Math 4610 Fundamentals of Computational Mathematics - Topic 12.

Most mathematical problems require the use of approximations as a part of the solution process. For example, the solution of the simple ordinary differential equation

$$\frac{dy}{dt} = -2 y$$

with initial condition, y(0) = 1, is the function

$$y(t) = e^{-2t}$$

You can check this on your own. This is a single term that seems nice and tidy for predicting values of the solution to the differential equation. However, due to the fact that the number e=2.71828... is an irrational number any evaluation will be an approximation at best. For certain values like t=0 the exponential can be evaluated exactly since $e^0=1$. However, for just about any other number all we can do is approximate the value based on mathematical formulas.

From any standard second semester engineering calculus course, an infinite series representation of the exponential function is given by

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \dots = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

Of course, this being an infinite series, the best we can do is sum a finite number of terms and neglect/truncate the rest of the infinite series.

Mathematically, we know that the series converges rapidly to an output value given any reasonable input value. It may take a few (or a lot of) terms, but a truncated series

$$e^x \approx \sum_{k=0}^{N} \frac{x^k}{k!}$$

for some, N > 0, can be used to approximate the exponential function. In this example, there are a couple of practical problems that still need to be addressed. First, if we truncate the infinite sum to a finite number of terms, N > 0, how good is the approximation? As we will see below, the truncation of the series can be analyzed mathematically using Taylor series expansions.

The second problem involves errors in number representation and errors in arithmetic operations on any/all computers. That is, due to the finite resources (memory/disk space) available on a computer, we will run into problems for either very small or very large input values to the exponential function.

The first problem is due to the truncation error which is an artifact of replacing a mathematically exact model with some approximation. For the example, once a value of N > 0 is chosen, the truncation uses a finite number of terms and creates an error dependent on an infinite number of neglected terms in the series. Truncation error in any given problem needs to be analyzed mathematically. The second problem is really beyond our control since it is due to the particular computer and operating system we are using. We will treat the problem of truncation error in this section and save the problem of round off error and machine precision for another topic in the near future.

A Definition Of Taylor Series And Taylor Series With Remainders:

In almost any calculus sequence, the topic of infinite series and in particular Taylor series is discussed. A definition for Taylor series is the following.

Definition 1 Suppose that the function, f, is a function with derivatives of all orders at a point, a, in the domain of f. Then the Taylor series of f about the point a is given by

$$f(x) \sim f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2 + \dots = \sum_{k=0}^{\infty} \frac{f^{(k)}}{k!} (x-a)^k$$

where $f^{(k)}(a)$ denotes the k^{th} derivative of f at a and $k! = k(k-1)(k-2)\dots(2)(1)$ is the k^{th} factorial and we use 0! = 1

Students should be able to produce the Taylor series of simple functions like the trigonometric functions or examples like $f(x) = \ln(1+x)$. If you are a little foggy on the details, there are examples all over the internet or you can refer to any book that presents topics in engineering calculus. In the next topic in the course a few helpful/standard examples will be reviewed.

An important note at this point in the presentation is that writing down a Taylor series representation does not guarantee the infinite series will converge for all points in the domain of a function. The geometric series will provide one such example. Part of the work on power series in a calculus course is to determine the interval of convergence. This is typically done via the ratio test which we will not cover here. Students should review these ideas if calculus seems to be in the distant past.

For some of the analysis of approximations it will be important to know how to apply the Taylor series with remainder. The definition we need is the following.

Definition 2 Suppose that the function, f, is a function with n+1 continuous derivatives at a point, a, in the domain of the function. Then, the Taylor series with remainder is

$$f(x) \sim \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} (x-a)^k + R_f(a,n)$$

where

$$R_f(a,n) = \frac{f^{n+1}(\xi)}{(n+1)!} (x-a)^{n+1}$$

and ξ is a point between x and a.

The remainder in this definition can be used to establish upper bounds on the truncation error as will be seen in the examples in this topic.

Increment Form of the Taylor Series:

Computational mathematicians should be able to use Taylor series with ease in the analysis of numerical methods. There are several different, but equivalent forms of the Taylor series. For the purposes in this course, we will use the h or increment form for Taylor series expansions. To get to the appropriate form, letting h = x - a in either the Taylor series definition or the Taylor series with remainder definition in the previous section. Substituting this change of variables and doing some simplification gives

$$f(a+h) \sim f(a) + f'(a)h + \frac{1}{2}f''(a)h^2 + \dots = \sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!} h^k$$

or using the Taylor series with remainder

$$f(a+h) \sim \sum_{k=0}^{N} \frac{f^{(k)}(a)}{k!} h^{k} + R_{f}(a, N)$$

where

$$R_f(a, N) = \frac{f^{N+1}(\xi)}{(N+1)!} h^{N+1}$$

This form allows us to analyze approximations of functions. As an example, let's consider the example at the beginning of the this topic.

Using the h-form of the Taylor series expansion for the natural exponential the solution of the differential equation can be represented as

$$y(a+h) = e^{-2(a+h)} \sim \sum_{k=0}^{N} \frac{y^{(k)}(a)}{k!} h^{N} + R_{y}(a, N)$$

and

$$R_y(a, N) = \frac{y^{N+1}(\xi)}{(N+1)!} h^{N+1}$$

To be a bit more specific, consider the case when N=3 and a=1.0. Then we can write

$$y(1.0+h) = y(1.0) + y'(1.0) h + \frac{1}{2!} y''(1.0) h^2 + \frac{1}{3!} y'''(1.0) h^3 + \frac{1}{4!} y^{(4)}(\xi) h^4$$

We can replace the derivatives in the expression using

$$y = e^{-2t}$$
 \rightarrow $y' = -2e^{-2t}$, $y'' = 4e^{-2t}$, $y''' = -8e^{-2t}$, $y'''' = 16e^{-2t}$

to obtain

$$y(1.0+h) = e^{-2} - 2e^{-2} h + 2e^{-2} h^2 - \frac{4}{3} e^{-2} h^3 + \frac{1}{24} e^{\xi} h^4$$

where ξ is a value between t=1 and t=1+h.

The first four terms in the last expression define a cubic polynomial which is called the Taylor polynomial of degree three. The Taylor polynomial defines an approximation of the solution. The last term accounts for truncating an infinite number of terms in the Taylor series. The remainder term will allow us to obtain a bound on the error in the approximation. That is, if we use

$$y(1.0+h) \approx e^{-2} - 2e^{-2} h + 2e^{-2} h^2 - \frac{4}{3} e^{-2} h^3$$

we are neglecting the remainder term. The error in this approximation is obtained by determining an upper bound on the absolute value of the remainder term. So, for our example with E denoting the error at t = 1,

$$E = \left| \frac{1}{24} e^{\xi} h^{4} \right| = \frac{1}{24} \left| e^{\xi} \right| h^{4} \le \frac{1}{24} \left| e^{0} \right| h^{4}$$

Note that $0 < e^{-2} < e^{0}$. As h is pushed towards zero, the error will be reduced proportional to h^{4} . If we were to choose h = 0.1 then the error will be bounded as

$$E \le \frac{1}{24} 10^{-4}$$

The question is whether or not the error is acceptable. If not, we may want to add more terms to the approximation.

We will do a lot of these types of computations throughout the semester. In particular, when we analyze root finding problems, we will use Taylor series to determine whether or not the truncation error will be reduced to zero in some sense and if this is the case, how fast the error is reduced.