Numerical Solution of Differential Equations
Problem Sheet 2

Stuart Golodetz

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1. Consider the Runge-Kutta method $y_{n+1} = y_n + h(\alpha k_1 + \beta k_2)$ where $k_1 = f(x_n, y_n)$ and $k_2 = f(x_n + \gamma h,\ y_n + \gamma h k_1)$, and where α, β, γ are real parameters.

   (a) Show that there is a choice of these parameters such that the order of the method is 2.

   (b) Suppose that a second-order method of the above form is applied to the initial value problem $y' = -\lambda y$, $y(0) = 1$, where λ is a positive real number. Show that the sequence $(y_n)_{n\geq 0}$ is bounded if and only if $h \leq \frac{2}{\lambda}$.
   (Hard; not compulsory!): Show further that, for such λ,

$$|y(x_n) - y_n| \leq \frac{1}{6}\lambda^3 h^2 x_n, \quad n \geq 0.$$

Answer

(a) The answer to this is almost exactly the same as the derivation in the lecture notes, with the proviso that the a_2 and b_{21} given there now satisfy the additional constraint $a_2 = b_{21}$: both are in fact equal to our parameter γ here.
We're required to show that the method is second-order accurate, i.e. that $T_n = O(h^2)$. So consider:

$$\begin{aligned} T_n &= \frac{y(x_{n+1}) - y(x_n)}{h} - \Phi(x_n, y(x_n); h) \\ &= \frac{y(x_{n+1}) - y(x_n)}{h} - \alpha f(x_n, y(x_n)) - \beta f(x_n + \gamma h,\ y(x_n) + \gamma h f(x_n, y(x_n))) \end{aligned}$$

Now, if we apply Taylor expansion to $y(x_{n+1})$, we get:

$$\begin{aligned} y(x_{n+1}) &= y(x_n + h) \\ &= y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(x_n) + O(h^3) \end{aligned}$$

Thus:

$$\frac{y(x_{n+1}) - y(x_n)}{h} = y'(x_n) + \frac{h}{2} y''(x_n) + O(h^2)$$

Hence:

$$\begin{aligned} T_n &= y'(x_n) + \frac{h}{2} y''(x_n) + O(h^2) \\ &\quad - \alpha f(x_n, y(x_n)) - \beta \underbrace{f(x_n + \gamma h,\ y(x_n) + \gamma h f(x_n, y(x_n)))}_{\phi} \end{aligned}$$

So far, so good. Now it gets a bit trickier. We want to use Taylor expansion to simplify the expression marked ϕ in the above. Using the formula for a Taylor series for a function of two variables, as per the notes, and writing f instead of $f(x_n, y(x_n))$ where appropriate for brevity, we derive that:

$$f(x_n + \gamma h,\ y(x_n) + \gamma h f) = f + [\gamma h f_x + \gamma h f f_y] + O(h^2)$$

Hence:

$$T_n = y'(x_n) + \frac{h}{2}y''(x_n) - \alpha f - \beta\left(f + \gamma h[f_x + f f_y]\right) + O(h^2)$$

Since $y'(x_n) = f$, we observe that:

$$T_n = (1-\alpha-\beta)y'(x_n) + h\left\{\frac{1}{2}y''(x_n) - \beta\gamma[f_x + f f_y]\right\} + O(h^2)$$

Now we want $T_n = O(h^2)$, so we try equating the h^0 and h^1 terms with 0 as follows: for the h^0 term, we have $1 - \alpha - \beta = 0$. For the h^1 term, we observe that $y'' = (y')' = \frac{df}{dx} = f_x + f_y y' = f_x + f_y f$ by the chain rule, hence we want to ensure that:

$$\begin{aligned} \frac{1}{2}(f_x + f_y f) - \beta\gamma(f_x + f_y f) &= 0 \\ \Rightarrow \qquad \beta\gamma &= \frac{1}{2} \end{aligned}$$

Given these constraints, $T_n = O(h^2)$ and hence the order of the method is 2, as required.

(b) We note the following:

$$\begin{aligned} y' &= -\lambda y \\ y_0 &= 1 \\ k_1 &= -\lambda y_n \\ k_2 &= -\lambda(y_n + \gamma h k_1) \\ &= -\lambda(y_n - \gamma h \lambda y_n) \\ &= \lambda y_n(\gamma h \lambda - 1) \\ y_{n+1} &= y_n + h(\alpha k_1 + \beta k_2) \\ &= y_n + h(\alpha(-\lambda y_n) + \beta(\lambda y_n(\gamma h\lambda - 1))) \\ &= y_n + h\lambda y_n(-\alpha + \beta(\gamma h \lambda - 1)) \\ &= y_n\left[1 + h\lambda(-\alpha + \beta(\gamma h\lambda - 1))\right] \end{aligned}$$

Now we know from our constraints above that $\beta\gamma = \frac{1}{2}$ and $-\alpha - \beta = -1$, so:

$$\begin{aligned} y_{n+1} &= y_n\left[1 + h\lambda(-\alpha + \frac{1}{2}h\lambda - \beta)\right] \\ &= y_n\left[1 + h\lambda(\frac{1}{2}h\lambda - 1)\right] \\ &= y_n\left[\frac{1}{2}h^2\lambda^2 - h\lambda + 1\right] \\ &= \frac{1}{2}y_n\left[(h\lambda)^2 - 2(h\lambda) + 2\right] \end{aligned}$$

Suppose $h > \frac{2}{\lambda}$. Then *for every value of* n:

$$y_{n+1} > \frac{1}{2}y_n\left[2^2 - 2(2) + 2\right] = y_n$$

Or in other words, the sequence $(y_n)_{n\geq 0}$ grows unboundedly as $n \to \infty$. Conversely, if $h \leq \frac{2}{\lambda}$, then $y_{n+1} \leq y_n$ and the sequence is bounded by $y_0 = 1$.

2. (a) What does it mean to say that a linear multistep method is *zero-stable*? Formulate an equivalent characterisation of zero-stability of a linear multistep method in terms of the roots of its first characteristic polynomial.

   (b) Define the truncation error of a linear multistep method.

   (c) Show that there is a value of the parameter b such that the linear multistep method defined by the formula $y_{n+3} + (2b - 3)(y_{n+2} - y_{n+1}) - y_n = hb(f_{n+2} + f_{n+1})$ is fourth-order accurate. Show further that the method is *not* zero-stable for this value of b.

Answer

(a) Following the lecture notes, if we say that a linear k-step method is zero-stable, we mean that when we apply it for an ODE $y' = f(x, y)$, there exists a constant K such that, for any two sequences $y_0, y_1, \ldots, y_{k-1}$ and $\hat{y_0}, \hat{y_1}, \ldots, \hat{y_{k-1}}$:

$$|y_n - \hat{y_n}| \leq K \max_{i\in[0,k-1]} |y_i - \hat{y_i}|$$

This is all very well and good, but it deserves a clearer (if far less precise (and not necessarily accurate!)) explanation in prose. What we're essentially saying here is this: suppose we generated two sequences of initial values using two different methods, then provided our k-step method is zero-stable, the (absolute) difference between any corresponding pair of subsequent approximate values (y_n and $\hat{y_n}$, say) that gets generated will be bounded by some constant multiple of the greatest (absolute) difference between a corresponding pair of the initial values. Roughly speaking, this means that the difference in output if we use different methods to generate the starting values will be bounded by some multiple of the greatest difference in the starting values generated, i.e. using our k-step method with the values generated only makes the problems we might have caused by using an inferior starting method worse by a constant factor : if the output's bad, it's because the starting method was bad, not because the k-step method was bad.

The lecture notes observe that this definition is inconvenient for checking zero-stability of a method, thus we formulate[1] the equivalent characterisation asked for. Given that the general equation for a linear multistep method is

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(x_{n+j}, y_{n+j})$$

we define its first characteristic polynomial ρ as

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

Given a linear multistep method for an ODE $y' = f(x, y)$, then, where f obeys a Lipschitz condition, we say that it is zero-stable iff all zeros (i.e. all values z s.t. $\rho(z) = 0$) of its first characteristic polynomial are inside the closed unit disk (i.e. $\{z : |z| \leq 1\}$), with any that lie on the unit circle being simple.

[1] Actually, when I say 'we formulate', I mean 'we find the appropriate formulation in the lecture notes and paraphrase it' : just for the sake of telling the absolute truth.

(b) As per the lecture notes, taking the general equation for a linear multistep method to be

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(x_{n+j}, y_{n+j})$$

the truncation error is defined as

$$T_n = \frac{\sum_{j=0}^{k} [\alpha_j y(x_{n+j}) - h\beta_j y'(x_{n+j})]}{h \sum_{j=0}^{k} \beta_j}$$

This isn't altogether surprising. Noting that $y'(x_{n+j}) = f(x_{n+j}, y_{n+j})$, we observe that the numerator of the truncation error is obtained by subtracting the right-hand side of the above equation from the left-hand side. The denominator is there for scaling purposes.

(c) i. Using the formula given and the general equation for linear multistep methods given in the lecture notes, we can work out what the values in the equation must have. In particular, we have that $k = 3$, $\alpha_3 = 1$, $\alpha_2 = 2b - 3$, $\alpha_1 = 3 - 2b$, $\alpha_0 = -1$, $\beta_3 = 0$, $\beta_2 = b$, $\beta_1 = b$ and $\beta_0 = 0$.
Now, the lecture notes use Taylor expansion to show that

$$T_n = \frac{1}{h \sum_{j=1}^{k} \beta_j} \left[\sum_{i=0}^{\infty} C_i h^i y^{(i)}(x_n) \right]$$

where, in particular

$$C_0 = \sum_{j=0}^{k} \alpha_j$$

and

$$C_1 = \sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j$$

and

$$C_q = \sum_{j=1}^{k} \frac{j^q}{q!} \alpha_j - \sum_{j=1}^{k} \frac{j^{q-1}}{(q-1)!} \beta_j$$

To show that our method is fourth-order accurate, therefore, we are simply required to show that there exists some value of b s.t. $C_0 = C_1 = C_2 = C_3 = C_4 = 0$ and $C_5 \neq 0$. Considering them in order:

$$C_0 = \sum_j = 0^3 \alpha_j = 1 + 2b - 3 + 3 - 2b + (-1) = 0$$

So any value of b would work so far. Continuing, we have:

$$C_1 = \sum_{j=1}^{3} j\alpha_j - \sum_{j=0}^{3} \beta_j = [3(1) + 2(2b - 3) + 1(3 - 2b)] - 2b = 3 + 2b - 3 - 2b = 0$$

So any value of b would still work.

$$
\begin{aligned}
C_2 &= \sum_{j=1}^{3} \frac{j^2}{2}\alpha_j - \sum_{j=1}^{3} j\beta_j \\
&= \left[\frac{1}{2}(3-2b) + \frac{4}{2}(2b-3) + \frac{9}{2}(1)\right] - [1(b) + 2(b) + 3(0)] \\
&= \frac{1}{2}[3 - 2b + 4(2b-3) + 9] - 3b \\
&= \frac{1}{2}[6b] - 3b \\
&= 0
\end{aligned}
$$

Again, any value of b would work.

$$
\begin{aligned}
C_3 &= \sum_{j=1}^{3} \frac{j^3}{6}\alpha_j - \sum_{j=1}^{3} \frac{j^2}{2}\beta_j \\
&= \frac{1}{6}[1(3-2b) + 8(2b-3) + 27(1)] - \frac{1}{2}[1(b) + 4(b) + 9(0)] \\
&= \frac{1}{6}[14b+6] - \frac{1}{2}[5b] \\
&= \frac{7b}{3} + 1 - \frac{5b}{2} \\
&= 1 - \frac{b}{6}
\end{aligned}
$$

Now we have a potential value for b, since by equating $1 - b/6$ to zero, we have that $b = 6$. Let's test this value:

$$
\begin{aligned}
C_4 &= \sum_{j=1}^{3} \frac{j^4}{24}\alpha_j - \sum_{j=1}^{3} \frac{j^3}{6}\beta_j \\
&= \frac{1}{24}[1(3-2b) + 16(2b-3) + 81(1)] - \frac{1}{6}[1(b) + 8(b) + 27(0)] \\
&= \frac{30b+36}{24} - \frac{9b}{6} \\
&= \frac{5b+6}{4} - \frac{9b}{6} \\
&= \frac{5(6)+6}{4} - \frac{9(6)}{6} \\
&= 9 - 9 \\
&= 0
\end{aligned}
$$

So this value of b works for C_4 as well. All that remains to be shown is that $C_5 \neq 0$ with this value of b. Well:

$$\begin{aligned}
C_5 &= \sum_{j=1}^{3} \frac{j^5}{120}\alpha_j - \sum_{j=1}^{3} \frac{j^4}{24}\beta_j \\
&= \frac{1}{120}[1(3-2b) + 32(2b-3) + 243(1)] - \frac{1}{24}[1(b) + 16(b) + 81(0)] \\
&= \frac{1}{120}[62b + 150] - \frac{17b}{24} \\
&= \frac{522}{120} - \frac{102}{24} \\
&= \frac{522 - 510}{120} \\
&= \frac{1}{10} \\
&\neq 0
\end{aligned}$$

So for $b = 6$, this linear multistep method is fourth-order accurate, as required.

ii. Now, what about zero-stability? Well, first of all observe that our method is now given by the formula:

$$y_{n+3} + 9(y_{n+2} - y_{n+1}) - y_n = 6h(f_{n+2} + f_{n+1})$$

Consider the first characteristic polynomial of this, namely:

$$\rho(z) = \sum_{j=0}^{k} \alpha_j z^j = z^3 + (2b-3)z^2 + (3-2b)z - 1 = z^3 + 9z^2 - 9z - 1$$

This is clearly zero when $z = 1$, so factor out $z - 1$:

$$z^3 + 9z^2 - 9z - 1 = (z-1)(z^2 + 10z + 1)$$

The quadratic $z^2 + 10z + 1$ has roots at $z \approx -0.101$ and $z \approx -9.899$. This latter root is quite clearly not in the closed unit disk, therefore by the root condition theorem, the method is not zero-stable when $b = 6$.

3. A linear multistep method $\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(x_{n+j}, y_{n+j})$, $n \geq 0$, for the numerical solution of the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$, on the mesh $\{x_j : x_j = x_0 + jh\}$ of uniform spacing $h > 0$ is said to be *absolutely stable* for a certain h if, when applied to the model problem $y' = \lambda y$, $y(0) = 1$, with $\lambda < 0$, on the interval $x \in [0, \infty)$, the sequence $(|y_n|)_{n \geq k}$ decays exponentially fast; i.e., $|y_n| \leq Ce^{-\mu n}$, $n \geq k$, for some positive constants C and μ.

(a) Show that a linear multistep method is absolutely stable for $h > 0$ if and only if all roots z of its *stability polynomial* $\pi(z; \bar{h}) = \rho(z) - \bar{h}\sigma(z)$, where ρ and σ are the first and second characteristic polynomial of the linear multistep method respectively and $\bar{h} = \lambda h$, belong to the open unit disk $D = \{z : |z| < 1\}$ in the complex plane.

(b) For each of the following methods find the range of $h > 0$ for which it is absolutely stable (when applied to $y' = \lambda y$, $y(0) = 1$, $\lambda < 0$, $x \in [0, \infty)$):

i. $y_{n+1} - y_n = hf(x_n, y_n)$;

ii. $y_{n+1} - y_n = hf(x_{n+1}, y_{n+1})$;

iii. $y_{n+2} - y_n = \frac{1}{3}h(f(x_{n+2}, y_{n+2}) + 4f(x_{n+1}, y_{n+1}) + f(x_n, y_n))$.

Answer

(a) TODO: I haven't the first idea where to start with this one...help!

(b)

i. Here we have $k = 1$, $\alpha_1 = 1$, $\alpha_0 = -1$, $\beta_1 = 0$ and $\beta_0 = 1$, so

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

and

$$\sigma(z) = \sum_{j=0}^{1} \beta_j z^j = 1$$

Thus the stability polynomial is:

$$\pi(z; \bar{h}) = \rho(z) - \bar{h}\sigma(z) = z - 1 - \bar{h} = z - 1 - \lambda h$$

From the previous part of the question, we know that the method is absolutely stable iff all roots of this polynomial belong to the open unit disk in the complex plane. Well, $z - 1 - \lambda h = 0$ when, and only when, $z = 1 + \lambda h$, so the method is absolutely stable iff $1 + \lambda h \in D$, where $D = \{z : |z| < 1\}$ is the open unit disk in the complex plane. This is the case exactly when $|1 + \lambda h| < 1$, i.e. (since $h > 0$ and $\lambda < 0$) when $\lambda h > -2$. (This last assertion follows by noting that $\lambda h < 0$, so $1 + \lambda h < 1$ for any h, whence we only require that $1 + \lambda h > -1$, i.e. $\lambda h > -2$.) So the method is absolutely stable for all values of h such that $h < -2/\lambda$, i.e. when $h < |2/\lambda|$. In other words, the answer is $(0, |2/\lambda|)$.

ii. Here we have $k = 1$, $\alpha_1 = 1$, $\alpha_0 = -1$, $\beta_1 = 1$ and $\beta_0 = 0$, so

$$\rho(z) = z - 1$$

as before, and

$$\sigma(z) = \sum_{j=0}^{1} \beta_j z^j = z$$

Thus the stability polynomial is:

$$\pi(z; \bar{h}) = \rho(z) - \bar{h}\sigma(z) = z - 1 - \bar{h}z = z - 1 - \lambda h z = z(1 - \lambda h) - 1$$

Now, this is zero when $z(1 - \lambda h) = 1$, i.e. when $z = \dfrac{1}{1 - \lambda h}$. This is in the open unit disk exactly when

$$\left| \frac{1}{1 - \lambda h} \right| < 1$$

Now, since $\lambda < 0$ and $h > 0$, we have that $\lambda h < 0$ and hence $1 - \lambda h > 1$. So our condition becomes

$$\frac{1}{1 - \lambda h} < 1$$

or

$$1 < 1 - \lambda h$$

But this is clearly satisfied for all values of $h > 0$, bearing in mind that we just saw this exact inequality above. So the answer is $(0, \infty)$.

iii. Here we have $k = 2$, $\alpha_2 = 1$, $\alpha_1 = 0$, $\alpha_0 = -1$, $\beta_2 = 1/3$, $\beta_1 = 4/3$ and $\beta_0 = 1/3$, so

$$\rho(z) = \sum_{j=0}^{2} \alpha_j z^j = z^2 - 1$$

and

$$\sigma(z) = \sum_{j=0}^{2} \beta_j z^j = \frac{1}{3}(z^2 + 4z + 1)$$

Thus the stability polynomial is:

$$\pi(z; \bar{h}) = \rho(z) - \bar{h}\sigma(z) = z^2 - 1 - \frac{1}{3}\bar{h}(z^2 + 4z + 1)$$

This has roots exactly when $3\pi(z; \bar{h})$ does, so multiply through to remove the annoying fraction, giving:

$$3\pi(z; \bar{h}) = 3z^2 - 3 - \bar{h}(z^2 + 4z + 1) = z^2(3 - \bar{h}) + z(-4\bar{h}) + (-3 - \bar{h})$$

We'll solve this using the usual quadratic formula to give:

$$\begin{aligned} z &= \frac{4\bar{h} \pm \sqrt{16\bar{h}^2 - 4 \cdot (3 - \bar{h}) \cdot (-3 - \bar{h})}}{2(3 - \bar{h})} \\ &= \frac{4\bar{h} \pm \sqrt{16\bar{h}^2 - 4 \cdot (\bar{h}^2 - 9)}}{2(3 - \bar{h})} \\ &= \frac{4\bar{h} \pm \sqrt{12\bar{h}^2 + 36}}{2(3 - \bar{h})} \\ &= \frac{4\bar{h} \pm \sqrt{12(\bar{h}^2 + 3)}}{2(3 - \bar{h})} \end{aligned}$$

Now, we want to find the intersection of the sets of values for h when each of these two roots is in the open unit disk. Starting with the positive root:

$$\begin{aligned} & \left| \frac{4\bar{h} + \sqrt{12(\bar{h}^2 + 3)}}{2(3 - \bar{h})} \right| < 1 \\ \Leftrightarrow\ & \frac{\left|4\bar{h} + \sqrt{12(\bar{h}^2 + 3)}\right|}{2(3 - \bar{h})} < 1 \qquad \text{since } \bar{h} = \lambda h < 0 \\ \Leftrightarrow\ & \left|4\bar{h} + \sqrt{12(\bar{h}^2 + 3)}\right| < 2(3 - \bar{h}) \end{aligned}$$

TODO: This is starting to look moderately long and unpleasant, I think I may have missed the point somewhere?