

1 - Taylor Series and the Mean Value Theorem of Derivatives

The numerical solution of engineering and scientific problems described by mathematical models often requires solving differential equations. Differential equations arise because they describe rates of change and technical people are interested in change. Often the mathematical models are so complicated that analytical solutions are not possible – at least by the tools commonly instilled in most engineers and scientists – so they must be solved numerically. This requires the approximation of derivatives. It is important to have some idea as to the accuracy of those approximations if the solutions obtained using those approximations are to be employed in designing equipment that may have terrible consequences if it fails.

The Taylor Series can be rearranged to yield approximations of derivatives from adjacent values of a function. The Mean Value Theorem of Derivatives allows one to make judgments about the accuracy of such approximations and how their accuracy may improve by decreasing the distance between adjacent values of the function used for the approximations.

The Taylor Series can also be used to approximate the value of a function at a nearby base value. The Mean Value Theorem of Derivatives is related to the Taylor Series in that the Mean Value Theorem concludes that any Taylor Series approximation may be made perfect by adding the next term left out of the approximation if it is evaluated at some point – unfortunately unknown – between the base value of the function and the value to which it is being extrapolated. However, it is this feature that provides for an approximation of the error in derivatives.

Richardson Extrapolation is the last topic covered in this chapter. It is a method of efficiently extrapolating the value of a function by getting a very accurate estimate of the first derivative. The key word here is *efficiently*. The goal of the science of numerical methods is to maximize accuracy and minimize computational effort. This is because computational effort translates to computer time and time is money.

There are several example MathCad files available. The first one extrapolates the $\ln(1.1)$ to $\ln(1.3)$. The second one finds the *unknown value* described by Mean Value Theorem that would make an estimate using the Taylor Series Approximation exact. Of course, this is only possible if one knows the exact value, which is the case in the example because the function is given.

Lastly, some Microsoft Word files contain inserted MathCad objects (i.e. – pasted in). If the computer you are using has MathCad available to it, double clicking on these objects will activate the object within Microsoft Word. If this is done, the MathCad Object can then be modified as you like and it will recalculate to your specifications. All SDSM&T lab computers have MathCad installed. Since your home computer probably does not have MathCad, these objects cannot be activated by doubling clicking on them. In some cases bit maps of MathCad and other application's output are available on the website. MathCad from MathSoft Inc. is available at greatly discounted rates for students. Please see your instructor if you are interested in this option.

1.1 - Taylor Series Approximation

The Taylor series is used for approximation of a function. If the value of the function is known at c , then the value of the function may be determined at x .

$$f(x) = f(c) + f'(c)(x-c) + \frac{f''(c)(x-c)^2}{2!} + \frac{f'''(c)(x-c)^3}{3!} + \dots \quad (1.1)$$

In general,

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(c)(x-c)^k}{k!} \quad (1.2)$$

If terms are left out of Taylor's Series then the result is an approximation and must be written as such.

$$f(x) \approx f(c) + f'(c)(x-c) + \frac{f''(c)(x-c)^2}{2!} \quad (1.3)$$

Example 1a

Given $\ln(1.1)$, find $\ln(1.3)$ using Taylor Series Approximation.

$$\text{Note } \frac{d \ln(x)}{dx} = \frac{1}{x}, \quad \frac{d^2 \ln(x)}{dx^2} = -\frac{1}{x^2}, \text{ etc.}$$

$$f(x) = \ln(c) + \frac{1}{c}(x-c) - \frac{1}{c^2} \frac{(x-c)^2}{2!} + \frac{1}{c^3} \frac{(x-c)^3}{3!} - \frac{1}{c^4} \frac{(x-c)^4}{4!} + \dots \quad (1.4)$$

$$\ln(1.3) = \ln(1.1) + \frac{1}{1.1}(1.3-1.1) - \frac{1}{1.1^2} \frac{(1.3-1.1)^2}{2} + \frac{2}{1.1^3} \frac{(1.3-1.1)^3}{6} - \dots \quad (1.5)$$

MathCad Computations

$$f(c) := \ln(c)$$

$$fn(x,c,n) := \sum_{k=0}^n \left[\frac{\frac{d^k}{dc^k} f(c) \cdot (x-c)^k}{k!} \right]$$

$$fn(1.3,1.1,4) = 0.26233$$

MatLab Function

```
function f=TaylorSeriesApproxOfLn(x,c,n)
f=log(c)
for i=1:n
    if i==1
        f=f+1/c*(x-c)
    else
        f=f-(-1)^i/c^i*factorial(i-1)*(x-c)^i /factorial(i)
    end
end
```

MatLab Results

```
>> TaylorSeriesApproxOfLn(1.3,1.1,4)

f =
    0.0953
f =
    0.2771
f =
    0.2606
f =
    0.2626
f =
    0.2623
ans =
    0.2623
```

1.2 - Mean Value Theorem

The Mean Value Theorem allows this expression to be written exactly by the addition of the next term evaluated at ξ as follows.

$$f(x) = f(c) + f'(c)(x-c) + \frac{f''(c)(x-c)^2}{2!} + \frac{f'''(\xi)(x-c)^3}{3!} \quad (1.6)$$

where $c < \xi < x$.

The Mean Value Theorem states that there will always be (providing the function is continuous) a value of ξ that lies between c and x that will make the approximation exact.

This is easily seen when only one term is used in the approximation such that

$$f(x) \approx f(c) \quad (1.7)$$

There is a slope of the function that if used will make the approximation exact and that slope is a slope of the function between x and c as shown in Figure 1. In the homework problems you are asked to determine the value of ξ for a particular function.

$$f(x) = f(c) + f'(\xi)(x - c)$$

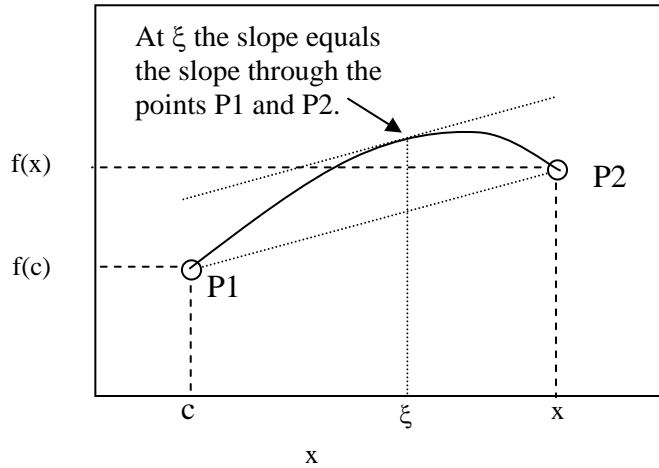


Figure 1. The Mean Value Theorem of Derivatives

1.3 - Taylor Series Using h

The Taylor Series is normally written as

$$f(x) = f(c) + f'(c)(x - c) + \frac{f''(c)(x - c)^2}{2!} + \frac{f'''(c)(x - c)^3}{3!} + \dots \quad (1.8)$$

In general,

$$f(x) = \sum_{k=0}^{\infty} \frac{f^k(c)(x - c)^k}{k!} \quad (1.9)$$

It is convenient to define the distance from c to x as h.

$$h = x - c.$$

If we then discontinue the use of c in favor of x, Eq. (1.8) becomes

$$f(x + h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \dots \quad (1.10)$$

where x replaces c and x + h replaces x as shown in Figure 2.

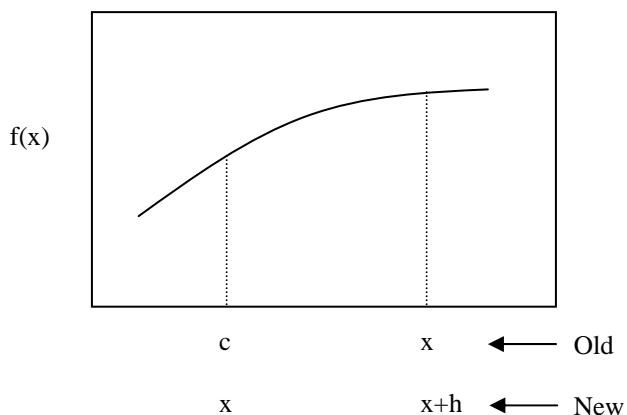


Figure 2. Comparison of previous notation and the new “h” notation

Example 1b. - Mean Value Theorem of Derivatives Problem

Find the value of ξ that makes the Taylor Series approximation in Eq. (1.11) exact for the function $f(x) = x^4 - 2x - 90$ where $x = 2$ and $c = 1.5$.

Solution

The Mean Value Theorem allows the following expression to be written where the last derivative term is evaluated at ξ .

$$f(x) = f(c) + f'(c)(x-c) + \frac{f''(c)(x-c)^2}{2!} + \frac{f'''(\xi)(x-c)^3}{3!} \quad (1.11)$$

where $c < \xi < x$.

In this example, three terms are used for the approximation of $f(x)$ and the fourth term using the third derivative at ξ makes the approximation $f(x)$ exact. Substituting into Eq. (1.1) gives

$$(x^4 - 2x - 90) = (c^4 - 2c - 90) + (4c^3 - 2)(x-c) + 12c^2(x-c)^2/2! + 24\xi(x-c)^3/3! \quad (1.12)$$

$$\xi = 1.625$$

MathCad Computation of ζ

$$x := 2$$

$$c := 1.5$$

$$\zeta := \frac{\left(\frac{4}{x^4} - 2 \cdot x - 90\right) - \left(\frac{4}{c^4} - 2 \cdot c - 90\right) - \left(4 \cdot c^3 - 2\right) \cdot (x - c) - 12 \cdot c^2 \cdot \frac{(x - c)^2}{2!}}{24 \cdot \frac{(x - c)^3}{3!}}$$

$$\zeta = 1.625$$

Note: $c < \zeta < x$

Then in general,

$$f(x+h) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)h^k}{k!} \quad (14)$$

1.4 - Derivative Approximations from Taylor Series

Taylor Series may be written as

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \dots \quad (1.13)$$

An approximation for the first derivative may be obtained by rearranging Eq. (1.13) to give

$$f'(x) = \frac{[f(x+h) - f(x)]}{h} - \frac{f''(\xi)h}{2!} \quad (1.14)$$

The last term, which arises from the Mean Value Theorem, is a measure of the error in the estimate of the derivative. That is,

$$f'(x) = \frac{[f(x+h) - f(x)]}{h} + O(h) \quad (1.15)$$

The function O is related to h to the first power as given in Eq. (16). Although the actual value of the error is unknown, it is known that the error is related to the first power of h . Therefore, if h were reduced by a factor of, say 10, the error in the derivative would be reduced by approximately a factor of 10. It

should go without saying that if the error were known, the derivative could simply be corrected using the known error. Since errors are important, any means of improving the estimation of the derivative is important. The next section presents just such an improvement in estimating the first derivative.

The estimation of the first derivative given in Eq. (1.15) is centered about $x = x + h/2$. That is, the two values of the function are located at x and $x + h$. Improved accuracy in the derivative might be expected were the derivative centered about x . This can be achieved by using approximations of the function at $x - h$ and $x + h$ as follows:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \dots \quad (1.16)$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \dots \quad (1.17)$$

Note that the sign of every other term is negative in Eq. (1.17) as required since the negative sign raised to an odd power gives a negative result.

Subtracting Eq. (1.17) from Eq. (1.16) gives a much improved approximation of the first derivative.

$$f'(x) = \frac{[f(x+h) - f(x-h)]}{2h} + O(h^2) \quad (1.18)$$

where

$$O(h^2) = \frac{f''(x)h^2}{2!} \quad (1.19)$$

indicates that the error in the approximation of this derivative varies with the square of the step size h . Therefore, if h were reduced by a factor of 10 the error in the derivative would be reduced by a factor of 100. The higher the power of h in $O(h^n)$ the more rapidly the estimation improves with decreasing step size.

An approximation of the second derivative may be obtained by adding Eq. (1.17) and Eq. (1.18) to give

$$f''(x) = \frac{[f(x+h) - 2f(x) + f(x-h)]}{h^2} + O(h^2) \quad (1.20)$$

Table 1 shows a summary of various approximations of derivatives and their corresponding Order of Error. The table may be extended to higher-order derivatives and higher order approximations.

1.5 - Richardson Extrapolation

Taylor Series may be written as

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \frac{f^{(5)}(x)h^5}{5!} + \dots \quad (1.21)$$

Table 1. Derivative Approximations

Derivative	Type	Order of Error	Approximation
1 st	Backward	O(h)	$\frac{f(x) - f(x-h)}{\Delta x}$
	Backward	O(h ²)	$\frac{f(x-2h) - 4f(x-h) + 3f(x)}{2\Delta x}$
	Central	O(h ²)	$\frac{f(x+h) - f(x-h)}{2\Delta x}$
	Forward	O(h)	$\frac{f(x+h) - f(x)}{\Delta x}$
	Forward	O(h ²)	$\frac{-3f(x) + 4f(x+h) - f(x+2h)}{2\Delta x}$
2 nd	Backward	O(h)	$\frac{f(x-2h) - 2f(x-h) + f(x)}{\Delta x^2}$
	Backward	O(h ²)	$\frac{-f(x-3h) + 4f(x-2h) - 5f(x-h) + 2f(x)}{\Delta x^2}$
	Central	O(h ²)	$\frac{f(x+h) - 2f(x) + f(x-h)}{\Delta x^2}$
	Forward	O(h)	$\frac{f(x) - 2f(x+h) + f(x+2h)}{\Delta x^2}$
	Forward	O(h ²)	$\frac{2f(x) - 5f(x-h) + 4f(x-2h) - f(x+3h)}{\Delta x^2}$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} - \frac{f^{(5)}(x)h^5}{5!} + \dots \quad (1.22)$$

An approximation for the first derivative may be obtained by subtracting Eq. (1.22) from (1.21) to give

$$f'(x) = \frac{[f(x+h) - f(x-h)]}{2h} - \frac{f'''(x)h^2}{3!} - \frac{f^{(5)}(x)h^4}{5!} - \dots \quad (1.23)$$

Now define for derivation convenience $\varphi(h)$

$$\varphi(h) = \frac{[f(x+h) - f(x-h)]}{2h} \quad (1.24)$$

so that Eq. (1.23) rearranged becomes

$$\varphi(h) = f'(x) + \frac{f''(x)h^2}{3!} + \frac{f'''(x)h^4}{5!} + \dots \quad (1.25)$$

Richardson eliminated the second order h term by evaluating the function φ at $\varphi\left(\frac{h}{2}\right)$

$$\varphi\left(\frac{h}{2}\right) = f'(x) + \frac{f''(x)(h/2)^2}{3!} + \frac{f'''(x)(h/2)^4}{5!} + \dots \quad (1.26)$$

and eliminating the term by combining Eqs. (1.25) and (1.26) as follows

$$\begin{aligned} \varphi(h) &= f'(x) + \frac{f''(x)h^2}{3!} + \frac{f'''(x)h^4}{5!} + \dots \\ -4 \left[\varphi\left(\frac{h}{2}\right) &= f'(x) + \frac{f''(x)(h/2)^2}{3!} + \frac{f'''(x)(h/2)^4}{5!} + \dots \right] \end{aligned} \quad (1.27)$$

Which establishes that the order of error is related to h^4 .

$$f'(x) = \left\{ \varphi\left(\frac{h}{2}\right) + \frac{1}{3} \left[\varphi\left(\frac{h}{2}\right) - \varphi(h) \right] \right\} + \frac{f'''(x)h^4}{4 \cdot 5!} + \dots \quad (1.28)$$

Richardson's Extrapolation Equation for the first derivative is then

$$f'(x) = \left\{ \varphi\left(\frac{h}{2}\right) + \frac{1}{3} \left[\varphi\left(\frac{h}{2}\right) - \varphi(h) \right] \right\} + O(h^4) \quad (1.29)$$

and approximated as

$$f'(x) \approx \left\{ \varphi\left(\frac{h}{2}\right) + \frac{1}{3} \left[\varphi\left(\frac{h}{2}\right) - \varphi(h) \right] \right\} \quad (1.30)$$

where

$$\varphi(h) = \frac{[f(x+h) - f(x-h)]}{2h} \quad (1.31)$$

and

$$\varphi\left(\frac{h}{2}\right) = \frac{\left[f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right) \right]}{2 \frac{h}{2}} \quad (1.32)$$

The power of this result should be clear since the order of error is now reduced from h^2 to h^4 by simply adding an additional evaluation of the function at $(x+h/2)$ and at $(x-h/2)$. This is an arithmetic increase in the number of calculations for a geometric increase in the accuracy. That is to say, the accuracy benefit outweighs the computational cost.

Example 1c - Richardson Extrapolation by MathCad

Estimate the derivative of $\sin(x)$ at $x=1$.

$$h := 0.1 \quad h2 := \frac{h}{2} \quad x := 1 \quad f(x) := \sin(x)$$

$$\phi(h) := \frac{f(x+h) - f(x-h)}{2 \cdot h}$$

$$\phi(h) = 0.53940225 \quad \phi(h2) = 0.54007721$$

These are the slopes found by the conventional central difference equation. Notice how cutting the step size in half improves the result.

Richardson Extrapolation

$f'(x) = \text{slope}$

$$\text{slope}(x) := \phi\left(\frac{0.1}{2}\right) + \frac{1}{3}\left(\phi\left(\frac{0.1}{2}\right) - \phi(0.1)\right)$$

$$\text{slope}(x) = 0.54030219$$

This slope obtained by Richardson Extrapolation is much more accurate since error is a function $O(h^4)$ rather than $O(h^2)$.

Analytical Solution

$$f'(x) = -\cos(x)$$

$$\cos(1) = 0.54030231$$

Eq. (1.30) may be written as

$$f'(x) \approx \frac{1}{3} \left[4\phi\left(\frac{h}{2}\right) - \phi(h) \right] \quad (1.33)$$

which will be interesting to compare with later topics such as Simpson's 1/3 Rule and 4th Order Runge-Kutta. They each involve the average of two *exterior* values, $f(x+h)$, $f(x-h)$ from $\phi(h)$, and four *center* values, $4\phi(h/2)$.