Research Article
Limit Cycle for the Brusselator by He's Variational Method

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He's variational method for finding limit cycles is applied to the Brusselator. The technique developed in this paper is similar to Kantorovitch's method in variational theory. The present theory can be applied not only to weakly nonlinear equations, but also to strongly ones, and the obtained results are valid for the whole solution domain.

1. Introduction

The Brusselator originates from a chemical reaction which consists of four steps:

$$\overline{A} \longrightarrow X, \quad \overline{B} + X \longrightarrow \overline{D} + Y, \quad 2X + Y \longrightarrow 3X, \quad X \longrightarrow \overline{E}, \tag{1.1}$$
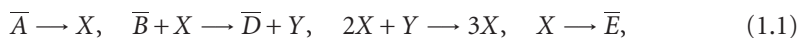
where $\overline{A}, \overline{B}, \overline{D}, \overline{E}, X$, and Y are all species. The differential equations given in dimensionless form for these species are

$$\dot{X} = A - (1 + B)X + X^2 Y, \tag{1.a}$$

$$\dot{Y} = BX - X^2 Y, \tag{2.a}$$

where all rate constants are assumed to be equal to 1, and the reactants $\overline{A}$ and $\overline{B}$ are assumed to be in large excess so that their concentrations do not change with time. The parameters A and B are the controllable parameters.

For this analysis, the dynamics of the Brusselator reaction can be described by a system of two ODEs. In dimensionless forms, they are

$$\dot{x} = A - (1 + B)x + x^2 y, \qquad (1.b)$$

$$\dot{y} = Bx - x^2 y, \qquad (2.b)$$

where $x, y \in \mathbb{R}$, and $A, B \in \mathbb{R}$ are constants with $A, B > 0$, x and y stand for the dimensionless concentrations of reference reactants.

System (1.b)-(2.b) has been extensively studied in a mathematical view [1–3], but rarely in an engineering approach. In engineering, we need a design formulation embodying the essential relationships needed by engineers who have to design practical systems.

System (1.b)-(2.b) has no possible small parameters, so the traditional perturbation methods [4] cannot be directly applied. Recently, some new perturbation methods and nonperturbative methods are proposed, for example, nonperturbative method [5], δ-method [6, 7], artificial small parameter method [8], homotopy perturbation method [9–14], variational iteration methods [15–18], perturbation-incremental method [21, 22], various modified Lindstedt-Poincare methods [23–25], a review of the recently developed analytical methods are given by He [19, 20].

The determination of amplitude and period of limit cycles is a crucial question in nonlinear problems [26–35]. Ji-Huan He suggested an energy approach to limit cycles [26, 27], it is a simple but powerful method. The method is similar to Kantorovitch's method in variational theory, so the method was called as He's variational method by D'Acunto [28, 29]. In this paper, we apply He's variational method to the Brusselator, revealing that the method is very effective and convenient.

2. An illustrative example

Generally speaking, limit cycles can be determined approximately in the form [4, 19, 20, 26, 27]

$$x = b + a(t)\cos\omega t + \sum_{n=1}^{m} (C_n \cos n\omega t + D_n \sin n\omega t), \qquad (2.1)$$

where b, C_n, and D_n are constants.

In order to best illustrate the theory, we consider Duffing equation as an illustrative example,

$$\dot{x} = y, \qquad (2.2)$$

$$\dot{y} = -x - \varepsilon x^3. \qquad (2.3)$$

Suppose that $x = a\cos\omega t$, where a is a constant. From (2.2), we have $y = -a\omega\sin\omega t$. Substituting the results into (2.3), we get the following residual:

$$R(t) = \dot{y} + x + \varepsilon x^3 = -a\omega^2 \cos\omega t + a\cos\omega t + \varepsilon a^3 \cos^3\omega t. \qquad (2.4)$$
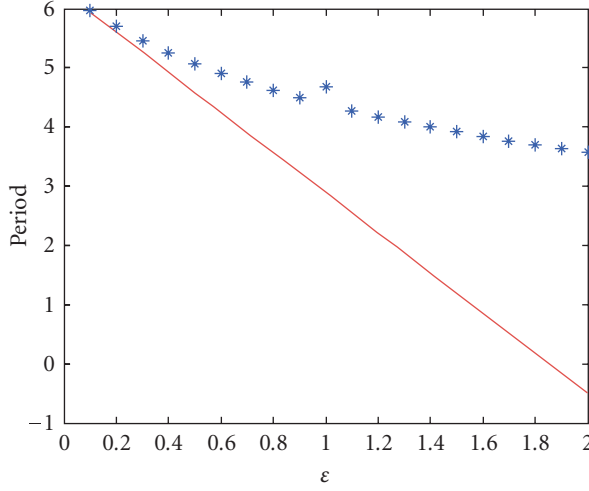
Figure 2.1. Comparison of perturbation period (T_{pert}) of Duffing equation (continuous line) with the exact one (T_{ex}) (discontinuous line).

In general, the residual might not be vanishingly small at all points. The best approximation for the solution is to minimize the residuum R, and the simplest method of obtaining the solution is the weighted residual method [26, 27], which requires that

$$\int_0^T R\cos\omega t\,dt = 0, \tag{2.5}$$

where T is the period.

From (2.5), we readily obtain the following result:

$$\omega = \sqrt{1 + \frac{3}{4}\varepsilon a^2}. \tag{2.6}$$

We, therefore, obtain the following approximate period:

$$T = \frac{2\pi}{\sqrt{1 + 0.75\varepsilon a^2}}. \tag{2.7}$$

In addition, from [4], we know that the perturbation solution is

$$T_{\text{pert}} = 2\pi\left(1 - \frac{3}{8}\varepsilon a^2\right), \quad \varepsilon \ll 1, \tag{2.8}$$

and the exact solution is

$$T_{\text{ex}} = \frac{4}{\sqrt{1 + \varepsilon a^2}} \int_0^{\pi/2} \frac{dx}{\sqrt{1 - k\sin^2 x}}, \quad k = \frac{\varepsilon a^2}{2(1 + \varepsilon a^2)}. \tag{2.9}$$
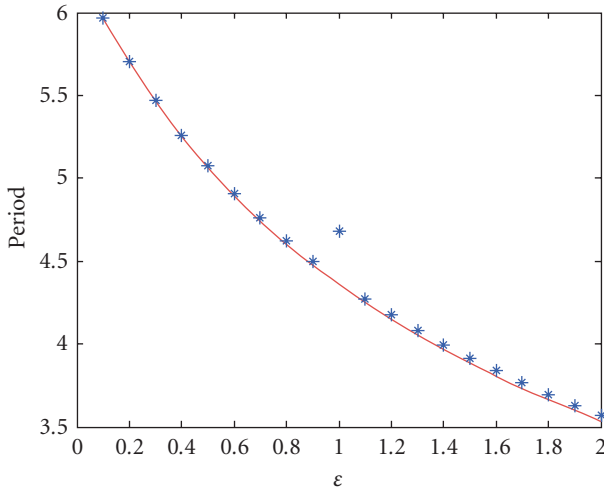
Figure 2.2. Comparison of our result (2.7) of Duffing equation with the exact one. Our result: continuous line; exact solution: discontinuous line.

From Figures 2.1 and 2.2, it is obvious that perturbation solution becomes invalid for large values of ε, however, our result is valid for the whole solution domain, that is, $0 < \varepsilon < \infty$. In case $\varepsilon \to \infty$, we have

$$\lim_{\varepsilon \to \infty} \frac{T_{\text{ex}}}{T} = \frac{2\sqrt{0.75}}{\pi} \int_0^{\pi/2} \frac{dx}{\sqrt{1 - 0.5 \sin^2 x}} = \frac{2\sqrt{0.75}}{\pi} \times 1.68575 = 0.929. \tag{2.10}$$

The 7.6% accuracy is remarkably good in view of the simplest trial function, $x = a \cos \omega t$, when $\varepsilon \to \infty$. The accuracy can be dramatically improved if we choose the trial function in the form $x = a \cos \omega t + b \cos 3\omega t$.

In order to improve the accuracy, we can begin with $x_0 = a \cos \omega t$, then from (2.3) we can obtain y_0; substituting y_0 into (2.2), the function x can be updated as x_1. The procedure can be continued before we use the weighted residual method to identify the frequency. The technique developed in this paper is similar to Kantorovitch's method in variational theory [4].

3. The Brusellator

To simplify the procedure, from (1.2) and (1.3) we can obtain the following equation:

$$\dot{y} = -\dot{x} + A - x. \tag{3.1}$$

System (1.b)-(2.b) is equivalent to (1.b) and (3.1), or (2.b) and (3.1). Now we begin with

$$x = a_0 \cos \omega t + a_1, \tag{3.2}$$

where a_0, a_1, and ω are unknown constants. Substituting (3.2) into (3.1) results in

$$\dot{y} = a_0 \omega \sin \omega t + A - a_0 \cos \omega t - a_1. \tag{3.3}$$

No secular terms in y requires that

$$a_1 = A. \tag{3.4}$$

Solving (3.3), we have

$$y = -a_0 \cos \omega t - \frac{a_0}{\omega} \sin \omega t + b, \tag{3.5}$$

where b is a constant to be further determined.

In view of (3.2) and (3.5), we obtain the following residuum:

$$\begin{aligned}
R &= -\dot{y} + Bx - x^2 y = -a_0 \omega \sin \omega t + a_0 \cos \omega t + B(a_0 \cos \omega t + A) \\
&\quad + (a_0 \cos \omega t + A)^2 \left(a_0 \cos \omega t + \frac{a_0}{\omega} \sin \omega t - b \right) \\
&= -a_0 \omega \sin \omega t + a_0 \cos \omega t + Ba_0 \cos \omega t + AB \\
&\quad + (a_0^2 \cos^2 \omega t + 2Aa_0 \cos \omega t + A^2) \left(a_0 \cos \omega t + \frac{a_0}{\omega} \sin \omega t - b \right) \\
&= -a_0 \omega \sin \omega t + a_0 \cos \omega t + Ba_0 \cos \omega t + AB \\
&\quad + (a_0^3 \cos^3 \omega t + 2Aa_0^2 \cos^2 \omega t + A^2 a_0 \cos \omega t) \\
&\quad + a_0^2 \frac{a_0}{\omega} \sin \omega t \cos^2 \omega t + 2Aa_0 \frac{a_0}{\omega} \sin \omega t \cos \omega t + A^2 \frac{a_0}{\omega} \sin \omega t \\
&\quad - ba_0^2 \cos^2 \omega t - 2Aa_0 b \cos \omega t - A^2 b.
\end{aligned} \tag{3.6}$$

In order to identify the constants a_0, b, and ω, we set

$$\begin{aligned}
\int_0^T R\, dt &= 0, \\
\int_0^T R \cos \omega t\, dt &= 0, \\
\int_0^T R \sin \omega t\, dt &= 0,
\end{aligned} \tag{3.7}$$

where T is the period.

From (3.7), we have

$$\begin{aligned}
AB + Aa_0^2 - \frac{1}{2} ba_0^2 - A^2 b &= 0, \\
a_0 + Ba_0 + \frac{3}{4} a_0^3 + A^2 a_0 - 2Aa_0 b &= 0, \\
-a_0 \omega + \frac{a_0^3}{4\omega} + A^2 \frac{a_0}{\omega} &= 0.
\end{aligned} \tag{3.8}$$

Solving (3.8), simultaneously, we have

$$b = \frac{(7/2)A^2 + B + 1 \pm \sqrt{-(15/4)A^4 + 3A^2(B-3) + (B+1)^2}}{4A},$$

$$a_0^2 = \frac{AB - A - A^3}{b - (5/4)A} = \frac{B - 1 - A^2}{(b/A) - (5/4)},$$

$$\omega = \sqrt{\frac{AB - A - A^3}{4b - 5A} + A^2}.$$

(3.9)

Note that b and a_0 are real numbers, so there are

$$\Delta = -\frac{15}{4}A^4 + 3A^2(B-3) + (B+1)^2 \geq 0,$$

$$\frac{B - 1 - A^2}{(b/A) - (5/4)} \geq 0.$$

(3.10)

By a simple analysis, we can obtain the following results.
(1) When $B > 1 + A^2$, the constant b can be finally determined as

$$b = \frac{(7/2)A^2 + B + 1 + \sqrt{-(15/4)A^4 + 3A^2(B-3) + (B+1)^2}}{4A}.$$

(3.11)

(2) When $B \leq 1 + A^2$ and $A^2 > 4$, the constant b can be finally determined as

$$b = \frac{(7/2)A^2 + B + 1 \pm \sqrt{-(15/4)A^4 + 3A^2(B-3) + (B+1)^2}}{4A}.$$

(3.12)

The approximate period can be written in the form

$$T = \frac{2\pi}{\sqrt{((AB - A - A^3)/(4b - 5A)) + A^2}},$$

(3.13)

where b is defined by (3.11) or (3.12).

4. Conclusion

To summarize, we can conclude from the results thus obtained that the method developed here is extremely simple in its principle, quite easy to use, and gives a very good accuracy in the whole solution domain, even with the simplest trial functions. Theoretically, any accuracy can be arrived at by suitable choice of trial functions or by iterations before weighted residual method is applied.

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