Numerical Methods KOM2722-AVE3842

Week 2

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Syllabus

Texts:

- An Introduction to Numerical Methods and Analysis, J. F. Epperson, Wiley, 2002
- Applied Numerical Methods with MATLAB, S.C. Chapra, 2012, McGrow-Hill

Lecture Notes

- We will use lecture notes of Asst. Prof. Birol Erol and Asst. Prof. Bahadır Çatalbaş prepared from textbooks.
- Lecture slides will be shared with students.

Grading:

- 60% Midterm + Homework
- 40% Final

Attendance

- At least 70%

Basic Tools of Calculus
Taylor's Theorem

Provides an approximation of $(n + 1)$ times differentiable function around a given point.

Suppose that we are working on a function f(x) that is continuous and has $(n + 1)$ continious derivatives on interval $(a, b]$.

Theorem (Taylor's Theorem with Remainder):

Let $f(x)$ have $n + 1$ continuous derivatives on $(a, b]$ for some $n \geq 0$ and let $x, x_0 \in [a,\ b]$, then

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

$$p_n(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)(x-x_0)^2}{2!} + \cdots = \sum_{k=0}^{n} \frac{(x-x_0)^k}{k!} f_{(x_0)}^{(k)}$$

The remainder

$$R_n(x) = \frac{1}{n!} \int_{x_0}^{x} (x - t)^n f^{(n+1)}(t) dt$$

*Every continuous function can be approximated by a polynomial of order n.

*Allow us to replace/obtain, in a computational setting, a much simple problem.

The remainder, the error term,

$$R_n(x) = \frac{(x-x_0)^{n+1}}{(n+1)!} f^{(n+1)}(c) for\ some\ c\ between\ x_0\ and\ x$$

$$and$$

$$\lim_{n \to \infty} R_n(x) = 0$$

Taylor's series for $x_0 = 0$ is called as Maclaurin series

Example: $f(x) = e^x$, find n^{th} order Taylor series expansion of $f(x)$ around $x = 0$

$$f^{(k)}(0) = 1$$

$$e^x = 1 + \underbrace{x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n}_{p_n(x)} + \underbrace{\frac{1}{(n+1)!}x^{n+1}e^{c_x}}_{R_n(x)}$$

$R_n(x)$, remainder c_x is an unknown point between x and 0.

Taylor's Theorem an approximation and an error estimate provides

Considering the problem of approximating the exponential function on the interval $[-1, 1]$

$$e^x = \underbrace{1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n}_{p_n(x)\ \text{Polynomial}} + \underbrace{\frac{1}{(n+1)!}x^{n+1}e^{c_x}}_{R_n(x),\ \text{remainder}}$$

c_x is an unknown point between x and 0.

Without lost of generality x can be any point in [-1, 1] then

c_x can be any point in [-1, 1]

For simplicity, let's denote polynomial by $p_n(x)$ and remainder by $R_n(x)$, so that the equation:

$$\mathrm{e}^x = p_n(x) + R_n(x)$$

Suppose that we want this approximation to be accurate within 10^{-6} absolute error. i.e.,

$|e^x - p_n(x)| \leq 10^{-6}$ for all x in the interval $[-1, 1]$.

$|e^x - p_n(x)| = |R_n(x)| \leq 10^{-6}$, if we make $|R_n(x)| \leq 10^{-6}$ the absolute error in approximation will be less that 10^{-6}.

In other words, we need make the **upper bound** less than 10^{-6}.

$$|R_n(x)| = \frac{|x^{n+1}e^{c_x}|}{(n+1)!} = \frac{|x|^{n+1}e^{c_x}}{(n+1)!} \qquad \text{(Note that: } e^z > 0 \text{ } \underline{\text{for all z.)}}$$

$$\leq \frac{e^{c_x}}{(n+1)!}, \text{ because } |x| \leq 1 \text{ for all } x \in [-1, 1]$$

$$\leq \frac{e}{(n+1)!}, \text{ because } e^{c_x} \leq e \text{ for all } x \in [-1, 1]$$

So that, if we find n such that $\frac{e}{(n+1)!} \leq 10^{-6}$ then we will have $|e^x - p_n(x)| = |R_n(x)| \leq 10^{-6}$.

$n = 9$ satisfies the desired accuracy.

Rolle's Theorem

Suppose that $y = f(x)$ is continuous at every point of the closed interval $[a, b]$ and differentiable at every point of its interior (a, b). If

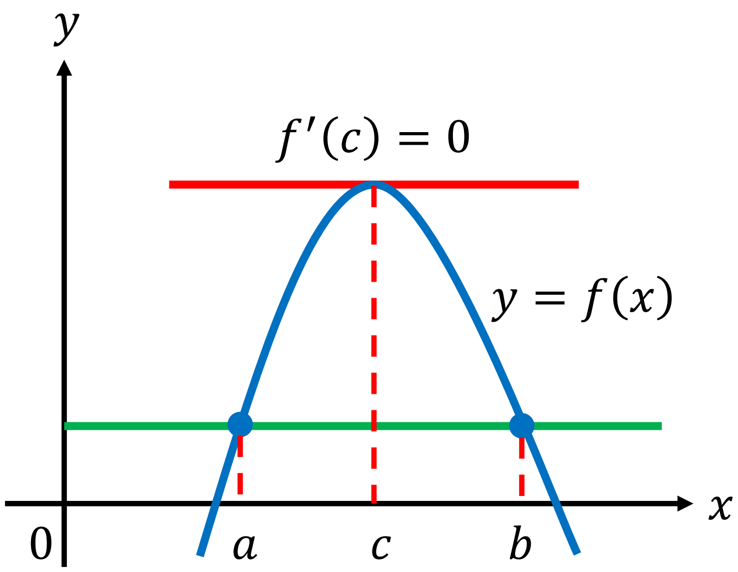
$$f(a) = f(b)$$

then there is at least one number c in (a, b) at which

$$f'(c) = 0.$$

Thus, there should be one place where tangent line should be horizontal

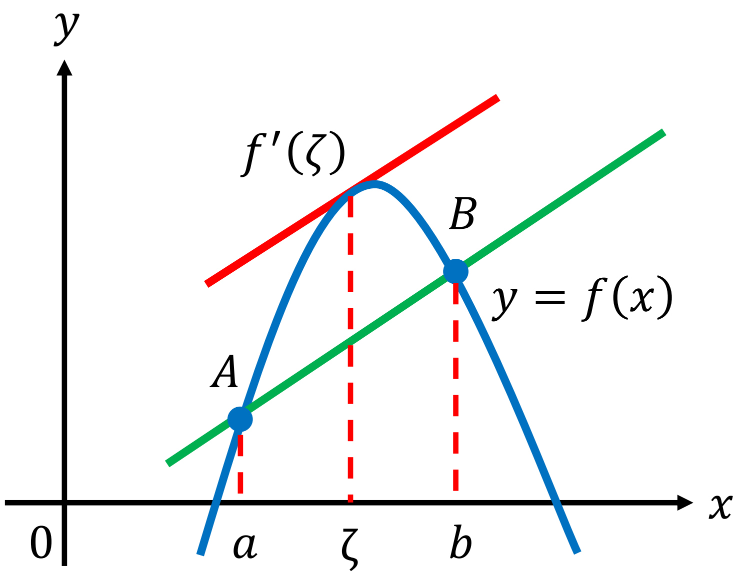
Note that it is also satisfied for functions intersect the x axis at two points; $f(a) = f(b) = 0$.



The Mean Value Theorem

Let f be a given function, continuous on closed interval $[a, b]$ and differentiable at every point of its interior (a, b). Then there exists a point $\zeta \in [a, b]$ such that

$$f'(\zeta) = \frac{f(b) - f(a)}{b - a}$$



The mean value theorem (MVT) states that between any two points on the graph of a differentiable function f there at least one place where the tangent line to the graph is parallel to line joining.

Consequences of MVT

MVT is used to prove many results

-> Let f be a function that is continuous and differentiable on $[a, b]$

if $f'(x) > 0$ for every x in $[a, b]$, the f is increasing on $[a, b]$

$f'(x) < 0$ decreasing

$f'(x) = 0$ constant

Proof:

Secant line intersection points for $\mathrm{y} = f(x)$: $\mathrm{A}\big(a, f(a)\big)$, $\mathrm{B}(b, f(b))$

Equation of secant line: $y - y_1 = m(x - x_1)$

Here $g(x)$ is the equation of secant line AB

$$g(x) - f(a) = \frac{f(b) - f(a)}{b - a}(x - a)$$

$$g(x) = \frac{f(b) - f(a)}{b - a}(x - a) + f(a) \qquad (1)$$

Let $h(x) = f(x) - g(x)$,

$$h(x) = f(x) - \left[\frac{f(b) - f(a)}{b - a}(x - a) + f(a)\right] \qquad from\ (1)$$

$h(a) = h(b) = 0$ and $h(x)$ is continuous on $[a, b]$ and differentiable on (a, b).

Thus applying Rolle's Theorem, there is some $\mathrm{x} = c$ in (a, b) such that $h'(c) = 0$

$$h'(x) = f'(x) - \frac{f(b) - f(a)}{b - a}$$

For some c in (a, b), $h'(c) = 0$. Thus,

$$h'(c) = f'(c) - \frac{f(b) - f(a)}{b - a} = 0$$

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

Intermediate Value Theorem

Let $f \in C([a, b])$ be given, and assume that W is a value between $f(a)$ and $f(b)$, that is, either $\mathrm{f}(a) \leq W \leq f(b)$, or $f(b) \leq W \leq f(a)$. Then there exists a point $c \in [a, b]$ such that $f(c) = W$.

* This theorem says that a certain point exists does not give us much information about its numerical value.

-> We will use this theorem as the basis for finding the roots.

Note: $C([a, b])$ — The set of functions f which are defined on the interval $[a, b]$, continuous on all of (a, b), and continuous from the interior of $[a, b]$ at the endpoints.

Extreme Value Theorem

Let $f \in C([a,b])$ be given; then there exists a point $m \in [a,b]$ such that $f(m) \leq f(x)$ for all $x \in [a,b]$, and a point $M \in [a,b]$ such that $f(M) \geq f(x)$ for all $x \in [a,b]$. Moreover, f achieves its maximum and minimum values on $[a,b]$ either at the endpoints a or b, or at a critical point.

The student should recall that a critical point is a point where the first derivative is either undefined or equal to zero.

Integral Mean Value Theorem

Let f and g both be in $C([a,b])$, and assume further that g does not change sign on $[a,b]$. Then there exists a point $\zeta \in [a,b]$ such that

$$\int_a^b g(t)f(t)dt = f(\zeta)\int_a^b g(t)dt$$

Discrete Average Value Theorem

Let $f \in C([a,b])$ and consider the sum,

$$S = \sum_{k=1}^{n} a_k f(x_k)\,,$$

Where each point $x_k \in [a,b]$, and the coefficients satisfy

$$a_k \geq 0, \qquad \sum_{k=1}^{n} a_k = 1$$

Then there exists a point $\eta \in [a,b]$ such that $f(\eta) = S$, i.e.,

$$f(\eta) = \sum_{k=1}^{n} a_k f(x_k)$$

Proof:

$$f(x_k) \leq f_M \Rightarrow S = \sum_{k=1}^{n} a_k f(x_k) \leq f_M \sum_{k=1}^{n} a_k = f_M$$

Error, Approximate Equality and Asymptotic Order

There are different error definitions such as measurement errors, modeling errors, etc. Here we concerned here only with the computational errors such as truncation error or approximation error (True Value = Approximation Error + Error).

We have already talked about the "error" made in a simple Taylor series approximation. It is time we got a little more precise.

Error

If A is a quantity we want to compute and A_h is an approximation to that quantity, then the error is the difference between the two:

$$error = A - A_h;$$

the absolute error is simply the absolute value of the error:

$$absolute\ error = |A - A_h|;$$

and the relative error normalizes by the absolute value of the exact value:

$$relative\ error = \frac{|A - A_h|}{|A|},$$

where we assume that $A \neq 0$.

Using a relative error protects us from misguiding the accuracy of an approximation for very large or very small numbers.

Approximate Equality

If two quantities are approximately equal to each other, we will use the notation "$\approx$" to denote this relationship, as in

$$A \approx B$$

This is an admittedly vague notion. Is $0.99 \approx 1$? Probably so. Is $0.8 \approx 1$? Maybe not.

$$\lim_{h \to 0} A_h = A \Rightarrow A_h \approx A \; for \; all \; "h" \; sufficiently \; small$$

$$\lim_{n \to \infty} A_n = A \Rightarrow A_n \approx A \; for \; all \; "n" \; sufficiently \; large$$

For example, the definition of derivative of function $y = f(x)$ is as follows:

$$\lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = f'(x)$$

We therefore conclude that, for h small enough,

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

Asymptotic Order (Big O notation)

Another notation of use is the so-called "Big O" notation, more formally known as asymptotic order notation. Suppose that we have a value y and a family of values $\{y_h\}$, each of which approximates this value,

$$y \approx y_h$$

for small values of h. If there exists a positive function $\beta(h)$, $\beta(h) \to 0$ as $h \to 0$, and a constant $C > 0$, independent of h, such that

$$|y - y_h| \leq C\beta(h)$$

for all h sufficiently small, then we say that

$$y = y_h + O\big(\beta(h)\big),$$

meaning that $y - y_h$ is “on the order of” $\beta(h)$. Here $\beta(h)$ is a function of the parameter h, and we assume that

$$\lim_{h \to 0} \beta(h) = 0$$

Example: $A = \int_0^\infty e^{-2x} dx\,,\ A_n = \int_0^n e^{-2x} dx$

Exact solution $\Rightarrow A = \frac{1}{2}$

Solution $of\ approximation \Rightarrow A_n = \frac{1}{2} - \frac{1}{2} e^{-2n}$

$$\Rightarrow A_n = A - \frac{1}{2} e^{-2n}$$

$$\Rightarrow A = A_n + \frac{1}{2} e^{-2n}$$

$$\Rightarrow A = A_n + O(\underbrace{e^{-2n}}_{\beta(n) = e^{-2n}})$$

Theorem: Let $y = y_h + O(\beta(h))$ and $\mathrm{z} = z_h + O(\gamma(h))$, with $b\beta(h) > \gamma(h)$ for all h near zero. Then

$$y + z = y_h + z_h + O(\beta(h) + \gamma(h))$$

$$y + z = y_h + z_h + O(\beta(h))$$

Horner's Rule

Up to now, we devoted some time to the construction of polynomial approximations to given functions. It might be good if we discussed the best way to evaluate those approximations efficiently.

The most efficient way to evaluate a polynomial is by nested multiplication. If we have

$$p_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n,$$

then we factor out each power of x as far as it will go, thus getting

$$p_n(x) = a_0 + x(a_1 + x(a_2 + \cdots + x(a_{n-1} + a_n x) \dots)).$$

In the first form –> we need to find powers of $x^2, x^3, \dots, x^n$

In the second form –> $(n+1)$ multiplications and n additions

Example: We could write

$$q(x) = 1 + x + 3x^2 - 6x^3$$

as

$$q(x) = 1 + x(1 + x(3 - 6x))$$

Difference Approximations To The Derivative

One of the simplest uses of Taylor's Theorem as a means of constructing approximations involves the use of difference quotients to approximate the derivative of a known function f . Intuitively, this is obvious from the definition of the derivative:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) + f(x)}{h} \Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h}$$

The challenge for us is to make this vague statement more precise (just how accurate is this approximation, in terms of the parameter h?)

Using Tylor's Theorem

$$f'(x) - \frac{f(x+h) - f(x)}{h} = f'(x) - \frac{hf'(x) + \frac{1}{2}h^2 f''(\zeta x, h)}{h}$$

$$= -\tfrac{1}{2} h f''(\zeta x, h)$$

Here the error is proportional to h.

Can we do better?

$$\Rightarrow f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(\zeta_1)$$

$$\Rightarrow f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) - \frac{1}{6}h^3 f'''(\zeta_2)$$

<u>Subtract</u>

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{1}{6}h^3 f'''(\zeta_1) - \frac{1}{6}h^3 f'''(\zeta_2)$$

Let us solve for $f'(x)$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}h^2 \frac{f'''(\zeta_1) + f'''(\zeta_2)}{2}$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}h^2 f'''(\zeta_x, h)$$

This estimate will tent to be better since $\underline{h^2 < h}$.

Forward difference approximation: $f'(x) = \frac{f(x+h)-f(x)}{h}$

Central difference approximation: $f'(x) = \frac{f(x+h)-f(x-h)}{2h}$

Example: $f(x) = e^x$, take derivative for $x = 1$, using $h = 1/8$

Exact Value:

$$f'(x) = e^x, f'(1) = e$$

Forward difference approximation:

$$f'(x) \approx \frac{e^{1.125} - e}{0.125} = 2.895480164$$

Central difference approximation:

$$f'(x) \approx \frac{e^{1.125} - e^{0.875}}{0.25} = 2.72536622$$

The error in first approximation is -0.177

in second approximation is $-7.084x10^{-3}$

Euler's Method For Initial Value Problems

One immediate application of difference methods for approximating derivatives is the approximate solution o f initial value problems for ordinary differential equations. The usual general form of such a problem is

$$y' = f(t, y), \qquad y(t_0) = y_0,$$

where f is a known function of t and y, and t_0 and y_0 are given values. The object in solving this problem is to find y as a function of t; in ordinary differential equations, there are different techniques for analytically solution ways but in some cases, it may not be easy or feasible.

From the last course, we can show that

$$f'(x) - \frac{f(x+h) - f(x)}{h} = -\frac{1}{2} h f''(\zeta_{x,h}) = O(h)$$

with Taylor series expansion.

For $y'(t) = f(t, y(t))$,

$$\frac{y(t+h) - y(t)}{h} = f(t, y(t)) + \frac{1}{2} h y''(t_h)$$

which can be simplified slightly to become

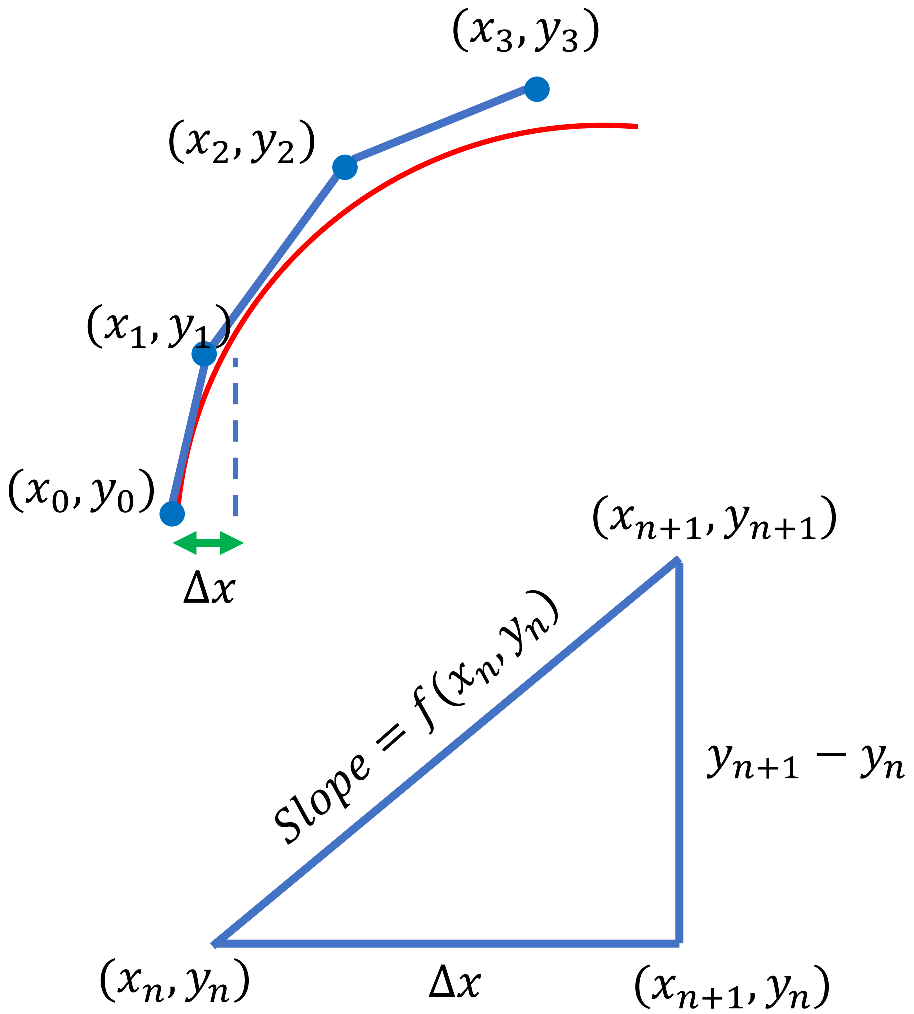
$$y(t+h) = y(t) + hf(t, y(t)) + \frac{1}{2} h^2 y''(t_h).$$

We will choose some small increment Δx

** The basic idea behind Euler's method is to start at the known initial point (x_0, y_0) and draw a line segment in the direction determined by the slope field until we reach the point (x_1, y_1) with x coordinate $x_1 = x_0 + \Delta x$

$$\frac{y_{n+1} - y_n}{\Delta x} = f(x_n, y_n)$$

$$y_{n+1} = y_n + f(x_n, y_n)\Delta \mathrm{x}$$



To approximate the solution of the initial-value problem

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

<u>Step 1:</u> Choose a nonzero number Δx to serve as an increment or step size along x-axis

$$x_1 = x_0 + \Delta x, x_2 = x_1 + \Delta x, \ldots.$$

<u>Step 2:</u> Compute successively,

$$\left.\begin{aligned} y_1 &= y_0 + f(x_0, y_0)\Delta x \\ y_2 &= y_1 + f(x_1, y_1)\Delta x \\ &\cdots \\ y_{n+1} &= y_n + f(x_n, y_n)\Delta x \end{aligned}\right\}$$

The number $y_1, y_2, \ldots, y_{n+1}$ are the approximations of $y(x_1), y(x_2), \ldots, y(x_{n+1})$

$$y_{n+1} = y_n + hf(t_n, y_n)$$

Example: $y' = -y + \sin(t)\,,\ y(0) = 1$

This has exact solution $y(t) = \frac{3}{2}e^{-t} + \frac{1}{2}(\sin(t) - \cos(t))$, found by using the kinds of methods taught in the usual ODE courses.

Let us apply Euler's method for $\Rightarrow h = 1/4$

Step 1: $h = 1/4$, so $t_1 = h = 1/4$ and y_0 is given as 1. Then,

$$y_1 = y_0 + hf(t_0, y_0)$$
$$= 1 + \frac{1}{4}(-1 + \sin(0)) = \frac{3}{4}$$

Thus, $y\left(\frac{1}{4}\right) \approx 0.75$, the error in this approximation

$$e_1 = y\left(\frac{1}{4}\right) - y_1 = 0.8074469434 - 0.75 = 0.0574469434$$

Step 2: We have $t_2 = 2h = \frac{1}{2}$ and $y_1 = 0.75$ from the Step 1. Then

$$y_2 = y_1 + hf(t_1, y_1) = \frac{3}{4} + \frac{1}{4}\left(-\frac{3}{4} + \sin\left(\frac{1}{4}\right)\right) = 0.624350 \approx y(\frac{1}{2})$$

$$e_2 = y\left(\frac{1}{2}\right) - y_2 = 0.7107174779 - 0.624350 = 0.08636$$