Variable Step Methods

1. Predictor-Corrector Methods
   - explicit and implicit methods
   - Adams-Bashforth/Adams-Moulton methods
   - relationship with Runge-Kutta methods
2. Multistep Methods
   - one step and multistep methods
   - stability
3. Variable Step Methods
   - formulas with different step sizes

MCS 471 Lecture 32
Numerical Analysis
Jan Verschelde, 4 November 2022

Variable Step Methods

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Euler's method and the modified Euler method

We consider the initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0.$$

1. Euler's method: $y_{n+1} = y_n + h f(x_n, y_n)$, $n = 0, 1, \ldots$

   We can immediately evaluate the right hand to obtain y_{n+1}.
   Euler's method is an *explicit method*.

2. the modified Euler method:

$$y_{n+1} = y_n + \frac{h}{2}\Big(f(x_n, y_n) + f(x_{n+1}, y_{n+1}) \Big), \quad n = 0, 1, \ldots$$

   We observe that y_{n+1} appears at the right hand side,
   the modified Euler method is an *implicit method*.

predictor-corrector methods

The method of Euler and the modified Euler method are used as a *predictor-corrector method*:

$$\begin{array}{lcrcl} \textit{predict} & : & \overline{y}_{n+1} & = & y_n + h f(x_n, y_n) \\ \textit{correct} & : & y_{n+1} & = & y_n + \dfrac{h}{2}\left(f(x_n, y_n) + f(x_{n+1}, \overline{y}_{n+1}) \right). \end{array}$$

In general,

1. the predictor is an explicit method,
2. the corrector is an implicit method.

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Adams-Bashforth/Adams-Moulton methods

The formulas are constructed so only one new function evaluation is needed in the next step. Points are equidistant: $x_n = x_0 + nh$, $h > 0$.

1. Adams-Bashforth methods are explicit, used to predict.

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} p(x)dx, \quad p(x_{n-i}) = f_{n-i}, \ i = 0, 1, \ldots k.$$

2. Adams-Moulton methods are implicit, used to correct.

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} p(x)dx, \quad p(x_{n+1-i}) = f_{n+1-i}, \ i = 0, 1, \ldots k.$$

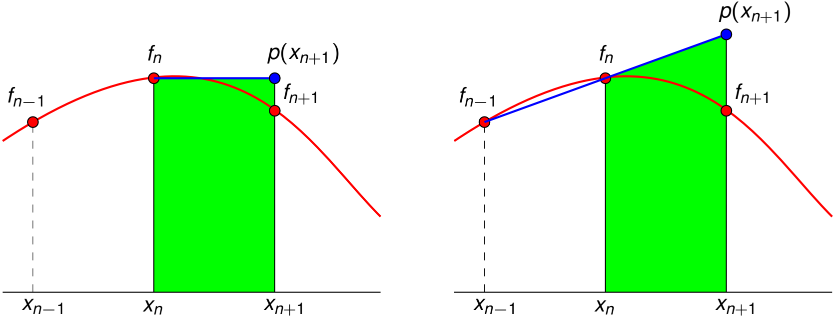
The parameter k is the same in the formulas in the pair.

The Adams-Moulton method uses one extra function evaluation.

Adams-Bashforth of orders 1 and 2

Interpolate at one point: $p(x) = f_n$ and $\displaystyle\int_{x_n}^{x_{n+1}} p(x)dx \approx hf_n$.

The forward Euler method:



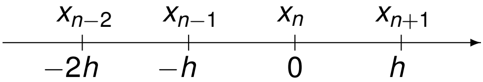
Use $\displaystyle p(x) = f_n + \frac{f_n - f_{n-1}}{x_n - x_{n-1}}(x - x_n) \Rightarrow y_{n+1} = y_n + \frac{h}{2}\left(3f_n - f_{n-1}\right)$.

Adams-Bashforth with 3 function evaluations

Determine the coefficients c_1, c_2, c_3 in

$$\int_{x_n}^{x_{n+1}} f(x, y(x))dx \approx c_1 f_n + c_2 f_{n-1} + c_3 f_{n-2}$$

so that the degree of precision is as high as possible.



The method of undetermined coefficients:

1. Take $x_n = 0$, $x_{n-1} = -h$, $x_{n-2} = -2h$.
2. Apply the rule to the basis functions, $f = 1, x, x^2$.
3. Solve the three conditions for c_1, c_2, and c_3.

using SymPy

```
using SymPy

h, c1, c2, c3, z = Sym("h, c1, c2, c3, z")
(xn, xnminus1, xnminus2) = (0, -h, -2*h)
rule(f) = c1*f(xn) + c2*f(xnminus1) + c3*f(xnminus2)

b1(x) = Sym("1")
b2(x) = x
b3(x) = x^2

rhs1 = SymPy.integrate(b1(z), (z, xn, xn+h))
rhs2 = SymPy.integrate(b2(z), (z, xn, xn+h))
rhs3 = SymPy.integrate(b3(z), (z, xn, xn+h))

eq1 = rule(b1) - rhs1
eq2 = rule(b2) - rhs2
eq3 = rule(b3) - rhs3

sol = SymPy.solve([eq1,eq2,eq3],[c1, c2, c3])
```

the output of `SymPy.solve`

```
$ julia adamsbashforth3.jl
The equations :
1*c1 + 1*c2 + 1*c3 - 1*h
-c2*h - 2*c3*h - h^2/2
c2*h^2 + 4*c3*h^2 - h^3/3
The solution :Dict{Any,Any}
(c1 => 23*h/12,c2 => -4*h/3,c3 => 5*h/12)
```

Then the 3-point Adams-Bashforth rule is

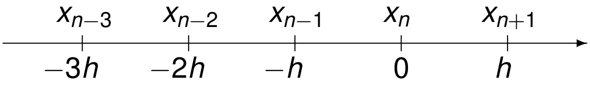
$$y_{n+1} = y_n + \frac{h}{12}\left(23f_n - 16f_{n-1} + 5f_{n-2}\right).$$

Adams-Bashforth with 4 function evaluations

Determine the coefficients c_1, c_2, c_3, c_4 in

$$\int_{x_n}^{x_{n+1}} f(x, y(x))dx \approx c_1 f_n + c_2 f_{n-1} + c_3 f_{n-2} + c_4 f_{n-3}$$

so that the degree of precision is as high as possible.



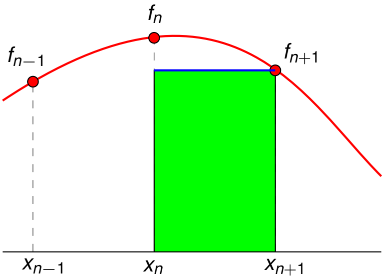
Exercise 1: Apply the method of undetermined coefficients to compute the weights c_1, c_2, c_3, c_4 so 1, x, x^2, x^3 are integrated correctly.

1. Define the equations in c_1, c_2, c_3, and c_4.
2. Solve the equations, e.g. with `SymPy`.
3. Write the 4-point Adams-Bashforth rule.

Adams-Moulton of orders 1 and 2

Interpolate at one point: $p(x) = f_{n+1}$ and $\displaystyle\int_{x_n}^{x_{n+1}} p(x)dx \approx hf_{n+1}$.

The backward Euler method:



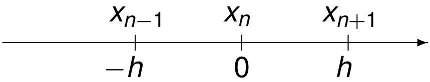
Use $p(x) = f_n + \dfrac{f_{n+1} - f_n}{x_{n+1} - x_n}(x - x_n) \Rightarrow y_{n+1} = y_n + \dfrac{h}{2}\left(f_n + f_{n+1}\right)$.

Adams-Moulton with 3 function evaluations

Determine the coefficients c_1, c_2, c_3 in

$$\int_{x_n}^{x_{n+1}} f(x, y(x))dx \approx c_1 f_{n+1} + c_2 f_n + c_3 f_{n-1}$$

so that the degree of precision is as high as possible.



The method of undetermined coefficients:

1. Take $x_{n+1} = h$, $x_n = 0$, $x_{n-1} = -h$.
2. Apply the rule to the basis functions, $f = 1, x, x^2$.
3. Solve the three conditions for c_1, c_2, and c_3.

using SymPy

```
using SymPy

h, c1, c2, c3, z = Sym("h, c1, c2, c3, z")
(xnplus1, xn, xnminus1) = (h, 0, -h)
rule(f) = c1*f(xnplus1) + c2*f(xn) + c3*f(xnminus1)

b1(x) = Sym("1")
b2(x) = x
b3(x) = x^2

rhs1 = SymPy.integrate(b1(z), (z, xn, xn+h))
rhs2 = SymPy.integrate(b2(z), (z, xn, xn+h))
rhs3 = SymPy.integrate(b3(z), (z, xn, xn+h))

eq1 = rule(b1) - rhs1
eq2 = rule(b2) - rhs2
eq3 = rule(b3) - rhs3

sol = SymPy.solve([eq1,eq2,eq3],[c1, c2, c3])
```

the output of SymPy.solve

```
$ julia adamsmoulton3.jl
The equations :
1*c1 + 1*c2 + 1*c3 - 1*h
c1*h - c3*h - h^2/2
c1*h^2 + c3*h^2 - h^3/3
The solution :Dict{Any,Any}
(c3 => -h/12,c1 => 5*h/12,c2 => 2*h/3)
```

Then the 3-point Adams-Moulton rule is

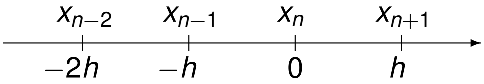
$$y_{n+1} = y_n + \frac{h}{12}\left(5f_{n+1} + 8f_n - f_{n-1}\right).$$

Adams-Moulton with 4 function evaluations

Determine the coefficients c_1, c_2, c_3, c_4 in

$$\int_{x_n}^{x_{n+1}} f(x, y(x))dx \approx c_1 f_{n+1} + c_2 f_n + c_3 f_{n-1} + c_4 f_{n-2}$$

so that the degree of precision is as high as possible.



Exercise 2: Apply the method of undetermined coefficients to compute the weights c_1, c_2, c_3, c_4 so 1, x, x^2, x^3 are integrated correctly.

1. Define the equations in c_1, c_2, c_3, and c_4.
2. Solve the equations, e.g. with `SymPy`.
3. Write the 4-point Adams-Moulton rule.

a predictor-corrector method

Applied to $\frac{dy}{dx} = f(x, y(x))$, $y(0) = y_0$, for some $h > 0$:

1. predict with the 3-point Adams-Bashforth rule:

$$\overline{y}_{n+1} = y_n + \frac{h}{12}\left(23f_n - 16f_{n-1} + 5f_{n-2}\right).$$

2. correct with the 3-point Adams-Moulton rule:

$$y_{n+1} = y_n + \frac{h}{12}\left(5f(x_{n+1}, \overline{y}_{n+1}) + 8f_n - f_{n-1}\right).$$

Observe that we do only one new function evaluation, at $f(x_{n+1}, \overline{y}_{n+1})$.

The local error is $\int_0^h x(x-h)(x-2h)dx = O(h^4)$.

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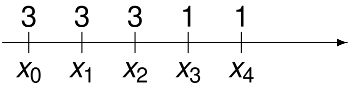
Runge-Kutta methods to start

A 3-stage Runge-Kutta method uses 3 function evaluations and has local error equal to $O(h^4)$.

The Runge-Kutta method is used in combination with the Adams-Bashforth/Adams-Moulton predictor corrector pair, at the start of the approximations:

1. at x_0, use the 3-stage Runge-Kutta for y_1,
2. at x_1, use the 3-stage Runge-Kutta for y_2,
3. at x_2, use the 3-stage Runge-Kutta for y_3,
4. at x_3, use the Adams-Bashforth to predict $\overline{y}_4$, and then correct with Adams-Moulton to obtain y_4.



count the number of function evaluations

The cost of solving an initial value problem is measured in the number of function evaluations.

Exercise 3:
Suppose we want to solve an initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(0) = y_0,$$

with a predictor-corrector method using three points in each step.

Calculate how many times we evaluate f to approximate $y(0.8)$, using step size $h = 0.1$.

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one step and multistep methods

Runge-Kutta methods are one step methods:

- y_{n+1} is computed by evaluation of f, and
- y_n, the value of the previous step.

Multistep methods use more than the previous y_n to compute the next y_{n+1}. For example:

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h b_1 f_n, \quad n = 0, 1, \ldots$$

The coefficients a_1, a_2, and b_1 are determined to obtain the highest order possible.

Multistep methods can be viewed as the application of interpolation of already computed values of the solution trajectory.

explicit and implicit two step methods

An implicit two step method with 3 function evaluations:

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h \left(b_0 f_{n+1} + b_1 f_n + b_2 f_{n-1} \right), \quad n = 0, 1, \ldots$$

The above method is implicit because f_{n+1} requires y_{n+1}.

If $b_0 = 0$, then

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h \left(b_1 f_n + b_2 f_{n-1} \right), \quad n = 0, 1, \ldots$$

is an explicit two step method with 2 function evaluations.

application of the Taylor expansion

$$\begin{aligned} y_{n+1} &= y(x_n + h) \\ &= y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{3!} y'''(x_n) + \frac{h^4}{4!} y''''(x_n) + O(h^5) \\ &= y_n + h\, y'_n + \frac{h^2}{2} y''_n + \frac{h^3}{3!} y'''_n + \frac{h^4}{4!} y''''_n + O(h^5) \end{aligned}$$

The known coefficients in the above expansion are compared with the Tayor expansion of

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h \left(b_0\, f_{n+1} + b_1\, f_n + b_2\, f_{n-1} \right),$$

which leads to conditions on the unknown a_1, a_2, b_0, b_1, and b_2.

two explicit two step methods of the same order

The conditions on a_1, a_2, b_0, b_1, and b_2 allow for choice.

- One choice of a solution to the conditions leads to

$$y_{n+1} = \frac{1}{2} y_n + \frac{1}{2} y_{n-1} + h \left(\frac{7}{4} f_n - \frac{1}{4} f_{n-1} \right),$$

  a two step explicit method with a local error of $O(h^4)$.

- Another choice of a solution yields

$$y_{n+1} = -y_n + 2 y_{n-1} + h \left(\frac{5}{2} f_n - \frac{1}{2} f_{n-1} \right),$$

  also a two step explicit method with a local error of $O(h^4)$.

Which method is better?

Variable Step Methods

a simple problem

Consider the simple initial value problem

$$\frac{dy}{dx} = 0, \quad y(0) = 0, \quad x \in [0, 1].$$

Obviously, the solution is $y \equiv 0$.

The application of

$$y_{n+1} = -y_n + 2y_{n-1} + h\left(\frac{5}{2}f_n - \frac{1}{2}f_{n-1}\right)$$

to this problem gives the formula

$$y_{n+1} = -y_n + 2y_{n-1} + h0, \quad n = 0, 1, \ldots$$

Of course, starting at zero will produce zero.

But there could be numerical solutions, other than zero.

other numerical solutions are possible

$$y_{n+1} = -y_n + 2y_{n-1} + h0, \quad n = 0, 1, \ldots$$

Substituting $y_n = c\lambda^n$ in the formula above yields

$$\begin{aligned} c\lambda^{n+1} + c\lambda^n - 2c\lambda^{n-1} &= 0 \\ c\lambda^{n-1}\left(\lambda^2 + \lambda - 2\right) &= 0. \end{aligned}$$

The roots of $\lambda^2 + \lambda - 2$ are $+1$ and -2.

For some nonzero constant c, other numerical solutions are

$$y = c \quad \text{and} \quad y = c(-2)^n.$$

By representation and roundoff errors, the values may y_n grow in size.

the stability of a method

A d-step method

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + \cdots + a_d y_{n-d+1} + h\left(\cdots \right), \quad n = 0, 1, \ldots$$

is *stable* if the roots of

$$x^d - a_1 x^{d-1} - a_2 x^{d-2} - \cdots - a_d$$

are bounded by one in absolute value and
all roots of absolute value equation to one are simple roots.

If one is the only root, then the method is *strongly stable*,
otherwise, it is *weakly stable*.

determine the stability of a method

Exercise 4:

Consider the explicit two step method

$$y_{n+1} = \frac{1}{2}y_n + \frac{1}{2}y_{n-1} + h\left(\frac{7}{4}f_n - \frac{1}{4}f_{n-1}\right), \quad n = 0, 1, \ldots$$

to solve an initial value problem.

1. Is this method stable? Justify.
2. If stable, is this method weakly or strongly stable? Justify.

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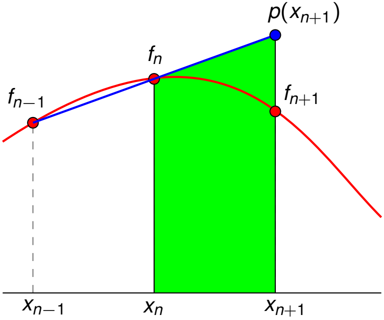
variable step methods

In a variable step method: $x_1 = x_0 + h_0$, $x_2 = x_1 + h_1$, $x_2 = x_2 + h_2$, ...

A variable step size Adams-Bashforth method of order 2:



$$p(x) = f_n + \frac{f_n - f_{n-1}}{x_n - x_{n-1}}(x - x_n)$$

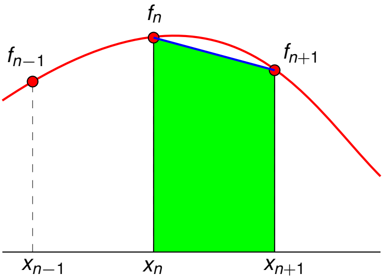
$$x_{n+1} - x_n = h_n$$

$$x_n - x_{n-1} = h_{n-1}$$

$$p(x_{n+1}) = f_n + \frac{f_n - f_{n-1}}{h_{n-1}} h_n$$

$$\begin{aligned} y_{n+1} &= y_n + \frac{h_n}{2}\Big(f_n + p(x_{n+1})\Big) \\ &= y_n + \frac{h_n}{2}\left(\left(2 + \frac{h_n}{h_{n-1}}\right) f_n - \left(\frac{h_n}{h_{n-1}}\right) f_{n-1}\right) \end{aligned}$$

a variable step Adams-Moulton method



Exercise 5:

Let $x_{n+1} = x_n + h_n$ and $x_n = x_{n-1} + h_{n-1}$.

Derive the formula for a variable step size Adams-Moulton method of order 2.

Initial Value Problems

A summary of five lectures follows.

1. Forward differences give Euler's method and the trapezoidal rule leads to the modified Euler method. Lipschitz continuity implies uniqueness of the solution.
2. A differential equation of order n is equivalent to a system of n first order equations. The eigenvalues of a linear system characterize solutions.
3. A p stage Runge-Kutta method uses p function evaluations and has $O(h^p)$ as global error.
4. To solve stiff equations, implicit methods are needed.
5. Explicit multistep methods using multiple function evaluations define predictors and correctors apply implicit multistep methods.