NTNU

TMA4215 Numerical Mathematics — Fall 2016

Problem Set 5

1 Let $\{t_i\}_{i=0}^n$ be a set of equidistant nodes, so that $t_i = t_0 + ih$ for $i = 1, 2, \dots, n$, where h is the distance between the nodes. Given a function f defined on an interval containing the nodes, with $f_i := f(t_i)$ for $i = 0, 1, \dots, n$, we can introduce *forward differences* recursively by

$$\Delta^0 f_i = f_i, \qquad \Delta f_i = f_{i+1} - f_i \qquad \text{and} \qquad \Delta^j f_i = \Delta\left(\Delta^{j-1} f_i\right) = \Delta^{j-1} f_{i+1} - \Delta^{j-1} f_i$$

for $i = 0, \dots, n$ and $j = 0, 1, \dots, n - i$. For example,

$$\Delta^2 f_0 = f_2 - 2f_1 + f_0 \qquad \text{and} \qquad \Delta^3 f_0 = f_3 - 3f_2 + 3f_1 - f_0.$$

Now let $t = t_0 + sh$, where $s \in \mathbb{R}$, be any point. In this exercise we want to establish that the polynomial p_n of degree n interpolating f in the nodes $\{t_i\}$ can be written as

$$p_n(t) = p_n(t_0 + sh) = f_0 + \sum_{j=1}^{n} \binom{s}{j} \Delta^j f_0, \tag{1}$$

where

$$\binom{s}{j} := \frac{s(s-1)\cdots(s-j+1)}{j!}$$

is a generalized binomial coefficient. Equation (1) is called *Newton's forward difference formula*.

a) Show by induction that

$$f[t_0, t_1, \dots, t_j] = \frac{\Delta^j f_0}{j!\,h^j} \qquad \text{for} \qquad j = 1, \dots, n, \tag{$\star$}$$

where $f[t_0, t_1, \dots, t_j]$ is a *forward divided difference* defined from

$$f[t_j] = f_j \quad \text{for} \quad j \in \{0, \dots, n\}$$

and

$$f[t_i, \dots, t_{i+j}] = \frac{f[t_{i+1}, \dots, t_{i+j}] - f[t_i, \dots, f_{i+j-1}]}{t_{i+j} - t_i}$$

for $j \in \{1, \dots, n\}$ and $i \in \{0, \dots, n - j\}$.

Solution. For $j = 1$ we have $f[t_0, t_1] = (f_1 - f_0)/h = \Delta f_0 / h$. Suppose now that ($\star$) holds for some $j \in \{1, \dots, n-1\}$. In particular,

$$f[t_1, \dots, t_{j+1}] = \frac{\Delta^j f_1}{j!\,h^j}$$

by an index shift. Hence,

$$f[t_0,\dots,t_{j+1}] = \frac{f[t_1,\dots,t_{j+1}] - f[t_0,\dots,t_j]}{(j+1)h} = \frac{\Delta^j f_1 - \Delta^j f_0}{(j+1)!\,h^{j+1}} = \frac{\Delta^{j+1} f_0}{(j+1)!\,h^{j+1}}.$$

b) Show that

$$\prod_{i=0}^{j-1}(t-t_i) = j!\,h^j\binom{s}{j} \qquad \text{for} \qquad j=1,\dots,n.$$

Solution. Since $t - t_i = (t_0 + sh) - (t_0 + ih) = (s-i)h$, we immediately get

$$\prod_{i=0}^{j-1}(t-t_i) = h^j s(s-1)\cdots(s-j+1) = j!\,h^j\binom{s}{j}.$$

c) Use the results from a) and b) to prove (1).

Solution. Recall that the unique polynomial $p_n \in \mathbb{P}_n$ interpolating f in the nodes $\{t_i\}$ can be given by Newton's divided difference formula

$$p_n(t) = f[t_0] + \sum_{j=1}^{n} f[t_0,\dots,t_j]\prod_{i=0}^{j-1}(t-t_i).$$

Inserting the expressions from a) and b) now gives (1).

Comment: Equivalently, it is possible to show *Newton's backward difference formula*. Backward differences on the sequence $\{f_i\}$ are defined by

$$\nabla^0 f_i = f_i, \qquad \nabla f_i = f_i - f_{i-1}, \qquad \nabla^j f_i = \nabla^{j-1} f_i - \nabla^{j-1} f_{i-1}, \qquad j = 1,2,\dots$$

Newton's backward difference formula is given by

$$p_n(t) = p_n(t_n + sh) = f_n + \sum_{j=1}^{n}(-1)^j\binom{-s}{j}\nabla^j f_n. \tag{2}$$

This expression is used to develop Adams methods; see the note on the webpage. In the next exercise, it is used to develop the so-called BDF-methods.

2 The *backward differentiation formulas* (BDFs) is a family of implicit linear k-step methods to the initial value problem

$$y' = f(t,y), \qquad y(t_0) = y_0,$$

where we assume that the starting values $y_1,\dots,y_{k-1}$ (in addition to y_0) are given with sufficient accuracy. To construct them, we first use (2) to find the polynomial $q \in \mathbb{P}_k$ interpolating all the previously computed points plus the new one, that is, the points

$$(t_{n-k+1}, y_{n-k+1}),\ \dots,\ (t_n, y_n),\ (t_{n+1}, y_{n+1}).$$

Then we replace y by q in the ODE and evaluate the corresponding equation at t_{n+1}, which yields the BDF

$$q'(t_{n+1}) = f(t_{n+1}, y_{n+1}).$$

a) Establish that a k-step BDF can be written as

$$\sum_{j=1}^{k} \delta_j^\star \nabla^j y_{n+1} = hf_{n+1},$$

and find an expression for $\delta_j^\star$.

Solution. From (2) we infer that

$$q(t) = q(t_{n+1} + sh) = y_{n+1} + \sum_{j=1}^{k} (-1)^j \binom{-s}{j} \nabla^j y_{n+1},$$

and so an application of the chain rule, using that

$$t(s) = t_{n+1} + sh \qquad \text{and} \qquad s(t) = \frac{t - t_{n+1}}{h},$$

results in

$$q'(t_{n+1}) = \frac{\mathrm{d}q(t(s))}{\mathrm{d}s}\bigg|_{s=0} \frac{\mathrm{d}s}{\mathrm{d}t}\bigg|_{t=t_{n+1}} = \sum_{j=1}^{k} (-1)^j \left(\frac{\mathrm{d}}{\mathrm{d}s} \binom{-s}{j} \bigg|_{s=0} \right) \nabla^j y_{n+1} \cdot \frac{1}{h}.$$

Thus we obtain the desired form with

$$\delta_j^\star = (-1)^j \frac{\mathrm{d}}{\mathrm{d}s} \binom{-s}{j} \bigg|_{s=0} = \frac{1}{j}.$$

b) Write down the methods for $k = 1, 2$ and 3 and check if they are zero-stable. Moreover, find their orders and the corresponding error constants.

Solution. Routine calculations yield that

$$\begin{aligned}
&\text{BDF1:} \quad && y_{n+1} - y_n = hf_{n+1} \qquad \text{(backward Euler);}\\
&\text{BDF2:} \quad && \tfrac{3}{2} y_{n+1} - 2y_n + \tfrac{1}{2} y_{n-1} = hf_{n+1};\\
&\text{BDF3:} \quad && \tfrac{11}{6} y_{n+1} - 3y_n + \tfrac{3}{2} y_{n-1} - \tfrac{1}{3} y_{n-2} = hf_{n+1}.
\end{aligned}$$

For example, the left-hand side in BDF2 is

$$\delta_1^\star \nabla y_{n+1} + \delta_2^\star \nabla^2 y_{n+2} = (y_{n+1} - y_n) + \tfrac{1}{2} \big(y_{n+1} - y_n - (y_n - y_{n-1}) \big)$$

before simplifying.

All three methods are zero-stable, because the roots of the characteristic polynomials are

$$\begin{aligned}
&\text{BDF1:} \quad && r_1 = 1;\\
&\text{BDF2:} \quad && r_1 = 1 \quad \text{and} \quad r_2 = \tfrac{1}{3};\\
&\text{BDF3:} \quad && r_1 = 1 \quad \text{and} \quad r_{2,3} = \tfrac{1}{22} \big(7 \pm \mathrm{i}\sqrt{39} \big).
\end{aligned}$$

For example, the characteristic polynomial of BDF3 is $\rho(r) = \frac{11}{6}r^3 - 3r^2 + \frac{3}{2}r - \frac{1}{3}$. (Note that we have to reindex first so that the subscripts start at n and not $n-2$.) As regards the order conditions for a k-step BDF, we compute the C_q's, which with the given indexing become

$$C_0 = \sum_{l=-k+1}^{1} \alpha_l \quad \text{and} \quad C_q = \frac{1}{q!}\sum_{l=-k+1}^{1} l^q \alpha_l - \frac{1}{(q-1)!} \quad \text{for} \quad q = 1, 2, \dots,$$

where we have used that only $\beta_1 (= 1)$ is nonzero. This gives

$$\begin{aligned}
&\text{BDF1:} \quad C_0 = C_1 = 0 && \text{and error constant} \quad C_2 = -\tfrac{1}{2}, \quad \text{so order 1;}\\
&\text{BDF2:} \quad C_0 = C_1 = C_2 = 0 && \text{and error constant} \quad C_3 = -\tfrac{1}{3}, \quad \text{so order 2;}\\
&\text{BDF3:} \quad C_0 = C_1 = C_2 = C_3 = 0 && \text{and error constant} \quad C_4 = -\tfrac{1}{4}, \quad \text{so order 3.}
\end{aligned}$$

c) Based on b), guess what the error constant would be for a general k-step BDF, and try to prove it.

Solution. We guess that the error constant is $C_{k+1} = -1/(k+1)$ in general. To prove this, we need to show two things, namely, that $C_0 = \cdots = C_k = 0$ and that C_{k+1} has the given value.

There are likely several ways to establish the result. One possible route may be to express the BDF in the typical form

$$\sum_{l=-k+1}^{1} \alpha_l \, y_{n+l} = h f_{n+1},$$

find the α_l's and verify the order conditions in b) algebraically, perhaps together with some induction argument. Explicitly, we can show that

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = \sum_{j=1}^{k} \frac{1}{j} \sum_{i=0}^{j} (-1)^i \binom{i}{j} y_{n+1-i} = \sum_{l=-k+1}^{1} \alpha_l \, y_{n+l},$$

with

$$\alpha_1 = \sum_{i=1}^{k} \frac{1}{i} \quad \text{and} \quad \alpha_l = (-1)^{1-l} \sum_{i=1-l}^{k} \frac{1}{i} \binom{i}{1-l} \quad \text{for} \quad l = -k+1, \dots, 0,$$

but the expressions look a bit unpleasant.

Instead, we take advantage of that the BDFs are established by means of interpolation polynomials and directly calculate the local truncation error $d_{n+1}(h)$. First we rewrite the BDF into the form

$$y_{n+1} + \big(h\, q'(t_{n+1}) - y_{n+1}\big) = h f_{n+1},$$

which yields that

$$\begin{aligned}
d_{n+1}(h) &= y(t_{n+1}) - \Big[h f\big(t_{n+1}, y(t_{n+1})\big) - h\, q'\big(t_{n+1}; y(t_{n-k+1}), \dots, y(t_{n+1})\big) + y(t_{n+1})\Big]\\
&= -h\Big[y'(t_{n+1}) - q'\big(t_{n+1}; y(t_{n-k+1}), \dots, y(t_{n+1})\big)\Big],
\end{aligned}$$

where $q(t_{n+1};\cdots)$ denotes the polynomial which interpolates the points

$$\big(t_{n-k+1}, y(t_{n-k+1})\big),\ \ldots,\ \big(t_n, y(t_n)\big),\ \big(t_{n+1}, y(t_{n+1})\big).$$

Remember now that the formula for the interpolation error is

$$y(t) - q(t;\cdots) = \frac{y^{(k+1)}\big(\xi(t)\big)}{(k+1)!}\pi_k(t),$$

where $\xi(t) \in (t_{n-k+1}, t_{n+1})$ and $\pi_k(t) = \prod_{i=0}^{k}(t - t_{n-k+1+i})$. Notice from the chain and product rules that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big\{y^{(k+1)}\big(\xi(t)\big)\,\pi_k(t)\Big\}\Big|_{t=t_{n+1}} &= y^{(k+2)}\big(\xi(t_{n+1})\big)\,\xi'(t_{n+1})\,\pi_k(t_{n+1}) + y^{(k+1)}\big(\xi(t_{n+1})\big)\,\pi_k'(t_{n+1})\\ &= y^{(k+1)}\big(\xi(t_{n+1})\big)\,k!\,h^k,\end{aligned}$$

because $\pi_k(t_{n+1}) = 0$ and

$$\pi_k'(t_{n+1}) = \prod_{i=0}^{k-1}(t_{n+1} - t_{n-k+1+i}) = \prod_{i=0}^{k-1}(k-i)\,h = k!\,h^k.$$

Hence,

$$y'(t_{n+1}) - q'(t_{n+1};\cdots) = \frac{1}{k+1}y^{(k+1)}\big(\xi(t_{n+1})\big)\,h^k,$$

and so

$$d_{n+1}(h) = -\frac{1}{k+1}y^{(k+1)}\big(\xi(t_{n+1})\big)\,h^{k+1}.$$

To complete, we Taylor-expand $y^{(k+1)}$ around t_n (status quo) to get

$$d_{n+1}(h) = -\frac{1}{k+1}y^{(k+1)}(t_n)\,h^{k+1} + \mathcal{O}(h^{k+2}),$$

and conclude that $C_0 = \cdots = C_k = 0$ and $C_{k+1} = -1/(k+1)$, as desired.

(Detail: We skipped issues of differentiability and remark that it is not obvious that $\xi(t)$ is differentiable.)

NB! BDF-methods with $k > 6$ are not zero-stable, and thus not convergent.