Calculus for the Life Sciences

Lecture Notes – Numerical Methods for Differential Equations

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Outline

Introduction

Introduction

- Differential Equations provide useful models
- Realistic Models are often Complex
- Most differential equations can **not** be solved exactly
- Develop numerical methods to solve differential equations

Pollution in a Lake 1

Pollution in a Lake

- Previously studied a simple model for **Lake Pollution**
- Complicate by adding time-varying pollution source
- Include periodic flow for seasonal effects
- Present numerical method to simulate the model

Pollution in a Lake

Non-point Source of Pollution and Seasonal Flow Variation

- Consider a non-point source, such as agricultural runoff of pesticide
  - Assume a pesticide is removed from the market
  - If the pesticide doesn't degrade, it leaches into runoff water
- Concentration of the pesticide in the river being time-varying
- Typically, there is an exponential decay after the use of the pesticide is stopped
  - Example of concentration

$$p(t) = 5\,e^{-0.002t}$$

Pollution in a Lake

Including Seasonal Effects

- River flows vary seasonally
- Assume lake maintains a constant volume, V
- Seasonal flow (time varying) entering is reflected with same outflowing flow
  - Example of sinusoidal annual flow

$$f(t) = 100 + 50\cos(0.0172t)$$

Pollution in a Lake

Mathematical Model: Use Mass Balance

The change in amount of pollutant =
Amount entering - Amount leaving

- Amount entering is concentration of the pollutant in the river times the flow rate of the river

$$f(t)p(t)$$

- Amount leaving a well-mixed lake is concentration of the pollutant in the lake times the flow rate of the river

$$f(t)c(t)$$

- The amount of pollutant in the lake, $a(t)$, satisfies

$$\frac{da}{dt} = f(t)p(t) - f(t)c(t)$$

Pollution in a Lake

Mathematical Model: Let the concentration be $c(t) = \frac{a(t)}{V}$

$$\frac{dc(t)}{dt} = \frac{f(t)}{V}(p(t) - c(t)) \quad \text{with} \quad c(0) = c_0$$

- Assume that the volume of the lake is 10,000 m^3 and the initial level of pollutant in the lake is $c_0 = 5$ ppm
- With $p(t)$ and $f(t)$ from before, model is

$$\frac{dc(t)}{dt} = (0.01 + 0.005\cos(0.0172t))(5\,e^{-0.002t} - c(t))$$

- Complicated, but an exact solution exists
- Show an easier numerical method to approximate the solution

Euler's Method 1

Initial Value Problem: Consider

$$\frac{dy}{dt} = f(t,y) \quad \text{with} \quad y(t_0) = y_0$$

- From the definition of the derivative

$$\frac{dy}{dt} = \lim_{h \to 0} \frac{y(t+h) - y(t)}{h}$$

- Instead of taking the limit, fix h, so

$$\frac{dy}{dt} \approx \frac{y(t+h) - y(t)}{h}$$

- Substitute into the differential equation and with algebra write

$$y(t+h) \approx y(t) + hf(t,y)$$

Euler's Method 2

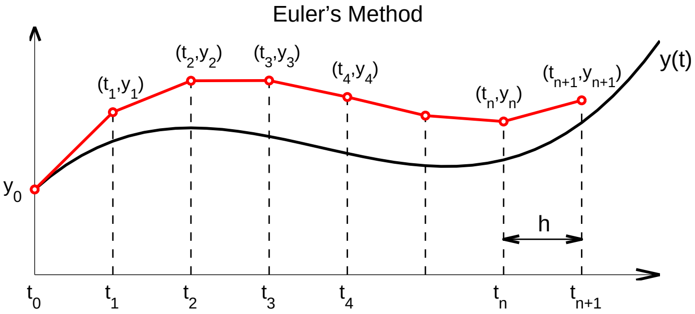
Euler's Method for a fixed h is

$$y(t+h) = y(t) + hf(t,y)$$

- Geometrically, Euler's method looks at the slope of the tangent line
  - The approximate solution follows the tangent line for a time step h
  - Repeat this process at each time step to obtain an approximation to the solution
- The accuracy of this method to track the solution depends on the length of the time step, h, and the nature of the function $f(t,y)$
- This technique is rarely used as it has very bad convergence properties to the actual solution

Euler's Method

Graph of Euler's Method



Euler's Method

Euler's Method Formula: Euler's method is just a discrete dynamical system for approximating the solution of a continuous model

- Let $t_{n+1} = t_n + h$
- Define $y_n = y(t_n)$
- The initial condition gives $y(t_0) = y_0$
- **Euler's Method** is the discrete dynamical system

$$y_{n+1} = y_n + h\,f(t_n, y_n)$$

- Euler's Method only needs the initial condition to start and the right hand side of the differential equation (the **slope field**), $f(t,y)$ to obtain the approximate solution

Malthusian Growth Example 1

Malthusian Growth Example: Consider the model

$$\frac{dP}{dt} = 0.2\,P \qquad \text{with} \qquad P(0) = 50$$

Find the exact solution and approximate the solution with Euler's Method for $t \in [0, 1]$ with $h = 0.1$

Solution: The exact solution is

$$P(t) = 50\,e^{0.2t}$$

Malthusian Growth Example 2

Solution (cont): The **Formula for Euler's Method** is

$$P_{n+1} = P_n + h\,0.2\,P_n$$

The initial condition $P(0) = 50$ implies that $t_0 = 0$ and $P_0 = 50$

Create a table for the Euler iterates

t_n	P_n
$t_0 = 0$	$P_0 = 50$
$t_1 = t_0 + h = 0.1$	$P_1 = P_0 + 0.1(0.2P_0) = 50 + 1 = 51$
$t_2 = t_1 + h = 0.2$	$P_2 = P_1 + 0.1(0.2P_1) = 51 + 1.02 = 52.02$
$t_3 = t_2 + h = 0.3$	$P_3 = P_2 + 0.1(0.2P_2) = 52.02 + 1.0404 = 53.0604$

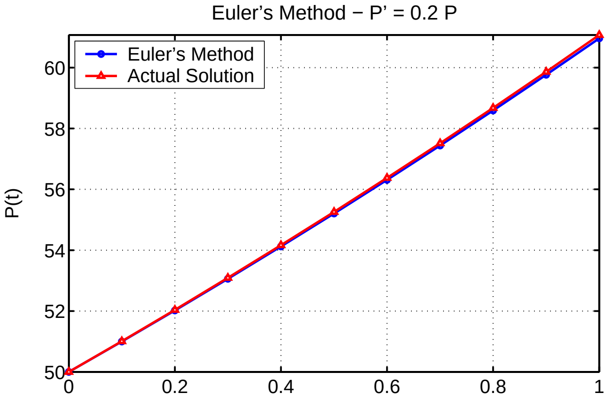
Malthusian Growth Example 3

Solution (cont): Iterations are easily continued - Below is table of the actual solution and the Euler's method iterates

t	Euler Solution	Actual Solution
0	50	50
0.1	51	51.01
0.2	52.02	52.041
0.3	53.060	53.092
0.4	54.122	54.164
0.5	55.204	55.259
0.6	56.308	56.375
0.7	57.434	57.514
0.8	58.583	58.676
0.9	59.755	59.861
1.0	60.950	61.070

Malthusian Growth Example

Graph of Euler's Method for Malthusian Growth Example



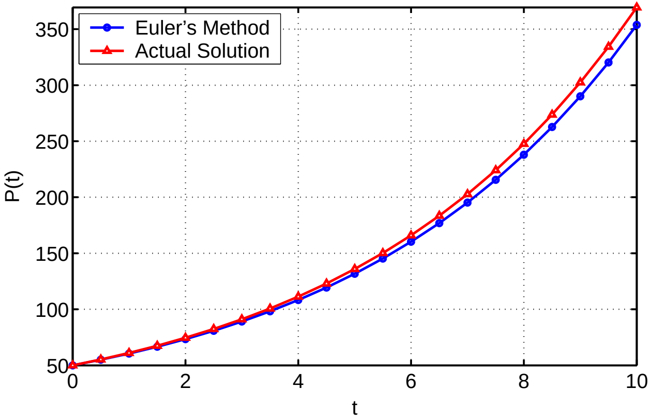
Malthusian Growth Example 5

Error Analysis and Larger Stepsize

- The table and the graph shows that Euler's method is tracking the solution fairly well over the interval of the simulation
- The error at $t = 1$ is only 0.2%
- However, this is a fairly short period of time and the stepsize is relatively small
- What happens when the stepsize is increased and the interval of time being considered is larger?

Malthusian Growth Example

Graph of Euler's Method with $h = 0.5$



There is a 9% error in the numerical solution at $t = 10$

Euler's Method with $f(t, y)$ 1

Euler's Method with $f(t, y)$: Consider the model

$$\frac{dy}{dt} = y + t \qquad \text{with} \qquad y(0) = 3$$

Find the approximate solution with Euler's Method at $t = 1$ with stepsize $h = 0.25$

Compare the Euler solution to the exact solution

$$y(t) = 4\,e^{t} - t - 1$$

Euler's Method with $f(t,y)$ 2

Solution: Verify the actual solution:

1. Initial condition:

$$y(0) = 4\,e^0 - 0 - 1 = 3$$

2. The differential equation:

$$\begin{aligned} \frac{dy}{dt} &= 4\,e^t - 1 \\ y(t) + t &= 4\,e^t - t - 1 + 1 = 4\,e^t - 1 \end{aligned}$$

Euler's formula for this problem is

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

Euler's Method with $f(t, y)$ 3

Solution (cont): Euler's formula with $h = 0.25$ is

$$y_{n+1} = y_n + 0.25(y_n + t_n)$$

t_n	Euler solution y_n
$t_0 = 0$	$y_0 = 3$
$t_1 = 0.25$	$y_1 = y_0 + h(y_0 + t_0) = 3 + 0.25(3 + 0) = 3.75$
$t_2 = 0.5$	$y_2 = y_1 + h(y_1 + t_1) = 3.75 + 0.25(3.75 + 0.25) = 4.75$
$t_3 = 0.75$	$y_3 = y_2 + h(y_2 + t_2) = 4.75 + 0.25(4.75 + 0.5) = 6.0624$
$t_4 = 1$	$y_4 = y_3 + h(y_3 + t_3) = 6.0624 + 0.25(6.0624 + 0.75) = 7.7656$

Euler's Method with $f(t,y)$ 4

Solution (cont): Error Analysis

- $y_4 = 7.7656$ corresponds to the approximate solution of $y(1)$
- The actual solution gives $y(1) = 8.87312$, so the Euler approximation with this large stepsize is not a very good approximation of the actual solution with a 12.5% error
- If the stepsize is reduced to $h = 0.1$, then Euler's method requires 10 steps to find an approximate solution for $y(1)$
- It can be shown that the Euler approximate of $y(1)$, $y_{10} = 8.37497$, which is better, but still has a 5.6% error

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Numerical Solution of the Lake Problem 1

Numerical Solution of the Lake Problem Earlier described a more complicated model for pollution entering a lake with an oscillatory flow rate and an exponentially falling concentration of the pollutant entering the lake via the river

- The initial value problem with $c(0) = 5 = c_0$

$$\frac{dc}{dt} = (0.01 + 0.005\,\cos(0.0172t))(5\,e^{-0.002t} - c(t))$$

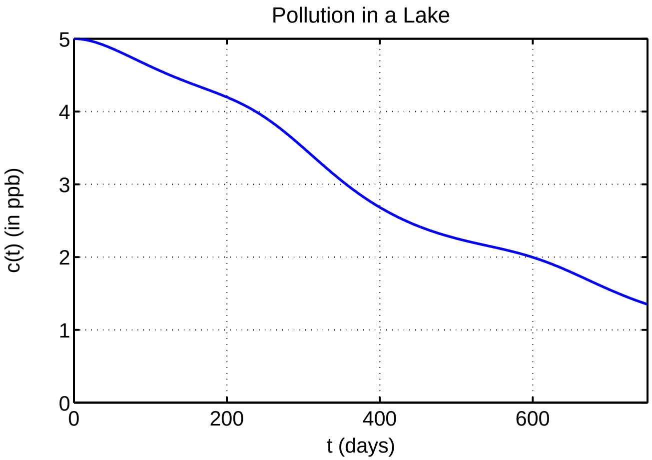
- The **Euler's formula** is

$$c_{n+1} = c_n + h(0.01 + 0.005\,\cos(0.0172t_n))(5\,e^{-0.002t_n} - c_n)$$

- The model was simulated for 750 days with $h = 1$

Numerical Solution of the Lake Problem 2

Graph of Simulation



Numerical Solution of the Lake Problem 3

Simulation: This solution shows a much more complicated behavior for the dynamics of the pollutant concentration in the lake

- Could you have predicted this behavior or determined quantitative results, such as when the pollution level dropped below 2 ppm?
- This example is much more typical of what we might expect from more realistic biological problems
- The numerical methods allow the examination of more complex situations, which allows the scientist to consider more options in probing a given situation
- Euler's method for this problem traces the actual solution very well, but better numerical methods are usually used

Euler Example A 1

Euler Example A: Consider the initial value problem

$$\frac{dy}{dt} = -2\,y^2 \qquad \text{with} \qquad y(0) = 2$$

Skip Example

- With a stepsize of $h = 0.2$, use Euler's method to approximate $y(t)$ at $t = 1$
- Show that the actual solution of this problem is

$$y(t) = \frac{2}{4\,t + 1}$$

- Determine the percent error between the approximate solution and the actual solution at $t = 1$

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Euler Example A 2

Solution: Euler's formula with $h = 0.2$ for this example is

$$y_{n+1} = y_n - h(2y_n^2) = y_n - 0.4\, y_n^2$$

t_n	y_n
$t_0 = 0$	$y_0 = 2$
$t_1 = t_0 + h = 0.2$	$y_1 = y_0 - 0.4y_0^2 = 2 - 0.4(4) = 0.4$
$t_2 = t_1 + h = 0.4$	$y_2 = y_1 - 0.4y_1^2 = -0.4 - 0.4(0.16) = 0.336$
$t_3 = t_2 + h = 0.6$	$y_3 = y_2 - 0.4y_2^2 = 0.336 - 0.4(0.1129) = 0.2908$
$t_4 = t_3 + h = 0.8$	$y_4 = y_3 - 0.4y_3^2 = 0.2908 - 0.4(0.08459) = 0.2570$
$t_5 = t_4 + h = 1.0$	$y_5 = y_4 - 0.4y_4^2 = 0.2570 - 0.4(0.06605) = 0.2306$

Euler Example A

Solution (cont): Verify that the solution is

$$y(t) = \frac{2}{4t+1} = 2(4t+1)^{-1}$$

- Compute the derivative

$$\frac{dy}{dt} = -2(4t+1)^{-2}(4) = -8(4t+1)^{-2}$$

- However, $-2\,(y(t))^2 = -2(2(4t+1)^{-1})^2 = -8(4t+1)^{-2}$
- Thus, the differential equation is satisfied by the solution that is given
- At $t = 1$, $y(1) = 0.4$
- The percent error is

$$100 \times \frac{y_{Euler}(1) - y_{actual}}{y_{actual}(1)} = \frac{100(0.2306 - 0.4)}{0.4} = -42.4\%$$

Euler Example B

Euler Example B: Consider the initial value problem

$$\frac{dy}{dt} = 2\frac{t}{y} \qquad \text{with} \qquad y(0) = 2$$

Skip Example

- With a stepsize of $h = 0.25$, use Euler's method to approximate $y(t)$ at $t = 1$
- Show that the actual solution of this problem is

$$y(t) = \sqrt{2\,t^2 + 4}$$

- Determine the percent error between the approximate solution and the actual solution at $t = 1$

Euler Example B

Solution: Euler's formula with $h = 0.25$ for this example is

$$y_{n+1} = y_n + h\left(\frac{2t_n}{y_n}\right) = y_n + 0.5\left(\frac{t_n}{y_n}\right)$$

t_n	y_n
$t_0 = 0$	$y_0 = 2$
$t_1 = t_0 + h = 0.25$	$y_1 = y_0 + 0.5t_0/y_0 = 2 + 0.5(0/2) = 2$
$t_2 = t_1 + h = 0.5$	$y_2 = y_1 + 0.5t_1/y_1 = 2 + 0.5(0.25/2) = 2.0625$
$t_3 = t_2 + h = 0.75$	$y_3 = y_2 + 0.5t_2/y_2 = 2.0625 + 0.5(0.5/2) = 2.1875$
$t_4 = t_3 + h = 1.0$	$y_4 = y_3 + 0.5t_3/y_3 = 2.1875 + 0.5(0.75/2) = 2.375$

Euler Example B 3

Solution (cont): Verify that the solution is

$$y(t) = (2t^2 + 4)^{0.5}$$

- Compute the derivative

$$\frac{dy}{dt} = 0.5(2t^2 + 4)^{-0.5}(4t) = 2t(2t^2 + 4)^{-0.5}$$

- However, $2t/y(t) = 2t/(2t^2 + 4)^{0.5} = 2t(2t^2 + 4)^{-0.5}$
- Thus, the differential equation is satisfied by the solution that is given
- At $t = 1$, $y(1) = \sqrt{6} = 2.4495$
- The percent error is

$$100 \times \frac{y_{Euler}(1) - y_{actual}}{y_{actual}(1)} = \frac{100(2.375 - 2.4495)}{2.4495} = -3.04\%$$

Time-varying Population Model 1

Time-varying Population Model: A Malthusian growth model with a time-varying growth rate is

$$\frac{dP}{dt} = (0.2 - 0.02\,t)P \qquad \text{with} \qquad P(0) = 5000$$

Skip Example

- With a stepsize of $h = 0.2$, use Euler's method to approximate $P(t)$ at $t = 1$
- Show that the actual solution of this problem is

$$P(t) = 5000\,e^{0.2t - 0.01t^2}$$

- Determine the percent error between the approximate solution and the actual solution at $t = 1$
- Use the actual solution to find the maximum population of this growth model and when it occurs

Time-varying Population Model 2

Solution: Euler's formula with $h = 0.2$ for this example is

$$P_{n+1} = P_n + h(0.2 - 0.02t_n)P_n$$

t_n	P_n
$t_0 = 0$	$P_0 = 5000$
$t_1 = t_0 + h = 0.2$	$P_1 = P_0 + 0.2(0.2 - 0.02t_0)P_0 = 5200$
$t_2 = t_1 + h = 0.4$	$P_2 = P_1 + 0.2(0.2 - 0.02t_1)P_1 = 5403.8$
$t_3 = t_2 + h = 0.6$	$P_3 = P_2 + 0.2(0.2 - 0.02t_2)P_2 = 5611.35$
$t_4 = t_3 + h = 0.8$	$P_4 = P_3 + 0.2(0.2 - 0.02t_3)P_3 = 5822.3$
$t_5 = t_4 + h = 1.0$	$P_5 = P_4 + 0.2(0.2 - 0.02t_4)P_4 = 6036.6$

Time-varying Population Model

Solution (cont): Verify that the solution is

$$P(t) = 5000\, e^{0.2t - 0.01t^2}$$

- Compute the derivative

$$\frac{dP}{dt} = 5000\, e^{0.2t-0.01t^2}(0.2 - 0.02\,t)$$

- However, $(0.2 - 0.02\,t)P(t) = 5000\, e^{0.2t-0.01t^2}(0.2 - 0.02\,t)$
- Thus, the differential equation is satisfied by the solution that is given
- At $t = 1$, $P(1) = 6046.2$
- The percent error is

$$100 \times \frac{P_{Euler}(1) - P_{actual}}{P_{actual}(1)} = \frac{100(6036.6 - 6046.2)}{6046.2} = -0.16\%$$

Time-varying Population Model

Solution (cont): Maximum of the population

- The **maximum** is when the derivative is equal to zero
- Because $P(t)$ is positive, the derivative is zero (growth rate falls to zero) when $0.2 - 0.02\,t = 0$ or $t = 10$ years
- This is substituted into the actual solution

$$P(10) = 5000\,e^{1} = 13,591.4$$

Improved Euler's Method

Improved Euler's Method: There are many techniques to improve the **numerical solutions of differential equations**

- Euler's Method is simple and intuitive, but lacks accuracy
- Numerical methods are available through standard software, like Maple or MatLab
- Some of the best are a class of single step methods called **Runge-Kutta methods**
- The simplest of these is called the Improved Euler's method
- Showing why this technique is significantly better than Euler's method is beyond the scope of this course

Improved Euler's Method 2

Improved Euler's Method Formula: This technique is an easy extension of Euler's Method

- The Improved Euler's method uses an average of the Euler's method and an Euler's method approximation to the function
- Let $y(t_0) = y_0$ and define $t_{n+1} = t_n + h$ and the approximation of $y(t_n)$ as y_n
- First approximate y by Euler's method, so define

$$ye_n = y_n + h\,f(t_n, y_n)$$

- The Improved Euler's formula starts with $y(t_0) = y_0$ and becomes the discrete dynamical system

$$y_{n+1} = y_n + \frac{h}{2}\left(f(t_n, y_n) + f(t_n + h, ye_n)\right)$$

Example: Improved Euler's Method

Example: Improved Euler's Method: Consider the initial value problem:

$$\frac{dy}{dt} = y + t \qquad \text{with} \qquad y(0) = 3$$

- The solution to this differential equation is

$$y(t) = 4\,e^{t} - t - 1$$

- Numerically solve this using Euler's Method and Improved Euler's Method using $h = 0.1$
- Compare these numerical solutions

Example: Improved Euler's Method 2

Solution: Let $y_0 = 3$, the Euler's formula is

$$y_{n+1} = y_n + h(y_n + t_n) = y_n + 0.1(y_n + t_n)$$

The Improved Euler's formula is

$$ye_n = y_n + h(y_n + t_n) = y_n + 0.1(y_n + t_n)$$

with

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{2}\left((y_n + t_n) + (ye_n + t_n + h)\right) \\ y_{n+1} &= y_n + 0.05\left(y_n + ye_n + 2\,t_n + 0.1\right) \end{aligned}$$

Example: Improved Euler's Method 3

Solution: Below is a table of the numerical computations

t	Euler's Method	Improved Euler	Actual
0	$y_0 = 3$	$y_0 = 3$	$y(0) = 3$
0.1	$y_1 = 3.3$	$y_1 = 3.32$	$y(0.1) = 3.3207$
0.2	$y_2 = 3.64$	$y_2 = 3.6841$	$y(0.2) = 3.6856$
0.3	$y_3 = 4.024$	$y_3 = 4.0969$	$y(0.3) = 4.0994$
0.4	$y_4 = 4.4564$	$y_4 = 4.5636$	$y(0.4) = 4.5673$
0.5	$y_5 = 4.9420$	$y_5 = 5.0898$	$y(0.5) = 5.0949$
0.6	$y_6 = 5.4862$	$y_6 = 5.6817$	$y(0.6) = 5.6885$
0.7	$y_7 = 6.0949$	$y_7 = 6.3463$	$y(0.7) = 6.3550$
0.8	$y_8 = 6.7744$	$y_8 = 7.0912$	$y(0.8) = 7.1022$
0.9	$y_9 = 7.5318$	$y_9 = 7.9247$	$y(0.9) = 7.9384$
1	$y_{10} = 8.3750$	$y_{10} = 8.8563$	$y(1) = 8.8731$

Example: Improved Euler's Method 4

Solution: Comparison of the numerical simulations

- It is very clear that the Improved Euler's method does a substantially better job of tracking the actual solution
- The Improved Euler's method requires only one additional function, $f(t, y)$, evaluation for this improved accuracy
- At $t = 1$, the Euler's method has a -5.6% error from the actual solution
- At $t = 1$, the Improved Euler's method has a -0.19% error from the actual solution