Numerical Analysis Mat 205

1. Errors:

- Absolute and Relative Errors,
- Round – off Errors,
- Truncation Errors,

2. Linear System of Equations:

- Gauss Elimination Method,
- Jacobi's Iteration Method,
- Gauss – Seidel Iteration Method.

3. Nonlinear Equations:

- Bisection Method,
- Newton – Raphson Method,
- Simple Iteration Method.

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4. Finite Differences and Interpolation:

- Finite Difference Operators,
- Difference Tables ,
- Newton's Forward Interpolation Formula ,
- Newton's Backward Interpolation Formula ,
- Lagrange's Interpolation Formula ,
- Newton's Divided Differences Interpolation Formula .

5. Numerical Differentiation:

- Derivatives Based on Newton's Forward Interpolation Formula ,
- Derivatives Based on Newton's Backward Interpolation Formula .

6. Numerical Integration :

- Trapezoidal Rule ,
- Simpson's Rule .

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7. Methods for First Order Ordinary Differential Equations :

- Euler's Method ,
- Modified Euler's Method ,
- Runge – Kutta Method of order Two ,
- Runge – Kutta Method of order Four .

References :

[1] R.L. Burden and J.D. Faires , Numerical Analysis , Ninth Edition , PWS Publishing , Boston , 2011 .

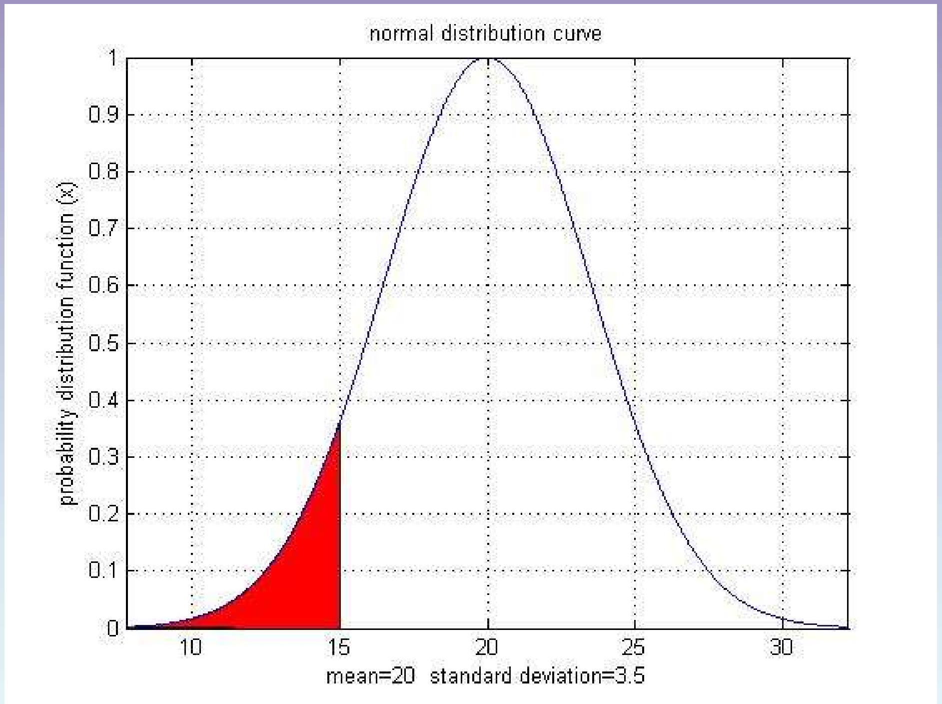
[2] S.C. Chapra and R.P. Canale . Numerical Methods for Engineers , Seventh Edition , McGraw – Hill , New York , 2015 .

[3] W. Gautschi , Numerical Analysis , Second Edition , Springer , New York , 2011 .

Why use Numerical Methods?

- To solve problems that cannot be solved exactly

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} e^{-\frac{u^2}{2}}\,du$$



Why measure errors?

1) To determine the accuracy of numerical results.
2) To develop stopping criteria for iterative algorithms.

Absolute Error

- Defined as the difference between the exact value in a calculation and the approximate value found using a numerical method etc.

Absolute Error = exact value – Approximate Value

Example—Absolute Error

The derivative, $f'(x)$ of a function $f(x)$ can be approximated by the equation,

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

If $f(x) = 7e^{0.5x}$ and $h = 0.3$

a) Find the approximate value of $f'(2)$

b) exact value of $f'(2)$

c) Absolute error for part (a)

Solution:

a) For $x = 2$ and $h = 0.3$

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3} \quad = 10.263$$

Solution (cont.)

b) The exact value of $f'(2)$ can be found by using our knowledge of differential calculus.

$$f(x) = 7e^{0.5x}$$

$$f'(x) = 7 \times 0.5 \times e^{0.5x}$$

$$= 3.5e^{0.5x}$$

So the exact value $f'(2)$ is of

$$f'(2) = 3.5e^{0.5(2)}$$

$$= 9.5140$$

Absolute error is calculated as $E_t =$ exact value – Approximate Value

$$= 9.5140 - 10.263 = -0.722$$

Relative Absolute Error

- Defined as the ratio between the Absolute error, and the exact value.

$$\text{Relative Absolute Error } (\in_t) = \frac{\text{Absolute Error}}{\text{exact Value}}$$

Example—Relative Absolute Error

Following from the previous example for Absolute error, find the relative Absolute error for $f(x) = 7e^{0.5x}$ at $f'(2)$ with $h = 0.3$

From the previous example,

$$E_t = -0.722$$

Relative Absolute Error is defined as

$$\in_t = \frac{\text{True Error}}{\text{True Value}}$$

$$= \frac{-0.722}{9.5140} = -0.075888$$

as a percentage,

$$\in_t = -0.075888 \times 100\% = -7.5888\%$$

Approximate Error

- What can be done if exact values are not known or are very difficult to obtain?
- Approximate error is defined as the difference between the present approximation and the previous approximation.

Approximate Error (E_a) = Present Approximation – Previous Approximation

Example—Approximate Error

For $f(x) = 7e^{0.5x}$ at $x = 2$ find the following,

a) $f'(2)$ using $h = 0.3$

b) $f'(2)$ using $h = 0.15$

c) approximate error for the value of $f'(2)$ for part b)

Solution:

a) For $x = 2$ and $h = 0.3$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

Solution: (cont.)

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3} = 10.263$$

b) For $x = 2$ and $h = 0.15$

$$f^{'}(2) \approx \frac{f(2 + 0.15) - f(2)}{0.15}$$

$$= \frac{f(2.15) - f(2)}{0.15}$$

Solution: (cont.)

$$= \frac{7e^{0.5(2.15)} - 7e^{0.5(2)}}{0.15}$$

$$= \frac{20.50 - 19.028}{0.15} = 9.8800$$

c) So the approximate error, E_a is

$$E_a = \text{Present Approximation} - \text{Previous Approximation}$$

$$= 9.8800 - 10.263$$

$$= -0.38300$$

Relative Approximate Error

- Defined as the ratio between the approximate error and the present approximation.

$$\text{Relative Approximate Error } (\in_a) = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$

Example—Relative Approximate Error

For $f(x) = 7e^{0.5x}$ at $x = 2$, find the relative approximate error using values from $h = 0.3$ and $h = 0.15$

Solution:

From Example 3, the approximate value of $f'(2) = 10.263$ using $h = 0.3$ and $f'(2) = 9.8800$ using $h = 0.15$

$E_a =$ Present Approximation – Previous Approximation

$$= 9.8800 - 10.263$$

$$= -0.38300$$

Solution: (cont.)

$$\in_a = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$

$$= \frac{-0.38300}{9.8800} = -0.038765$$

as a percentage,

$$\in_a = -0.038765 \times 100\,\% = -3.8765\,\%$$

Absolute relative approximate errors may also need to be calculated,

$$\left|\in_a\right| = |-0.038765| = 0.038765 \text{ or } 3.8765\%$$

How is Absolute Relative Error used as a stopping criterion?

If $|\in_a| \leq \in_s$ where $\in_s$ is a pre-specified tolerance, then no further iterations are necessary and the process is stopped.

If at least *m* significant digits are required to be correct in the final answer, then

$$|\in_a| \leq 0.5 \times 10^{2-m}\%$$

Table of Values

For $f(x) = 7e^{0.5x}$ at $x = 2$ with varying step size, h

h	$f'(2)$	$\lvert \in_a \rvert$	m
0.3	10.263	N/A	0
0.15	9.8800	3.877%	1
0.10	9.7558	1.273%	1
0.01	9.5378	2.285%	1
0.001	9.5164	0.2249%	2

Sources of numerical error

1) Round off error

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1) Truncation error

خطأ ناتج عن الاقتطاع

Round off Error

- Caused by representing a number approximately

$$\frac{1}{3} \cong 0.333333$$

$$\sqrt{2} \cong 1.4142...$$

Truncation error

- Error caused by truncating or approximating a mathematical procedure.

Example of Truncation Error

Taking only a few terms of a Maclaurin series to approximate e^x

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots\dots\dots\dots\dots\dots\dots$$

If only 3 terms are used,

$$Truncation\ \ Error = e^x - \left(1 + x + \frac{x^2}{2!}\right)$$

Example 1 —Maclaurin series

Calculate the value of $e^{1.2}$ with an absolute relative approximate error of less than 1%.

$$e^{1.2} = 1 + 1.2 + \frac{1.2^2}{2!} + \frac{1.2^3}{3!} + \dots\dots\dots\dots\dots\dots$$

n	$e^{1.2}$	E_a	$\left\|\in_a\right\|\%$
1	1	—	—
2	2.2	1.2	54.545
3	2.92	0.72	24.658
4	3.208	0.288	8.9776
5	3.2944	0.0864	2.6226
6	3.3151	0.020736	0.62550

6 terms are required.

Another Example of Truncation Error

Since

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \cdots$$

Using a finite *h*= Δx to approximate $f'(x)$

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

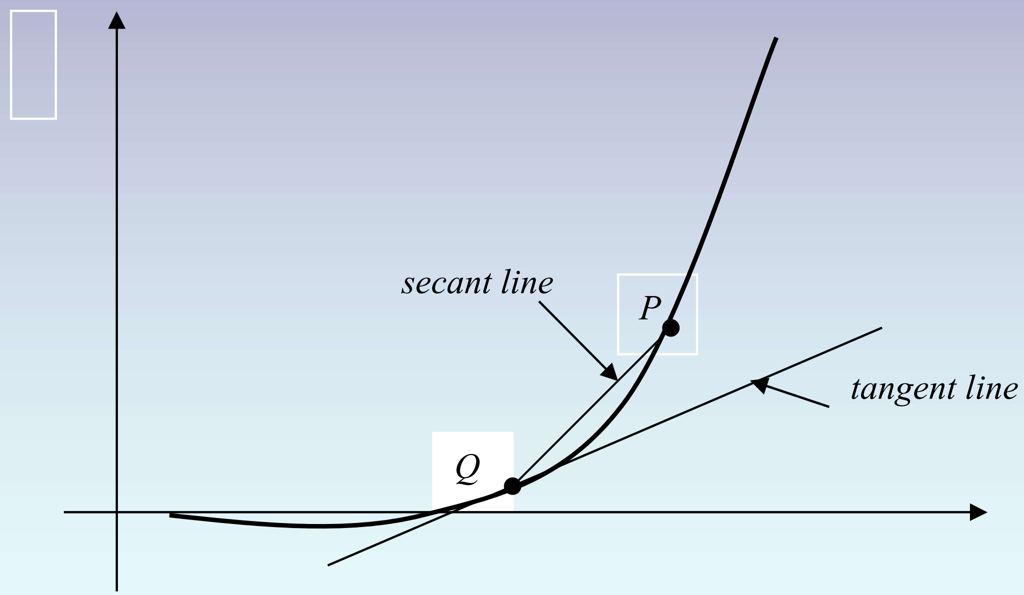


Figure 1. Approximate derivative using finite Δx

Example 2 —Differentiation

Find $f'(3)$ for $f(x) = x^2$ using $f'(x) \approx \dfrac{f(x+\Delta x) - f(x)}{\Delta x}$

and $\Delta x = 0.2$

$$f^{'}(3) = \frac{f(3+0.2) - f(3)}{0.2}$$

$$= \frac{f(3.2) - f(3)}{0.2} = \frac{3.2^2 - 3^2}{0.2} = \frac{10.24 - 9}{0.2} = \frac{1.24}{0.2} = 6.2$$

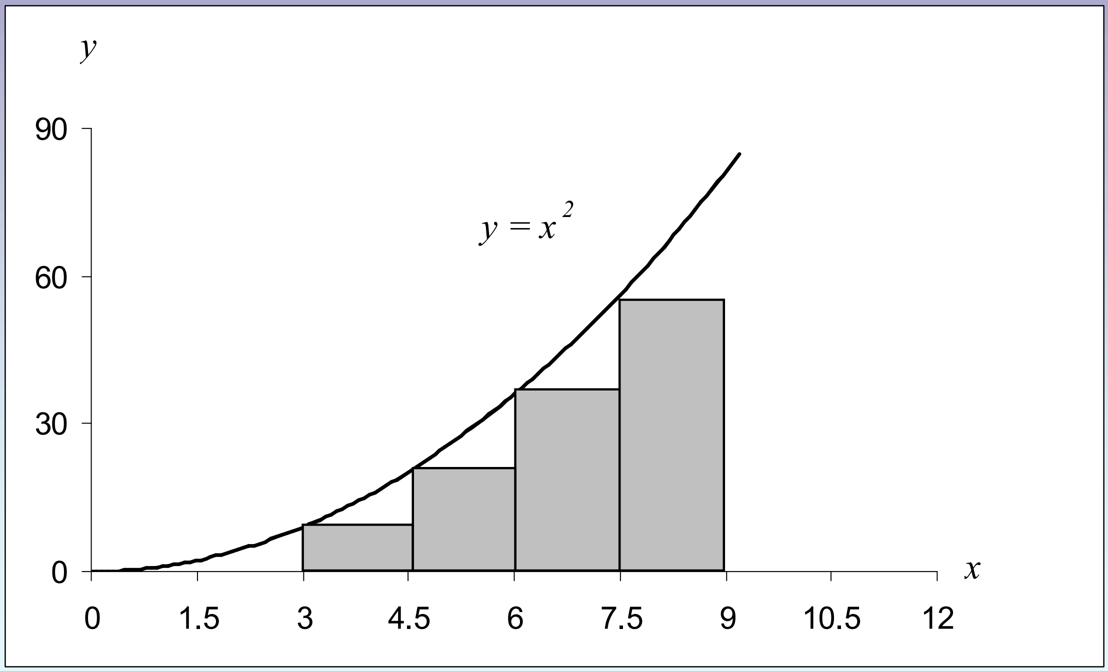
The actual value is

$$f^{'}(x) = 2x, \quad f^{'}(3) = 2 \times 3 = 6$$

Truncation error is then, $6 - 6.2 = -0.2$

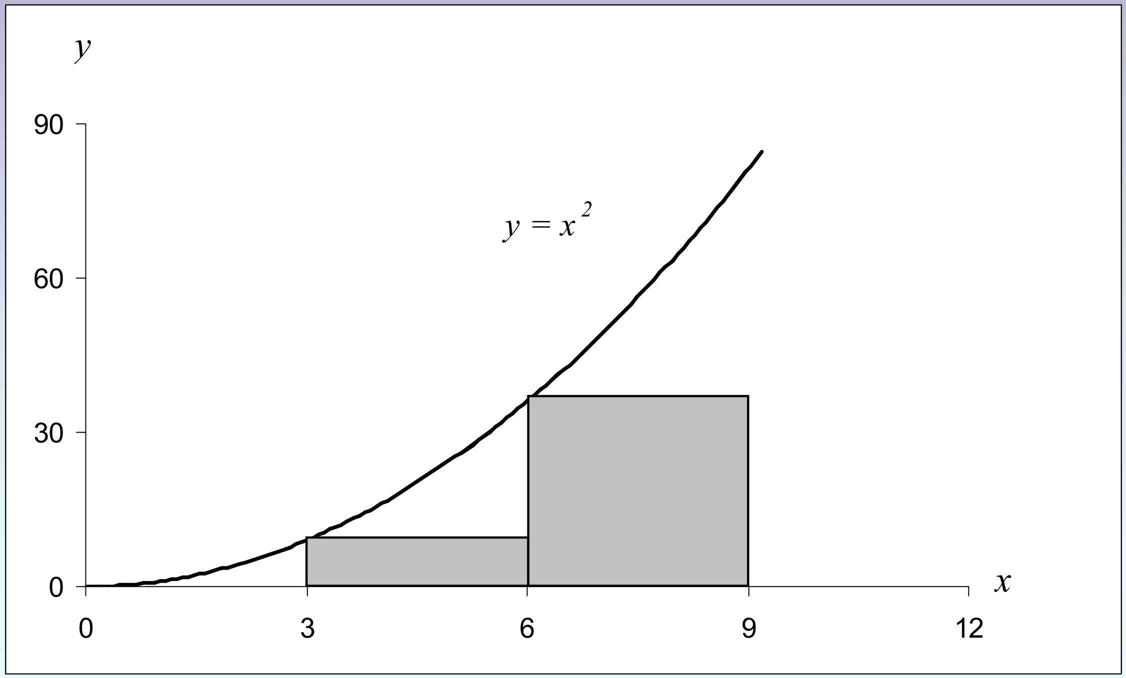
Another Example of Truncation Error

Using finite rectangles to approximate an integral.



Example 3 — Integration

Use two rectangles of equal width to approximate the area under the curve for $f(x) = x^2$ over the interval $[3,9]$



$$\int_3^9 x^2 dx$$

Integration example (cont.)

Choosing a width of 3, we have

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$$\int_3^9 x^2 dx = (x^2)\Big|_{x=3}(6-3) + (x^2)\Big|_{x=6}(9-6)$$

$$= (3^2)3 + (6^2)3$$

$$= 27 + 108 = 135$$

Actual value is given by

$$\int_3^9 x^2 dx = \left[\frac{x^3}{3}\right]_3^9 = \left[\frac{9^3 - 3^3}{3}\right] = 234$$

Truncation error is then

$$234 - 135 = 99$$

Propagation of Errors

In numerical methods, the calculations are not made with exact numbers. How do these inaccuracies propagate تنتشر through the calculations?

Example 1:

Find the bounds for the propagation in adding two numbers. For example if one is calculating $X+Y$ where

$$X = 1.5 \pm 0.05$$
$$Y = 3.4 \pm 0.04$$

Solution

Maximum possible value of $X = 1.55$ and $Y = 3.44$

Maximum possible value of $X + Y = 1.55 + 3.44 = 4.99$

Minimum possible value of $X = 1.45$ and $Y = 3.36$.

Minimum possible value of $X + Y = 1.45 + 3.36 = 4.81$

Hence

$$4.81 \leq X + Y \leq 4.99$$

Propagation of Errors In Formulas

If f is a function of several variables $X_1, X_2, X_3, \ldots\ldots., X_{n-1}, X_n$ then the maximum possible value of the error in f is

$$\Delta f \approx \left|\frac{\partial f}{\partial X_1}\Delta X_1\right| + \left|\frac{\partial f}{\partial X_2}\Delta X_2\right| + \ldots\ldots. + \left|\frac{\partial f}{\partial X_{n-1}}\Delta X_{n-1}\right| + \left|\frac{\partial f}{\partial X_n}\Delta X_n\right|$$

Example 2:

Subtraction of numbers that are nearly equal can create unwanted inaccuracies. Using the formula for error propagation, show that this is true.

Solution

Let

$$z = x - y$$

Then

$$\begin{aligned} |\Delta z| &= \left|\frac{\partial z}{\partial x}\Delta x\right| + \left|\frac{\partial z}{\partial y}\Delta y\right| \\ &= |(1)\Delta x| + |(-1)\Delta y| \\ &= |\Delta x| + |\Delta y| \end{aligned}$$

So the relative change is

$$\left|\frac{\Delta z}{z}\right| = \frac{|\Delta x| + |\Delta y|}{|x - y|}$$

For example if

$$x = 2 \pm 0.001$$
$$y = 2.003 \pm 0.001$$

$$\left|\frac{\Delta z}{z}\right| = \frac{|0.001| + |0.001|}{|2 - 2.003|}$$

$$= 0.6667$$
$$= 66.67\%$$

General Taylor Series

The general form of the Taylor series is given by

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \cdots$$

provided that all derivatives of *f(x)* are continuous and exist in the interval *[x,x+h]*

If we have the value of the function at a single point, and the value of all its derivatives at that single point, then we can get the value of the function at any other point

Example—Taylor Series

Find the value of $f(6)$ given that $f(4) = 125$, $f'(4) = 74$, $f''(4) = 30$, $f'''(4) = 6$ and all other higher order derivatives of $f(x)$ at $x = 4$ are zero.

Solution:

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2!} + f'''(x)\frac{h^3}{3!} + \cdots$$

If $x = 4$ Then $h = 6 - 4 = 2$

Solution: (cont.)

Since the higher order derivatives are zero,

$$f(4+2)=f(4)+f'(4)2+f''(4)\frac{2^2}{2!}+f'''(4)\frac{2^3}{3!}$$

$$f(6)=125+74(2)+30\left(\frac{2^2}{2!}\right)+6\left(\frac{2^3}{3!}\right)$$

$$=125+148+60+8$$

$$=341$$

Note that to find $f(6)$ exactly, we only need the value of the function and all its derivatives at some other point, in this case $x=4$

Special case of Taylor series

The **Maclaurin series** is simply the Taylor series about the point $x=0$

$$f(x+h)=f(x)+f'(x)h+f''(x)\frac{h^2}{2!}+f'''(x)\frac{h^3}{3!}+f''''(x)\frac{h^4}{4}+f'''''(x)\frac{h^5}{5}+\cdots$$

$$f(0+h)=f(0)+f'(0)h+f''(0)\frac{h^2}{2!}+f'''(0)\frac{h^3}{3!}+f''''(0)\frac{h^4}{4}+f'''''(0)\frac{h^5}{5}+\cdots$$

Derivation for Maclaurin Series for e^x

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Since $f(x) = e^x$, $f'(x) = e^x$, $f''(x) = e^x$,..., $f^n(x) = e^x$ and

$$f^n(0) = e^0 = 1$$

the Maclaurin series is then

$$f(h) = (e^0) + (e^0)h + \frac{(e^0)}{2!}h^2 + \frac{(e^0)}{3!}h^3 \ldots$$

$$= 1 + h + \frac{1}{2!}h^2 + \frac{1}{3!}h^3 \ldots$$

So,

$$f(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$$

Error in Taylor Series

The Taylor polynomial of order *n* of a function *f(x)* with *(n+1)* continuous derivatives in the domain [*x,x+h]* is given by

$$f(x+h)=f(x)+f'(x)h+f''(x)\frac{h^2}{2!}+\cdots+f^{(n)}(x)\frac{h^n}{n!}+R_n(x)$$

where the remainder is given by

$$R_n(x)=\frac{(x-h)^{n+1}}{(n+1)!}f^{(n+1)}(c)$$

where $x<c<x+h$

that is, c is some point in the domain [x,x+h]

Example—error in Taylor series

The Taylor series for e^x at point $x = 0$ is given by

$$e^h = 1 + h + \frac{1}{2!}h^2 + \frac{1}{3!}h^3 \ldots$$

It can be seen that as the number of terms used increases, the error bound decreases and hence a better estimate of the function can be found.

How many terms would it require to get an approximation of e^1 (*h=1*) within a magnitude of Absolute error of less than 10^{-6}.

Solution:

Using $(n+1)$ terms of Taylor series gives error bound of

$$R_n(x) = \frac{(x-h)^{n+1}}{(n+1)!} f^{(n+1)}(c) \qquad x = 0, h = 1, f(x) = e^x$$

$$R_n(0) = \frac{(0-1)^{n+1}}{(n+1)!} f^{(n+1)}(c)$$

$$= \frac{(-1)^{n+1}}{(n+1)!} e^c$$

Since

$$x < c < x+h$$
$$0 < c < 0+1$$
$$0 < c < 1$$

$$\frac{1}{(n+1)!} < |R_n(0)| < \frac{e}{(n+1)!}$$

Solution: (cont.)

So if we want to find out how many terms it would require to get an approximation of e^1 within a magnitude of Absolute error of less than 10^{-6}

$$\frac{e}{(n+1)!} < 10^{-6}$$

$$(n+1)! > 10^6 e$$

$$(n+1)! > 10^6 \times 3$$

But 10!=3628800

$$n \geq 9$$

So 9 terms or more are needed to get a Absolute error less than 10^{-6}