Numerical Methods and Modeling in Biomedical Engineering

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Lecture materials are available on Blackboard and lecture’s website: http://tiny.cc/z26j2x
Requirements

• Knowledge on multivariable calculus, linear algebra, some basics on differential equations including ordinary differential equations (ODEs) and partial differential equations (PDEs).

• Know how to use MATLAB®, or other numerical software you prefer.

• Do we need computer lab for those who want to deepen their MATLAB’s skill?
Grading

- Homework 30%
- Midterm project 30%
- Final project 35%
- Presence (quizzes) 5%

- Individual and group homework
- Midterm and final exams: group projects

- Be on time to class
- No cell phone disruptions or electronic device distractions
- Turn in homework on time
Software

(1) MATLAB
http://www.bu.edu/tech/services/support/desktop/distribution/mathsci/matlab/

Or, some alternative
(2) Octave → https://www.gnu.org/software/octave/

(3) SciLab → http://www.scilab.org/

(4) Python
The Octave language is quite similar to Matlab so that most programs are easily portable.
SciLab

Initialization:
Chargement de l'environnement de travail

```
--> a = rand(10, 10)
```

```
column 1 to 5
 0.2113249 0.5608486 0.3076091 0.5015342 0.2806498
 0.7560439 0.6623569 0.9329616 0.4268588 0.1280058
 0.0002211 0.7264507 0.2166008 0.2693125 0.7783129
 0.3303271 0.1985144 0.312642 0.6325745 0.2119030
 0.6658311 0.5442573 0.3414361 0.4051954 0.1121355
 0.6283918 0.2320748 0.2922267 0.9184708 0.6858986
 0.8947452 0.2312237 0.5684429 0.4037334 0.1531217
 0.6857310 0.2146423 0.826472 0.4818509 0.6970851
 0.8782685 0.8833888 0.3321719 0.2639556 0.8415518
 0.0683740 0.6525135 0.5935059 0.4148104 0.4062025

column 6 to 10
 0.4094825 0.3873779 0.5376230 0.5878720 0.6488563
 0.8784126 0.9222899 0.1199926 0.4829179 0.9923191
 0.1138360 0.9481814 0.2256303 0.2226665 0.5050420
 0.1998338 0.3453377 0.6274093 0.8400896 0.7485507
 0.5618661 0.3760119 0.7608433 0.1205996 0.4104059
 0.5896177 0.7340941 0.0485566 0.2855364 0.6084526
 0.6853980 0.2625761 0.6723950 0.8607315 0.8544211
 0.8906225 0.4993494 0.2017173 0.8494102 0.0642647
 0.5042213 0.2638578 0.3911574 0.5257061 0.9279083
 0.3493615 0.5253563 0.8300317 0.9931210 0.9262344
```

```
## What will be covered

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What are numerical methods?

Techniques by which mathematical problems (from real life problems e.g. in biology, physics, economy) are formulated so that they can be solved with arithmetic operations.

They provide approximations to the problems in question.
Why study numerical methods?


Final project group 2 Fall 2014 (Jawde, Huang, Weber, Yao)
Most (> 99.9%) of real world problems in science and engineering are too complex and sophisticated to be solved analytically (exactly), hence they can only be solved \textit{numerically} (approximately).
Errors and Numerical Series
Errors

- Computers use a base-2 representation
  \[ 1 0 1 0 1 1 0 1 \]

- Computers cannot precisely represent certain exact
  base-10 numbers. Non-integer numbers, such as
  \( \pi = 3.1415926535 \ldots \), \( e = 2.718281 \ldots \), or
  \( \sqrt{7} \) are cumbersome and can’t be expressed by a fixed
  number of significant figures.

- The discrepancy creates an error usually referred to as
  **round-off error** or **rounding error**
Errors

Round-off error is the difference between an approximation of a number used in computation and its exact value\(^1\).

Suppose \(\tilde{a}\) is an approximation to the (nonzero) exact value \(a\), then:

Absolute error

\[
\epsilon_a = |a - \tilde{a}|
\]

Relative error

\[
\epsilon_r = \frac{|a - \tilde{a}|}{|a|}
\]

1 = http://mathworld.wolfram.com/RoundoffError.html
Errors

Example:

The value of $\pi = 3.141592653589\ldots$ is to be stored on a base-10 system that allows 7 significant figures.

Chopping approximation $\Rightarrow \pi = 3.141592$
Absolute error $= |3.1415926535 - 3.141592|$
$= 0.000000653\ldots$

Rounding approximation $\Rightarrow \pi = 3.141593$
Absolute error $= |3.1415926535 - 3.141593|$
$= 0.000000346\ldots$
Fractional numbers in computers are usually represented using floating-point form:

\[ m \cdot b^e \]

- \( m \): mantissa
- \( b \): base of the number system being used
- \( e \): exponent

Example: in a floating-point base-10 system that allows only 4 decimal places to be stored, the quantity \( \frac{1}{34} = 0.029411765 \) would be stored as \( 0.2941 \times 10^{-1} \)

- Allows both fractions and very large numbers to be expressed on the computer
- Takes up more space
- Takes longer time to process
- Source of round-off error
In Matlab’s Command Window type in:

```matlab
>> a=0.0000123454981202
```

By default, Matlab displays numeric output as 5-digit scaled, fixed point values. Now change the display format to 15-digit scaled fixed point by typing:

```matlab
>> format long
```

and type the value of `a` again.

*These format settings only affect how numbers are displayed, not how Matlab computes or saves them.*
Numerical Error

• For numerical methods, the true value of a function is known from its analytical solution.

• However, in real-world applications, it is impossible to know the true value of a function \textit{a priori}.

• Hence, the percentage relative error:

\[ \varepsilon_r = \frac{|\text{current approx.} - \text{previous approx.}|}{|\text{current approx.}|} \times 100\% \]  

(1.1)
Maclaurin’s series

Let the power series for \( f(x) \) be

\[
f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \ldots
\]

where \( a_0, a_1, a_2, \ldots \) are constants.

At \( x = 0 \)

\[
f(0) = a_0, \text{ or } a_0 = f(0)
\]

\[
f'(x) = a_1 + 2a_2 x + 3a_3 x^2 + 4a_4 x^3 + \ldots
\]

\[
f'(0) = a_1, \text{ or } a_1 = f'(0)
\]
\[ f''(x) = 2a_2 + 6a_3x + 12a_4x^2 + \ldots \]
\[ f''(0) = 2a_2 = 2!a_2, \text{ or } a_2 = \frac{f''(0)}{2!} \]
\[ f'''(x) = 6a_3 + 24a_4x + \ldots \]
\[ f'''(0) = 6a_3 = 3!a_3, \text{ or } a_3 = \frac{f'''(0)}{3!} \]

Substituting for \(a_0, a_1, a_2, \ldots\) in \(f(x)\) gives:

\[
f(x) = f(0) + xf'(0) + \frac{x^2}{2!}f''(0) + \frac{x^3}{3!}f'''(0) + \ldots
\]

(1.2)
The resultant Maclaurin’s series must be convergent

\[ f(x) = f(0) + xf'(0) + \frac{x^2}{2!}f''(0) + \frac{x^3}{3!}f'''(0) + \ldots \]

(1) \( f(0) \neq \infty \)

(2) \( f'(0), f''(0), f'''(0), \ldots \neq \infty \)

(3) The resultant Maclaurin’s series must be convergent
Using Maclaurin’s series, at some point $Q$ in Figure above:

$$f(h) = f(0) + hf'(0) + \frac{h^2}{2!}f''(0) + \ldots$$
Example 1.1

Using Maclaurin series, determine the first four terms of the power series for \( \cos(x) \).
Example 1.1

Solution:
The constants needed for Maclaurin series are

\[ f(x) = \cos(x) \quad f(0) = \cos(0) = 1 \]
\[ f'(x) = -\sin(x) \quad f'(0) = -\sin(0) = 0 \]
\[ f''(x) = -\cos(x) \quad f''(0) = -\cos(0) = -1 \]
\[ f'''(x) = \sin(x) \quad f'''(0) = \sin(0) = 0 \]
\[ f^{iv}(x) = \cos(x) \quad f^{iv}(0) = \cos(0) = 1 \]
\[ f^{v}(x) = -\sin(x) \quad f^{v}(0) = -\sin(0) = 0 \]
Example 1.1

Hence, the power series

\[ f(x) = f(0) + x f'(0) + \frac{x^2}{2!} f''(0) + \frac{x^3}{3!} f'''(0) + \cdots \]

\[ \cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \]
Taylor series

If the y-axis and origin are moved \( a \) units to the left, the equation of the same curve relative to the new axis becomes \( y = f(a + x) \) and the function value at \( P \) is \( f(a) \).

At point \( Q \):

\[
f(a + h) = f(a) + hf'(a) + \frac{h^2}{2!} f''(a) + \cdots
\] (1.3)
Taylor series provides a means to predict a function value at one point \((x_{i+1})\) in terms of the function value and its derivatives at another point \((x_i)\):

\[
f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \ldots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n
\]

(1.4)

where:

\[
R_n = \frac{f^{(n+1)}(\xi)}{(n + 1)!}h^{n+1}
\]

\(n = \text{order of derivative}\)

\[h = x_{i+1} - x_i = \Delta x\]
Since $h = x_{i+1} - x_i$, sometimes Taylor series are written in ways that look a little different from eqn. (1.3) but in reality are completely equivalent, such as

\[
f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)f'(x_i) + \frac{1}{2!}(x_{i+1} - x_i)^2 f''(x_i) + \cdots + \frac{1}{n!}(x_{i+1} - x_i)^n f^n(x_i) + R_n
\]

(1.5)

If we want to predict a function backward, at point $(x_{i-1})$ in terms of the function and its derivatives at point $(x_i)$ where $h = x_i - x_{i-1}$, then

\[
f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!} f''(x_i) - \frac{h^3}{3!} f'''(x_i) + \cdots + \frac{h^n}{n!} f^n(x_i) + R_n
\]

(1.6)
Example 1.2

Use zero-through third-order Taylor series expansion to predict $f(3)$ for

$$f(x) = 25x^3 - 6x^2 + 7x - 88$$

using a base point at $x = 1$. Compute the true percent relative error for each approximation.
Example 1.2

Use zero-through third-order Taylor series expansion to predict \( f(3) \) for

\[
f(x) = 25x^3 - 6x^2 + 7x - 88
\]

using a base point at \( x = 1 \). Compute the true percent relative error for each approximation.

Solution

The true value of the function \( f(x) \) at \( x = 3 \) is \( f(3) = 554 \), which is the value that we are going to predict/approximate.

For \( n = 0 \), the Taylor series approximation is

\[
f(x_{i+1}) \approx f(x_i)
\]

\[
f(x_{i+1}) \approx 25(1)^3 - 6(1)^2 + 7(1) - 88 = -62
\]

and relative error \( \epsilon_r = \frac{|554 - (-62)|}{554} \times 100\% = 111.19\% \)
For \( n = 1 \), the first derivative is \( f'(x) = 75x^2 - 12x + 7 \), and the first order Taylor series approximation

\[
f(x_{i+1}) \approx f(x_i) + f'(x_i)h
\]

\[
f(x_{i+1}) \approx -62 + [75(1)^2 - 12(1) + 7](2) = 78
\]

and relative error \( \varepsilon_r = \frac{|554 - 78|}{554} \times 100\% = 85.92\% \)

For \( n = 2 \), the second derivative is \( f''(x) = 150x - 12 \), and the second order Taylor series approximation

\[
f(x_{i+1}) \approx f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2
\]

\[
f(x_{i+1}) \approx 78 + \left( \frac{150(1) - 12}{2!} \right)(2)^2 = 354
\]

and relative error \( \varepsilon_r = \frac{|554 - 354|}{554} \times 100\% = 36.10\% \)
For $n = 3$, the third derivative is $f'''(x) = 150$, and the third order Taylor series approximation

$$f(x_{i+1}) \approx f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3$$

$$f(x_{i+1}) \approx 354 + \frac{150}{3!}(2)^3 = 554$$

The Taylor series expansion to the third order derivative yields an exact estimate at $x_{i+1} = 3$,

hence, the remainder term is $R_3 = \frac{f^{(4)}(\xi)}{4!}h^4 = 0$
Taylor series can be used to estimate truncation errors.

The notion of truncation errors usually refers to errors introduced when a more complicated mathematical expression is “replaced” with a more elementary formula.

From the Taylor series expansion

\[ f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \ldots + R_n \]

we truncate the series after the first derivative term

\[ f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + R_1. \]
Truncation Errors

Rearranging the equation gives us

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

first-order approximation  \hspace{1cm} \text{truncation error}

Using

\[ R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!} (x_{i+1} - x_i)^{n+1} \]

for \( n = 1 \), we get

\[ \frac{R_1}{x_{i+1} - x_i} = \frac{f''(\xi)}{2!} (x_{i+1} - x_i) \]

or

\[ \frac{R_1}{x_{i+1} - x_i} = O(x_{i+1} - x_i) \]  \hspace{1cm} (1.7)
The problem with evaluating $f(x)$ is unknown because $x$ is unknown. We can overcome this if:

- $\tilde{x}$ is close to $x$, and
- $f(\tilde{x})$ is continuous and differentiable

We use Taylor series to compute $f(x)$ near $f(\tilde{x})$

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x}) + \frac{f''(\tilde{x})}{2}(x - \tilde{x})^2 + \ldots$$
**Error Propagation**

Dropping the second- and higher-order terms and rearranging gives us

\[ f(x) - f(\tilde{x}) \approx f'(\tilde{x})(x - \tilde{x}) \]

or

\[ \Delta f(\tilde{x}) = |f'(\tilde{x})| \Delta \tilde{x} \quad (1.8) \]

where

\[ \Delta f(\tilde{x}) = |f(x) - f(\tilde{x})| \quad \text{represents an estimate of the error of the function } f(x) \]

\[ \Delta \tilde{x} = |x - \tilde{x}| \quad \text{represents an estimate of the error of } x \]

This enables us to approximate the error in \( f(x) \) given the derivative of a function and an estimate of the error in \( x \).
Taylor series with two variables $x$ and $y$ can be described from the figure on the left. We want to determine a function at point B from a function and its derivatives at point A. The coordinates at both points are different, where:

- at A $\rightarrow$ function $f = f(a, b)$
- at B $\rightarrow$ function $f = f(a+\Delta x, b+\Delta y)$

also:

- at C $\rightarrow$ function $f = f(a, b+\Delta y)$
- at D $\rightarrow$ function $f = f(a+\Delta x, b)$
Taylor Series for Functions with More than One Variable

First we relate $f(a+\Delta x, b+\Delta y)$ at point B to the functions and its derivatives at point C. This involves changing only the $x$ coordinate while keeping $y$ constant, hence it is a typical one-dimensional approximation:

$$f(a + \Delta x, b + \Delta y) = f(a, b + \Delta y) + \frac{\partial f(a, b + \Delta y)}{\partial x} \Delta x$$

$$+ \frac{1}{2!} \frac{\partial^2 f(a, b + \Delta y)}{\partial x^2} \Delta x^2 + \cdots \quad (1.9)$$

Now we need approximation for the first term on the right hand side of eqn. (1.9), which is approximation at point C derived from function and its derivative at point A.
That is,

\[ f(a, b + \Delta y) = f(a, b) + \frac{\partial f(a, b)}{\partial y} \Delta y + \frac{1}{2!} \frac{\partial^2 f(a, b)}{\partial y^2} \Delta y^2 + \ldots \]  

(1.10)

All derivatives on the right hand side of eqn. (1.10) are evaluated at \((x = a, y = b)\). Now we turn our attention back to eqn. (1.9) and look at the second term on the right hand side where it involves derivative \(\partial f/\partial x\) evaluated at \((a, b+\Delta y)\) which needs to be expressed in terms of what is happening at \((x = a, y = b)\). We do this by defining

\[ g(x, y) = \frac{\partial f(x, y)}{\partial x} \]  

(1.11)
Then we write the Taylor series for $g(a, b+\Delta y)$ in complete analogy with that for $f$ in eqn. (1.10):

$$\frac{\partial f(a, b + \Delta y)}{\partial x} = g(a, b + \Delta y)$$

$$= g(a, b) + \frac{\partial g(a, b)}{\partial y} \Delta y + \frac{1}{2!} \frac{\partial^2 g(a, b)}{\partial y^2} \Delta y^2 + \cdots$$

$$= \frac{\partial f(a, b)}{\partial x} + \frac{\partial^2 f(a, b)}{\partial y \partial x} \Delta y + \cdots$$  

(1.12)

We need an approximation for the third term of eqn. (1.10), that is

$$\frac{\partial^2 f(a, b + \Delta y)}{\partial y^2} = \frac{\partial^2 f(a, b)}{\partial y^2}$$

(1.13)
Now, substituting eqns. (1.10), (1.12), and (1.13) into eqn. (1.9) and rearranging yields

\[
f(a + \Delta x, b + \Delta y) = f(a, b) + \left( \frac{\partial f(a, b)}{\partial x} \Delta x + \frac{\partial f(a, b)}{\partial y} \Delta y \right) \\
+ \frac{1}{2!} \left( \frac{\partial^2 f(a, b)}{\partial x^2} \Delta x^2 + 2 \frac{\partial^2 f(a, b)}{\partial x \partial y} \Delta x \Delta y + \frac{\partial^2 f(a, b)}{\partial y^2} \Delta y^2 \right) \\
+ \cdots
\]

(1.14)

which is the Taylor series for 2 variables (2 dimension) up to second order terms.
Taylor Series for Functions with More than One Variable

If all second-order and higher terms are dropped and rearrange, we get

$$f(a + \Delta x, b + \Delta y) - f(a, b) = \left| \frac{\partial f}{\partial x} \right| \Delta x + \left| \frac{\partial f}{\partial y} \right| \Delta y$$

$$\Delta f(x, y) = \left| \frac{\partial f}{\partial x} \right| \Delta x + \left| \frac{\partial f}{\partial y} \right| \Delta y$$

where

- $\Delta x$ is the estimate of the error in $x$
- $\Delta y$ is the estimate of the error in $y$
References


• Higher Engineering Mathematics, John Bird.

• All You Wanted To Know About Mathematics but Were Afraid To Ask, Louis Lyons.