Rational Approximants to the Solution of the Brusselator System compared to the Adomian Decomposition Method

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Abstract

Brusselator is an initial value problem which serves as a theoretical model in chemical kinetics. Here it is solved by applying a rational approximation to the variables that represent concentrations. The problem transfers to the solution of simple nonlinear algebraic systems. A symbolic manipulation package is given that deals with this issue. Comparisons with the results from the Adomian decomposition method are very promising.

Mathematics Subject Classification: 65L05, 65L99

Keywords: Decomposition Method, Brusselator system, Mathematica

1 Introduction

Brusselator model was introduced by Lefever and Nicolis [2] and has the following general form:

\[
\begin{align*}
\frac{\partial x}{\partial t} &= a + x^2y - (b + 1)x, \\
\frac{\partial y}{\partial t} &= bx - x^2y.
\end{align*}
\] (1)

where \(a > 0\) and \(b > 0\) are constants. It is one of the simplest but most fundamental models which displays biological and chemical oscillations. \(x\) and \(y\) represent concentrations of two substances. Suppose that we have the following initial conditions:

\[x(0) = N_1, \quad y(0) = N_2.\]
2 The New method

Let us consider that the solution has the following rational forms:

\[ x(t) = \frac{N_1 + \sum_{j=1}^{n} c_j t^j}{1 + \sum_{j=1}^{n} c_{j+n} t^j} \]

and

\[ y(t) = \frac{N_2 + \sum_{j=1}^{n} d_j t^j}{1 + \sum_{j=1}^{n} d_{j+n} t^j} \]

Assuming \( a = 0, b = -1, N_1 = 1, N_2 = 1, n = 2 \) and by applying the above expressions to the first of equations in (1) we get:

\[
\begin{pmatrix}
-1 - c_1 + t^2 c_2^2 - 2tc_2 + 2t^3 c_1 c_2 + t^4 c_2 + c_3 - 2tc_3 - 2t^2 c_1 c_3 - t^2 c_2 c_3 \\
-2t^3 c_2 c_3 + 2tc_4 - 2t^2 c_4 + t^2 c_1 c_4 - 2t^3 c_1 c_4 - 2t^4 c_2 c_4 + td_1 \\
+2tc_1 d_1 + t^3 c_1^2 d_1 + 2t^3 c_2 d_1 + 2t^4 c_1 c_2 d_1 + t^5 c_2^2 d_1 + t^2 d_2 + 2t^3 c_1 d_2 \\
+ t^4 c_2 d_2 + 2t^4 c_2 d_2 + 2t^5 c_1 c_2 d_2 + t^6 c_2^2 d_2 - 2td_3 - tc_1 d_3 - 2t^2 c_1 d_3 \\
-2t^2 c_2 d_3 - 2t^3 c_2 d_3 + tc_3 d_3 - 2t^2 c_3 d_3 - 2t^3 c_1 c_3 d_3 - t^3 c_2 c_3 d_3 \\
-2t^4 c_2 c_3 d_3 + 2t^2 c_4 d_3 - 2t^3 c_1 c_4 d_3 - 2t^4 c_1 c_4 d_3 \\
-2t^5 c_2 c_4 d_3 - 2t^2 d_4 - t^2 c_1 d_4 - 2t^3 c_1 d_4 - 2t^3 c_2 d_4 - 2t^4 c_2 d_4 \\
+ t^2 c_3 d_4 - 2t^3 c_3 d_4 - 2t^4 c_1 c_3 d_4 - t^4 c_2 c_3 d_4 - 2t^5 c_2 c_3 d_4 \\
+ 2t^3 c_1 d_4 - 2t^4 c_1 d_4 + t^4 c_1 c_4 d_4 - 2t^5 c_1 c_4 d_4 - 2t^6 c_2 c_4 d_4
\end{pmatrix}
\]

\[(1 + tc_3 + t^2 c_4)^2 (1 + td_3 + t^2 d_4)\]

Expanding the numerator in powers of \( t \) up to third order we have to solve the following four equations.

\[-1 - c_1 + c_3 = 0,\]
\[-2c_2 - 2c_3 + 2c_4 + d_1 - 2d_3 - c_1 d_3 + c_3 d_3 = 0,\]
\[
\begin{pmatrix}
c_1^2 - 2c_1 c_3 - c_2 c_4 - 2c_4 + c_1 c_4 + c_1 d_1 + d_2 - 2c_1 d_3 \\
-2c_2 d_3 - 2c_3 d_3 + 2c_4 d_3 - 2d_4 - c_1 d_4 + c_3 d_4
\end{pmatrix}
= 0,
\]
\[
\begin{pmatrix}
2c_1 c_2 - 2c_2 c_3 - 2c_1 c_4 + c_1^2 d_1 + 2c_2 d_1 + 2c_1 d_2 \\
-2c_2 d_3 - 2c_1 c_3 d_3 - c_2 c_3 d_3 - 2c_4 d_3 + c_1 c_4 d_3
\end{pmatrix}
= 0
\]

Again, substituting the rational approximations of \( x(t) \) and \( y(t) \) in the second of equations (1) we conclude to another four equations in the coefficients \( c_i \) and \( d_i, i = 1, 2, 3, 4 \):
Rational Approximation to the Brusselator system

\[ d_1 - d_3 = 0, \]
\[ c_1 - c_3 + d_1 + 2c_3d_1 + 2d_2 - d_3 - 2c_3d_3 - 2d_4 = 0, \]
\[
\begin{pmatrix}
  c_1^2 + c_2 - c_1c_3 - c_4 + 2c_1d_1 + c_3^2d_1 + 2c_4d_1 + d_2 \\
  + 4c_3d_2 - 2c_3d_3 - c_3^2d_3 - 2c_4d_3 + d_1d_3 \\
  + d_2d_3 - d_3^2 - d_4 - 4c_3d_4 - d_1d_4
\end{pmatrix} = 0,
\]
\[
\begin{pmatrix}
  2c_1c_2 - c_2c_3 - c_1c_4 + c_1^2d_1 + 2c_2d_1 + 2c_3c_4d_1 + 2c_1d_2 \\
  + 2c_3^2d_2 + 4c_4d_2 + c_1^2d_3 - 2c_1c_3d_3 - 2c_4d_3 - 2c_3c_4d_3 \\
  + 2c_1d_1 + d_2 + 2c_3d_2d_3 - c_2d_3^2 - c_3d_3^2 - 2c_4d_3 \\
  - 2c_2^2d_4 - 4c_4d_4 + d_1d_4 - 2c_3d_1d_4 - 2d_3d_4
\end{pmatrix} = 0
\]

Solving the eight equations for the eight coefficients we get the following rational approximations of the solution.

\[ x(t) = \frac{1 - t - t^2}{1 + \frac{3t}{4} + \frac{t^2}{2}}, \]
\[ y(t) = \frac{1 + t + t^2}{1 + t + \frac{t^2}{2}}. \]

This technique can be automatized by a MATHEMATICA program for any values of \( a, b, N_1, N_2 \), and \( n \).

\[
\text{Bruss}[a_, b_, n1_, n2_, n_] := \\
\text{Module}[\{c, j1, x, y, equ, so\}, \\
\quad x = \left( n1 + \text{Sum}[c[j1]*t^j1, \{j1, 1, n\}] \right) / \left( 1 + \text{Sum}[c[j1 + n]*t^j1, \{j1, 1, n\}] \right); \\
\quad y = \left( n2 + \text{Sum}[d[j1]*t^j1, \{j1, 1, n\}] \right) / \left( 1 + \text{Sum}[d[j1 + n]*t^j1, \{j1, 1, n\}] \right); \\
\quad equ = \text{Join}[ \\
\quad \text{Series}[\text{Numerator}[\text{Factor}[\text{D}[x, t] - a - x^2*y + (b + 1)*x]], \{t, 0, 2*n - 1\}][[3]], \\
\quad \text{Series}[\text{Numerator}[\text{Factor}[\text{D}[y, t] - b*x + x^2*y]], \{t, 0, 2*n - 1\}][[3]]]; \\
\quad so = \text{NSolve}[\{\text{equ} == \text{Table}[0, \{j1, 1, 4*n\}], \\
\quad \text{Variables}[\text{equ}], \text{WorkingPrecision} -> 16]; \\
\quad x = x / . so; y = y / . so; \\
\quad \text{Return}[\{x, y\}] 
\]

Thus by simple try we have

\text{In}[1] := \text{Bruss}[0, 1, 1, 1, 2]
and propose the approximations Ayati [1] proposed ninth order polynomials instead.

\[ \begin{align*}
\text{Out}[1] &:= \left\{ \left\{ \frac{1 - t + t^2}{1 + t + \frac{t^2}{2}} \right\}, \left\{ \frac{1 + t + t^2}{1 + t + \frac{t^2}{2}} \right\} \right\} \\
\text{In}[2] &: \text{Bruss}[0, 1, 1, 1, 4] \\
\text{Out}[2] &:= \left\{ \left\{ \frac{1 + 3189t + 2464t^2 + 926t^3 + 2660t^4}{1 + 2444t + 340t^2 + 1913t^3 + 51960t^4}, \frac{1 + 3189t + 2464t^2 + 926t^3 + 2660t^4}{1 + 2444t + 340t^2 + 1913t^3 + 51960t^4} \right\} \right\} 
\end{align*} \]

3 Numerical Results

To illustrate the new method we comparing the results of this method with the results of Adomian decomposition method. Here are two examples given in [1].

**Example 1:** Take \( a = 0, b = 1, N_1 = 1, N_2 = 1 \). For this example we we propose the approximations

\[
x(t) = \frac{1 + 3189t + 2464t^2 + 926t^3 + 2660t^4}{1 + 2444t + 340t^2 + 1913t^3 + 51960t^4} \\
y(t) = \frac{1 + 9127t + 299t^2 + 299t^3 + 1724t^4}{1 + 8660 + 1724t^2 + 64700t^4} 
\]


\[
x(t) = 1 - t + \frac{t^3}{2} - \frac{3t^4}{8} + \frac{3t^5}{20} + \frac{7t^6}{240} - \frac{37t^7}{240} + \frac{7t^8}{40} - \frac{1813t^9}{17280},
\]

and

\[
y(t) = 1 + \frac{t^2}{2} - \frac{t^3}{2} + \frac{t^4}{4} - \frac{3t^5}{40} + \frac{13t^6}{240} + \frac{3t^7}{20} - \frac{299t^8}{1920} + \frac{1477t^9}{17280}.
\]

<table>
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<th>( t )</th>
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<th>( y )</th>
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<th>( y )</th>
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In Table– 1 we summarize the true errors observed by both methods in logarithmic scale. It is obvious that more than a digit was gained by our proposal with less computational cost.

**Example 2:** Consider system (1), by the coefficients

\[ N_1 = 2, \quad N_2 = 3, \quad a = 0.02 \quad \text{and} \quad b = 0.1 \]

Using the MATHEMATICA package we get:

\[
x(t) = \frac{\left(2 - 25.18018291568923t + 164.9557457647571t^2 \right) \left(-589.4802065148397t^3 + 1230.249861992605t^4 \right) \left(-1196.290424543237t^5 + 430.81271384133558t^6 \right)}{1 - 17.50009145784462t + 153.4438219403956t^2 \left(-788.4557008211359t^3 + 2498.515618435320t^4 \right) \left(-4529.39599571568t^5 + 3715.805143053156t^6 \right)}
\]

and

\[
y(t) = \frac{\left(3 - 52.03420633647790t + 397.6413042804737t^2 \right) \left(-1599.73061718659t^3 + 3127.223972517517t^4 \right) \left(-1189.811693306206t^5 - 3615.66504320403t^6 \right)}{1 - 13.41140211215930t + 91.40525311899800t^2 \left(-324.6942330262930t^3 + 582.9386069057401t^4 \right) \left(-129.5221005957941t^5 - 632.7008182557557t^6 \right)}
\]

J. Biazar and Z. Ayati [1] proposed twelfth order polynomials. The errors observed by both methods are summarized in Table– 2.

**Table 2: Errors for Example– 2.**

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<td>-2.22</td>
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It is remarkable that more than five digits of accuracy is gained by our method.

**ACKNOWLEDGEMENTS.** This research was accomplished while the author was on Sabbatical at the University of Peloponnese.
References


Received: November, 2008