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A Unified Approach for the Order Verification of Numerical Methods

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Abstract

In this paper, we will present a unified numerical technique for the order verification of the error in numerical methods. Four examples are presented to illustrate the approach which include the order verification of the errors in Taylor polynomial approximation, the 5-point forward numerical differentiation formula, the composite Simpson method, and the 4-stage explicit Runge-Kutta method. The approach is very convenient for teaching the order of various numerical methods at the undergraduate level and is suitable for utilizing technology as a tool.

Keywords: Numerical methods, order verification, asymptotic expansion, perturbation solution.

1 Introduction

Taylor polynomial approximation and numerical methods are core topics in the undergraduate Mathematics curriculum. Verifying the order of the approximation's error of such problems plays a central role in the teaching of such methods.

Recently, the order verification of solutions to differential equations has been investigated in a number of papers. Khuri and Xie [5] used a numerical method to verify the order of the asymptotic expansion of Duffing's equation. Deeba and Xie [4] utilized an analogous technique for the verification of order of the asymptotic expansion of Van der Pol's equation. Khuri [6] examined the numerical order verification of the asymptotic expansion of a nonlinear differential equation arising in general relativity.

In this paper, a unified numerical technique will be discussed for finding and verifying the order of accuracy of a given numerical method. The technique that we will introduce is general and unified and thus enjoys wide applicability in numerical methods. The unified technique can be implemented as long as the exact, asymptotic [7], perturbation [1, 2, 8], and/or the numerical solution [3] is also available.

The unified order verification approach is first introduced and then tested on a number of numerical methods. The examples discussed, include the order verification of the following numerical methods:

1. *Taylor Polynomial Approximation*

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We will consider the Taylor polynomial $P_n(x)$ of degree n that approximates a given function $f(x)$ at $x = x_0 + h$.

$$f(x) \approx P_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}\,(x - x_0)^k \tag{1.1}$$

2. Numerical Differentiation

We will consider the following 5-point forward formula that estimates the first derivative of a given function $f(x)$ at the point $x = x_0$.

$$\begin{aligned} f'(x_0) \;\approx\; & \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + \right. \\ & \left. 16f(x_0+3h) - 3f(x_0+4h)\right] \end{aligned} \tag{1.2}$$

3. Numerical Integration

In a third example, we will discuss the order of the error in the composite Simpson method which approximates the definite integral from $x = a$ to $x = b$ of a given function $f(x)$. It is given by the formula:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4\sum_{n=1}^{N/2} f(x_{2n-1}) + 2\sum_{n=1}^{N/2\,-1} f(x_{2n}) + f(x_N)\right] \tag{1.3}$$

where $x_i = a + ih$ for $i = 0, 1, 2, ...N$ and $h = \dfrac{b-a}{N}$.

4. Numerical solution of the initial-value problem:

$$y' = f(x, y), \quad y(x_0) = y_0$$

Finally, we will verify the order of the error in the most common 4-stage explicit Runge-Kutta method given by:

$$y_{n+1} = y_n + \frac{h}{6}\,(k_1 + 2k_2 + 2k_3 + k_4) \tag{1.4}$$

$$\begin{aligned} k_1 &= f(x_n,\ y_n) & k_2 &= f\left(x_n + \frac{h}{2},\ y_n + \frac{1}{2}hk_1\right) \\ k_3 &= f\left(x_n + \frac{h}{2},\ y_n + \frac{1}{2}hk_2\right) & k_4 &= f\left(x_n + h,\ y_n + hk_3\right) \end{aligned} \tag{1.5}$$

to approximate the solution $y(x)$ of the initial-value problem at $x_0 + h$, the end of one step of length h.

Verifying the order of the errors in numerical methods, particularly Taylor polynomial approximation, is usually difficult for students to understand and thus does not receive much focus or interest in the undergraduate curriculum. In this paper we present a unified simple approach for verifying the order which is very convenient for students to apply and comprehend. Most of the symbolic and numerical computations have been performed using the computer algebra system - Maple. In fact, any software which keeps track of enough significant digits can be utilized.

The balance of this paper is organized as follows. In Section 2, the unified numerical technique for the order verification of the error in Taylor polynomial approximation and other more general numerical methods is described. In section 3 the technique is implemented for several numerical examples. In section 4 we give an error analysis and the Maple code for the order verification of Taylor approximation. In section 5 we give a conclusion that briefly summarizes the paper's content.

2 Order Verification Approach

In this section, the unified verification of order approach is described. We assume that the numerical, perturbation, asymptotic expansion, or analytical solution exists for a given problem.

First, we will introduce the method and implement it to verify the order of the error in Taylor's polynomial approximation. Then, in the second subsection, we will show how the method can be applied for other numerical methods.

2.1 Order verification for Taylor polynomial approximation

Let f be a function such that f and its first n derivatives are continuous on the closed interval I and let $f^{(n+1)}(x)$ exist on the interior of I. Then for x_0 and x in I we have

$$f(x) = P_n(x) + R_n(x)$$

where $P_n(x)$ is the nth degree Taylor Polynomial centered at x_0 given by

$$P_n(x) = f(x_0) + \frac{f'(x_0)}{1!}\,(x - x_0) + \frac{f''(x_0)}{2!}\,(x - x_0)^2 + ... + \frac{f^{(n)}(x_0)}{n!}\,(x - x_0)^n \tag{2.6}$$

and R_n is a remainder term that depends on x, denoting the difference between the Taylor polynomial of degree n and the original function $f(x)$.

If both x_0 and $x = x_0 + h$ lie in I, then we have the following Taylor expansion about x_0:

$$f(x_0 + h) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}\,h^k + R_n(h) \tag{2.7}$$

The remainder term $R_n(h)$ can be estimated by Mh^{n+1} for sufficiently small h, as expressed in the relationship:

$$R_n(h) = \frac{f^{(n+1)}(x_0^*)}{(n+1)!}\,h^{n+1} \approx Mh^{n+1}, \qquad x_0 \le x_0^* \le x_0 + h$$

for sufficiently small h. Hence the remainder $R_n(h)$ will be replaced by $E_n(h) = Mh^{n+1}$, where M is a constant.

To verify the order of the error in Taylor's polynomial approximation about x_0 we proceed as follows:

$$f(x_0 + h) = P_n(x_0 + h) + Kh^{n+1} \tag{2.8}$$

or equivalently

$$|E_n(h)| = |f(x_0 + h) - P_n(x_0 + h)| = |K||h|^{n+1} \tag{2.9}$$

Taking the logarithm for both sides yields

$$\log |E_n(h)| = \log |K| + (n + 1) \log |h| \tag{2.10}$$

Next, we graph $\log |E_n(h)|$ versus $\log |h|$ for several different values of h. These points should approximately lie on a straight line. Using linear least-square approximation we can determine the best fitted line $y = ax + b$ for the points $\{(\log |h|,\ \log |E_n(h)|)\}$. We can then obtain the order of the error in the approximation which is the slope of the line, that is, $a = n + 1$. It is worth pointing out that the y-intercept equals $b = \log K$, where K is the absolute value of the error constant.

2.2 Order verification for general numerical method

For a more general numerical method, let $A(h)$ denote an approximation obtained by using a specified numerical method with a specified step size h. If $T(h)$ is the corresponding true value of the given step size h, then the error $E(h) \equiv |A(h) - T(h)|$ can be estimated by

$$E(h) = K|h|^M, \tag{2.11}$$

where M is the order of the error in the numerical method and K is the absolute value of the error constant. To find the order M we follow the same scheme used for polynomial approximation by taking the logarithm of both sides of equation (2.11). We obtain

$$\log [E(h)] = \log K + M \log |h| \tag{2.12}$$

We note from equation (2.12) that the value of $\log E(h)$ as a function of $\log |h|$ is linear with slope M and y-intercept equals to $\log K$. Thus, in order to verify the order of the error in the numerical method, we graph $\log E(h)$ versus $\log |h|$ for several different values of $|h|$; the points $\{(\log |h|,\ \log |E(h)|)\}$ should approximately lie on a straight line. Using linear least-square approximation, we obtain the best fitted line $y = ax + b$ for these points. Then, we obtain the order of the error which is the slope of the line, namely, $M = a$. Note that the absolute value of the error constant is equal to $K = e^b$.

3 Examples

In this section, we will give four examples to illustrate the technique described in the previous section. In the first example, the order verification of the error in Taylor polynomial is verified by considering three different cases of polynomial approximations: two Maclaurin polynomials and one Taylor about $x_0 = 1$. In the last three examples, the order of the errors are verified for numerical methods in differentiation, integration, and solution of initial-value problems, respectively. The order of the error of each method is verified by manipulating the unified technique described in the previous section.

Example 1. (Order verification of Taylor polynomial)

(i) Consider the Taylor polynomial:

$$A(h) = h - \frac{1}{6}h^3 + \frac{1}{120}h^5 \tag{3.13}$$

that approximates the function $f(x) = \sin x$ near the point $x_0 = 0$.

In order to verify the order of the Taylor polynomial given in (3.13), let $T(h) = f(h) = \sin h$ and then we use 15 significant digits to calculate the set of points $\{(\log(h_i), \log|E(h_i)|)\}_{i=1}^{10}$, where

$$h_i = 0.02i \qquad \text{for} \qquad i = 1, 2, 3, ..., 10.$$

Figure 1. shows a graph of these points and the best fitted line for the specified points is determined to be

$$y = -8.5262206593 + 6.9996607358\ x \tag{3.14}$$

We conclude from the equation (3.14) of the best fitted line that the order M of the error in the Taylor polynomial is equal to the slope of the line, that is, $M = 7$. Further the error constant is given by

$$K = e^{-8.5262206593} \approx 1.982 \times 10^{-4}$$

which agrees with the actual error constant $\dfrac{f^{(7)}(x_0^*)}{7!} \approx \dfrac{1}{7!} = 1.984 \times 10^{-4}$.

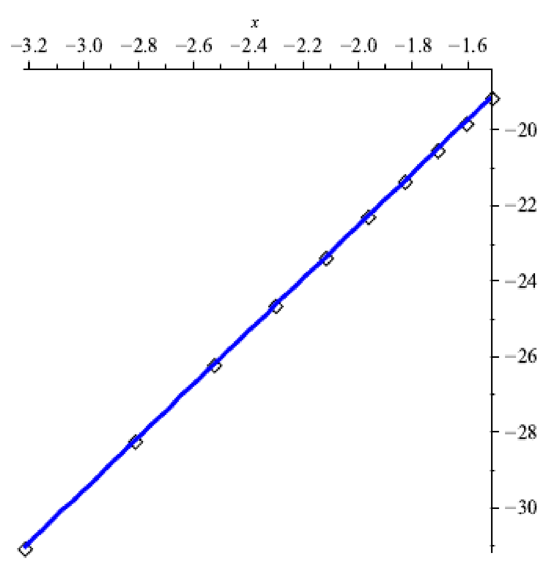

Figure 1. Fitted line for order verification of Taylor polynomial (3.13).

(ii) Consider the Taylor polynomial:

$$A(h) = h^2 - \frac{1}{6}h^6 + \frac{1}{120}h^{10} - \frac{1}{5040}h^{14} \tag{3.15}$$

that approximates the function $f(x) = \sin(x^2)$ near the point $x_0 = 0$.

Let $T(h) = \sin(h^2)$, then following the same steps as in part (i) and using 35 significant digits yields the following best fitted line:

$$y = -12.8018644234 + 17.9999861866\, x \tag{3.16}$$

From the equation (3.16), we conclude that the order M of the error in the Taylor polynomial is equal to approximately $M = 18$. The error constant is given by

$$K = e^{-12.8018644234} \approx 2.7556 \times 10^{-6},$$

which agrees with the actual error constant $\dfrac{f^{(18)}(x_0^*)}{18!} \approx \dfrac{1}{362880} = 2.7557 \times 10^{-6}$. For the choice of $h_i = 0.02i,\ i = 1, 2, ..., 10$ and 15 significant digits, Maple fails to obtain the best fitted line. The effect of the choice of stepsize h and the number of significant digits will be discussed in Section 4.

(iii) Consider the Taylor polynomial:

$$A(h) = e\left[1 + \frac{1}{2}h + \frac{1}{48}h^3 - \frac{5}{384}h^4\right] \tag{3.17}$$

that approximates the function $f(x) = e^{\sqrt{x}}$ near the point $x_0 = 1$.

Let $T(h) = f(x_0 + h) = f(1 + h) = e^{\sqrt{1+h}}$. Following the same steps as in part (i) using 15 significant digits, the best fitted line for the specified points will be

$$y = -3.9319940563 + 4.9224946719\, x \tag{3.18}$$

Hence we conclude that the order of the error in the Taylor polynomial (3.17) is approximately $M = 5$. The error constant is

$$K = e^{-3.9319940563} \approx 1.96045 \times 10^{-2}.$$

Example 2. (Order verification of a numerical differentiation formula)

Consider the 5-point forward differentiation formula:

$$A(h) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)\right] \tag{3.19}$$

that approximates $f'(x)$ at the point $x_0 = 1$, where $f(x) = e^x$. To verify the order of the error in the formula (3.19), let $T(h) = f'(h) = e^h$ and we use 15 significant digits to calculate the set of points $\{(\log(h_i), \log|E(h_i)|)\}_{i=1}^{10}$, where

$$h_i = 0.01\, i \qquad \text{for} \qquad i = 1, 2, 3, ..., 10.$$

Figure 2. shows the plot of the points $\{(\log(h_i),\ \log|E(h_i)|)\}_{i=1}^{10}$ and the best fitted line for these points which is

$$y = -0.2265056964 + 4.0951612247\, x \tag{3.20}$$

From the equation (3.20) representing the best fitted line, we observe that the order of the error in the 5-point forward differentiation formula is given by the slope of the line. More specifically, the order of the error is $M = 4$ and the error constant

$$K = e^{-0.2265056964} \approx 0.79732.$$

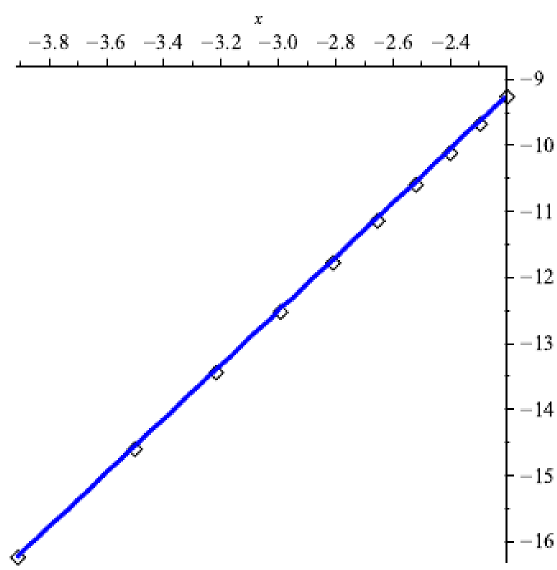

Figure 2. Fitted line for order verification of the 5-point numerical differentiation.

Example 3. (Order verification of a numerical integration formula)

Consider the composite Simpson's formula:

$$A(h) = \frac{h}{3}\left[f(x_0) + 4\sum_{n=1}^{N/2} f(x_{2n-1}) + 2\sum_{n=1}^{N/2-1} f(x_{2n}) + f(x_N)\right] \tag{3.21}$$

that approximates the integral $T(h) = \displaystyle\int_0^1 f(x)\,dx$ where

$$f(x) = e^{x^2}, \quad x_i = ih, \quad i = 0, 1, 2, ..., N \quad \text{and} \quad h = \frac{1}{N}.$$

The order of the error in the formula (3.21) can be determined by using 15 significant digits to calculate the set of points $\{(\log(h_i), \log|E(h_i)|)\}_{i=1}^{10}$, where

$$h_i = \frac{1}{8+2i} \qquad \text{for} \qquad i = 1, 2, 3, ..., 10$$

and

$$E(h) = |A(h) - T(h)|.$$

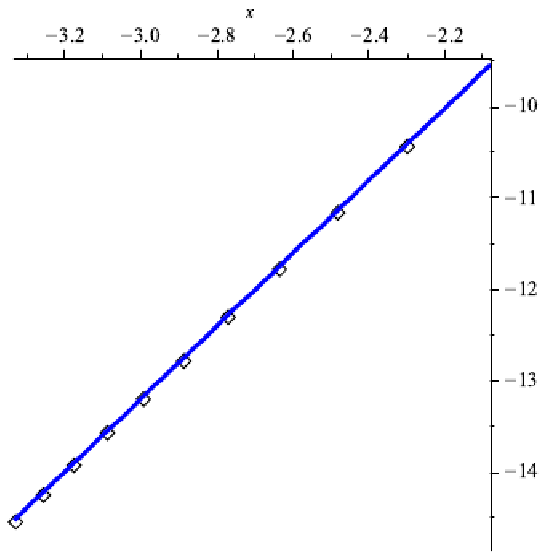

Figure 3. Fitted line for order verification of the composite Simpson's rule.

The best fitted line for the set of points, which is shown in Figure 3, is given by:

$$y = -1.2439014509 + 3.9863619506\, x \tag{3.22}$$

Clearly, the best fitted line equation (3.22) shows that the error in the composite Simpson's rule is of order $M = 4$ and the error constant is

$$K = 10^{-1.2439014509} \approx 0.288254.$$

Example 4. (Order verification of a numerical method for solving an initial-value problem)

Consider the 4-stage explicit Runge-Kutta method:

$$A(h) = y_0 + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{3.23}$$

where

$$\begin{aligned} k_1 &= f(x_0, y_0), & k_2 &= f\left(x_0 + \frac{h}{2}, y_0 + \frac{1}{2}hk_1\right), \\ k_3 &= f\left(x_0 + \frac{h}{2}, y_0 + \frac{1}{2}hk_2\right), & k_4 &= f\left(x_0 + h, y_0 + hk_3\right), \end{aligned} \tag{3.24}$$

that estimates the value $T(h) = y(h) = e^h$ of the solution of the initial-value problem

$$y' = y, \qquad y(0) = 1. \tag{3.25}$$

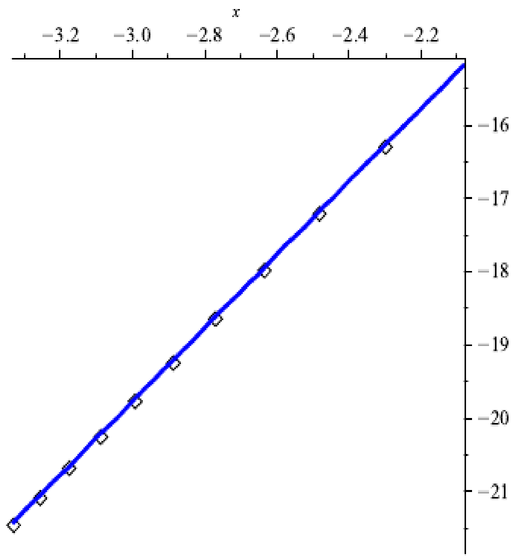

Figure 4. Fitted line for order verification of the 4-stage explicit R-K method.

The order of the error in the formula (3.23) can be confirmed by using 15 significant digits to calculate the set of points $\{(\log(h_i), \log|E(h_i)|)\}_{i=1}^{10}$, where

$$h_i = \frac{1}{8+2i} \qquad \text{for} \qquad i = 1, 2, 3, ..., 10$$

and

$$E(h) = |A(h) - T(h)| \, .$$

The best fitted line for the set of points, which is shown in Figure 4, is found to be:

$$y = -4.7490897218 + 5.0098653465\, x \tag{3.26}$$

From the latter linear equation it is obvious that the 4-stage explicit Runge-Kutta method has local truncation error $E(h) = Kh^5$. Since the method has order p if its local truncation error has order $p+1$, hence we conclude that the method has order 4. Further, the error constant equals to

$$K = e^{-4.7490897218} \approx 8.6595 \times 10^{-3}.$$

4 Error Analysis and Maple code

In this section, example $1(iii)$ is chosen to explore the unified order verification approach. More specifically, we will investigate the effect of the number of points and the significant digits on the accuracy of the estimated orders and error constants. The approach will be applied for different choices of the number of significant digits, points, and bounds for the stepsize. We have used the following Maple code for the Taylor approximation $A(h) \approx e^{\sqrt{x}}$ (where n is the number of points used, a is the step increment, and $Digits$ is the number of significant digits):

D	min h	n	max h	$y = \log K + Mx$
10	0.02	10	0.20	$-4.246 + 4.749x$
15	0.02	10	0.20	$-3.932 + 4.922x$
20	0.02	10	0.20	$-3.932 + 4.922x$
10	0.02	15	0.30	$-4.160 + 4.787x$
15	0.02	15	0.30	$-3.977 + 4.904x$
20	0.02	15	0.30	$-3.978 + 4.904x$
10	0.01	10	0.10	$-6.794 + 3.751x$
15	0.01	10	0.10	$-3.835 + 4.959x$
20	0.01	10	0.10	$-3.835 + 4.959x$
10	0.01	15	0.15	$-5.755 + 4.085x$
20	0.01	15	0.15	$-3.868 + 4.949x$

Table 1: Fitted lines for the Taylor polynomial (3.17).

$n := 10;\ \ min := 0.02;\ \ a := 0.02;$
$Digits := 10;$
$f := x -> \ exp(sqrt(x));$
$x[0] := 1;$
$T_v := h_v -> \ f(x[0] + h_v);$
$M_v := h_v -> \ e + \frac{e}{2}h_v + \frac{e}{48}h_v^3 + \frac{5e}{384}h_v^4;$
$for\ k\ from\ 1\ to\ n + 1\ do$
$h := min + a * k;$
$T[k] := T_v(h);$
$A[k] := evalf(M_v(h));$
$E[k] := evalf(abs|T[k] - A[k]|);$
$x[k] := log(h);$
$y[k] := log(E[k]);$
$end\ do$

Then, we have applied Maple's *stats[fit, leastsquare]* syntax (Version 11), that is found in the *stats* library, to find the best fitted line for the sequence of points $\{(x[i],\ y[i])\}_{i=1}^{n}$. The following table contains the fitted lines for different values of the number of points n. From Table 1 we observe that when the number of points is increased, the estimated orders are improved only when the significant digits are also increased. A similar argument is applied when the stepsize h is decreased. Hence, it is recommended to use a number of points that gives a reasonable stepsize h (10 to 15 points with $0.01 \leq h \leq 0.20$ and at least 15 significant digits). On the other hand, using higher significant digits will keep or improve the accuracy. The actual value for the error order is $M = 5$ and for the error constant is $K = \frac{f^{(5)}(c)}{5!}$, where $x_0 < c < x_0 + h$. Since $x_0 = 1$ and the average value of $h \approx 0.1$, we may consider $-4.106 \leq \log K \leq -3.670$. Similar recommendations also holds for other numerical methods.

5 Conclusion

In this paper, we have presented a general approach for the order verification of the errors in Taylor polynomial approximations as well as other more general numerical methods. The technique was tested by verifying the error for several familiar numerical methods that normally arise in the undergraduate curriculum. Four examples were selected and presented to illustrate the approach including Taylor polynomial approximation, the 5-point forward numerical differentiation formula, the composite Simpson's rule and the 4-stage explicit Runge-Kutta method. Other numerical methods such as Newton's method for solving equations and Gaussian integration can also be considered.

The unified approach was explored using one of the examples to investigate the effect of the number of points and significant digits on the accuracy of the estimated orders and error constants. Suggestions for the choice of such numbers as well as reasonable stepsize h were given.

Understanding and verifying the error of Taylor approximations as well as numerical methods does not get much attention by students possibly because it is difficult to apprehend or too complicated. The approach offers a simple alternative and unified technique that manipulates technology as a tool. Thus, it is convenient to teach and include this approach in the undergraduate mathematics curriculum.

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