Computational Physics
Lecture 11 – Evaluating Finite Difference Methods

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Slides available from https://bb.imperial.ac.uk/

Outline

Goals

By the end of this lecture, you should be able to

- Determine if a given finite difference equation is actually a consistent representation of the DE you want to solve
- Determine the expected numerical accuracy of a given finite difference method
- Evaluate the stability properties of a finite differencing scheme

Outline

1. Consistency
2. Accuracy
3. Stability & Convergence

Make sure you are solving the right ODE...

Given a finite difference expression, you can work out what DE it actually exactly corresponds to.
$\rightarrow$ always a good consistency check to do before you run off writing and optimising code!

Start with your finite difference expression – e.g. for the Euler Method:

$$y(x_n + h) \approx y(x_n) + h\,f(x_n, y_n) \tag{1}$$

Taylor expand the lefthand side around $x = x_n$:

$$y(x_n) + y'(x_n)h + \frac{y''(x_n)}{2}h^2 + \frac{y'''(x_n)}{3!}h^3 + \ldots \approx y(x_n) + h\,f(x_n, y_n) \tag{2}$$

Make sure you are solving the right ODE. . .

$$y(x_n) + y'(x_n)h + \frac{y''(x_n)}{2}h^2 + \frac{y'''(x_n)}{3!}h^3 \;\; + \ldots \approx y(x_n) + h\,f(x_n, y_n)$$

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$$\cancel{y(x_n)} + y'(x_n)\cancel{h} + \frac{y''(x_n)}{2}h^{\cancel{2}} + \frac{y'''(x_n)}{3!}h^{\cancel{3}2} + \ldots \approx \cancel{y(x_n)} + h\,f(x_n, y_n)$$

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$$
\begin{gathered}
y(x_n) + y'(x_n)h + \frac{y''(x_n)}{2}h^2 + \frac{y'''(x_n)}{3!}h^3 + \ldots \approx y(x_n) + h\,f(x_n, y_n) \\
\cancel{y(x_n)} + y'(x_n)\cancel{h} + \frac{y''(x_n)}{2}h^{\cancel{2}} + \frac{y'''(x_n)}{3!}h^{\cancel{3}2} + \ldots \approx \cancel{y(x_n)} + h\,f(x_n, y_n) \\
y'(x_n) = f(x_n, y_n) - \frac{y''(x_n)}{2}h - \frac{y'''(x_n)}{3!}h^2 - \ldots
\end{gathered}
$$

Make sure you are solving the right ODE...

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$$y'(x_n) = f(x_n, y_n) - \frac{y''(x_n)}{2}h - \frac{y'''(x_n)}{3!}h^2 - \ldots$$

$\Longrightarrow$ same as the desired DE $y'(x) = f(x, y)$ to order $\mathcal{O}(h)$.

This **modified differential equation** is the one that the finite difference scheme is actually solving.

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$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \ldots$$

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$$
\begin{aligned}
y(x+h) &= y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \dots \\
&= y(x) + hy'(x) + \mathcal{O}(h^2)
\end{aligned}
$$

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Question: So how are these equivalent?

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Question: So how are these equivalent?

Answer: global (total) error is the sum of error in each step:

$$\textbf{global error} \approx \text{local error} \times \text{number of steps}$$

Assuming we have properly normalised variables so that x varies over the unit interval or thereabouts, these terms are of order

$$\mathcal{O}(\text{local error}) \times \mathcal{O}(\text{number of steps}) = \mathcal{O}(h^2) \times \mathcal{O}(1/h) = \mathcal{O}(h)$$

Make sure you are getting a precise result. . .

$\rightarrow$ A method is "*n*th-order" if it has local error $\mathcal{O}(h^{n+1})$ and global error $\mathcal{O}(h^n)$.

$\Longrightarrow$ Euler Method is a first-order finite difference scheme.

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$\implies$ Euler Method is a first-order finite difference scheme.

Also remember that floating-point roundoff error accumulates as you keep taking each step:

$\rightarrow$ with roundoff error μ at each step, actual error at each step is $\mathcal{O}(\mu + h^2)$

$\rightarrow$ global error is then actually $\mathcal{O}(\frac{\mu}{h} + h)$

$\implies$ there is no gain in taking h arbitrarily small – actually there is a 'sweet spot' when $h \sim \sqrt{\mu}$

Outline

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Take error at step n to be ϵ_n:

$$\tilde{y}_n = y_n + \epsilon_n, \tag{3}$$

Stability requires that the error from each step decreases or stays steady from step to step:

$$\left| \frac{\epsilon_{n+1}}{\epsilon_n} \right| \leq 1 \tag{4}$$

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Only stable methods converge — unstable ones diverge as you take more steps.

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You can work this out by substituting the finite difference rule into the expression for the $n+1$th value

$$\tilde{y}_{n+1} = y_{n+1} + \epsilon_{n+1}, \tag{5}$$

and linearising the resulting expression about $y = y_n$, then rearranging to get an expression for $\epsilon_{n+1}/\epsilon_n$.

Stability

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1. Take the expression for the error on the $n+1$th value:

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Now substitute in the finite difference rule for the Euler Method:

$$\tilde{y}(x_n + h) = \tilde{y}(x_n) + h\,f(x_n, \tilde{y}_n) \tag{7}$$

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$$\begin{aligned} \tilde{y}(x_n+h) &= \tilde{y}(x_n) + h\,f(x_n,\tilde{y}_n) && (7) \\ &= y(x_n) + \epsilon_n + h\,f(x_n, y_n+\epsilon_n) && (8) \end{aligned}$$

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This gives

$$y(x_n + h) + \epsilon_{n+1} = y(x_n) + \epsilon_n + h\, f(x_n, y_n + \epsilon_n) \tag{9}$$

Stability

2. Now linearise this expression

$$y(x_n + h) + \epsilon_{n+1} = y(x_n) + \epsilon_n + h\,f(x_n, y_n + \epsilon_n) \qquad (10)$$

around $y = y_n$.

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$$y(x_n + h) + \epsilon_{n+1} = y(x_n) + \epsilon_n + h\, f(x_n, y_n + \epsilon_n) \qquad (10)$$

around $y = y_n$. To first order in ϵ_n, we have

$$f(x_n, y_n + \epsilon_n) = f(x_n, y_n) + \epsilon_n \frac{\partial f}{\partial y}(x_n) + \mathcal{O}(\epsilon_n^2). \qquad (11)$$

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Therefore, the linearised version is

$$\begin{aligned} y(x_n + h) + \epsilon_{n+1} = \quad & y(x_n) + \epsilon_n + h\left[f(x_n, y_n) + \epsilon_n \tfrac{\partial f}{\partial y}(x_n)\right. \\ & \left. + \mathcal{O}(\epsilon_n^2)\right] \end{aligned} \qquad (12)$$

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So, we can rewrite the linearised expression as just

$$\epsilon_{n+1} + \mathcal{O}(h^2) = \epsilon_n \left[1 + h\frac{\partial f}{\partial y}(x_n)\right] + \mathcal{O}(\epsilon_n^2) \tag{15}$$

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Dropping the higher-order terms, this is

$$\frac{\epsilon_{n+1}}{\epsilon_n} \approx 1 + h\frac{\partial f}{\partial y}(x_n). \tag{16}$$

Stability

So, for stability we therefore require

$$\left|\frac{\epsilon_{n+1}}{\epsilon_n}\right| \approx \left|1 + h\frac{\partial f}{\partial y}(x_n)\right| \leq 1. \tag{17}$$

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i.e. $$h \leq -\frac{2}{\partial f/\partial y(x_n)} \tag{19}$$

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Let’s explore the stability of the Euler method in a real example – Jupyter notebook

Note that none of the topics covered today says anything about ***efficiency***.

That is where more advanced methods come in – which is what the next 3 lectures are about.

Housekeeping

- Assignment ongoing – tomorrow’s lab the last chance to ask extended questions
- Friday: Solving ODE Initial Value Problems