ME 539 – Applied Numerical Methods for Mechanical Engineers

Text

Steven C. Chapra and Raymond P. Canale, *Numerical Methods for Engineers, 7th Edition*, McGraw-Hill, 2014.

References

Curtis F. Gerald, *Applied Numerical Analysis, 2nd Edition*, Addison-Wesley, 1980

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Section 1 – Introduction

Numerical methods are techniques by which complex mathematical problems are formulated so that they can be solved with simple arithmetic operations. There are many such methods, but they share one common characteristic: they always involve large amounts of tedious arithmetic operations, making them ideal for computer applications.

Numerical methods differ from the more traditional, analytical approaches to mathematics. Analytical mathematics tend to focus on the solution techniques themselves, and not so much on the problem formulation or the interpretation of the results. In addition, the number and types of applied mathematical problems encountered in applied fields such as engineering that have closed-form solutions are very limited. Numerical methods focus on the problem formulation and the close interpretation of the results in order to validate both the model and the results themselves.

In this course we will become familiar with numerical techniques covering the following topics:

- Roots of equations
- Systems of linear equations
- Optimization
- Curve fitting
- Numerical differentiation and integration
- Ordinary differential equations
- Partial differential equations

We will make extensive use of computer programming, using both Excel and Matlab as programming environments.

1.1 Approximations and Round-off Errors

All numerical methods involve the approximation and round-off of numbers, and it will be extremely important for us to be able to quantify the effect these approximations have on the results of our calculations.

The ***significant digits*** of a number are those that can be used with confidence, usually corresponding to a certain number of digits known precisely, plus one estimated digit.

Accuracy refers to how closely a computed or measured value agrees with its true value. ***Precision*** is related to repeatability and refers to how closely individual computed or measured values agree with each other. Often we will have to make decisions to accept lower levels of accuracy in order to efficiently solve problems. The techniques we choose must be sufficiently accurate to meet the requirements of a particular problem and must be precise enough to meet the requirements of engineering design. We will often use the term ***error*** to both inaccuracy and imprecision.

1.2 Definitions of Error

There are two basic types of errors inherent in numerical methods. ***Truncation errors*** are those that result when approximations are used to represent exact mathematical procedures. ***Round-off errors*** results when numbers with limited significant figures are used to represent exact numbers. Both types of error can be formulated as:

True value = approximation + error

or

E_t = True value – approximation

where E_t is the true error. The relative error is defined as

$$\varepsilon_t = \frac{true\_error}{true\_value} \tag{1.2.1}$$

In the application of numerical methods, exact values are known when we have an analytical solution to compare. Instead, we will normalize the error to the best available estimate of the true value, that is, the approximation itself:

$$\varepsilon_a = \frac{approximate\_error}{approximation} \tag{1.2.2}$$

In addition, we need to estimate the error without knowing the true value. Certain numerical methods involve iterative calculations, where a calculation is made based on the results of a previous calculation to computer better and better approximations:

$$\varepsilon_a = \frac{current\_approximation - previous\_approximation}{current\_approximation} \tag{1.2.3}$$

Errors can be either positive or negative. Normally we are not concerned with the sign but whether it is smaller than some pre-specified percent tolerance, ε_s. Calculations are performed until the absolute value of the relative approximate error falls below the tolerance:

$$\left|\varepsilon_a\right| < \varepsilon_s \tag{1.2.4}$$

To find a result that is correct to at least n significant digits:

$$\varepsilon_s = (0.5 \times 10^{2-n})\% \tag{1.2.5}$$

1.3 Round-Off Errors

Without going into too much detail, computers (and calculators) retain only a fixed number of significant figures during calculations. This leads to what is known as ***round-off error***. The following aspects are always important to keep in mind when performing computer or calculator calculations:

- ***There is a limited number of quantities that may be represented.*** Only pre-defined types of numbers can be stored in computers, and each type has a defined range associated with it. Any attempt to use numbers outside of these ranges results in *overflow errors*.
- ***There are only a finite number of quantities that can be represented within the range***. Due the fact that computers use a fixed number of significant figures, the degree of precision is limited. Clearly, irrational numbers cannot be precisely represented but most rational numbers also cannot be represented precisely either. These types of errors are called *quantizing errors*.
- ***The interval between numbers increases as the numbers grow in magnitude***. Floating-point representations preserve significant digits, but this feature also means that quantizing errors are proportional to the magnitude of the number being represented.

Even though round-off errors can be significant, most engineering calculations can be carried out with more than acceptable precision on most computers and calculators. When precision is of the utmost importance, the use of extended precision quantities can greatly mitigate the effects of round-off errors and is recommended.

1.4 Truncation Errors and the Taylor Expansion

The Taylor Series

The Taylor Series is an important mathematical tool used to approximate the values of a function, and we will make extensive use of its properties. Recall from calculus that if a function f and its $n+1$ derivatives are continuous in the vicinity of a point x_i, then its value at a nearby point x_{i+1} can be expressed as

$$\begin{aligned} f(x_{i+1}) &= f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 \\ &\quad + \frac{f^{(3)}(x_i)}{3!}(x_{i+1} - x_i)^3 + \frac{f^{(4)}(x_i)}{4!}(x_{i+1} - x_i)^4 + R_n \end{aligned} \tag{1.4.1}$$

where the remainder term accounts for the rest of the terms of the infinite series

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{(n+1)} \tag{1.4.2}$$

The subscript n denotes that this is an nth-order approximation and ξ is a value that lies between point x_i and point x_{i+1}. Note that this remainder is an exact representation of the error that would be a result of using a finite number of terms of the Taylor Series.

We will often simplify the Taylor series to be defining a *step size* $h = x_{i+1} - x_i$ and writing Eq. (1.4.1) as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + R_n \tag{1.4.3}$$

where the remainder (1.4.2) is now given as

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1} \tag{1.4.4}$$

In general, nth-order Taylor expansions are exact for nth-order polynomials. For other differentiable and continuous functions, such as exponentials and transcendental functions, a finite number of terms does not exactly represent the function. Each additional term adds some improvement to the approximation. The assessment of how many terms to include in order to be "close enough" for a given problem is the essence of numerical analysis.

Even though the Taylor Series will be the basis of a number of techniques we will study, its use has two important drawbacks. First, the value of ξ is not known exactly, only that it is between the values x_i and x_{i+1}. This means that we will rarely be able to precisely know the error in our approximations. Secondly, since we will often not know the function that we are approximating (if we did, there would be no need to approximate it!), and its derivatives will also be unknown. However, the properties of the Taylor Series are very useful in estimating the errors associated with a numerical technique, particularly truncation errors.

In any numerical technique, we have control over certain parameters of the analysis. One of the most important is the step size h. We can look at Eq. (1.4.2) as $R_n = O(h^{n+1})$, which means that the truncation error is "of order" h^{n+1}, that is, it is proportional to h^{n+1}. This gives us a guideline with which to change an analysis to increase accuracy and reduce error.

As an example of how this is used in numerical analysis, estimate the first derivative of the function f in the vicinity of x_i. By Eq. (1.4.3)

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + R_1$$

solving for the first derivative gives

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \frac{R_1}{h}$$

using Eq (1.4.2) gives

$$\frac{R_1}{h} = \frac{f^{(2)}(\xi)}{h(n+1)!}h^2 = O(h)$$

Therefore, the estimate of the first derivative has a truncation error of *O(h)*, which means that the approximation is proportional to the step size *h*. Consequently, if we halve the step size, we would expect to halve the truncation error. This particular approximation for the first derivative is called the *first forward difference*.

Numerical Differentiation

The Taylor expansion of a function can be represented by:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + + \frac{f^{(3)}(x_i)}{3!}h^3 \cdots \qquad (1.4.5)$$

The Taylor Series can also be expanded backwards to calculate a previous value based on a current value.

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots \qquad (1.4.6)$$

which can be used to show the first backward difference:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

Subtracting E1 (1.4.6) from (1.4.5) and solving for the first derivative yields the *centered difference* approximation:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \qquad (1.4.7)$$

Note that this error term is proportional to h^2, so that if we halve the step size, the error is quartered.

Error Propagation

Using the first-order Taylor Series, it can be shown the errors associated with common mathematical operations using inexact numbers $\tilde{u}$ and $\tilde{v}$ can be summarized as

Operation		**Estimated Error**
Addition	$\Delta(\tilde{u} + \tilde{v})$	$\Delta(\tilde{u}) + \Delta(\tilde{v})$
Subtraction	$\Delta(\tilde{u} - \tilde{v})$	$\Delta(\tilde{u}) + \Delta(\tilde{v})$

Multiplication	$\Delta(\tilde{u}\tilde{v})$	$\lvert\tilde{u}\rvert\Delta(\tilde{v})+\lvert\tilde{v}\rvert\Delta(\tilde{u})$
Division	$\Delta(\frac{\tilde{u}}{\tilde{v}})$	$\frac{\lvert\tilde{u}\rvert\Delta(\tilde{v})+\lvert\tilde{v}\rvert\Delta(\tilde{u})}{\lvert\tilde{v}\rvert^2}$

Stability and Condition
The *condition* of a mathematical problem is a measure of its sensitivity to changes in its input values. A computation is *numerically unstable* if the uncertainty of the input values is grossly magnified by the numerical method.

Using a first-order Taylor Series,

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x-\tilde{x})$$

The *relative error of f(x)* is

$$\frac{f(x)-f(\tilde{x})}{f(\tilde{x})} \cong \frac{f'(\tilde{x})(x-\tilde{x})}{f(\tilde{x})}$$

The *relative error of x* is

$$\frac{x-\tilde{x}}{\tilde{x}}$$

The *condition number* is the ratio of these relative errors

$$Condition\_number = \frac{\tilde{x}f'(\tilde{x})}{f(\tilde{x})} \tag{1.4.7}$$

and is a measure of how the uncertainty in *x* is magnified in *f(x)*. A value of 1 means that the function's relative error matches the relative error in *x*. A value greater than 1 means that the relative error is amplified; values less than one mean that the error is attenuated. Functions with large condition numbers are said to be *ill-conditioned*.

1.5 Total Numerical Error

The ***total numerical error*** is the summation of the truncation and round-off errors. In general, the way to minimize round-off errors is to increase the number of significant figures used in the calculation. Round-off error increases due to subtractive cancellation and as the number of calculations in an analysis becomes larger. Truncation error can be reduced by decreasing the step size, which leads to increased numbers of calculations and an increase in round-off errors.

Numerical errors can be controlled with certain general guidelines:

- Avoid subtracting two nearly-equal numbers to avoid subtractive cancellation
- Work with the smallest numbers first and progressively include the largest

- The use of numerical experiments and sensitivity analyses may provide insight to numerical strategies
- Performing the analysis with different modeling and numerical techniques may provide more confidence in the final results.

Blunders
Gross errors, or *blunders*, are sometimes unavoidable. Sources of blunders are mainly based in human imperfection and include errors of the modeling process and incorrect programming. We will frequently mention techniques with which to avoid blunders and check our numerical calculations.

Formulation Errors
Formulation or modeling errors are due to incomplete mathematical models. It is important to note that formulation errors cannot be resolved with increased numerical analysis. Poorly conceived models cannot yield useful results, no matter how sophisticated the analysis techniques.

Data Uncertainty
All physical data is subject to variation and uncertainty, and always exhibits both inaccuracy and imprecision. Where such variation is important to interpret the results in a meaningful way, the analysis must be carried out with data that is described in statistical terms, usually consisting of a central measure and the degree of spread about that central measure.

1.6 Example – Calculation of Archimedes's Constant (π)

$\pi \approx 22/7$, $\varepsilon < 1.3 \times 10^{-3}$

$\pi \approx 355/113$, $\varepsilon < 2.7 \times 10^{-3}$

Standard Gregory-Liebnitz series: $\pi = 4\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k-1}$

Telescoping Gregory-Liebnitz series: $\pi = 8\sum_{k}^{\infty} \frac{1}{[2(2k-1)]^2 - 1}$

Vieta's Product: $\pi = 4R_0 \prod_{k=1}^{\infty} \frac{1}{R_k}, R_k = \sqrt{\frac{1+R_{k-1}}{2}}, R_0 = \sqrt{\frac{1}{2}}$