Predictor-corrector methods

Multistep methods

Predictor-corrector methods

A simple example

CN method:

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + \frac{h}{2}(\mathbf{f}(x_k, \overline{\mathbf{y}}_k) + \mathbf{f}(x_{k+1}, \overline{\mathbf{y}}_{k+1})).$$

This method is an implicit one. If $h \leq 2/L$ (L is the Lipschitz constant), then the equation has a unique solution for $\overline{\mathbf{y}}_{k+1}$. $\overline{\mathbf{y}}_{k+1}$ can be computed by fixed point iteration:

$$\overline{\mathbf{y}}_{k+1}^{(s+1)} = \overline{\mathbf{y}}_k + \frac{h}{2}(\mathbf{f}(x_k, \overline{\mathbf{y}}_k) + \mathbf{f}(x_{k+1}, \overline{\mathbf{y}}_{k+1}^{(s)})).$$

Problems:

- When to stop the iteration?
- $\mathbf{f}(x, \overline{\mathbf{y}})$ must be computed many times.
- What is a good choice for $\overline{\mathbf{y}}_{k+1}^{(0)}$?

A simple example

Solution: Let us apply an explicit method to obtain a good guess for $\overline{\mathbf{y}}_{k+1}^{(0)}$.

For example, we can use the explicit Euler method. That is we set

$$\overline{\mathbf{y}}_{k+1}^{(0)} = \overline{\mathbf{y}}_k + h\mathbf{f}(x_k, \overline{\mathbf{y}}_k).$$

Iterating only once we obtain the method

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + \frac{h}{2}(\mathbf{f}(x_k, \overline{\mathbf{y}}_k) + \mathbf{f}(x_{k+1}, \overline{\mathbf{y}}_k + h\mathbf{f}(x_k, \overline{\mathbf{y}}_k)),$$

which is an explicit method.

Advantage of this technique: What is the order of this method? The EE method is first order, the CN method is second order, but the combined method above is second order. This is the Heun method ($b = 1/2$), which is second order indeed.

The idea of predictor-corrector methods

The application of an explicit and an implicit method after each other.

- **Predictor:** An explicit method that predicts a good starting value for the iteration in the case of an implicit method.
- **Corrector:** The applied implicit method, with which we correct the value of $\overline{\mathbf{y}}_{k+1}$.

Multistep methods

General form of s-step methods

$$
\begin{aligned}
& a_s y_{k+1} + a_{s-1} y_k + \ldots + a_0 y_{k-(s-1)} \\
= h(b_s \underbrace{f_{k+1}}_{f(x_{k+1}, y_{k+1})} & + b_{s-1} \underbrace{f_k}_{f(x_k, y_k)} + \ldots + b_0 \underbrace{f_{k-(s-1)}}_{f(x_{k-(s-1)}, y_{k-(s-1)})})
\end{aligned}
$$

- $a_s \neq 0$, because it is used to calculate y_{k+1}.
- If $b_s = 0$, then the method is explicit, otherwise it is implicit.
- To start the method we need the values $y_0, \ldots, y_{s-1}$. These can be calculated with a sufficiently accurate one-step method (e.g. with some RK methods).

Adams methods

If $a_s = 1$, $a_{s-1} = -1$ and $a_k = 0$ $(k = s-2, \dots, 0)$, then the method is called Adams method. The explicit Adams methods are called Adams-Bashforth methods (John Couch Adams (1819 - 1892, English), astronomer, mathematician; Francis Bashforth (1819 - 1912, English), mathematician), and the implicit ones Adams-Moulton methods (Forest Ray Moulton (1872 - 1952, USA), astronomer).
Construction:

$$\int_{x_k}^{x_{k+1}} y'(x)\,\mathrm{d}x = \int_{x_k}^{x_{k+1}} f(x, y(x))\,\mathrm{d}x$$

$$y_{k+1} - y_k = \int_{x_k}^{x_{k+1}} \sum_{j=k-s+1}^{k(AB),\ k+1(AM)} \underbrace{f(x_j, y_j)}_{f_j} l_j(x)\,\mathrm{d}x,$$

$$= \sum_{j=k-s+1}^{k(AB),\ k+1(AM)} f_j \int_{x_k}^{x_{k+1}} l_j(x)\,\mathrm{d}x$$

where l_j $(j = k-s+1, \dots, k(AB), k+1(AM))$ is the jth characteristic Lagrange polynomial to the points $x_{k-s+1}, \dots, x_k(AB), x_{k+1}(AM)$.

Adams methods

The maximal order Adams–Bashforth formulas:

Steps	Formula	Order
1	$y_{k+1} = y_k + hf_k$ (EE)	1
2	$y_{k+1} = y_k + \frac{h}{2}(3f_k - f_{k-1})$	2
3	$y_{k+1} = y_k + \frac{h}{12}(23f_k - 16f_{k-1} + 5f_{k-2})$	3
4	$y_{k+1} = y_k + \frac{h}{24}(55f_k - 59f_{k-1} + 37f_{k-2} - 9f_{k-3})$	4
5	$y_{k+1} = y_k + \frac{h}{720}(1901f_k - 2774f_{k-1} + 2616f_{k-2} - 1274f_{k-3} + 251f_{k-4})$	5

The maximal order Adams–Moulton formulas:

Steps	Formula	Order
1	$y_{k+1} = y_k + hf_{k+1}$ (IE)	1
1	$y_{k+1} = y_k + \frac{h}{2}(f_{k+1} + f_k)$ (CN)	2
2	$y_{k+1} = y_k + \frac{h}{12}(5f_{k+1} + 8f_k - f_{k-1})$	3
3	$y_{k+1} = y_k + \frac{h}{24}(9f_{k+1} + 19f_k - 5f_{k-1} + f_{k-2})$	4
4	$y_{k+1} = y_k + \frac{h}{720}(251f_{k+1} + 646f_k - 264f_{k-1} + 106f_{k-2} - 19f_{k-3})$	5

Backward differentiation formulas (BDF)

If $b_s = 1$ and $b_k = 0$ $(k = s-1, \dots, 0)$, then the method is called backward differentiation formula - BDF.

Construction:

We start with the differential equation at the point x_{k+1}

$$y'(x_{k+1}) = f(x_{k+1}, y(x_{k+1})).$$

The right hand side is approximated by $f(x_{k+1}, y_{k+1}) = f_{k+1}$, and on the left hand side we apply a backward difference formula.

The maximal order BDF methods:

Steps	Formula	Order
1	(IE) $y_{k+1} - y_k = hf_{k+1}$	1
2	$\frac{3}{2}y_{k+1} - 2y_k + \frac{1}{2}y_{k-1} = hf_{k+1}$	2
3	$\frac{11}{6}y_{k+1} - 3y_k + \frac{3}{2}y_{k-1} - \frac{1}{3}y_{k-2} = hf_{k+1}$	3
4	$\frac{25}{12}y_{k+1} - 4y_k + 3y_{k-1} - \frac{4}{3}y_{k-2} + \frac{1}{4}y_{k-3} = hf_{k+1}$	4
5	$\frac{137}{60}y_{k+1} - 5y_k + 5y_{k-1} - \frac{10}{3}y_{k-2} + \frac{5}{4}y_{k-3} - \frac{1}{5}y_{k-4} = hf_{k+1}$	5

Consistency

We calculate h·LTE (let we develop the Taylor expansion at $z = x_{k-s+1}$):

$$\begin{aligned}
h \cdot LTE =& a_s y(x_{k+1}) + \ldots + a_0 y(x_{k-s+1}) \\
&- h(b_s f(x_{k+1}, y(x_{k+1})) + \ldots + b_0 f(x_{k-s+1}, y(x_{k-s+1}))) = \\
=& \sum_{i=0}^{s} \left(a_i y(z+ih) - hb_i \underbrace{f(z+ih, y(z+ih))}_{y'(z+ih)} \right) \\
=& \sum_{i=0}^{s} a_i (y(z) + y'(z)ih + y''(z)(ih)^2/2 + \ldots) \\
&- h \sum_{i=0}^{s} b_i (y'(z) + y''(z)ih + y'''(z)(ih)^2/2 + \ldots) \\
=& d_0 y(z) + d_1 y'(z)h + d_2 y''(z)h^2 + \ldots,
\end{aligned}$$

Consistency

where

$$d_0 = \sum_{i=0}^{s} a_i$$

$$d_1 = \sum_{i=0}^{s} (i a_i - b_i)$$

$$\vdots$$

$$d_j = \sum_{i=0}^{s} \left(\frac{i^j a_i}{j!} - \frac{i^{j-1} b_i}{(j-1)!} \right)$$

$$\vdots$$

Thus we have

$$\mathsf{LTE} = d_0 y(z) \frac{1}{h} + d_1 y'(z) + d_2 y''(z) h + d_3 y'''(z) h^2 + \dots .$$

Consistency

From the form of the local truncation error it follows the following result directly.

Thm. 148. The multistep method is consistent iff $d_0 = d_1 = 0$. If the solution y is in C^{m+1} and

$$d_0 = \ldots = d_m = 0 \ (m \geq 1)$$

and

$$d_{m+1} \neq 0,$$

then the local truncation error is $O(h^m)$, thus the consistency order of the method is m.

Example. The AB5 and AM4 methods have consistency order 5.

Example. The method $y_{k+1} - y_{k-1} = \frac{h}{3}(f_{k+1} + 4f_k + f_{k-1})$ has consistency order 4. $a_2 = 1, a_1 = 0, a_0 = -1,\ b_2 = 1/3, b_1 = 4/3, b_0 = 1/3.$ Thus $d_0 = \ldots = d_4 = 0$ és $d_5 = -1/90.$

Consistency

What is the maximal achievable consistency order?

The method has $2s+1$ free coefficients (because the coefficients are unique only up to a nonzero constant multiplier). There is some hope that we can choose the coefficients in such a way that $d_0 = \ldots = d_{2s} = 0$ ($2s+1$ equations and $2s+1$ unknowns).

Theorem

(Dahlquist (1956)) The system of equations $d_0 = \ldots = d_{2s} = 0$ has always a solution up to a nonzero constant multiplier. Thus, with an s-step method, we can achieve a consistency order as high as $2s$. (For explicit methods, the achievable highest order is $2s-1$ (b_s must be zero). For AB methods: s, and for AM methods: $s+1$.)

Germund Dahlquist, 1925-2005, Swedish

Stability

Def. 150. An s-step method is called to be (zero)stable if there are two constants $K > 0$ and $h_0 > 0$ independent of the step size such that for $0 < h < h_0$ we have

$$|y_k - \hat{y}_k| \leq K \max\{|y_0 - \hat{y}_0|, \ldots, |y_{s-1} - \hat{y}_{s-1}|\}, \; k = s, \ldots, N_h,$$

that is starting the scheme from two different sets of initial values, the difference of the solutions remains bounded on finite intervals. ($\hat{y}_k$ is the sequence produced with the hatted values.)

Thm. 151. An s-step method is stable iff all zeros of the so-called first characteristic polynomial $\zeta(z) = a_s z^s + \ldots + a_1 z + a_0$ lie in the closed complex unit circle centered at the origin and the zeros on the boundary are sigle.

Thm. 152. (Equivalence theorem) Let us suppose that the solution of the initial value problem is in C^{r+1}, moreover, let us suppose that the multistep method has consistency order r. Then the stability is a necessary and sufficient condition of the convergence. The order of the convergence is r.

Example.
EE, IE: $\zeta(z) = z - 1$, thus the methods are stable, they are also consistent (order is 1), and these imply that they are convergent with order 1.

Theorem
The Adams methods are convergent and their convergence order equals the order of their consistency.

Proof: $\zeta(z) = z^s - z^{s-1} = z^{s-1}(z-1)$. Thus, the method is always stable. The other part of the theorem follows from the equivalence theorem. ■

Stability

Theorem

There are valid the following so-called Dahlquist's (first and second) barriers (indicated by blue and extended by some previously discussed results).

s: number of steps of the method	Impicit	Explicit
The greatest possible consistency order	$2s$	$2s-1$
The greatest possible consistency order of a stable method	$s+1$ (s odd) $s+2$ (s even)	s
The greatest possible order of an A-stable method	2	-
The greatest possible order of a convergent Adams method	$s+1$ (AM)	s (AB)

A not stable method

$$y_{n+1} + 4y_n - 5y_{n-1} = h(4f_n + 2f_{n-1})$$

This 2-step method is explicit and third order, thus it cannot be stable. This can be verified on the test equation $y' = 0$, $y(0) = 0$.

Then for $y_0 = 0$ and $y_1 = \varepsilon_h$ we have

$$y_n = (1 - (-5)^n)\varepsilon_h/6.$$

The numerical solution at $x = 1$ is $(n = 1/h)$

$$(1 - (-5)^{1/h})\varepsilon_h/6.$$

With the choice $y_0 = 0$ and $y_1 = 0$ we obtain zero. This shows that the method cannot be stable.

Solution of boundary value problems

Solution of boundary value problems

Initial value problems: The values of all the unknown functions are known at the same fixed point.

Boundary value problems: The values of the unknown functions are known at more different points (generally at the two ends of an interval).

Example. The equation of the deflection of a rod:

$$EIy''(x) + P\cos(y(x)) = 0,\ \ y(0) = 0, y(L) = 0.$$

$$\Downarrow$$

$$\begin{aligned} y_1' &= y_2,\ \ y_1(0) = y_1(L) = 0, \\ y_2' &= -\frac{P}{EI}\cos(y_1). \end{aligned}$$

Boundary value problems

Let us consider the two-point boundary value problems in the form

$$y'' = f(x, y, y'), \quad y(a) = A, \ y(b) = B,$$

where $a < b$ and $x \in [a, b]$.

Theorem

Assume that f is continuous, the derivative with respect to the second argument is continuous and positive, the derivative with respect to the third argument is continuous and bounded. Then the boundary value problem has a unique solution.

Example. The problem $y'' = -y$, $y(0) = 3$, $y(\pi) = 7$ has no solution.

Shooting method

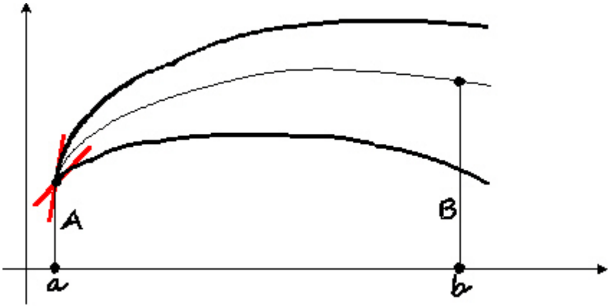
Shooting (garden hose) method

Let us rewrite the problem to an initial values problem

$$
\begin{aligned}
y_1' &= y_2, \quad y_1(a) = y(a) = A, \\
y_2' &= f(x, y_1, y_2), \quad y_2(a) = y'(a) =: D,
\end{aligned}
$$

where we have replaced the unknown value $y_2(a) = y'(a)$ by a fixed real number D.

Let us denote the solution of the above problem by $y(x; D)$. If $y(b; D) = B$, then $y(x; D)$ solves the original boundary value problem. Otherwise, we choose another value D. This can be done in a systematic way.



Shooting method

We have to solve the nonlinear equation

$$y(b; D) - B = 0$$

for the parameter D.

We can use the previously studied methods to find the appropriate D.

- Bisection method,
- Newton's method.

Finite difference method

Finite difference method (matrix method)

$$y'' = f(x, y, y'),\ y(a) = A,\ y(b) = B$$

Let us define an equidistant mesh on $[a, b]$. Let the length of the subintervals be $h = (b - a)/(n + 1)$, thus $x_i = a + ih$ $(i = 0, \ldots, n + 1)$.

Let y_i denote $(i = 0, \ldots, n + 1)$ the approximations of the exact solution at x_i. Let us replace the derivatives of the solution to finite difference approximations:

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} = f\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right),$$

moreover let $y_0 = A$ and $y_{n+1} = B$. If f is nonlinear, then the solution is difficult. We must use one of the solvers for nonlinear systems of equations (Newton's method, fixed point iteration).

Finite difference method

Let us investigate only linear equations, that is the boundary value problems in the form:

$$y''(x) = u(x) + v(x)y + w(x)y', \; y(a) = A, \; y(b) = B$$

Then the finite difference method results in the problem ($u(x_i) = u_i$, $v(x_i) = v_i$, $w(x_i) = w_i$):

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} = u_i + v_i y_i + w_i \frac{y_{i+1} - y_{i-1}}{2h}, \tag{6}$$

moreover $y_0 = A$ and $y_{n+1} = B$. After rearrangement we obtain

$$y_0 = A,$$

$$\overbrace{\left(\frac{1}{h^2} + \frac{w_i}{2h}\right)}^{a_i} y_{i-1} \overbrace{- \left(\frac{2}{h^2} + v_i\right)}^{b_i} y_i + \overbrace{\left(\frac{1}{h^2} - \frac{w_i}{2h}\right)}^{c_i} y_{i+1} = u_i$$

$$y_{n+1} = B,$$

Finite difference method

In order to obtain the approximations y_i, we have to solve the linear system:

$$\begin{bmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & b_{n-1} & c_{n-1} \\ & & & a_n & b_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix} = \begin{bmatrix} u_1 - a_1 A \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n - c_n B \end{bmatrix}.$$

Assume that $\inf v > 0$ and $w \not\equiv 0$ is a bounded function on $[a,b]$. Moreover, let us assume that the step size h is sufficiently small, that is $h \leq 2/\sup_{x\in[a,b]}\{|w(x)|\}$.

Then the matrix is strictly diagonally dominant, that implies that the system can be solved using the Gaussian elimination.

Convergence

Def. 156. The previous scheme for the solution of the boundary value problem is convergent if $\max_{i=1,\dots,n}|y_i - y(x_i)| = O(h^r)$ $(r \geq 0)$ provided that $h \to 0$ $(n \to \infty)$, moreover r is the order of the convergence.

Theorem

If $y \in C^4$ then the investigated scheme is convergent with convergence order 2.

Proof. Let us compute first the LTE at the point x_i:

$$\tau_i = \frac{y(x_{i-1}) - 2y(x_i) + y(x_{i+1})}{h^2} - u_i - v_i y(x_i) - w_i \frac{y(x_{i+1}) - y(x_{i-1})}{2h}$$

$$= \frac{h^2}{12} y''''(\xi) - w_i \frac{h^2}{6} y'''(\eta).$$

That is with a positive constant C we have

$$|\tau_i| \leq h^2 M_3 C.$$

Thus the method is consistent and the order of the consistency is 2.

Convergence

Let us subtract the scheme (6) from the inequility obtained for the LTE. Let us intruduce the notation $e_i = y(x_i) - y_i$ for the error at the point x_i. We obtain the linear system of equations:

$$\frac{e_{i-1} - 2e_i + e_{i+1}}{h^2} - v_i e_i - w_i \frac{e_{i+1} - e_{i-1}}{2h} = \tau_i,$$

that is componentwisely

$$\begin{bmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & b_{n-1} & c_{n-1} \\ & & & a_n & b_n \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_{n-1} \\ e_n \end{bmatrix} = \begin{bmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_{n-1} \\ \tau_n \end{bmatrix}.$$

Convergence

The matrix of the system is the -1 multiple of an M-matrix. The main diagonal is negative, the other elements are nonnegative, and the main diagonal is strictly dominant. We can apply the estimation for the inverses of M-matrices. Together with the expression for the LTE τ_i, we obtain that

$$\left\| \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_{n-1} \\ e_n \end{bmatrix} \right\|_\infty \le \frac{1}{\inf_{x\in[a,b]} v(x)} \left\| \begin{bmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_{n-1} \\ \tau_n \end{bmatrix} \right\|_\infty \le \frac{M_3 h^2 C}{\inf_{x\in[a,b]} v(x)}.$$

This shows second order convergence. ■