equation with the following initial condition [4]

\[ i \frac{\partial \psi(X,t)}{\partial t} = -\frac{1}{2} \nabla^2 \psi + V_d(X)\psi + \beta_d |\psi|^2 \psi, \quad X \in \mathbb{R}^d, \quad t \geq 0, \]  

(3)

\[ \psi(X,0) = \psi^0(X), \quad X \in \mathbb{R}^d. \]  

(4)

Where \( V_d(X) \) is the trapping potential and \( \beta_d \) is a real constant. For solving Eq. (3) with initial condition (4) by VIM, its correction functional can be written down as follows:

\[ \psi_{n+1}(X,t) = \psi_n(X,t) + \int_0^t \lambda(\xi)(i \frac{\partial \psi_n(X,\xi)}{\partial \xi} + \frac{1}{2} \nabla^2 \tilde{\psi}_n - V_d(X) \tilde{\psi}_n - \beta_d |\tilde{\psi}_n|^2 \tilde{\psi}_n) d\xi \]  

(5)
To make this correction functional stationary, knowing $\delta \psi_n (X, 0) = 0$, we have:

$$\delta \psi_{n+1}(X, t) = \delta \psi_n (X, t) + i \int_0^t \lambda (\xi) (\delta \psi_n (X, \xi))' d\xi = 0.$$ 

Its stationary conditions can be determined as follows:

$$\lambda'(\xi) = 0, \quad 1 + i\lambda(\xi)|_{\xi=t} = 0.$$ 

From which Lagrange multiplier can be identified as $\lambda = i$, and the following iteration formula is obtained,

$$\psi_{n+1}(X, t) = \psi_n (X, t) + i \int_0^t \lambda (\xi) (i \frac{\partial \psi_n (X, \xi)}{\partial t} + \frac{1}{2} \nabla^2 \psi_n - V_d (X) \psi_n - \beta_d |\psi_n|^2 \psi_n) d\xi$$

Beginning with $\psi_0 = \psi(X, 0) = \psi^0 (X)$, the approximate solution of (3) can be determined by iterative formula (6).

## 3 Examples

**Example 1.** Consider the following one-dimensional Schrodinger equation with the following initial condition [4]:

$$i \frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} - |\psi|^2 \psi,$$

Corresponding iterative formula (6) for this example can be derived as:

$$\psi_{n+1}(x, t) = \psi_n (x, t) + i \int_0^t (i \frac{\partial \psi_n (x, t)}{\partial t} + \frac{1}{2} \frac{\partial^2 \psi_n}{\partial x^2} - |\psi_n|^2 \psi_n) d\xi$$

Starting with $\psi_0 (x, t) = e^{ix}$, by iterative formula (8), we derive the following results:

$$\psi_1(x, t) = e^{ix} \left(1 + \frac{1}{2} it\right),$$
$$\psi_2(x, t) = e^{ix} \left(1 + \frac{1}{2} it - \frac{1}{8} it^2 + \frac{1}{12} it^3 - \frac{1}{32} it^4\right),$$
$$\psi_3(x, t) = e^{ix} \left(1 + \frac{1}{2} it - \frac{1}{8} it^2 - \frac{1}{48} it^3 - \frac{1}{96} it^4 + \cdots \right),$$
$$\vdots$$
$$\psi_n(x, t) = e^{ix} \left(1 + \frac{1}{11} \left(\frac{1}{2} it\right) + \frac{1}{21} \left(\frac{1}{2} it\right)^2 + \frac{1}{31} \left(\frac{1}{2} it\right)^3 + \cdots \right).$$

Thus, we have:

$$\psi(x, t) = \lim_{n \to \infty} \psi_n (x, t) = e^{ix} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} it\right)^n = e^{i(x+\frac{1}{2} t)}.$$
which is an exact solution. Its worth to point that, the result of example 1 is exactly the same Adomain decomposition method [4].

**Example 2.** Let’s solve the following two-dimensional Schrodinger equation [5]:

\[ i \frac{\partial \psi(x,t)}{\partial t} = - \frac{1}{2} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + V(x,y)\psi + |\psi|^2 \psi, \]  \hspace{1cm} (9)

where \( V(x,y) = 1 - \sin^2 x \sin y. \) By using the He’s variational iteration method, we have:

\[ \psi_{n+1}(x,y,t) = \psi_n(x,y,t) + \]

\[ i \int_0^t \left[ i \frac{\partial \psi_n(x,t)}{\partial t} + \frac{1}{2} \left( \frac{\partial^2 \psi_n}{\partial x^2} + \frac{\partial^2 \psi_n}{\partial y^2} \right) - V(x,y)\psi_n - |\psi_n|^2 \psi_n \right] d\xi, \]  \hspace{1cm} (10)

Considering the initial approximation \( \psi_0(x,y,t) = \sin x \sin y. \) And applying variational iteration formula (10), other terms of the sequence are computed as follows:

\[ \psi_1(x,y,t) = \sin x \sin y (1 - 2it), \]
\[ \psi_2(x,y,t) = \sin x \sin y (1 - 2it + \frac{1}{6}t^2 + \cdots), \]
\[ \psi_3(x,y,t) = \sin x \sin y (1 - 2it - 2t^2 + \cdots), \]
\[ \vdots \]
\[ \psi_n(x,y,t) = \sin x \sin y (1 + \frac{(2it)^n}{n!} + \frac{(2it)^2}{2!} + \frac{(2it)^3}{3!} + \cdots), \]

Therefore, we have:

\[ \psi(x,y,t) = \lim_{n \to \infty} \psi_n(x,y,t) \]
\[ = \sin x \sin y \sum_{n=0}^{\infty} \frac{(-2it)^n}{n!} \]
\[ = \sin x \sin y e^{-2it} \]

In this example we have also derived the exact solution.

**Example 3.** Consider the following three-dimensional Schrodinger equation with the following initial condition [5]:

\[ i \frac{\partial \psi(x,y,z,t)}{\partial t} = - \frac{1}{2} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V(x,y,z)\psi + |\psi|^2 \psi, \]  \hspace{1cm} (11)

Corresponding iterative formula (6) for this example can be derived as:

\[ \psi_{n+1}(x,y,z,t) = \psi_n(x,y,z,t) + \]

\[ i \int_0^t \left[ i \frac{\partial \psi_n(x,z,t)}{\partial t} + \frac{1}{2} \left( \frac{\partial^2 \psi_n}{\partial x^2} + \frac{\partial^2 \psi_n}{\partial y^2} + \frac{\partial^2 \psi_n}{\partial z^2} \right) - V(x,y,z)\psi_n - |\psi_n|^2 \psi_n \right] d\xi \]  \hspace{1cm} (12)
Starting with $\psi_0(x,t) = \sin x \sin y \sin z$, by iterative formula (12), we derive the following results:

\begin{align*}
\psi_1(x,t) &= \sin x \sin y \sin z \left(1 - \frac{5}{2}it\right), \\
\psi_2(x,t) &= \sin x \sin y \sin z \left(1 + \frac{1}{2}it + \frac{3}{8}t^2 + \cdots\right), \\
\psi_3(x,t) &= \sin x \sin y \sin z \left(1 - \frac{5}{2}it - \frac{25}{8}t^2 + \cdots\right), \\
\vdots & \\
\psi_n(x,t) &= \sin x \sin y \sin z \left(1 + \frac{1}{1!} \left(-\frac{5it}{2}\right) + \frac{1}{2!} \left(-\frac{5it}{2}\right)^2 + \frac{1}{3!} \left(-\frac{5it}{2}\right)^3 + \cdots\right).
\end{align*}

Thus, we have:

$$\psi(x,y,z,t) = \lim_{n \to \infty} \psi_n(x,y,z,t) = \sin x \sin y \sin z \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{5it}{2}\right)^n$$

Therefore, $\psi(x,y,z,t) = \sin x \sin y \sin z e^{-\frac{5}{2}it}$, which is an exact solution.

### 4 Conclusion

In this paper, the variational iteration method has been successfully applied to finding the solution of a Schrodinger equation. This method is a powerful tool for solving the large amount of the problems. Using the variational iteration method, we obtained exact solution for Schrodinger equation. It can be concluded that the He’s variational iteration method is very powerful and efficient technique in finding exact solutions for wide classes of problems. The main advantage of the VIM over decomposition procedure of Adomian [14] is that the former method provides the solution of the problem without calculating Adomian’s polynomials.

### References


https://doi.org/10.1016/s0096-3003(97)10147-3

https://doi.org/10.1016/j.amc.2004.10.066

Received: January 15, 2009; Accepted: March 11, 2009
Published: March 19, 2017