AN AUTOMATIC SCHEME ON THE HOMOTOPY ANALYSIS METHOD FOR SOLVING NONLINEAR ALGEBRAIC EQUATIONS

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Abstract. In this paper, an automatic scheme coupled with homotopy analysis method is presented for solving nonlinear algebraic equations. The experimental results show the potential and limitations of the new method and imply directions for future work.

Keywords: nonlinear algebraic equations; iterative method; homotopy analysis method.

1. Introduction

Many practical problems in all fields of science, engineering, or applied mathematics give rise to the need to solve nonlinear algebraic equations (NAE). Typical examples that involve NAE include: calculation of chemical equilibrium by minimization of Gibbs energy or using equilibrium constants, continuous operation of

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some reactors (such as continuous stirred tank reactors, CSTR), heat exchanger calculations (where logarithmic mean temperature difference is used), calculation of the parameters of activity coefficient equations (such as the Van Laar and Wilson equations), solving various equations of state for specific volume or compressibility factor and calculation of the minimum reflux ratio using the Underwood equations [13].

Many powerful algorithms and codes for solving NLE have been developed in recent years. So far, almost all iterative techniques require the prior one or more initial guesses for the desired root and may fail to converge when the initial guess in far from the required solution. Achieving convergence in an efficient manner in these situations has become a real challenge.

The Homotopy Analysis Method (HAM) is based on the classic homotopy theory and it is a general method for solving nonlinear problems. HAM was developed by Shijun Liao from 1990s to 2010s, together with contributions of many other researchers in theory and applications [7]–[11]. The basic ideas of the HAM are described in Appendix A.

The HAM method has demonstrated promise in the arena of analytical solutions of equations. Abbasbandy and et al. [3] have been successfully extended HAM to the iterative numerical solution of algebraic equations. Indeed the inherent flexibility and generality of the HAM method makes this a challenging task. The successful theoretical development of this methodology forms a core accomplishment of the work by Awawdeh [5]. Awawdeh developed the methodology for the iterative numeric solution of multivariate system of nonlinear algebraic equations.

In this work, an automatic homotopy analysis method (AHAM) is presented for a single NAE. Some problems were selected to illustrate the performance of our algorithms in solving NAE. The calculations were done using Matlab 7. Our comparison of the methods is based upon the number of iterations. We use the following stopping criterion for our computer programs:

$$|x_{k+1} - x_k| < \epsilon,$$

where $\epsilon = 2.22e - 16$ is a Matlab constant.

2. Iterative methods for solving nonlinear equations

Consider the nonlinear algebraic equation

$$f(x) = 0, \tag{1}$$

where p is a simple root of it and $f \in C^n$ on an interval containing p as $[a, b]$. Let $p_0 \in [a, b]$ be an approximation to the solution p of (1) such that $f\,'(p_0) \neq 0$.

Consider the n^{th} Taylor polynomial for $f(x)$ expanded about p_0, and evaluated at $x = p_0 - \beta$,

$$f(p_0 - \beta) = f(p_0) - \beta f'(p_0) + \frac{\beta^2}{2} f''(p_0) + \cdots + (-1)^n \frac{\beta^n}{n!} f^{(n)}(p_0) + O(\beta^{n+1}).$$

We are looking for β such that

$$0 = f(p_0 - \beta) \simeq f(p_0) - \beta f'(p_0) + \frac{\beta^2}{2} f''(p_0) + \cdots + (-1)^n \frac{\beta^n}{n!} f^{(n)}(p_0),$$

or what amounts to the same as

$$\frac{f(p_0)}{f'(p_0)} = \beta - \frac{\beta^2}{2} \frac{f''(p_0)}{f'(p_0)} + \frac{\beta^3}{6} \frac{f'''(p_0)}{f'(p_0)} + \cdots + (-1)^{n+1} \frac{\beta^n}{n!} \frac{f^{(n)}(p_0)}{f'(p_0)}. \tag{2}$$

By setting

$$\lambda_1 = \frac{f(p_0)}{f'(p_0)} \quad \textit{and} \quad \lambda_m = \frac{(-1)^{m+1}}{m!} \frac{f^{(m)}(p_0)}{f'(p_0)} \quad \text{for} \quad m \geq 2,$$

Equation (2) reduces to

$$\mathcal{N}(\beta) = \beta + \lambda_2 \beta^2 + \lambda_3 \beta^3 + \cdots + \lambda_n \beta^n - \lambda_1 = 0.$$

We will apply the HAM to approximate β. To this end, let $\hbar \neq 0$ an auxiliary parameter and $\mathcal{L}$ an auxiliary linear operator with the property $\mathcal{L}[f(x)] = 0$ when $f(x) = 0$. Then by using $q \in [0, 1]$ as an embedding parameter, we construct such a homotopy

$$\mathcal{H}(w(q); \beta_\circ, \hbar, q) = (1 - q)\mathcal{L}(w(q) - \beta_0) - q\hbar \mathcal{N}(w(q)), \tag{3}$$

where β_0 is an initial guess of β. It should be emphasized that we have great freedom to choose the initial guess β_0, the auxiliary linear operator $\mathcal{L}$ and the non-zero auxiliary parameter $\hbar$. Enforcing the homotopy (3) to be zero, i.e.,

$$\mathcal{H}(w(q); \beta_\circ, \hbar, q) = 0,$$

we have the so-called zero-order deformation equation

$$(1 - q)\mathcal{L}(w(q) - \beta_0) = q\hbar \mathcal{N}(w(q)). \tag{4}$$

When $q = 0$, the zero-order deformation Equation (4) becomes

$$w(0) = \beta_0, \tag{5}$$

and when $q = 1$, it is equivalent to

$$w(1) = \beta. \tag{6}$$

Thus, according to (5) and (6), as the embedding parameter q increases from 0 to 1, $w(q)$ varies continuously from the initial approximation β_0 to the exact solution β. By Taylor's theorem, $w(q)$ can be expanded in a power series of q as follows

$$w(q) = \beta_0 + \sum_{m=1}^{\infty} \beta_m q^m, \tag{7}$$

where

$$\beta_m = \frac{1}{m!}\frac{d^m w(q)}{dq^m}|_{q=0}.$$

If the initial guess β_0, the auxiliary linear parameter $\mathcal{L}$ and the nonzero auxiliary parameter $\hbar$ are properly chosen so that the power series (7) converges at $q = 1$, then we have the series solution

$$\beta = w(1) = \beta_0 + \sum_{m=1}^{\infty}\beta_m. \tag{8}$$

The governing equation of β_m can be derived by differentiating the zero-order deformation Equation (4) m times with respective to q and then dividing by $m!$ and finally setting $q = 0$. We have the so-called m^{th}-order deformation equation

$$\mathcal{L}\left(\beta_m - \chi_m\beta_{m-1}\right) = \hbar\Big(\beta_{m-1} + \lambda_2\sum_{k=0}^{m-1}\beta_k\beta_{m-1-k} + \cdots + \lambda_n\sum_{r_1=0}^{m-1}\beta_{m-r_1-1}\sum_{r_2=0}^{r_1}\beta_{r_1-r_2} \cdots \sum_{r_{n-2}=0}^{r_{n-3}}\beta_{r_{n-3}-r_{n-2}}\sum_{r_{n-1}=0}^{r_{n-2}}\beta_{r_{n-2}-r_{n-1}}\beta_{r_{n-1}}\Big) - \hbar(1-\chi_m)\lambda_1,$$

where

$$\chi_m = \begin{cases} 0, & m \le 1, \\ 1, & m > 1. \end{cases}$$

Choosing the operator $\mathcal{L}$ as an identity operator, we have for $m \geqslant 1$ that

$$\beta_m = (\hbar+\chi_m)\beta_{m-1}+\hbar\lambda_2\sum_{k=0}^{m-1}\beta_k\beta_{m-1-k} + \cdots + \hbar\lambda_n\sum_{r_1=0}^{m-1}\beta_{m-r_1-1}\sum_{r_2=0}^{r_1}\beta_{r_1-r_2} \cdots \sum_{r_{n-2}=0}^{r_{n-3}}\beta_{r_{n-3}-r_{n-2}}\sum_{r_{n-1}=0}^{r_{n-2}}\beta_{r_{n-2}-r_{n-1}}\beta_{r_{n-1}}] - \hbar(1-\chi_m)\lambda_1. \tag{9}$$

Some cases will be discussed for various values of n:

Case [n=2] In this case, equation (9) reduces to

$$\beta_m = (\hbar + \chi_m)\beta_{m-1} + \hbar\lambda_2\sum_{k=0}^{m-1}\beta_k\beta_{m-1-k} - \hbar(1-\chi_m)\lambda_1.$$

Setting $\beta_0 = \lambda_1$, and, taking the zero-order approximation of β in (8), we can obtain

$$p = p_0 - \beta \simeq p_0 - \beta_0 = p_0 - \frac{f(p_0)}{f'(p_0)}. \tag{10}$$

We can write down the iteration form of (10) as follows

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)},$$

which is again Newton-Raphson method. Using first-order approximation of β in (8), we get that

$$p = p_0 - \beta \simeq p_0 - (\beta_0 + \beta_1) = p_0 - \frac{f(p_0)}{f'(p_0)} + \hbar \frac{f^2(p_0) f''(p_0)}{2f'^3(p_0)}. \tag{11}$$

The iteration form of (11) can be given as follows

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} + \hbar \frac{f^2(x_n) f''(x_n)}{2f'^3(x_n)}, \tag{12}$$

which is the Householder's iteration.

Case [n=3] Here, equation (9) becomes

$$\begin{aligned} \beta_m &= (\hbar + \chi_m)\beta_{m-1} + \hbar\lambda_2 \sum_{k=0}^{m-1} \beta_k \beta_{m-1-k} \\ &+ \hbar\lambda_3 \sum_{i=0}^{m-1} \beta_{m-i-1} \sum_{j=0}^{i} \beta_j \beta_{i-j} - \hbar(1-\chi_m)\lambda_1. \end{aligned} \tag{13}$$

Setting $\beta_0 = \lambda_1$ and taking the first-order approximation of β in (8), we get

$$p = p_0 - \beta \simeq p_0 - \beta_0 = p_0 - \frac{f(p_0)}{f'(p_0)}. \tag{14}$$

We can write down the iteration form of (14) as follows

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)},$$

which is the Newton-Raphson method. Using second-order approximation of β in (8), we obtain

$$\begin{aligned} p &= p_0 - \beta \simeq p_0 - (\beta_0 + \beta_1) \\ &= p_0 - \frac{f(p_0)}{f'(p_0)} + \hbar \frac{f^2(p_0) f''(p_0)}{2f'^3(p_0)} - \hbar \frac{f^3(p_0) f'''(p_0)}{6f'^4(p_0)}. \end{aligned} \tag{15}$$

The iteration form of (15) can be given as follows

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} + \hbar \frac{f^2(x_n)}{2f'^3(x_n)} \left(f''(x_n) - \frac{f(x_n) f'''(x_n)}{3f'(x_n)} \right), \tag{16}$$

which is the same as MADM [1] and MHPM [2] when $\hbar = -1$.

The proposed method (16) provides us with a family of iterative formulas in auxiliary parameter $\hbar$. This provides a convenient way to control convergence given by the technique. Liao [7], [11] suggested some ways to choose a fixed proper value of $\hbar$ such as the $\hbar-$curves.

The parameter $\hbar$ will not remain fixed. We will renew $\hbar$ after computing x_{n+1} by using any iterative formula for solving $f(x) = 0$. As an application to demonstrate the idea, the Chen-Li exponential iterative formula having quadratic convergence discussed in [6], [12]

$$x_{n+1} = x_n \exp(-\frac{f(x_n)}{x_n f'(x_n)}), \tag{17}$$

will be used.

Let $x_0,\ \hbar_0$ be initial guesses of p and $\hbar$. Iteration formula (16) can be written as

$$x_{n+1} = a_n + \hbar_n b_n, \tag{18}$$

where

$$\begin{aligned} a_n &= x_n - \frac{f(x_n)}{f'(x_n)}, \\ b_n &= \frac{f^2(x_n)}{2f'^3(x_n)} \left(f''(x_n) - \frac{f(x_n) f'''(x_n)}{3f'(x_n)} \right). \end{aligned} \tag{19}$$

We will renew $\hbar_n$ after computing x_{n+1} by applying Chen-Li exponential iterative formula (17) on $F(\hbar) = f(a_n + \hbar b_n) = 0$ with $\hbar_0 = \exp(-\frac{f(a_0)}{f'(b_0)b_0})$ as follows

$$\begin{aligned} \hbar_{n+1} &= \hbar_n \exp(-\frac{F(\hbar_n)}{\hbar_n F'(\hbar_n)}) \\ &= \hbar_n \exp(-\frac{f(a_n + \hbar_n b_n)}{\hbar_n f'(a_n + \hbar_n b_n) b_n}). \end{aligned} \tag{20}$$

3. Numerical examples

Some problems were selected in order to demonstrate the performance of algorithm (18-20), automatic homotopy analysis method (AHAM), as a novel solver for nonlinear algebraic equations. We present the results of AHAM with the classical Newton's method (NM), Adomian method (ADM) [1] and homotopy perturbation method (HPM) [2].

Example 1. Consider the equation

$$x^2 - e^x - x + 5 = 0$$

with the solution $p = 1.906180$. The numerical results are shown in Table 1.

Table 1. Numerical results of the solutions in Example 1

method	$x_0 = 40$	$x_0 = 100$
	iter	*iter*
NM	43	102
ADM	30	70
HPM	30	70
HAM	3	19

Example 2. Consider the equation

$$\ln(x^2 + 1) - e^{0.4x} = 0$$

with the solution $p = -0.982012$. Some numerical results are listed in Table 2.

Table 2. Numerical results of the solutions in Example 2

method	$x_0 = 40$	$x_0 = 100$
	iter	*iter*
NM	37	87
ADM	11	*Divergent*
HPM	11	*Divergent*
HAM	6	6

Example 3. Consider the equation

$$5x^3 - xe^x - 1 = 0$$

with the solution $p = 4.704594$. With $x_0 = 14$ and $x_0 = 70$, we will obtain Table 3. Note that the equation in this example has another solution $p = 0.837177$, which can be obtained using algorithm (18-20), with $x_0 = 2$, after nine iterations.

Table 3. Numerical results of the solutions in Example 3

method	$x_0 = 14$	$x_0 = 70$
	iter	*iter*
NM	15	72
ADM	11	49
HPM	11	49
HAM	5	12

4. Conclusion

The AHAM algorithms are very effective and efficient which provide highly accurate results in less number of iterations as compared to some well-known existing methods. It is shown to have significant advantages over the traditional methods in terms of flexibility, convergence and possibly speed. One of the disadvantages of the algorithms that it require the computation of high derivatives. But, The practical relevance of these methods increases since computer aided formulae manipulation facilities became a common tool in numerical analysis. HAM algorithms contain the parameter $\hbar$ which can be used to ensure and accelerate the convergence. In this work, an efficient method to get the value of $\hbar$, automatically, is presented.

Appendix A: Basic idea of HAM

To show the basic idea of HAM, let us consider the following equation

$$\mathcal{N}\left(y(t)\right) = 0,$$

where $\mathcal{N}$ is a nonlinear operator, $y(t)$ is unknown function and t the independent variable. 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 [7] constructs the so-called zero-order deformation equation

$$(1-q)\mathcal{L}\left(\phi(t;q) - y_0(t)\right) - qhH(t)\mathcal{N}[\phi(t;q)], \quad (21)$$

where $q \in [0,1]$ is the embedding parameter, $y_0(t)$ an initial guess of the exact solution $y(t)$, $h \neq 0$ an auxiliary parameter, $H(t) \neq 0$ an auxiliary function, $\phi(t;q)$ is a unknown function, and $\mathcal{L}$ is an auxiliary linear operator with the property $\mathcal{L}\left(y(t)\right) = 0$ when $y(t) = 0$. Then using $q \in [0,1]$ as an embedding parameter, It should be emphasized that we have great freedom to choose the initial guess $y_0(t)$, the auxiliary linear operator $\mathcal{L}$, the non-zero auxiliary parameter h, and the auxiliary function $H(t)$. Obviously, when $q = 0$ and $q = 1$, it holds

$$\phi(t;0) = y_0(t), \qquad \phi(t;1) = y(t).$$

Thus, as q increases from 0 to 1, the solution $\phi(t;q)$ varies continuously from the initial approximation $y_0(t)$ to the exact solution $y(t)$. Expanding $\phi(t;q)$ in Taylor series with respect to q, one has

$$\phi(t;q) = y_0(t) + \sum_{m=1}^{\infty} y_m(t) q^m \quad (22)$$

where

$$y_m(t) = \frac{1}{m!}\frac{\partial^m \phi(t;q)}{\partial q^m}|_{q=0}.$$

If the initial guess $y_0(t)$, the auxiliary linear parameter $\mathcal{L}$, the nonzero auxiliary parameter h, and the auxiliary function $H(t)$ are properly chosen so that the power series (22) converges at $q = 1$, one has

$$y(t) = y_0(t) + \sum_{m=1}^{\infty} y_m(t). \tag{23}$$

Define the vector

$$\overrightarrow{y}_n(t) = \{y_0(t), y_1(t), y_2(t), \ldots, y_n(t)\}.$$

Differentiating the zero-order deformation equation (21) m times with respective to q and then dividing by $m!$ and finally setting $q = 0$, we have the so-called mth-order deformation equation

$$\mathcal{L}\left(y_m(t) - \chi_m y_{m-1}(t)\right) = hH(t)\mathcal{R}_m(\vec{y}_{m-1}(t)) \tag{24}$$

where

$$\mathcal{R}_m(\vec{y}_{m-1}(t)) = \frac{1}{(m-1)!}\frac{\partial^{m-1}\mathcal{N}\left(\phi(t;q)\right)}{\partial q^{m-1}}$$

and

$$\chi_m = \begin{cases} 0, & m \leq 1 \\ 1, & m > 1 \end{cases}.$$

It should be emphasized that $y_m(t)$ for $m \geq 1$ is governed by the linear equation (24) with the linear boundary conditions that come from the original problem, which can be easily solved by symbolic computation software such as Matlab and Mathematica.

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