

The background of the slide is a dense, repeating pattern of small circles in two colors: a dark blue and a light yellow. These circles are arranged in a grid-like fashion, with some circles missing or faded to create a textured, halftone-like effect. The pattern is uniform across the entire slide.

CHEE 3602 – Topic 7: Ordinary differential equations

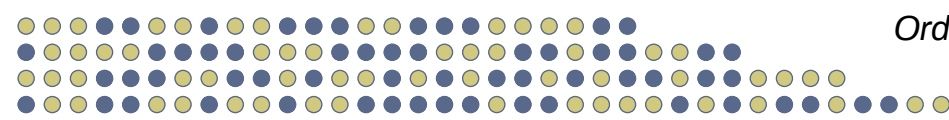
Stanislav Sokolenko
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The background of the slide is a dense, repeating pattern of small circles in two colors: a dark blue and a light yellow. The circles are arranged in a grid-like fashion, with some circles missing or faded to create a subtle, abstract pattern.

Adams-Bashforth methods

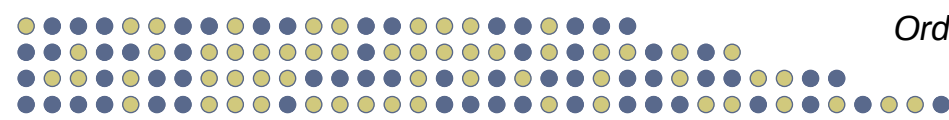
Multiple points

- 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:

$$\nabla^{(0)}f_i = f_i$$

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

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

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

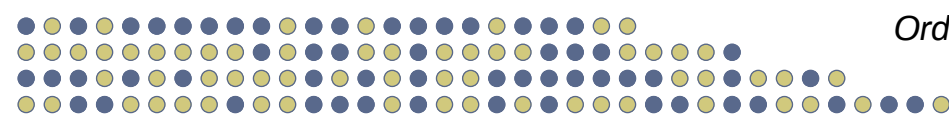
Backward difference polynomial

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:

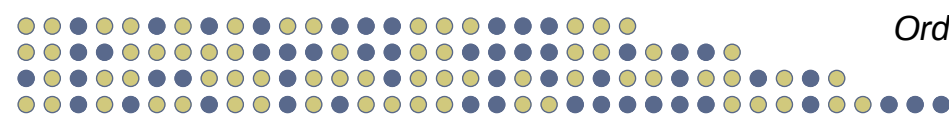
$$\frac{dy}{dx} = f(x, y)$$

$$dy = f(x, y)dx$$

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

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

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

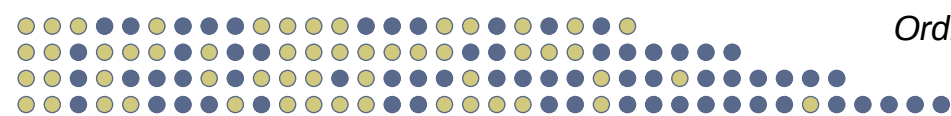


Formulation

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

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

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



0 order approximation

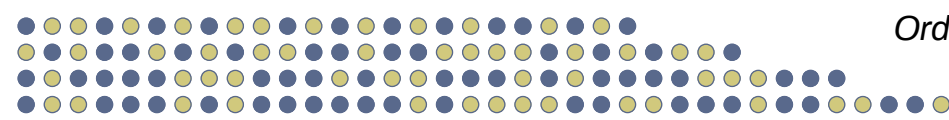
Using $P_0(s) = y'_i$:

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

Recall the chain rule to change dx to ds :

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

Which is just another way of expressing the Euler method.



1st order approximation

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

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

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

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

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

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

2nd order approximation

Example 4

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

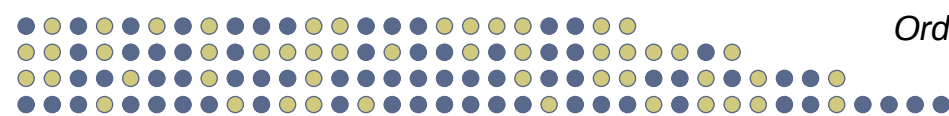


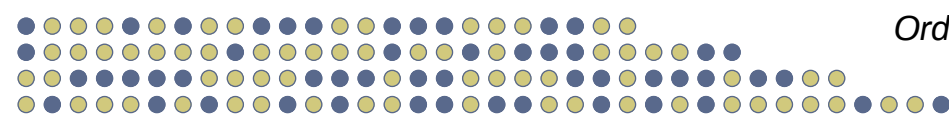
Table of coefficients

All Adams-Bashforth equations take the same general form:

$$y_{i+1} = y_i + (a_1 y'_i + a_2 y'_{i-1} + a_3 y'_{i-2} + \dots)h$$

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.



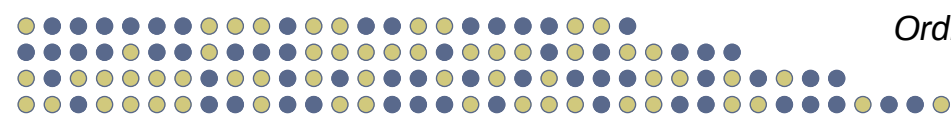
Example

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.

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



A note on error

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

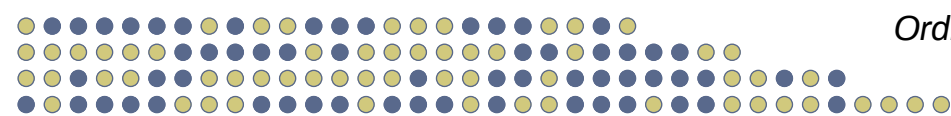
Taylor series expansion:

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

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!