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Letter to the Editor

Analysis of jump phenomena using Padé approximations

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1. Introduction

An investigation of jump (blow-up) phenomena is of a particular importance from both theoretical and practical points of view. We would only like to address the combustion problem, various problems in biology (an increase of population), buckling of construction and so on [1–6]. In order to understand and explain the mentioned phenomena, the various asymptotical methods are used, and in particular, the matched asymptotic procedure [1,3], geometric asymptotics [4], Whitham method [6,7], or boundary layers approach [8].

As it has been shown in Ref. [2], the jump phenomena can often be described using a concept of rational functions. This observation immediately suggests applying Padé approximations (PAs) [9–11]. For instance, PAs have been so successfully applied in the theory of solitons, that even a new term called “padeon” has been created [12–16]. In fact, the “direct Hirota method” used for construction of solitons has its source in the application of PA [17,18]. Note that PA can be successively applied also in many other cases, where the so-called solution localization appears.

Consider PAs which allow one to perform, to some extent, the most natural continuation of the power series. Let

$$F(\varepsilon) = \sum_{i=0}^{\infty} C_i \varepsilon^i,$$

$$F_{mn}(\varepsilon) = \sum_{i=0}^m a_i \varepsilon^i \left(1 + \sum_{i=1}^n b_i \varepsilon^i \right),$$

where the coefficients a_i , b_i are determined from the following condition: the first $(m+n)$ components of the expansion of the rational function $F_{mn}(\varepsilon)$ in a Maclaurin series coincide with the first components of the series $F(\varepsilon)$. Then F_{mn} is called the $PA[m, n]$. The set of F_{mn} functions

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for different m and n forms the Padé table. The diagonal PAs ($m = n$) are most widely used in practice. Note that a PA is unique when m and n are specified.

To construct the PAs, it is necessary to solve only systems of linear algebraic equations. Comparing the coefficients of $\varepsilon^0, \varepsilon^1, \varepsilon^2, \dots, \varepsilon^{m+n}$, the system of linear algebraic equations can be obtained from the following equality:

$$(c_0 + c_1\varepsilon + \dots + c_{m+n}\varepsilon^{m+n}) \left(1 + \sum_{i=1}^n b_i\varepsilon^i \right) = \sum_{i=0}^m a_i\varepsilon^i. \quad (1)$$

PAs perform a meromorphic continuation of the function given in the form of the power series, and for this reason, it allows one to achieve success in the cases where analytic continuation cannot be applied. If the PA sequence converges to a given function, then the roots of its denominators tend to singular points. It allows one to determine the singularities and then to perform the analytic continuation.

For instance, if the truncated series has the form

$$f(\varepsilon) = 1 + a\varepsilon + b\varepsilon^2 + \dots,$$

then diagonal PA is governed by the formula

$$PA[1, 1] = \frac{a + (a^2 - b)\varepsilon}{a - b\varepsilon}. \quad (2)$$

Using only two terms of the series, the following formula can be used:

$$PA[0, 1] = \frac{1}{1 - a\varepsilon}. \quad (3)$$

Now consider as an example the following boundary value problem:

$$y'' - y + 2y^3 = 0, \quad (4)$$

$$y(0) = 1, \quad (5)$$

$$y(\infty) = 0, \quad (6)$$

which has the exact solution

$$y = \cosh(x). \quad (7)$$

A solution in the form of a Dirichlet series may be written as

$$y = Ce^{-x}\varphi(x), \quad C = \text{const}, \quad (8)$$

where

$$\varphi(x) = 1 - \frac{1}{4}C^2e^{-2x} + \frac{1}{16}C^4e^{-4x} + \dots \quad (9)$$

Applying formula (2) to truncated series (9), and assuming

$$a = \frac{1}{4}C^2e^{-2x}, \quad b = \frac{1}{16}C^4e^{-4x}, \quad \varepsilon = e^{-2x}$$

from Eq. (8), one obtains

$$y = \frac{4C}{4e^x + C^2e^{-x}}. \quad (10)$$

Observe that solution (10) satisfies decaying conditions (6). From condition (5) one finds $C = 2$ and solution (10) overlaps with exact solution (6).

In order to illustrate an application of PA to blow-up problems, consider the following model problem:

$$\frac{dx}{dt} = \alpha x + \varepsilon x^2, \quad x(0) = 1,$$

where $0 < \varepsilon \ll \alpha \ll 1$.

The exact solution to this boundary value problem has the form

$$x(t) = \frac{\alpha \exp(\alpha t)}{(\alpha + \varepsilon - \varepsilon \exp(\alpha t))}. \quad (11)$$

For $t \rightarrow \ln[(\alpha + \varepsilon)/\varepsilon]$, the solution goes to infinity (blow-up of the solution appears). A regular asymptotics of the form

$$x(t) = \exp(\alpha t) \Psi(t), \quad (12)$$

where

$$\Psi(t) = 1 - \varepsilon \alpha^{-1} [1 - \exp(\alpha t)] + \dots \quad (13)$$

cannot describe the mentioned phenomenon. Using PA (3) for truncated series (13), and taking $\alpha = \alpha^{-1}[1 - \exp(\alpha t)]$, one obtains exact solution (11).

2. Analytical analysis

The combustion model is governed by

$$\dot{y} = y^2(1 - y), \quad (14)$$

$$y(0) = \varepsilon. \quad (15)$$

This problem will be investigated for $\varepsilon \ll 1$.

Numerical simulation of Eqs. (14) and (15) using the Runge–Kutta fourth order algorithm is shown in Fig. 1 for different values of ε . Observe that approximately for t^* , a sudden jump of solution occurs which possesses the two following properties. First, decreasing ε , the solution shape $y(t)$ approaches a unit step function form. Second, to the left of value t^* , the function $y(t)$ approaches almost horizontally the value of zero, whereas for $t > t^*$, this function is also horizontal and close to 1 for sufficiently small ε (see Fig. 1(c)).

The aim of this paper is to predict an occurring threshold for $t = t^*$ and to obtain analytical solutions for $t < t^*$ (zone I) and $t > t^*$ (zone II) by matching them at the point $t = t^*$.

First the following regular asymptotic expansion is used:

$$y = \sum_{i=0}^{\infty} \varepsilon^i y_i. \quad (16)$$

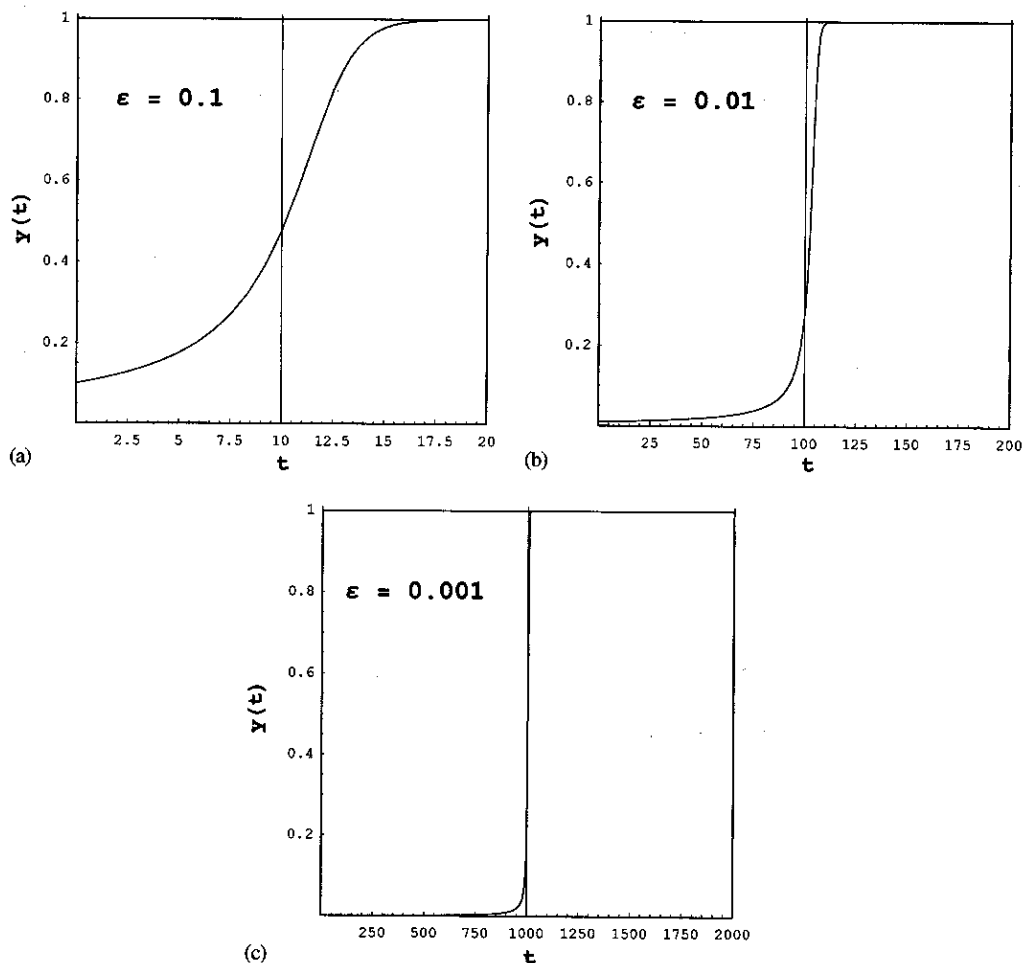


Fig. 1. Numerical solutions to Eq. (1) for different initial values: (a) $\varepsilon = 0.1$; (b) $\varepsilon = 0.01$; (c) $\varepsilon = 0.001$.

Substituting Eq. (16) into Eqs. (14) and (15), the problem is reduced to a set of initial problems:

$$\dot{y}_0 = y_0^2(1 - y_0), \quad (17)$$

$$y_0 = 1, \quad (18)$$

$$\dot{y}_1 = 0, \quad y_1 = C \equiv \text{const.}, \quad (19)$$

$$\dot{y}_2 = y_1^2, \quad y_2 = C^2 t, \quad (20)$$

$$\dot{y}_3 = y_1^3 + 2y_0 y_2, \quad y_3 = C^3(t - 1)t, \quad (21)$$

$$\dot{y}_4 = -3y_1^2 y_2 + y_2^2 + 2y_1 y_3, \quad y_4 = 5C^4(t - 1)t, \quad (22)$$

$$\dot{y}_5 = -3y_1y_2^2 - 3y_1^2y_3 + 2y_2y_3 + 2y_1y_4, \quad y_5 = C^5t(14t^2 - 21t + 3), \quad (23)$$

$$\dot{y}_6 = -y_2^3 - 6y_1y_2y_3 + y_3^2 - 3y_1^2y_4 + 2y_2y_4 + 2y_1y_5, \quad y_6 = 14C^6t^3(3t^2 - 6t + 2). \quad (24)$$

The results have been obtained using the “Mathematica” package (see Appendix A).

Eq. (16) has the solution $y_0 = 1$, which corresponds to a being sought function for $t \rightarrow \infty$. This part of the solution will be taken into further analysis. The constant C is defined from initial condition (14)

$$y_1 + \varepsilon y_2 + \varepsilon^2 y_3 + \dots = 1 \quad \text{for } t = 0,$$

which gives $C = 1$.

Now apply the PA to show that using this approximation gives the possibility to predict the observed numerical jump of the solution $y(t)$ occurring for $t = t^*$ with high accuracy. First the PA is briefly introduced and calculated “by hand”, whereas higher order PA will be calculated using the PA build using “Mathematica”. The function y will be approximated by the following rational one:

$$y_1 + \varepsilon y_2 + \varepsilon^2 y_3 + \varepsilon^3 y_4 + \dots = \frac{y_1 + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3 + \dots}{1 + b_1\varepsilon + b_2\varepsilon^2 + b_3\varepsilon^3 + \dots}, \quad (25)$$

where a_i and b_i are unknown coefficients.

According to the construction of the PA, expression (25) is transformed into the form

$$(y_0 + \varepsilon y_1 + \varepsilon^2 y_2 + \dots)(1 + b_1\varepsilon + b_2\varepsilon^2) = y_0 + a_1\varepsilon + a_2\varepsilon^2 + \dots.$$

Comparing the terms of the same powers of ε , one obtains

$$\begin{aligned} \varepsilon^0: \quad & y_1 = y_1, \\ \varepsilon^1: \quad & y_1 b_1 + y_2 = a_1, \\ \varepsilon^2: \quad & y_1 b_2 + y_2 b_1 + y_3 = a_2, \\ \varepsilon^3: \quad & y_1 b_3 + y_2 b_2 + y_3 b_1 + y_4 = a_3. \end{aligned} \quad (26)$$

Observe that the fraction to the right-hand side of Eq. (25) is finite and a number of unknowns $a_1, \dots, a_n, b_1, \dots, b_m$ are equal to $m + n$. Therefore, $m + n$ equations are taken from the infinite number of equations generated by series (16).

From Eq. (26) one gets

$$a_1 = C, \quad a_2 = C^2, \quad b_1 = -C(t - 1) \quad (27)$$

and $PA[2,1]$ has the form

$$PA[2, 1] = C\varepsilon \frac{1 + C\varepsilon}{(1 - C(t - 1)\varepsilon)}.$$

Here by $PA[m,n]$ is denoted the PA having $(m + 1)$ terms in the numerator, and having $(n + 1)$ terms in the denominator. This result has been verified using “Mathematica” (see Appendix B), where in addition, $C = 1$ has been obtained.

In a similar way to that corresponding to zone I, one can also construct different PA. They have the following forms:

$$PA[2, 1] = \frac{\varepsilon(-2 + \varepsilon t)}{2 + t\varepsilon[-3 + (2 + t)\varepsilon]}$$

$$PA[3, 1] = \frac{\varepsilon[2 + (-2 - \varepsilon(3 + (2 + t)\varepsilon))]}{2 + t[-2 + (-5 + 2t\varepsilon)]}$$

The threshold value t^* is found by a condition that the denominators are equal to zero. The following analytical values have been found:

$$t_{[2,1]}^* = -1 + \frac{1}{\varepsilon}, \quad (28)$$

$$t_{[2,2]}^* = \frac{3 - 2\varepsilon + \sqrt{1 + 4\varepsilon(\varepsilon - 3)}}{2\varepsilon}, \quad (29)$$

$$t_{[3,1]}^* = \frac{2 + 5\varepsilon + \sqrt{4 + \varepsilon(4 + 25\varepsilon)}}{4\varepsilon}. \quad (30)$$

The numerical values of t^* for three different values of ε are shown in Table 1.

Observe that in the case of $\varepsilon = 0.1$, there is an imaginary value of $t_{[2,2]}^*$ for Eq. (29), and also for $P[2, 2]$ and $P[3, 1]$, Eqs. (29) and (30) include only one solution (in fact, there exist two real solutions).

Therefore, the use of PA gave explanations to the observed numerical jumps of the $y(t)$ solution (see Fig. 1).

Now construct a solution in zone II ($t > t^*$). Since in this zone the solution is close to 1, the following change of variables is introduced:

$$y = 1 + \tilde{x} \quad (31)$$

and from Eq. (14) one obtains

$$\dot{\tilde{x}} = -\tilde{x}(1 + \tilde{x})^2, \quad (32)$$

where $\tilde{x} \ll 1$. The further procedure is similar to the case related to zone I. It is efficient to introduce an artificial small parameter δ . First, use this parameter for asymptotical splitting, and

Table 1
Numerical values of t^* obtained using PA

Equation number	ε		
	0.1	0.01	0.001
(18)	11.0	101.0	1001.0
(19)	x	102.08518	1002.008
(20)	11.640965	101.51492	1001.5015

Table 2
Values of t^* and t_0 obtained using PA

Padé approximations	Time constants	ε		
		0.1	0.01	0.001
PA[2,1]	t^*	24.945	945.722	31110.408
	t_0	24.213	944.100	31107.647
PA[3,1]	t^*	16.514	424.669	0641.779
	t_0	16.299	424.188	9640.571
PA[2,2]	t^*	16.514	424.669	9641.779
	t_0	16.299	424.188	9640.571

finally take $\delta = 1$. Then, apply the classical perturbation method assuming the solution

$$\tilde{x} = \delta x_0 + \delta^2 x_1 + \delta^3 x_2 + \dots \quad (33)$$

Substituting Eq. (33) to Eq. (32), one gets the following set of differential equations:

$$\begin{aligned} \frac{dx_0}{dt} &= -x_0, & x_0 &= e^{-(t-t_0)}, \\ \frac{dx_1}{dt} &= -x_1 - 2x_0, & x_1 &= 2e^{-2(t-t_0)}, \\ \frac{dx_2}{dt} &= -x_2 - x_0^3 - 4x_0x_1, & x_2 &= \frac{9}{2}e^{-3(t-t_0)}, \\ \frac{dx_3}{dt} &= -x_3 - 3x_0^2x_1 - 2x_1^2 - 4x_0x_2, & x_3 &= \frac{32}{8}e^{-4(t-t_0)}, \\ \frac{dx_4}{dt} &= -x_4 - 3x_0x_1^2 - 3x_0^2x_2 - 4x_1x_2 - 4x_0x_3, & x_4 &= \frac{625}{24}e^{-5(t-t_0)}. \end{aligned}$$

The value at time instant t_0 defines a temporarily unknown constant, which will be estimated during a matching process. The values of t^* and t_0 obtained using PA are shown in Table 2.

Now, having two solutions \bar{y} and \tilde{y} which are valid for zones I and II, correspondingly, they will be matched. The matching conditions have the form

$$\bar{y} = \tilde{y}, \quad \frac{d\bar{y}}{dt} = \frac{d\tilde{y}}{dt} \quad \text{for } t = t_0.$$

3. Numerical results

The obtained results are presented in the following figures, where a continuous curve corresponds to the exact (numerical) solution, a dashed curve corresponds to an asymptotic series, and a dense-dashed curve corresponds to a PA for $\varepsilon = 0.1; 0.01; 0.001$. Fig. 2 includes the

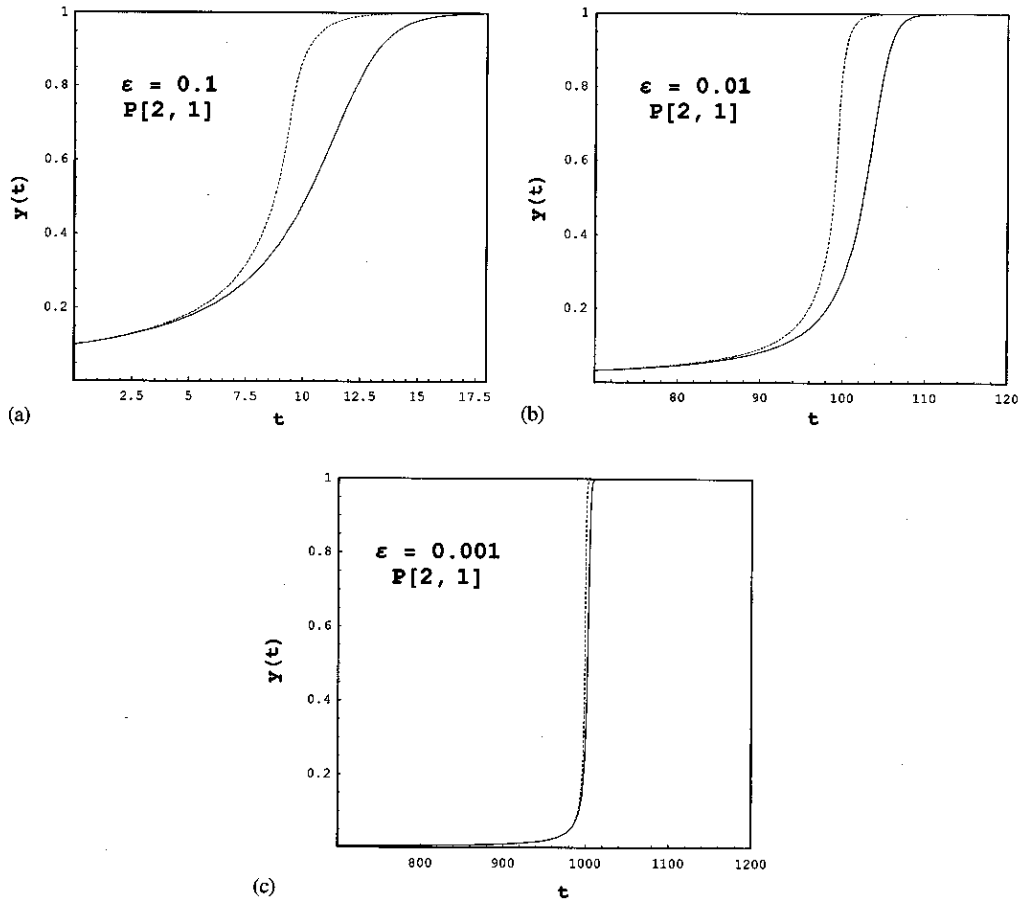


Fig. 2. Numerical, asymptotical and PA solutions for different values of ε : (a) 0.1; (b) 0.01; (c) 0.01 ($PA[2,1]$).

approximation $PA[2,1]$, Fig. 3 includes the approximation $P[3,1]$, whereas Fig. 4 includes the approximation $PA[2,2]$.

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Appendix A. Analytical solution using the classical perturbation technique

$$y_a = \varepsilon y_0 + \varepsilon^2 y_1 + \varepsilon^3 y_2 + \varepsilon^4 y_3 + \varepsilon^5 y_4 + \varepsilon^6 y_5;$$

$$y_{0p} = \text{Coefficient}[y_a^2(1-y_a) // \text{Expand}, \varepsilon^1]$$

0

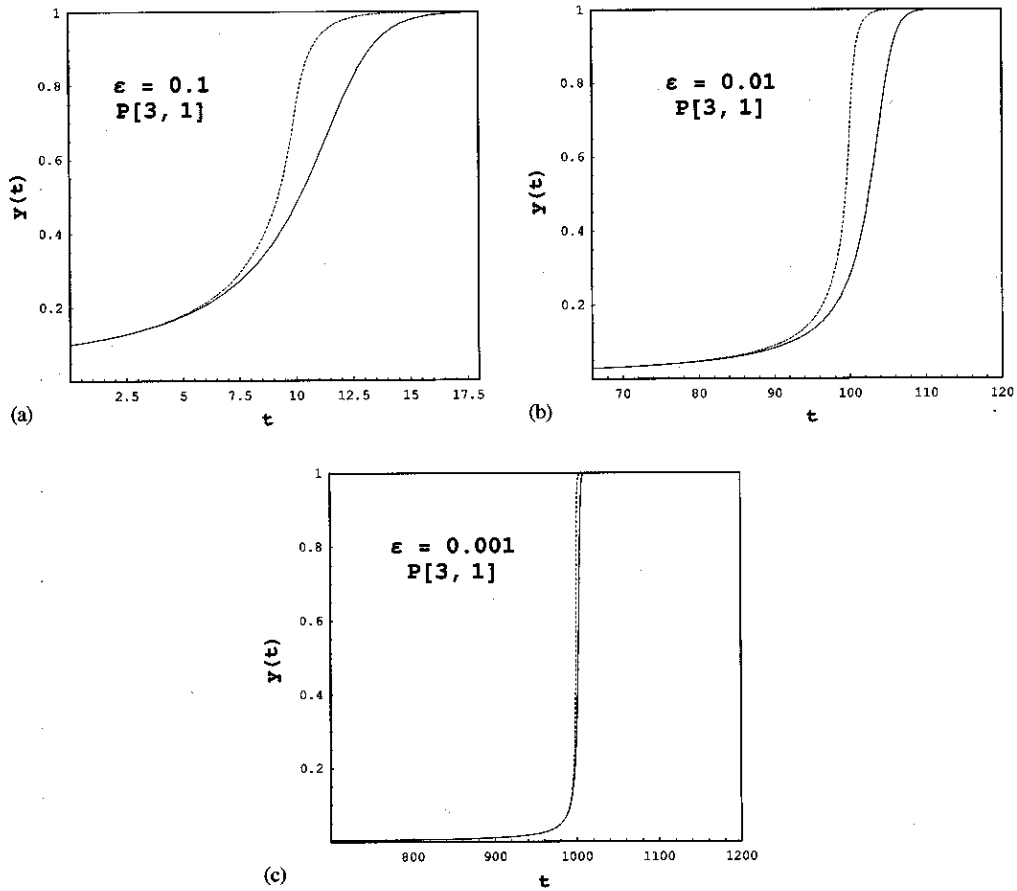
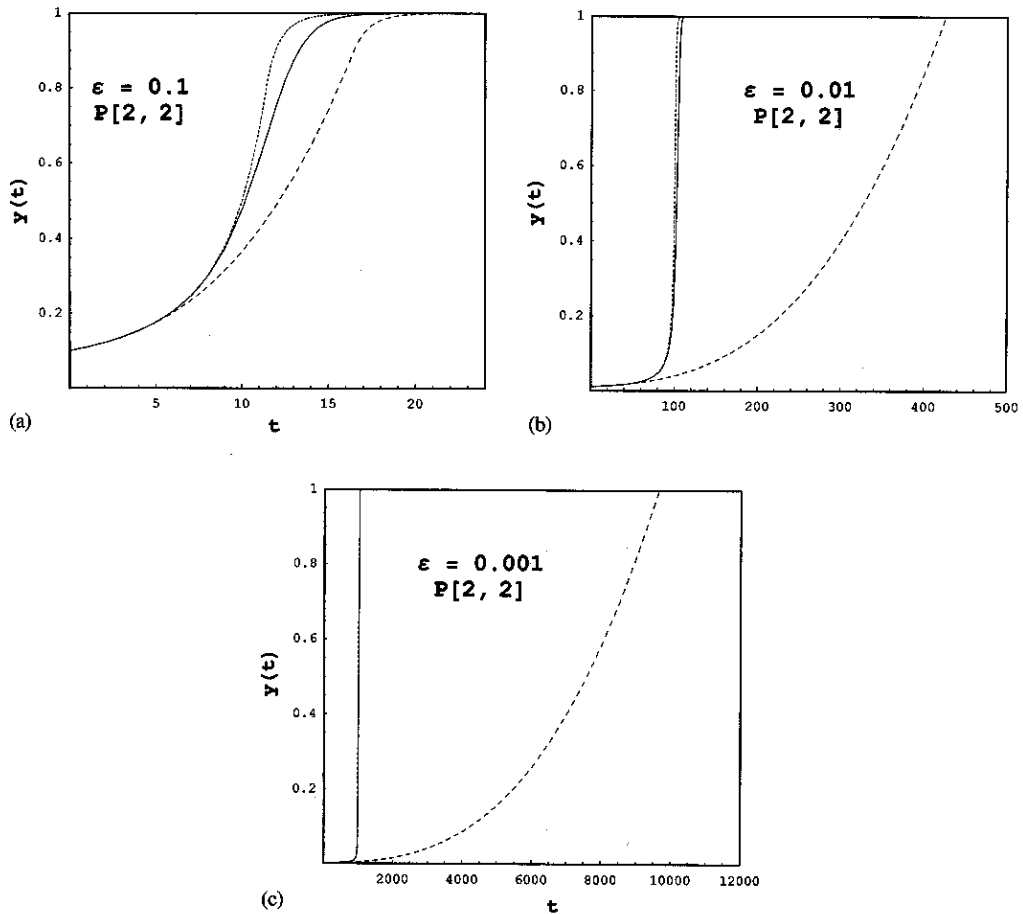


Fig. 3. Same as in Fig. 2 ($PA[3,1]$).

$$\begin{aligned}
 & y1p = \text{Coefficient}[ya^2(1-ya) // \text{Expand}, \epsilon^2] \\
 & y_0^2 \\
 & y2p = \text{Coefficient}[ya^2(1-ya) // \text{Expand}, \epsilon^3] \\
 & -y_0^3 + 2y_0y_1 \\
 & y3p = \text{Coefficient}[ya^2(1-ya) // \text{Expand}, \epsilon^4] \\
 & -3y_0^2y_1 + y_1^2 + 2t_0y_2 \\
 & y4p = \text{Coefficient}[ya^2(1-ya) // \text{Expand}, \epsilon^5] \\
 & -3y_0^2y_1^2 - 3y_0^2y_2 + 2y_1y_2 + 2y_0y_3 \\
 & y5p = \text{Coefficient}[ya^2(1-ya) // \text{Expand}, \epsilon^6] \\
 & -y_1^3 - 6y_0y_1y_2 + y_2^2 - 3y_0^2y_3 + 2y_1y_3 + 2y_0y_4 \\
 & y_0 = C \\
 & y1p \\
 & C \\
 & C^2 \\
 & y_1 = \int y1p dt // \text{Simplify}
 \end{aligned}$$

Fig. 4. Same as in Fig. 2 ($PA[2,2]$).

$$y_{2P} = y_{2P} // \text{Simplify}$$

$$C^2 t$$

$$C^3(-1 + 2t)$$

$$y_2 = \int y_{2P} dt // \text{Simplify}$$

$$y_{3P} = y_{3P} // \text{Simplify}$$

$$C^3(-1 + t)t$$

$$C^4 t(-5 + 3t)$$

$$y_3 = \int y_{3P} dt // \text{Simplify}$$

$$y_{4P} = y_{4P} // \text{Simplify}$$

$$C^4 \left(-\frac{5t^2}{3} + t^3 \right)$$

$$C^5 t(3 - 13t + 4t^2)$$

$$y_4P = \int y_{4P} dt // \text{Simplify}$$

$$\frac{1}{6} C^5 t^2(9 - 26t + 6t^2)$$

Appendix B. Padé[2,1]

<<Calculus 'Pade';

Pade [ya, {ε, 0, 2, 1}]/FullSimplify

$$\frac{C\varepsilon(1 + C\varepsilon)}{-1 + C(-1 + t)\varepsilon}$$

Computation of constant C

$$\text{Solve} \left[\left(\frac{C\varepsilon(1 + C\varepsilon)}{-1 + C(-1 + t)\varepsilon} / \cdot \{t \rightarrow 0\} \right) = \varepsilon, C \right]$$

{{C→1}}

Point of a jump

$$\text{Solve}[-1 + C(-1 + t)\varepsilon = 0, t] / \cdot \{C \rightarrow 1\}$$

$$\left\{ \left\{ t \rightarrow -\frac{-1 - \varepsilon}{\varepsilon} \right\} \right\}$$

$$-\frac{-1 - \varepsilon}{\varepsilon} / \cdot \{\varepsilon \rightarrow 0.1\}$$

11.

$$-\frac{-1 - \varepsilon}{\varepsilon} / \cdot \{\varepsilon \rightarrow 0.1\}$$

101.

$$-\frac{-1 - \varepsilon}{\varepsilon} / \cdot \{\varepsilon \rightarrow 0.1\}$$

1001.

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