Journal of Approximation Theory and Applied Mathematics, 2013 Vol. 2

Solving ODEs and DAEs with a Wavelet Collocation Method with Examples from the Chemical Reaction Kinetics

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Abstract

In this paper we apply a Wavelet Collocation Method to solve numerically an ODE and a DAE. This Method can be used in multiple cases, even for boundary value problems, PDEs or IEs. The examples we use belongs to the chemical reaction kinetic and the DAE is a test problem, which could be written as a stiff ODE.

Introduction

In the wavelet theory a scaling function ϕ is used wich belongs to a MSA (multi scale analysis with the following properties:

$$\ldots \subset V_{-1} \subset V_0 \subset V_1 \subset \ldots \subset L^2(R),$$

$\{\phi_{j,k}(t)\}_{k\in Z}$ is an orthonormal basis of V_j.

We use the following Approximation function

$$y_j(t) := \sum_{k=k_{\min}}^{k_{\max}} c_k \cdot \phi_{j,k}(t) \quad \text{, with } \phi \in C^1(R).$$

In the following examples it is shown how to recognize a bad approximation without knowing the exact solution.

We use

$$y_j(t) := \sum_{k=k_{\min}}^{k_{\max}} c_k \phi_{j,k}(t)$$

Since the approximation segment is not alway symmetrical to $t = 0$.

In the following chapters we always determine c by minimizing the function

$$Q(c) = \sum_{i=1}^{m} (y_j'(t_i) - f(y_j(t_i), t_i))^2 + (y_j(t_0) - y_0)^2$$

or

$$(1) \qquad Q(c) = \sum_{i=1}^{m} \left\| y_j'(t_i) - f(y_j(t_i), t_i) \right\|_2^2 + \left\| y_j(t_0) - y_0 \right\|_2^2 .$$

in case of a system. Analogous we can apply this method to DEAs, which shows the second example.

If f is a system, we can use

$$y_j(t) = \left(\sum_{k=k_{\min}}^{k_{\max}} c_{k,1}\phi_{j,k}(t), \sum_{k=k_{\min}}^{k_{\max}} c_{k,2}\phi_{j,k}(t), \ldots, \sum_{k=k_{\min}}^{k_{\max}} c_{k,n_f}\phi_{j,k}(t) \right)^T ,$$

if y consists of n_f components. For the i-th component of y we use y_i, but also $y^{(i)}$ if we want to avoid a confusion with y_j.

The ‘collocation‘ points t_i are defined by $t_i = t_0 + i \cdot h$ with

(2) $$h = \frac{t_{end} - t_0}{m} \text{ and } m \geq |k_{max} - k_{min}| .$$

For test purposes in simulations we chose different m.

Therefore we can compare

$$Q_{\min} = \sum_{i=1}^{m} \left\| y_j'(t_i) - f(y_j(t_i), t_i) \right\|_2^2 + \left\| y_j(t_0) - y_0 \right\|_2^2$$

with

$$Q_a = \sum_{i=1}^{m_a} \left\| y_j'(\tau_i) - f(y_j(\tau_i), \tau_i) \right\|_2^2 + \left\| y_j(t_0) - y_0 \right\|_2^2 \text{ with } \tau_i = t_0 + i \cdot h/a,$$

$m_a = a \cdot m$ provided a is an integer (see examples in the following chapters and [12]). If $Q_a >> Q_{min}$ than m should be increased.

Generally a good starting value for m is $m = |k_{max} - k_{min}|$ provided nothing is known about the solution. This has been shown in numerous simulations. For functions with extreme slopes or curvatures a bigger m is appropriate.

Example 1: System in Chemical Reaction Kinetics

in chemical reaction kinetics the Shell problem is given by the following differential equation system:

$y_1' = -p_1y_1y_2 + p_2y_3 + p_7y_3y_7 + p_9y_6y_7 - p_8y_1y_8 - p_{10}y_1y_9$
$y_2' = -p_1y_1y_2 + p_2y_3 - p_5y_2y_5 + p_6y_6$
$y_3' = p_1y_1y_2 - p_2y_3 - p_3y_3 + p_4y_4y_5 - p_7y_3y_7 + p_8y_1y_8 + p_{11}y_6y_8 - p_{12}y_3y_9$
$y_4' = p_3y_3 - p_4y_4y_5$
$y_5' = p_3y_3 - p_5y_2y_5 - p_4y_4y_5 + p_6y_6$
$y_6' = p_5y_2y_5 - p_6y_6 - p_9y_6y_7 - p_{11}y_6y_8 + p_{10}y_1y_9 + p_{12}y_3y_9$
$y_7' = -p_7y_3y_7 - p_9y_6y_7 + p_8y_1y_8 + p_{12}y_1y_9$
$y_8' = p_7y_3y_7 - p_8y_1y_8 - p_{11}y_6y_8 + p_{12}y_3y_9$
$y_9' = p_9y_6y_7 + p_{11}y_6y_8 - p_{10}y_1y_9 - p_{12}y_3y_9$.

The following results refer to the start vector:

$$y(0) = (0, 3, 0, 0, 0.01, 0, 1, 0, 0)^T .$$

The Shell-Problem originates from the Shell-Laboratories in Amsterdam (see [19]). The following parameter vector is used:

$$p = (0.299, 0.218, 49.5, 0.000363, 0.962, 47.8, 1000, 900, 700, 1260, 7000, 14000)^T$$

Following setup was chosen: $j = 1$, $k_{min} = -5$, $k_{max} = 20$ approximation interval $I = [0, 5]$. Therefore we have (20+5+1)·9 = 234 coefficients! For collocation points we chose

$$t_i = 1/20 \cdot i\text{, } with\ i = 1,\ldots,100$$

whereby m was set to 100.

The iteration (Mathematica function FindMinimum, Version 8) was stopped before the norm of the gradient was smaller than the tolerance ‘AccuracyGoal’ of Mathematica (because the step size was smaller than the tolerance ‘PrecisionGoal’).

The results were

$$Q_{min} \approx 1.50724 \cdot 10^{-9} \text{ and } Q_2 \approx 1.56389 \cdot 10^{-9}.$$

The largest deviation was at t_0. Without the term $\left\| y_j(t_0) - y_0 \right\|_2^2$ in Q there would be:

$$Q_{min} \approx 4.80455 \cdot 10^{-12} \quad \text{and} \quad Q_2 \approx 6.14072 \cdot 10^{-11}.$$

Here the biggest deviation is at $y^{(6)}$:

i	$\lvert y_j^{(i)}(t_0) - y^{(i)}(t_0)\rvert$
1	2.29951×10^{-9}
2	5.11224×10^{-10}
3	2.49557×10^{-8}
4	5.04493×10^{-15}
5	1.52255×10^{-7}
6	0.0000387611
7	1.41979×10^{-9}
8	1.41324×10^{-8}
9	2.25085×10^{-9}

Table 1: $\lvert y_j^{(i)}(t_0) - y^{(i)}(t_0)\rvert$

The following graph of $y_j^{(6)} - y^{(6)}$ in a small section at the beginning of the approximation area (y was numerically calculated using the Mathematica function NDSolve). There it can be seen that the deviation is relatively large in the beginning.

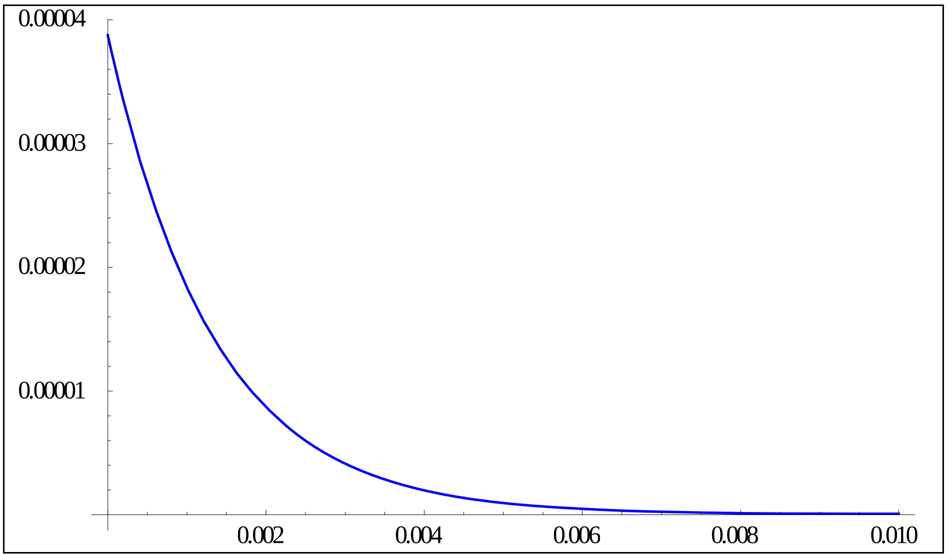

Figure 1. Graph of $y_j^{(6)} - y^{(6)}$

Up next is the graph of d with $d(t) = \|y_j'(t) - f(y_j(t),t)\|_2^2$:

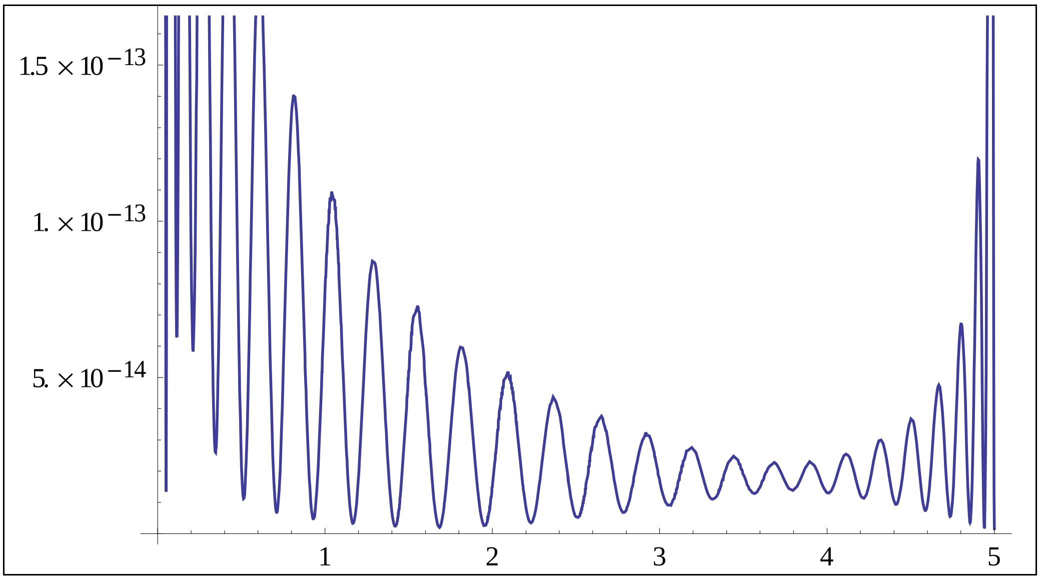

Figure 2. Graph of d

Up next the graphs of $y_j^{(i)} - y^{(i)}$:

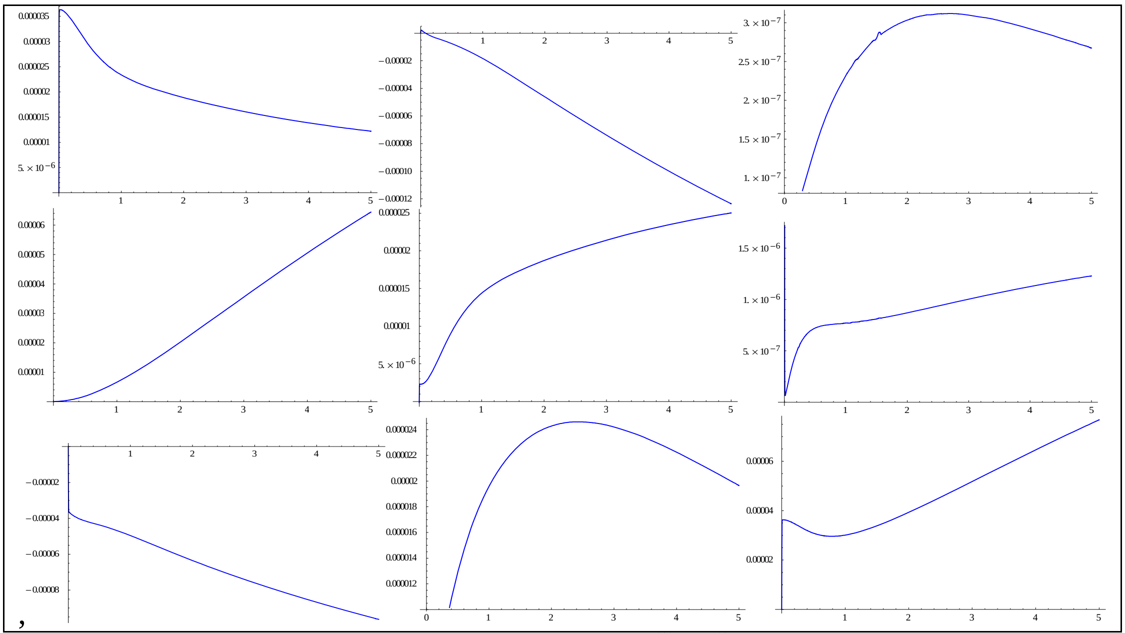

Figure 3. Graphs of $y_j^{(i))} - y^{(i)}$

And finally the graphs of $y_j^{(i)}$ and $y^{(i)}$ (graphically there can no difference be seen):

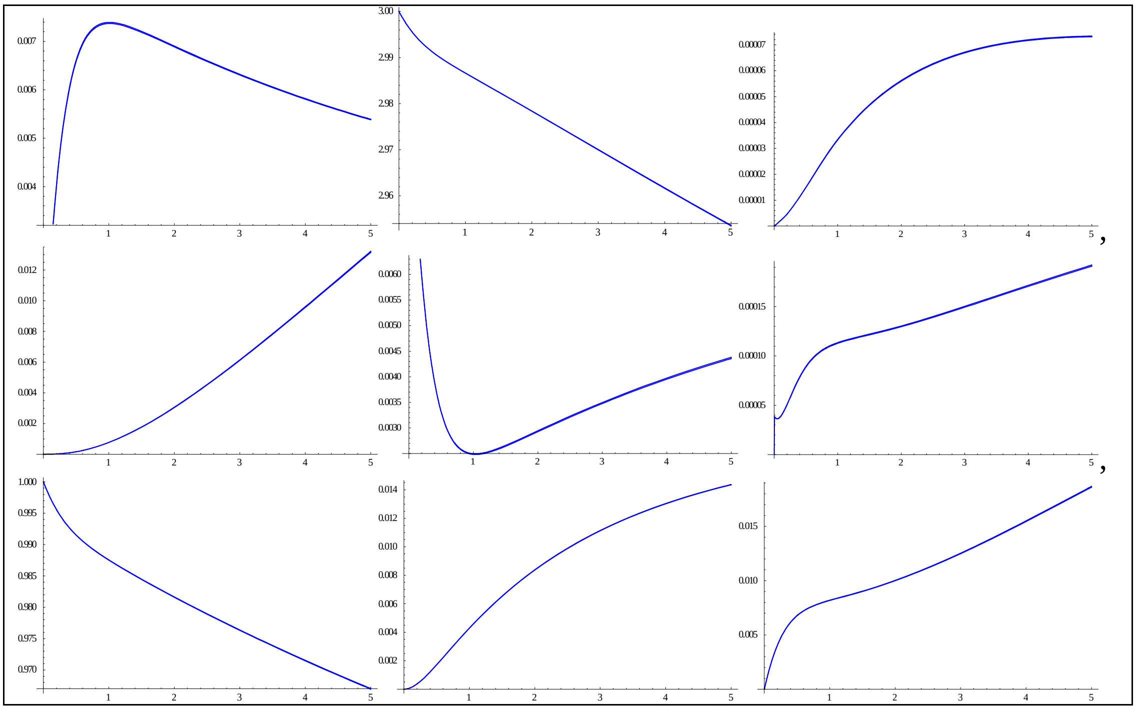

Figure 4. Graphs of $y_j^{(6)} - y^{(6)}$

Example 2: Differential Algebraic Equation (DAE)

The next example is a differential algebraic equation (DAE) which can be written as a differential equation. This equation is also used later used in parameter identification (see chapter 7.2, example from H.H. Robertson)

From that follows the following system of differential equations

$y_1' = -p_1 y_1 + p_3 y_2 y_3$
$y_2' = p_1 y_1 - p_3 y_2 y_3 - p_2 y_2^2$
$1 = y_1 + y_2 + y_3$

with $p = (0.04, 3\cdot 10^7, 10^4)^T$. The starting vector was set to $y(0) = (1, 0, 0)^T$.

The following function is going to be minimized:

$$Q(c) = \sum_{i=1}^{m} \left\| F(y_j'(t_i), y_j(t_i), t_i) \right\|_2^2 + \left\| y_j(t_0) - y_0 \right\|_2^2 .$$

At it $F(y'', y', t_i) = (y_1' + p_1 y_1 - p_3 y_2 y_3, y_2' - p_1 y_1 + p_3 y_2 y_3 + p_2 y_2^2, 1 - y_1 - y_2 - y_3)^T$.

Here it is shown that the method of approximation using wavelet bases can generally be applied to differential algebraic equations or boundary value problems.

In this problem y_2 has an extreme curvature in the beginning (that can be seen in the following graph at [0, 0.1]).

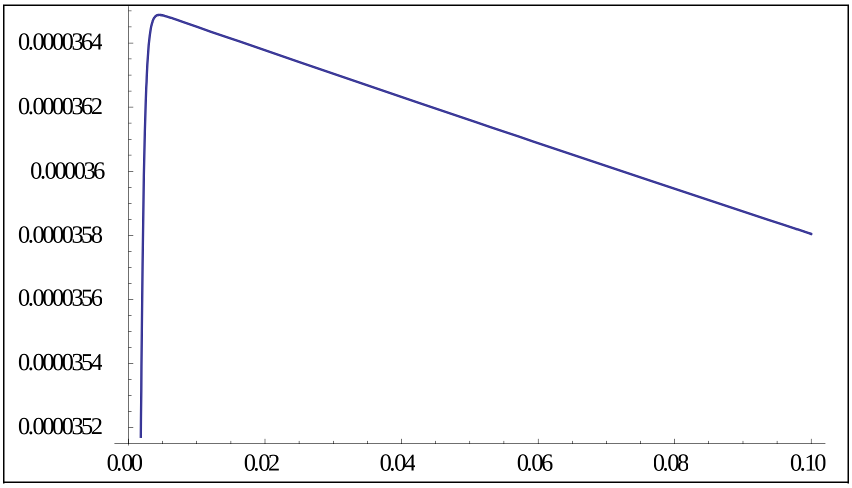

Figure 5. Graph of *y*

Following setup was chosen: $j = 1$, $k_{min} = -5$, k_{max} = approximation interval $I = [0, 5]$.

The iteration (Mathematica funktion FindMinimum, Version 8) was stopped before the norm of the gradient was smaller than the tolerance ‘AccuracyGoal’ of Mathematica (because the step size was smaller than the tolerance ‘PrecisionGoal’).

The results were

$$\mathrm{Q}_{\mathrm{min}} \approx 1.33891 \cdot 10^{-9} \text{ and } \mathrm{Q}_2 \approx 1.46643 \cdot 10^{-9}.$$

The largest deviation was at t_0. Without the term $\left\| y_j(t_0) - y_0 \right\|_2^2$ in Q there would be:

$$Q_{min} \approx 5.42071 \cdot 10^{-12} \text{ and } Q_2 \approx 1.32919 \cdot 10^{-10}.$$

Up next is the graph of d with $d(t) = \|F(y_j'(t),(y_j(t),t)\|_2^2$:

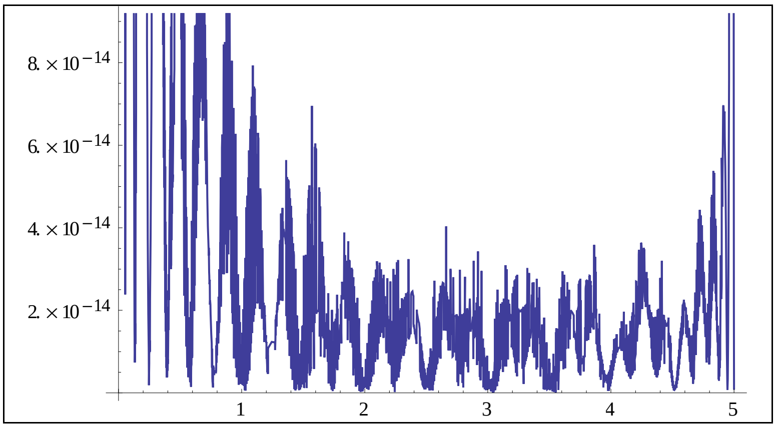

Figure 6. Graph of d

Below is the graph of $y_j^{(i)} - y^{(i)}$ (y was numerically calculated using the Mathematica function NDSolve).

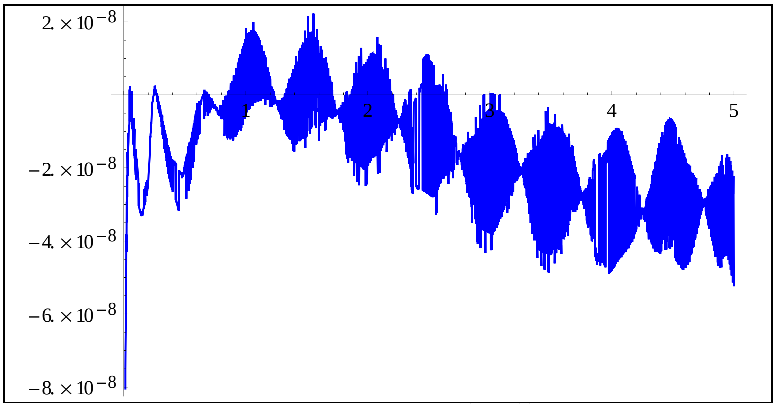

Figure 7. Graph of $y_j^{(1)} - y^{(1)}$

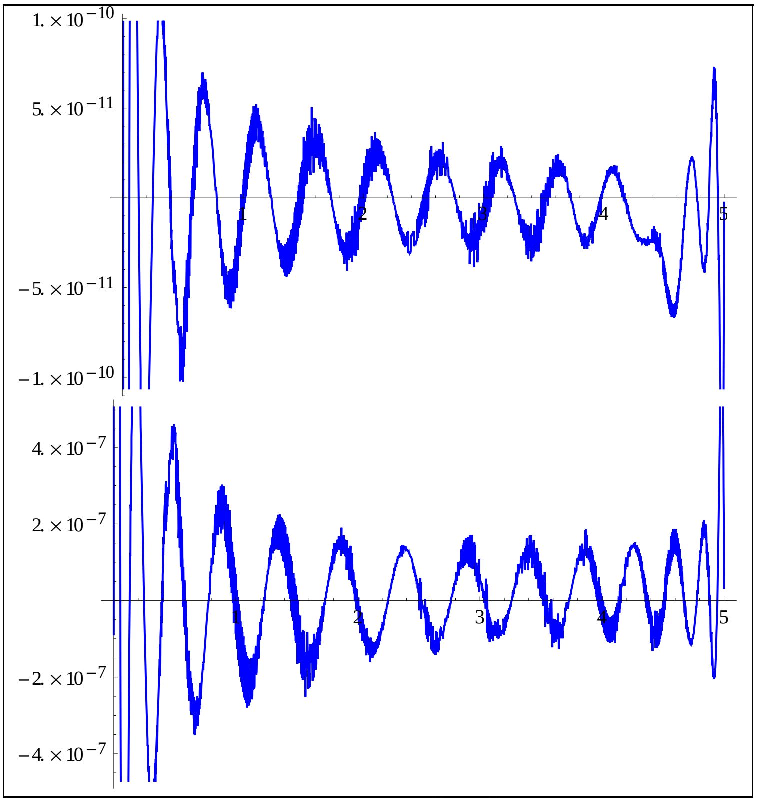

Figure 7. Graphs of $y_j^{(i)} - y^{(i)}$ *for* $i = 2,3$

And finally the graphs of $y_j^{(i)}$ and $y^{(i)}$ (graphically there can no difference be seen):

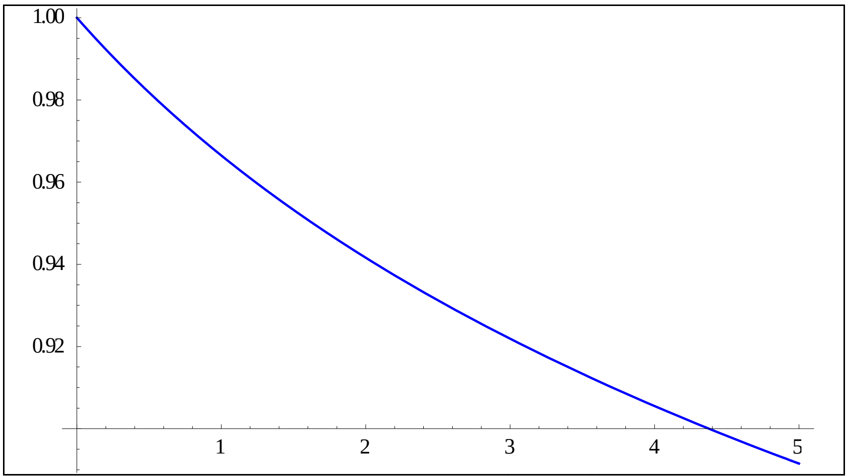

Figure 8. Graphs of $y_j^{(1)}$ and $y^{(1)}$

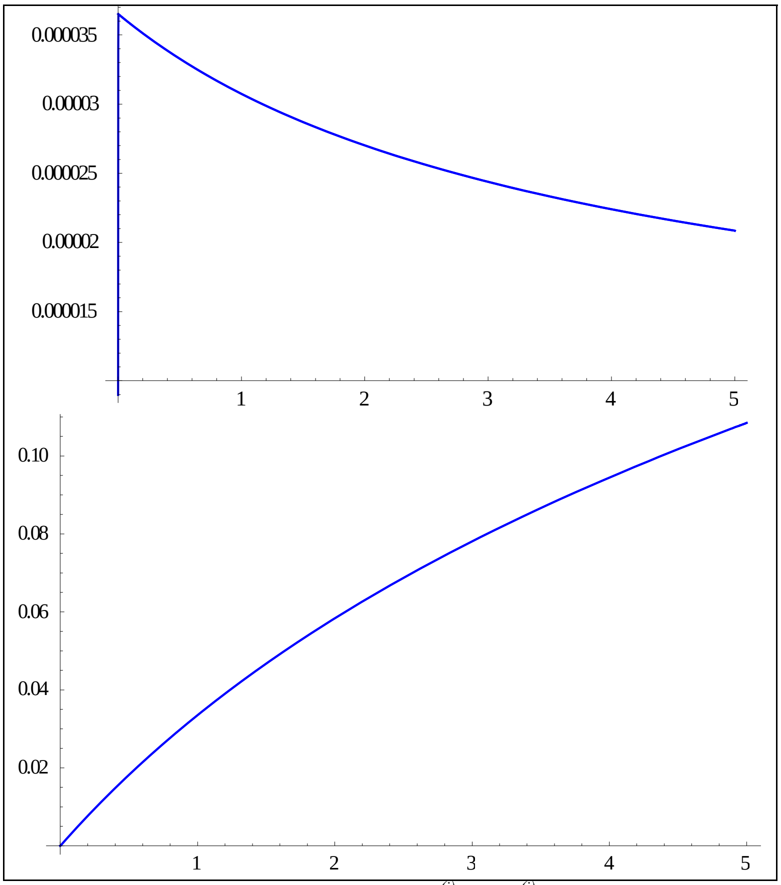

Figure 9**.** Graphs of $y_j^{(i)}$ and $y^{(i)}$ *for* $i = 2,3$

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