Scientific Computing HW 4

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Problem 1. Pf. The characteristic polynomial is

$$\rho(z) = z^k + \sum_{j=0}^{k-1} \alpha_j z^{k-1-j}$$

and the recurrence is

$$u_{n+1} + \sum_{j=0}^{k-1} \alpha_j u_{n-j} = 0$$

Define a linear operator $D := r\frac{\mathrm{d}}{\mathrm{d}r}$. Then for all n and l,

$$D[n^l r^n] = r\frac{\mathrm{d}}{\mathrm{d}r} n^l r^n = rn^l n r^{n-1} = n^{l+1} r^n$$

so that in particular,

$$n^l r^n = D[n^{l-1} r^n] = D^2[n^{l-2} r^n] = \ldots = D^l[r^n] \quad (1.1)$$

Plug $u_n = n^l r^n$ into the LHS of the recurrence, apply (1.1) to each term, then use the linearity of D.

$$u_{n+1} + \sum_{j=0}^{k-1} \alpha_j u_{n-j} = (n+1)^l r^{n+1} + \sum_{j=0}^{k-1} \alpha_j (n-j)^l r^{n-j} = D^l[r^{n+1}] + \sum_{j=0}^{k-1} \alpha_j D^l[r^{n-j}] = D^l\left[r^{n+1} + \sum_{j=0}^{k-1} \alpha_j r^{n-j} \right]$$

$$= D^l\left[r^{n-k+1}\left(r^k + \sum_{j=0}^{k-1} \alpha_j r^{k-1-j} \right) \right] = D^l[r^{n-k+1} \rho(r)] = D^l[0] = 0$$

Problem 2. Pf. We first establish a lemma. For the $(k-1) \times k$ matrix

$$\begin{bmatrix} \lambda & -1 & & & \\ & \lambda & -1 & & \\ & & \ddots & \ddots & \\ & & & \lambda & -1 \end{bmatrix}$$

The submatrix formed by deleting the jth column has determinant $(-1)^{k-j}\lambda^{j-1}$. To see this, write the

submatrix in block form.

$$M := \begin{bmatrix} \lambda & -1 & & & & & & \\ & \lambda & -1 & & & & & \\ & & \ddots & \ddots & & & 0_{(j-1)\times(k-j)} & \\ & & & \lambda & -1 & & & \\ & & & & \lambda & & & \\ & & & & & -1 & & \\ & & & & & \lambda & -1 & \\ & 0_{(k-j)\times(j-1)} & & & & & \ddots & \ddots \\ & & & & & & & \lambda & -1 \end{bmatrix}$$

Using the fact that

$$\det \begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix} = \det(B)\det(C)$$

we have $\det M = \lambda^{j-1}(-1)^{k-j}$.

We now aim to show $\det(\lambda I - A) = \rho(\lambda)$.

$$\lambda I - A = \begin{bmatrix} \lambda & -1 & & & \\ & \lambda & -1 & & \\ & & \ddots & \ddots & \\ & & & \lambda & -1 \\ \alpha_{k-1} & \alpha_{k-2} & \dots & \alpha_1 & \lambda+\alpha_0 \end{bmatrix}$$

Expanding over row k, starting at column k, and using the above lemma,

$$\det(\lambda I - A) = (\lambda+\alpha_0)(-1)^{k-k}\lambda^{k-1} + \sum_{j=1}^{k-1}(-1)^{k+k-j}\alpha_j(-1)^{k-k+j}\lambda^{k-j-1} = \lambda^k + \alpha_0\lambda^{k-1} + \sum_{j=1}^{k-1}(-1)^{2k}\alpha_j\lambda^{k-j-1}$$

$$= \lambda^k + \alpha_0\lambda^{k-1} + \sum_{j=1}^{k-1}\alpha_j\lambda^{k-j-1} = \lambda^k + \sum_{j=0}^{k-1}\alpha_j\lambda^{k-j-1} = \rho(\lambda)$$

Problem 3. Note: For explicit matrix norm computations we will use the Euclidean norm

$$\|A\| = \left[\sum_{i,j} A_{ij}^2\right]^{1/2}$$

Pf. Write the Jordan form of A.

$$A = SJS^{-1}, \quad J = \text{diag}(J_1, J_2, \dots, J_s), \quad J_q = r_q I_{m_q} + N_q, \quad N_q \overset{m_q \times m_q}{=} \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & & \ddots & \ddots \\ & & & & 0 & 1 \end{bmatrix}$$

For all p,

$$A^p = SJ^pS^{-1}, \quad J^p = \text{diag}(J_1^p, J_2^p, \dots, J_s^p)$$

so we seek a bound on $\|J^p\|$, where $J = rI + N$ is a Jordan block for an eigenvalue r with multiplicity m (we temporarily use J to denote a single block instead of the whole matrix).

If $m = 1$ then $J = [r]$, and since ρ satisfies the root condition, $|r| \leq 1$, giving

$$\|J^p\| = |r|^p \leq 1$$

Now say $m > 1$, so that $|r| < 1$ by the root condition. If $r = 0$ then $J = N$, hence $\|J^p\| = 0$ for all $p \geq m$. Now say $r \neq 0$. For $p \geq m$,

$$J^p = (rI + N)^p = \sum_{j=0}^{p} \binom{p}{j} r^{p-j} N^j = \sum_{j=0}^{m} \binom{p}{j} r^{p-j} N^j$$

$$\implies \|J^p\| \leq \sum_{j=0}^{p} \binom{p}{j} |r|^{p-j} \|N^j\|$$

Fix j with $0 \leq j \leq m$. We establish a bound on $\binom{p}{j}|r|^{p-j}$. Note

$$\binom{p}{j}|r|^{p-j} = \frac{p!}{j!(p-j)!}|r|^p|r|^{-j} = \frac{1}{|r|^j j!}|r|^p \prod_{i=0}^{j-1}(p-i) = \frac{1}{|r|^j j!} \cdot \frac{\prod_{i=0}^{j-1}(p-i)}{|1/r|^p}$$

Considering the fraction in the RHS as $p \to \infty$, the denominator, an exponential in p with base $|1/r| > 1$, grows faster than the numerator, a polynomial in p. This means $\binom{p}{j}|r|^{p-j}$ tends to 0 as $p \to \infty$, hence it has a bound M_j independent of p.

Writing small powers of N,

$$N^0 = I = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & \ddots & \ddots \\ & & & 0 & 1 \end{bmatrix}, \quad N^2 = \begin{bmatrix} 0 & 0 & 1 & \\ & 0 & 0 & 1 \\ & & 0 & \ddots & 1 \\ & & & 0 & 0 \end{bmatrix}, \quad N^3 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ & 0 & 0 & 0 & 1 \\ & & 0 & 0 & 0 \\ & & & 0 & 0 \end{bmatrix}$$

we see that for $0 \leq j \leq m$,

$$\|N^j\| = \left[\sum_{i,j}(N^j)_{ij}^2 \right]^{1/2} = [m-j]^{1/2} \leq m^{1/2}$$

We now have a bound on $\|J^p\|$ independent of p. Here we re–introduce the subscript q.

$$\|J_q^p\| \leq \max \left[\|J_q^1\|, \|J_q^2\|, \ldots, \|J_q^{m-1}\|, \sum_{j=0}^{m_q} M_{q,j} m_q^{1/2} \right] =: K_q$$

Looking at the whole Jordan matrix J,

$$\|J^p\| = \sum_{q=1}^{s} \|J_q^p\| \leq \sum_{q=1}^{s} K_q$$

Thus

$$\|A^p\| \leq \|S\| \|S^{-1}\| \sum_{q=1}^{s} K_q$$

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Problem 4. Plug the supposed solution U_n into the LHS of the recurrence.

$$U_{n+1} = A^{n-k+2}U_{k-1} + h\sum_{j=0}^{n+1-k} A^j G_{n-j} = A^{n-k+2}U_{k-1} + hG_n + h\sum_{j=1}^{n+1-k} A^j G_{n-j}$$

$$= A^{n-k+2}U_{k-1} + hG_n + h\sum_{j=0}^{n-k} A^{j+1} G_{n-j-1}$$

Plug the solution into the RHS.

$$AU_n + hG_n = A^{n-k+2}U_{k-1} + h\sum_{j=0}^{n-k} A^{j+1} G_{n-j-1} + hG_n$$

The two expressions are equal, so U_n indeed solves the recurrence.

Problem 5.

(a) **Pf.** For BDF2, the interpolant is

$$p(t) = y_{n+1} + y[t_{n+1}, t_n](t - t_{n+1}) + y[t_{n+1}, t_n, t_{n-1}](t - t_{n+1})(t - t_n)$$

The derivative of the last term at t_{n+1} is

$$\frac{d}{dt}\Big|_{t=t_{n+1}} (t - t_{n+1})(t - t_n) = (t - t_n) + (t - t_{n+1})\Big|_{t=t_{n+1}} = 2t_{n+1} - t_n - t_{n+1} = t_{n+1} - t_n = h_n$$

and so

$$p'(t_{n+1}) = y[t_{n+1}, t_n] + y[t_{n+1}, t_n, t_{n-1}]h_n$$

Equating this with $f_{n+1} := f(t_{n+1}, u_{n+1})$ gives the BDF2 method.

$$\frac{u_{n+1} - u_n}{h_n} + \frac{\frac{u_{n+1}-u_n}{h_n} - \frac{u_n - u_{n-1}}{h_{n-1}}}{h_n + h_{n-1}} h_n = f_{n+1}$$

From $h_n = t_{n+1} - t_n$ and $\omega = \frac{h_n}{h_{n-1}}$,

$$1 + \omega = 1 + \frac{h_n}{h_{n-1}} = \frac{h_{n-1} + h_n}{h_{n-1}} \implies (1+\omega)^2 = \frac{1}{h_{n-1}^2}\left[h_{n-1}^2 + h_n^2 + 2h_{n-1}h_n\right] \quad (5.1)$$

$$1 + 2\omega = 1 + 2\frac{h_n}{h_{n-1}} = \frac{h_{n-1} + 2h_n}{h_{n-1}} \quad (5.2)$$

From (5.1) and (5.2),

$$\frac{(1+\omega)^2}{1+2\omega} = \frac{h_{n-1}}{h_{n-1} + 2h_n}\frac{1}{h_{n-1}^2}\left[h_{n-1}^2 + h_n^2 + 2h_{n-1}h_n\right] = \frac{1}{h_{n-1} + 2h_n}\left[h_{n-1} + \frac{h_n^2}{h_{n-1}} + 2h_n\right]$$

$$= h_{n-1}(1 + 2\omega)\left[h_{n-1} + \frac{h_n^2}{h_{n-1}} + 2h_n\right] \quad (5.3)$$

Now multiply the method by $h_n(h_n + h_{n-1})$.

$$(u_{n+1} - u_n)(h_n + h_{n-1}) + \left[\frac{u_{n+1} - u_n}{h_n} - \frac{u_n - u_{n-1}}{h_{n-1}}\right]h_n^2 = h_n(h_n + h_{n-1})f_{n+1}$$

Collect coefficients of the following terms. Rewrite them using (5.2) and (5.3).

$$u_{n+1}: \quad h_n + h_{n-1} + \frac{h_n^2}{h_n} = 2h_n + h_{n-1} \overset{(5.2)}{=} h_{n-1}(1 + 2\omega)$$

$$u_n: \quad -(h_n + h_{n-1}) + \left[-\frac{1}{h_n} - \frac{1}{h_{n-1}}\right] h_n^2 = -\left[2h_n + h_{n-1} + \frac{h_n^2}{h_{n-1}}\right] \overset{(5.3)}{=} -h_{n-1}(1 + 2\omega)\frac{(1+\omega)^2}{1 + 2\omega}$$

$$u_{n-1}: \quad \frac{h_n^2}{h_{n-1}} = h_{n-1}\omega^2$$

Putting these together, the method is

$$h_{n-1}(1 + 2\omega)u_{n+1} - h_{n-1}(1 + 2\omega)\frac{(1+\omega)^2}{1 + 2\omega}u_n + h_{n-1}\omega^2 = h_n(h_n + h_{n-1})f_{n+1}$$

Divide by $h_{n-1}(1 + 2\omega)$.

$$u_{n+1} - \frac{(1+\omega)^2}{1 + 2\omega}u_n + \frac{\omega^2}{1 + 2\omega}u_{n-1} = h_n\frac{\frac{h_n}{h_{n-1}} + 1}{1 + 2\omega}f_{n+1} = h_n\frac{1 + \omega}{1 + 2\omega}f_{n+1}$$

(b) From the LHS of the method, define

$$\rho(z) := z^2 - \frac{(1+\omega)^2}{1 + 2\omega}z + \frac{\omega^2}{1 + 2\omega}$$

By Vieta's formulas, the roots r, s of ρ satisfy

$$r + s = \frac{(1+\omega)^2}{1 + 2\omega} = \frac{1 + \omega^2 + 2\omega}{1 + 2\omega} = \frac{\omega^2}{1 + 2\omega} + 1$$

$$rs = \frac{\omega^2}{1 + 2\omega}$$

From these we see

$$r = \frac{\omega^2}{1 + 2\omega}, \quad s = 1$$

Since $\omega < 1 + \sqrt{2}$,

$$w^2 < (1 + \sqrt{2})^2 = 1 + 2 + 2 \cdot \sqrt{2} = 1 + 2(1 + \sqrt{2}) = 1 + 2\omega \implies 0 \le r = \frac{\omega^2}{1 + 2\omega} < 1 \implies |r| < 1$$

This leaves $s = 1$ as the only root with modulus 1, and it has multiplicity 1. Thus ρ satisfies the root condition, hence the method is stable.

Problem 6. Code: `https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/hw4.ipynb`

A timestep of $h = 10^{-3}$ was used. The CPU time for DIRK2 was about 2.673 seconds, while the CPU time for BDF2 was about 2.015 seconds. The time evolution of the individual components is shown below.