CHEE 3602 – Topic 7: Ordinary differential equations

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Euler method

Euler method

The Euler method is convenient for introducing the general method to solving ODEs.

But, it is far too inaccurate for practical use and is only useful as a building block for more advanced techniques.

Euler method

The analytical derivative can be approximated as a finite difference:

$$f(x, y) = \frac{\mathrm{d}y}{\mathrm{d}x} \approx \frac{\Delta y}{\Delta x}$$

So, given some arbitrary point (x_i, y_i):

$$f(x_i, y_i) \approx \frac{y_{i+1} - y_i}{\Delta x}$$

$$y_{i+1} = y_i + f(x_i, y_i)\Delta x$$

$$y_{i+1} = y_i + f(x_i, y_i)h$$

Where Δx (also known as the step size h) should be as small as possible to ensure accuracy.

Algorithm summary

1. Select a step size h
2. Select a starting point x_i where the value of y_i is known
3. Calculate the derivative at x_i from the problem statement — note that $\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y)$ is given
4. Calculate new $y_{i+1} = y_i + f(x_i)h$ at $x_{i+1} = x_i + h$
5. Repeat until x_n equals to or exceeds desired value (which will depend on specific application/problem)

The overall output is a set of (x, y) points that approximates the true (but unknown) function $y(x)$.

Example

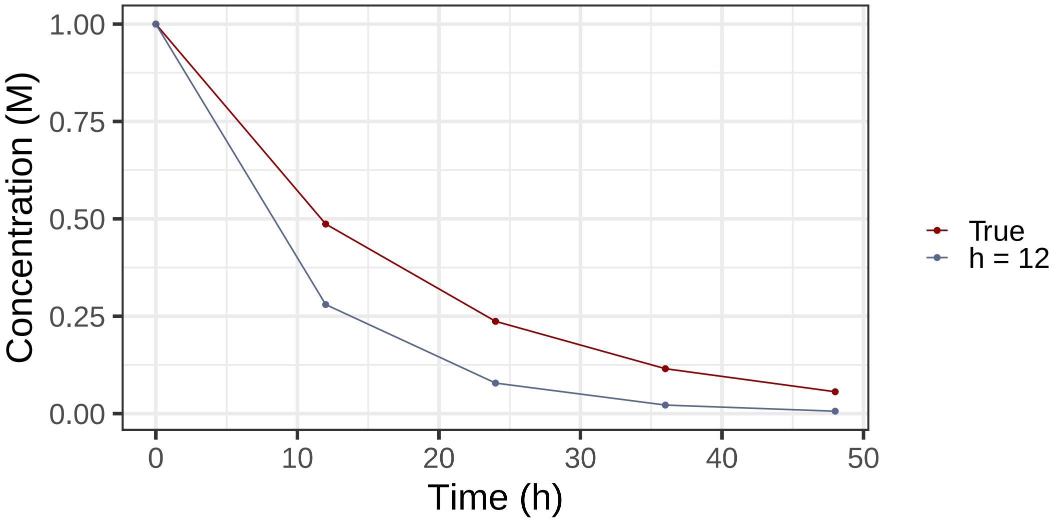
Example 2

Given a first order decay rate of 0.06 h^{-1} and a starting concentration of 1 M at 0 hours, find the concentration of compound A at 12, 24, 36, and 48 hours using the Euler method.

$$\frac{dC_A}{dt} = -0.06C_A$$

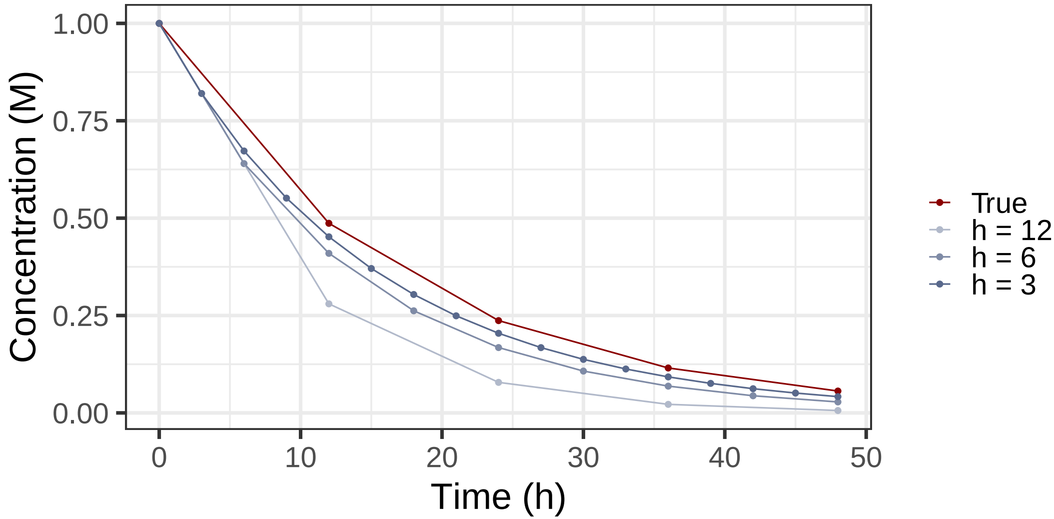
Accuracy

The equation from the previous example can be integrated directly to compare the estimate and true values:



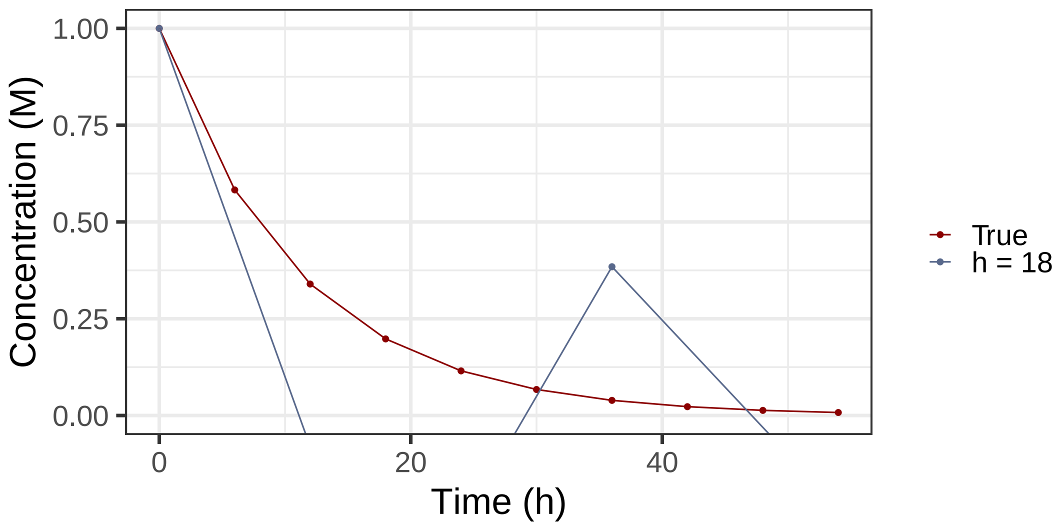
Accuracy

What happens if h changes?



Stability

Look what happens to the Euler method if h gets too big:



This oscillation is an indicator of instability.

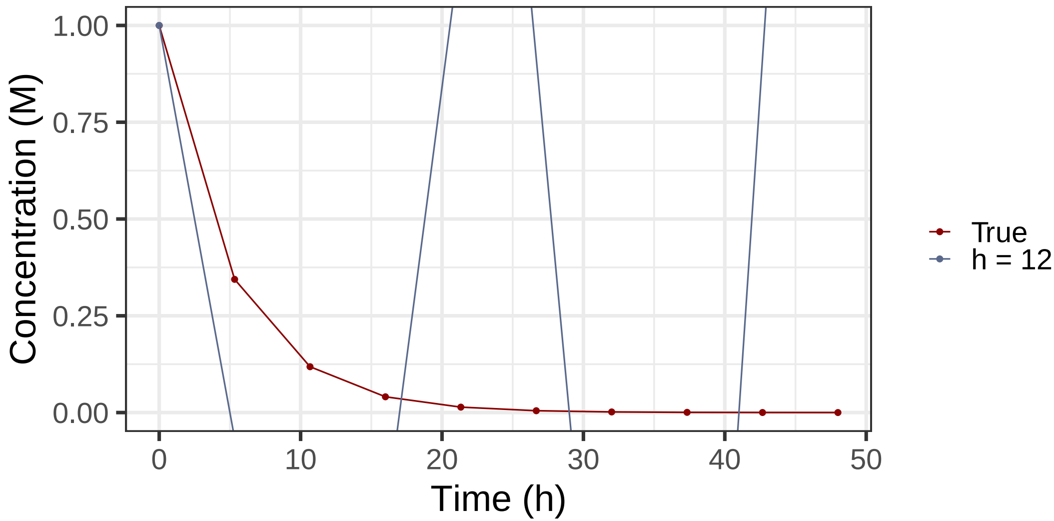
Stability

ODE stability analysis is a whole topic of numerical methods that will not be covered in this course.

In principle, an unstable solution is one that results in an unbounded solution when the true function is bounded — often observed as oscillations where no oscillations ought to be.

Stability

To see the effect of a relatively big step size, consider a faster decay rate:



And note the oscillations.

Stiffness

- In general, stability can be ensured by using small step sizes
- However, some types of problems place extreme demands on step size
  - known as stiff
- Unfortunately, it is not always known ahead of time which problems will be stiff

Stiffness

Although one definition of a stiff problem is literally "a problem that exhibits an unusual amount of instability" (which is not particularly helpful), one source of instability is large differences in the "timescale" of different terms:

$$y(t) = e^{-10t} sin(t) + e^{-0.1t}$$

The implicit approach

One way to deal with instability (without decreasing step size) is to use an implicit approach.

Recall the Euler method equation:

$$y_{i+1} = y_i + f(x_i, y_i)h$$

This approach is called explicit because the right hand side can be calculated directly (explicitly)

Alternatively, the implicit method is used to solve for the derivative at the unknown point:

$$y_{i+1} = y_i + f(x_{i+1}, y_{i+1})h$$

The implicit approach

Compare the explicit and implicit methods starting from the point $(0, 1)$ using the ODE equation from the slides above and $h = 0.1$:

$$f(x, y) = -0.06y$$

Explicit:

$$y_{i+1} = y_i + f(x_i, y_i)h$$
$$y_{i+1} = 1 - 0.06(1)0.1$$

Implicit:

$$y_{i+1} = y_i + f(x_{i+1}, y_{i+1})h$$
$$y_{i+1} = 1 - 0.06y_{i+1}0.1$$

The implicit approach

Whereas the explicit approach allows for direct calculation, the implicit equation requires some re-arranging to solve for y_{i+1}:

$$
\begin{aligned}
y_{i+1} &= y_i + f(x_{i+1}, y_{i+1})h \\
&= 1 - 0.06y_{i+1}0.1 \\
y_{i+1} + 0.06y_{i+1}0.1 &= 1 \\
y_{i+1}(1 + (0.06).1) &= 1 \\
y_{i+1} &= \frac{1}{1 + (0.06)0.1} \\
&= 0.994
\end{aligned}
$$

In practice

Note that the “re-arranging” in the previous slide made use of algebra that was specific to the particular problem.

Name one numerical method that can be used to solve the general equation — regardless of what $f(x, y)$ is:

$$y_{i+1} = y_i + f(x_{i+1}, y_{i+1})h$$

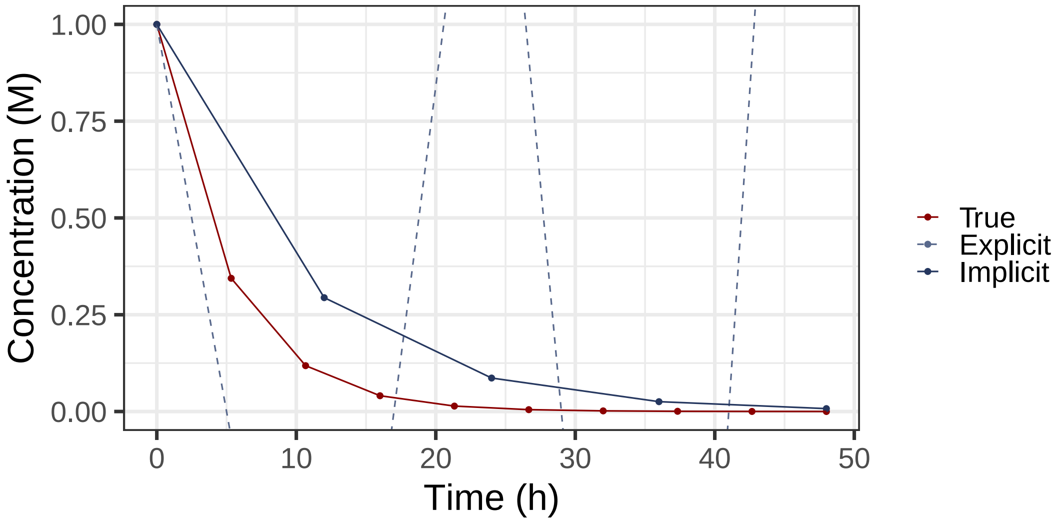
In practice

The implicit approach requires solving a (likely nonlinear) equation at every single step — resulting in a much slower process.

But (low order) implicit methods guarantee stability.

In practice

Going back to the previous example:



Clearly, the implicit method is much more stable.

Example

Example 3

Given a first order decay rate of 0.06 h^{-1} and a starting concentration of 1 M at 0 hours, find the concentration of compound A at 12, 24, 36, and 48 hours using the implicit Euler method.

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = -0.06C_A$$

Leaving Euler methods behind

Although the Euler methods were useful for demonstrating the core principles of solving ODEs, there are much better methods available for solving ODEs. The next two subsections will introduce two general improvements: the use of multiple points and adaptive step sizes.