Homotopy Analysis Method for a Nonlinear Chemistry Problem

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Abstract: In this paper, the Homotopy Analysis Method (HAM) is used for solving a system of nonlinear ordinary differential equations which often appear in chemical applications. HAM contains the auxiliary parameter \( h \) which provides us with a convenient way to adjust and control convergence region and rate of solution series. Moreover, HAM provides us with great freedom to choose the best base function, such as exponential functions, fractional functions and so on. In this paper, we choose two different base functions to illustrate the merit of this freedom.

Key words: Homotopy analysis method - system of nonlinear ordinary differential equations

INTRODUCTION

The homotopy analysis method [3, 4] was first proposed by Liao in 1992. The HAM was further developed and improved by Liao for nonlinear problems in [5], for solving solitary waves with discontinuity in [6], for series solutions of nano boundary layer flows in [7], for nonlinear equations in [8] and many other subjects. This technique has been successfully applied to many nonlinear problems such as heat transfer analysis of the steady flow of a fourth grade fluid [10], solitary wave solutions to the Kuramoto–Sivashinsky equation [11], heat transfer analysis of unsteady boundary layer flow [12], approximate solutions of singular two-point BVPs [13], 2-dimensional steady slip flow in microchannels [14], singular IVPs of Emden–Fowler type [15], heat radiation equations [16] and so on. ([17-22] for more applications of HAM).

The remaining structure of this article is organized as follows. Section 2 is a brief basic for the calculus of variation theory. Section 3 briefly reviews a mathematical basis of the homotopy analysis method used for this study. Two illustrative examples are documented in Section 4. These examples intuitively describe ability and reliability of the method. A conclusion and future directions for research are all summarized in the last section.

THE HOMOTOPY ANALYSIS METHOD

To illustrate the basic concept of homotopy analysis method, we consider the following general nonlinear system

\[ N[u(t)] = 0, \quad i = 1, 2, ..., n \]

where \( N \) are nonlinear operators, \( x \) denotes independent variable, \( u \) are unknown functions, respectively. For simplicity, we ignore all boundary or initial conditions, which can be treated in the similar way. By means of generalizing the traditional homotopy method, Liao constructs the so-called zero-order deformation equation

\[ (1 - p)L[\phi(t;p) - u_{i,0}(t)] = phH(t)N[\phi(t;p)], \quad i = 1, 2, ..., n \]

(2)

where \( p \in [0,1] \) is the embedding parameter \( h \neq 0 \) is a nonzero auxiliary parameter, \( H(t) \neq 0 \) is an auxiliary function, \( L_1 \) are auxiliary linear operators, \( u_i(0) \) are initial guess of \( u_i(t) \), \( \phi(t;p) \) are unknown functions.
respectively. It is important that one has great freedom to choose auxiliary things in HAM. Obviously, when \( p = 0 \) and \( p = 1 \), it holds

\[
\phi_i(t;0) = u_{i,0}(t), \quad \phi_i(t;1) = u_i(t), \quad i = 1, 2, ..., n
\]

respectively. Thus as \( p \) increases from 0 to 1, the solution \( \phi_i(t;p) \) varies from the initial guess \( u_{i,0}(t) \) to the solution \( u_i(t) \). Expanding \( \phi_i(t;p) \) in Taylor series with respect to \( p \) about \( p = 0 \), one has

\[
\phi_i(t;p) = \phi_i(t;0) + \sum_{m=1}^{\infty} \frac{\partial^m \phi_i(t;p)}{\partial p^m} \bigg|_{p=0} \cdot u_i(t), \quad i = 1, 2, ..., n
\]

where

\[
u_{i,m}(t) = \frac{1}{m!} \frac{\partial^m \phi_i(t;p)}{\partial p^m} \bigg|_{p=0}, \quad i = 1, 2, ..., n
\]

If the auxiliary linear operator, the initial guess, the auxiliary parameter \( h \) and the auxiliary function are so properly chosen, the series (3) converges at \( p = 1 \), one has

\[
u_i(t) = u_{i,0}(t) + \sum_{m=1}^{\infty} u_{i,m}(t), \quad i = 1, 2, ..., n
\]

which must be one of solutions of original nonlinear equation, as proved by Liao. The governing equation can be deduced from the zero-order deformation equation. Define the vector

\[
u_i(t) = \left\{ u_{i,0}(t), u_{i,1}(t), ..., u_{i,n}(t) \right\}
\]

Differentiating Eq. (2), \( m \) times with respect to the embedding parameter \( p \) and then setting \( p = 0 \) and finally dividing them by \( m! \), we have the so-called \( m \)-th-order deformation equation

\[
L_i[\nu_i(t)] = h H_i(t) R_i[\nu_{i,m-1}(t)], \quad i = 1, 2, ..., n
\]

where

\[
R_{i,m}(\nu_{i,m-1}) = \frac{1}{m!} \frac{\partial^m N_i[\phi_i(t;p)]}{\partial p^m} \bigg|_{p=0}, \quad i = 1, 2, ..., n
\]

and

\[
\chi_m = \begin{cases} 
0, & m \leq 1 \\
1, & m > 1
\end{cases}
\]

APPLICATIONS

In this section we consider a system representing a nonlinear reaction, which is taken from [1, 2]:

\[
\begin{align*}
u &= -u, \\
v &= u - v^2, \\
w &= v^2
\end{align*}
\]

with the boundary conditions

\[
u(0) = 1, \quad v(0) = 0, \quad w(0) = 0
\]

We assume two different base functions for this problem.

First approach: Exponential functions: We assume that the solution of the equation (6) can be expressed by a set of base functions

\[
\{e^{\nu_i}, \quad n = 0, 1, 2, ... \}
\]

in the form

\[
u = \sum_{i=0}^{\infty} c_{1,i} e^{\nu_i}, \quad v = \sum_{i=0}^{\infty} c_{2,i} e^{\nu_i}, \quad w = \sum_{i=0}^{\infty} c_{3,i} e^{\nu_i}
\]

where \( c_{1,i} \) and \( c_{3,i} \) are coefficients to be determined. This provides us with the so-called rule of solution expression, i.e., the solution of (6) must be expressed in the same form as (8) and the other expressions must be avoided. According to (6) and (8), we choose the linear operator

\[
L_i[\nu_i(t;p)] = \frac{\partial \phi_i(t;p)}{\partial p} + \phi_i(t;p), \quad i = 1, 2, 3
\]

with the property

\[
L_i[e^{\nu_i}] = 0, \quad i = 1, 2, 3
\]

where \( c_1 c_2 c, c_2 \) and \( c_3 c_3 \) are constants. From (6), we define nonlinear operators

\[
N_i[\phi_i(t;p)] = \frac{\partial \phi_i(t;p)}{\partial p} + \phi_i(t;p)
\]

\[
N_i[\phi_2(t;p)] = \frac{\partial \phi_2(t;p)}{\partial p} - \phi_2(t;p) + (\phi_2(t;p))^2
\]

\[
N_i[\phi_3(t;p)] = \frac{\partial \phi_3(t;p)}{\partial p} - (\phi_3(t;p))^2
\]

According to (7) and the rule of solution expression (8), it is straightforward that the initial approximations should be in the form \( u_0(t) = 1, v_0(t) = 0 \)
and \( w_0(t) = 0 \). From (4), the general zero-order deformation equations are as follow:

\[
\begin{align*}
(1 - p)L_1[\phi(t;p) - u_0(t)] &= p\beta H(t)N[\phi_1(t;p)] \\
(1 - p)L_2[\phi(t;p) - v_0(t)] &= p\beta H(t)N[\phi_2(t;p)] \\
(1 - p)L_3[\phi(t;p) - w_0(t)] &= p\beta H(t)N[\phi_3(t;p)]
\end{align*}
\]

with the initial conditions

\[
\phi_1(t;0) = u_0(t), \quad \phi_2(t;0) = v_0(t), \quad \phi_3(t;0) = w_0(t)
\]

From (5) and (6):

\[
\begin{align*}
R_m(\tilde{u}_{m-1}) &= u_m^\prime + u_{m-1} \\
R_m(\tilde{v}_{m-1}) &= v_m^\prime - v_{m-1} + \sum_{i=0}^{m-1} v_i v_{m-1-i} \\
R_m(\tilde{w}_{m-1}) &= w_m^\prime - \sum_{i=0}^{m-1} w_i v_{m-1-i}
\end{align*}
\]

where the prime denotes differentiation with respect to the similarity variable \( x \). Now, the solution of the \( m \)-th-order deformation equation (4) becomes:

\[
\begin{align*}
u_m(t) &= \xi_m u_{m-1}(t) + hL_1^{-1}[H(t)R_m(\tilde{u}_{m-1})] + c_1e^t \\
v_m(t) &= \xi_m v_{m-1}(t) + hL_2^{-1}[H(t)R_m(\tilde{v}_{m-1})] + c_2e^t \\
w_m(t) &= \xi_m w_{m-1}(t) + hL_3^{-1}[H(t)R_m(\tilde{w}_{m-1})] + c_3e^t
\end{align*}
\]

where the constants \( c_i \)'s are determined by the initial condition

\[
\begin{align*}
u_m(0) = 0, \quad v_m(0) = 0, \quad w_m(0) = 0
\end{align*}
\]

Therefore, the series solution can be expressed as

\[
\begin{align*}
\tilde{u}(t) &= u_0(t) + \sum_{m=1}^{\infty} u_m(t) \\
\tilde{v}(t) &= v_0(t) + \sum_{m=1}^{\infty} v_m(t) \\
\tilde{w}(t) &= w_0(t) + \sum_{m=1}^{\infty} w_m(t)
\end{align*}
\]

According to the rule of solution expression denoted by (8) and from Eq. (9), the auxiliary function \( H(t) \) should be in the form \( H(t) = \psi^k \), where \( k \) is an integer. It is found that we had to set \( k = 0 \), which uniquely determines the corresponding auxiliary function \( H(t) = 1 \).

It is obvious from Fig. 1 that to adjust and control the convergence region of solution series, the auxiliary parameter \( h_0 \) should be chosen as \( h = -1 \). The residual of approximate solution

\[
\begin{align*}
\tilde{u} &= \sum_{m=1}^{20} u_m(t), \quad \tilde{v} = \sum_{m=1}^{20} v_m(t)
\end{align*}
\]

is shown for second equation of 6 in Fig. 2 and for third equation of 6 in Fig. 3. For first equation of 6 the solution is exact.
Second approach: Polynomial functions: In this section we assume that the solution of the equation (6) can be expressed by a set of base functions

\[ \{t^n, \ n = 0,1,2,...\} \]

in the form

\[ u = \sum_{i=0}^{\infty} c_{i1} t^i, \quad v = \sum_{i=0}^{\infty} c_{i2} t^i, \quad w = \sum_{i=0}^{\infty} c_{i3} t^i \]  

(9)

where \( c_{i1}, c_{i2}, \) and \( c_{i3} \) are coefficients to be determined. This provides us with the so-called rule of solution expression, i.e., the solution of (6) must be expressed in the same form as (9) and the other expressions must be avoided. According to (6) and (9), we choose the linear operator

\[ L_i[\phi(t;p)] = \frac{\partial \phi(t;p)}{\partial t}, \quad i = 1,2,3 \]

with the property

\[ L_i[\zeta_i] = 0, \quad i = 1,2,3 \]

where \( c_1, c_2, c_1, c_2 \) and \( c_3, c_3 \) are constants. We choose the initial approximation

\[ u_0(t) = 0, \quad v_0(t) = 0, \quad w_0(t) = 0 \]

Therefore we have the following higher order deformation equation:

\[ u_m(t) = \sum u_m, u_{m-1}(t) + h L_{1i}[H(t)R_{m}(\tilde{u}_{m-1})] + c_i \]
\[ v_m(t) = \sum v_m, v_{m-1}(t) + h L_{2i}[H(t)R_{m}(\tilde{v}_{m-1})] + c_2 \]
\[ w_m(t) = \sum w_m, w_{m-1}(t) + h L_{3i}[H(t)R_{m}(\tilde{w}_{m-1})] + c_3 \]

where the constants \( \zeta_i's \) are determined by the initial condition

\[ u_m(0) = 0, \quad v_m(0) = 0, \quad w_m(0) = 0 \]

Therefore, the series solution can be expressed as

\[ u(t) = u_0(t) + \sum u_m(t) \]
\[ v(t) = v_0(t) + \sum v_m(t) \]
\[ w(t) = w_0(t) + \sum w_m(t) \]

According to the rule of solution expression denoted by (9) and from Eq. (10), the auxiliary function \( H(t) \) should be in the form \( H(t) = t^k \), where \( k \) is an integer. It is found that we had to set \( k = 0 \), which uniquely determines the corresponding auxiliary function \( H(t) = 1 \). It is obvious from Fig. 4 that to adjust and control the convergence region of solution series, the auxiliary parameter \( h_0 \) should be chosen as \( h_0 = -1 \). The residual of approximate solution
CONCLUSION

The ordinary differential equations which arise from engineering problems are usually nonlinear and such equations are difficult to estimate numerically or analytically. In this paper the homotopy analysis method was applied to solve a system of nonlinear ordinary differential equations which often appear in chemical applications. In the frame of HAM, the solution can be represented by two kinds of base function. HAM contains the auxiliary parameter which provides us with a convenient way to adjust and control convergence region and rate of solution series. Moreover, the solution of a given nonlinear problem can be expressed by many different base functions and thus can be more efficiently approximated by a better set of base function. From the residual it is observed that our present results are in good agreement with the exact solution. In this regard the homotopy analysis method is found to be a very useful analytic technique to get highly accurate and purely analytic solution to such kind of problems.

REFERENCES