CHEE 3602 – Topic 7: Ordinary differential equations

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Adams-Bashforth methods

Multiple points

- Recall that the explicit Euler method only uses information about a single (x_i, y_i) point to calculate $f(x, y)$ used to find (x_{i+1}, y_{i+1})
- But previously calculated points can offer useful information
- The Newton polynomial formulation can be used to fit an interpolating polynomial to multiple points at once
  - effectively, the explicit Euler method uses a 0 order polynomial

Backward difference

Whereas the previous topics have tended to use the forward difference, the ODE problem is best suited to a backward difference — using some "current" point i and $n-1$ previous points estimate point $i+1$.

Backward difference

The backward difference uses the ∇ symbol instead of the Δ symbol and steps backward rather than forward:

$$
\begin{aligned}
\nabla^{(0)} f_i &= f_i \\
\nabla^{(1)} f_i &= \nabla^{(0)} f_i - \nabla^{(0)} f_{i-1} \\
&= f_i - f_{i-1} \\
\nabla^{(2)} f_i &= \nabla^{(1)} f_i - \nabla^{(1)} f_{i-1} \\
&= (f_i - f_{i-1}) - (f_{i-1} - f_{i-2}) \\
&= f_i - 2f_{i-1} + f_{i-2} \\
\nabla^{(3)} f_i &= \nabla^{(2)} f_i - \nabla^{(2)} f_{i-1} \\
&= \ldots
\end{aligned}
$$

Backward difference polynomial

The backward difference polynomial is very similar to the forward difference one:

$$P_n(s) = \nabla^{(0)} f_i + s\nabla^{(1)} f_i + \frac{s(s+1)}{2!}\nabla^{(2)} f_i + \frac{s(s+1)(s+2)}{3!}\nabla^{(3)} f_i + \dots$$

Where s is defined in the same way as before:

$$s = \frac{x - x_i}{h}$$

Formulation

All Adams-Bashforth methods stem from the same basic derivation from the standard ODE form:

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

$$\mathrm{d}y = f(x,y)\mathrm{dx}$$

$$\int_{y_i}^{y_{i+1}} \mathrm{dy} = \int_{x_i}^{x_{i+1}} f(x,y)\mathrm{dx}$$

Replace $f(x,y)$ with y' — the derivative of y with respect to x such that taking the integral yields y:

$$\int_{y_i}^{y_{i+1}} \mathrm{dy} = \int_{\mathrm{x_i}}^{\mathrm{x_{i+1}}} \mathrm{y'dx}$$

Formulation

$$\int_{y_i}^{y_{i+1}} \mathrm{dy} = \int_{x_i}^{x_{i+1}} y' \mathrm{dx}$$

$$y_{i+1} - y_i = \int_{x_i}^{x_{i+1}} y' \mathrm{dx}$$

$$y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} y' \mathrm{dx}$$

y and y' are unknown, but y' can be replaced with an interpolated polynomial using the backward difference:

$$y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} (y_i' + s\nabla^{(1)} y_i' + \frac{s(s+1)}{2} \nabla^{(2)} y_i' + \ldots) \mathrm{dx}$$

0 order approximation

Using $P_0(s) = y_i'$:

$$y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} (y_i')\mathrm{dx}$$

Recall the chain rule to change dx to ds:

$$\begin{aligned} y_{i+1} &= y_i + \int_0^1 y_i' h \mathrm{ds} \\ &= y_i + y_i' h \end{aligned}$$

Which is just another way of expressing the Euler method.

1st order approximation

Using $P_1(s) = y_i' + s\nabla^{(1)} y_i$:

$$y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} (y_i' + s\nabla^{(1)} y_i')\mathrm{dx}$$

$$y_{i+1} = y_i + \int_0^1 (y_i' + s\nabla^{(1)} y_i') h \mathrm{ds}$$

$$= y_i + (y_i' s + \frac{s^2}{2}\nabla^{(1)} y_i')\Big|_{s=0}^{1} h$$

$$= y_i + (y_i' + \frac{1}{2}(y_i' - y_{i-1}'))h$$

$$= y_i + (\frac{3}{2}y_i' - \frac{1}{2}y_{i-1}')h$$

2nd order approximation

Example 4

Derive the 2nd order Adams-Bashforth equation by using a 2nd order backward Newton polynomial.

Table of coefficients

All Adams–Bashforth equations take the same general form:

$$y_{i+1} = y_i + (a_1 y_i' + a_2 y_{i-1}' + a_3 y_{i-2}' + \ldots)h$$

It is not necessary to derive these constants every time, simply read them from a table:

Order	a_1	a_2	a_3	a_4	a_5
0	1				
1	$\frac{3}{2}$	$-\frac{1}{2}$			
2	$\frac{23}{12}$	$-\frac{4}{3}$	$\frac{5}{12}$		
3	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{3}{8}$	
4	$\frac{1901}{720}$	$-\frac{1387}{360}$	$\frac{109}{30}$	$-\frac{637}{360}$	$\frac{251}{720}$

Multi-point implicit methods

A similar set of equations can be derived for higher order implicit methods — referred to as Adams-Moulton equations.

But these are outside the scope of the course.

Example

Example 5

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 6, 12, 18, and 24 hours using a 2nd order Adams-Bashforth method.

Note, you will have to use lower order methods until you have enough points for the full 2nd order.

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

A note on error

The Euler method is equivalent to a basic Taylor series expansion and is therefore $O(h^2)$ accurate.

Taylor series expansion:

$$f(x+h) = f(x) + hf'(x) + O(h^2)$$

Euler method:

$$y_{i+1} = y_i + f(x_i, y_i)h + O(h^2)$$

Note that $f()$ in the two equation means different things.

A note on error

- The Euler method is just a 0-order interpolation
  - which corresponds to a local error of $O(h^2)$
- Every increase in polynomial order corresponds to an increase in the order of the local error
  - so a 2nd-order estimate (using 3 points) has a local error of $O(h^4)$
- But the global estimate combines the error of multiple steps, reducing the order of the local error estimate by 1
  - so a 2nd-order estimate (using 3 points) has a global error of $O(h^3)$
  - while the Euler method is $O(h)$ globally

A note on error

Unless told otherwise, assume that any mention of $O(h^n)$ is global!