THE UNIVERSITY OF SYDNEY
MATH3076 AND MATH3976 (ADVANCED)

Mathematical Computing	Numerical Methods	2012

Lecturer: *D. J. Ivers*

Set 5 — Initial Value Problems for ODE's

For the week beginning Monday 28^{th} May.

* — tutorial question; A — advanced; S — supplementary

1* (a) Attached is a listing of the file `rk4.inc` containing an incomplete main program `rk4main`, which calls the subroutine `rk4`. Subroutine `rk4` implements the classical fourth-order Runge-Kutta method over one interval of width h to solve the initial value problem

$$\frac{dy}{dt} = f(t, y)\,, \quad y(t_0) = y_0\,.$$

Note the use of the `open` statement,

```
open (unit=8, file=output, status='unknown')
```

in the main program to open a file and connect it to unit 8. The name of the file is given by the character variable `output`, which is input from the keyboard. The main program writes t and y into unit 8 every `nprint` steps, where `nprint` is an `integer` read in with t_0, y_0, t_n and n. The `nprint` feature is implemented using the intrinsic function `mod(j,nprint)`, which gives the remainder of `j` divided by `nprint`.

Copy the file `$mc3nm/rk4.inc` to `rk4.f90` in your directory and complete the main program to do n steps from t_0 to $t_n = t_0 + nh$, where h is the step-size. Determine h from t_0,t_n and n.

(b) Test your program by solving the simple initial value problem

$$\frac{dy}{dt} = -2ty\,, \quad y(0) = 1\,,$$

($0 \le t \le 4$) and then comparing with the analytic solution. Plot your results using funplot.

(c) Modify your program to solve

$$\frac{dy}{dt} = -A(y - \sin t) + \cos t\,, \quad y(0) = 1\,,$$

on $[0, 3.5]$ with $A = 1000$. What stepsize must you take? Plot your results.

(d) Write a simple program to solve the initial value problem in Part (c) using the backward Euler (1-step Gear) method and the linearity of the differential equation,

$$y_{n+1} = y_n + hf(t_{n+1}, y_{n+1}) .$$

Take $A = 1000$. How does the stepsize compare with Part (c). What happens if $A = 10000$?

Solution.

See set5q1.ans.

2. Given the initial value problem

$$y' = -2ty\,, \qquad y(0) = 1\,,$$

find y when $t = 0.2$ by the following methods:

(a) analytically;

(b) Taylor series (find answer to four decimal places);

(c) Euler's method, with

(*i*) $h = 0.2$ and

(*ii*) $h = 0.1$;

(d) two-stage second-order Runge-Kutta method, with $h = 0.2$;

(e) classical four-stage fourth-order Runge-Kutta method, with $h = 0.2$;

(f) Euler-trapezoidal predictor-corrector method, with $h = 0.2$. The trapezoidal corrector is

$$y_{k+1} = y_k + \frac{1}{2}\{f(t_k, y_k) + f(t_{k+1}, y_{k+1})\} .$$

Give the results for

(*i*) one and

(*ii*) two applications of the corrector.

[Anwers: (a) $y = e^{-t^2}$, $y(0.2) = 0.9607894.$; (b) Six terms gives 0.96080; (c) (i) 1, (ii) 0.98; (d) 0.96; (e) 0.9607893; (f) (i) 0.96, (ii) 0.9616.]

Solution.

(a) Separate variables, $dy/y = -2dx/x$, and integrate, $\ln y = -2\ln x + \ln c = \ln x^2 + \ln c$. Exponentiate, $y = ce^{x^2}$. Evaluate the constant of integration c; the initial condition, $y = 1$ at $x = 0$, gives $c = 1$.

(b) Since

$$\begin{aligned}
y' &= -2xy \\
y'' &= -2y - 2xy' \\
y^{(3)} &= -2y' - 2y' - 2xy'' = -4y' - 2xy'' \\
y^{(4)} &= -4y'' - 2y'' - 2xy^{(3)} = -6y'' - 2xy^{(3)} \\
y^{(5)} &= -8y^{(3)} - 2xy^{(4)}\,,
\end{aligned}$$

$$\begin{aligned}
y'(0) &= -2\times 0\times 1 = 0\\
y''(0) &= -2\times 1 - 2\times 0\times 0 = -2\\
y^{(3)}(0) &= -4\times 0 - 2\times 0\times -2 = 0\\
y^{(4)}(0) &= -6\times -2 - 2\times 0\times 0 = 12\\
y^{(5)}(0) &= -8\times 0 - 2\times 0\times 12 = 0\,.
\end{aligned}$$

Hence the Taylor series for y about $x = 0$ is

$$y = 1 - \frac{2}{2!}x^2 + \frac{12}{4!}x^4 + O(x^6) = 1 - x^2 + \frac{1}{2}x^4 + O(x^6)\,.$$

Thus

$$y(0.2) = 1-(0.2)^2+\frac{1}{2}(0.2)^4+O(0.2)^6 = 1-0.04+0.0008+O(x^6) \approx 0.9608\,.$$

The first neglected term in is in fact $-(0.2)^6/3! = -0.00001066666\ldots$.

(c) (*i*) $h = 0.2$.

$$\begin{aligned}
x_1 &= x_0 + h = 0.0 + 0.2\\
&= 0.2\\
y_1 &= y_0 + hf(x_0, y_0)\\
&= y_0 + h(-2x_0y_0)\\
&= 1.0 + 0.2\times(-2\times 0.0\times 1.0)\\
&= 1.0\,.
\end{aligned}$$

(*ii*) $h = 0.1$.

$$\begin{aligned}
x_1 &= x_0 + h = 0.0 + 0.1\\
&= 0.\\
y_1 &= y_0 + hf(x_0, y_0)\\
&= y_0 + h(-2x_0y_0)\\
&= 1.0 + 0.1\times(-2.0\times 0.0\times 1.0)\\
&= 1.0\\
x_2 &= x_1 + h = 0.1 + 0.1\\
&= 0.2\\
y_2 &= y_1 + hf(x_1, y_1) = y_1 + h(-2x_1y_1)\\
&= 1.0 + 0.1\times(-2.0\times 0.1\times 1.0)\\
&= 0.98\,.
\end{aligned}$$

(d) The two-stage second-order Runge-Kutta method with $b = \frac{1}{2}$. $h = 0.2$.

$$\begin{aligned}
k_1 &= hf(x_0, y_0) \\
&= h(-2x_0 y_0) \\
&= 0.2 \times (-2.0 \times 0.0 \times 1.0) \\
&= 0 \\
k_2 &= hf(x_0 + h, y_0 + k_1) \\
&= h\{-2(x_0 + h)(y_0 + k_1)\} \\
&= 0.2 \times (-2.0 \times 0.2 \times 1.0) \\
&= -0.08 \\
y_1 &= y_0 + \frac{1}{2}(k_1 + k_2) \\
&= 1.0 + \frac{1}{2}(0.0 - 0.08) \\
&= 0.96\,.
\end{aligned}$$

(e) The classical four-stage fourth-order Runge-Kutta method. $h = 0.2$.

$$\begin{aligned}
k_1 &= hf(x_0, y_0) \\
&= h(-2x_0 y_0) \\
&= 0.2 \times (-2.0 \times 0.0 \times 1.0) \\
&= 0 \\
k_2 &= hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1) \\
&= h\{-2(x_0 + \frac{1}{2}h)(y_0 + \frac{1}{2}k_1)\} \\
&= 0.2 \times (-2.0 \times 0.1 \times 1.0) \\
&= -0.04 \\
k_3 &= hf(x_0 + h\frac{1}{2}, y_0 + \frac{1}{2}k_2) \\
&= h\{-2(x_0 + \frac{1}{2}h)(y_0 + \frac{1}{2}k_2)\} \\
&= 0.2 \times (-2.0 \times 0.1 \times 0.98) \\
&= -0.0392 \\
k_4 &= hf(x_0 + h, y_0 + k_3) \\
&= h\{-2(x0 + h)(y_0 + k_3)\} \\
&= 0.2 \times (-2.0 \times 0.2 \times 0.9608) \\
&= -0.076864 \\
y_1 &= y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
&= 1.0 + \frac{1}{6} \times (0 - 2.0 \times 0.04 - 2.0 \times 0.0392 - 0.076864) \\
&= 0.9607893\,.
\end{aligned}$$

(f) The Euler-predictor trapezoidal-corrector method. $h = 0.2$. Euler predictor:

$$\begin{aligned} y_1^{(0)} &= y_0 + hf(x_0, y_0) \\ &= y_0 + h(-2x_0y_0) \\ &= 1.0 + 0.2 \times (-2.0 \times 0.0 \times 1.0) \\ &= 1.0\,. \end{aligned}$$

Trapezoidal corrector (this is equivalent to the second-order Runge-Kutta method in Part (d)):

$$\begin{aligned} y_1^{(1)} &= y_0 + \frac{1}{2}h\{f(x_0, y_0) + f(x_1, y_1^{(0)})\} \\ &= y_0 + \frac{1}{2}h\{(-2x_0y_0) + (-2x_1y_1^{(0)})\} \\ &= 1.0 + \frac{1}{2} \times 0.2 \times \{(-2.0 \times 0.0 \times 1.0) + (-2.0 \times 0.2 \times 1.0)\} \\ &= 0.96 \\ y_1^{(2)} &= y_0 + \frac{1}{2}h\{f(x_0, y_0) + f(x_1, y_1^{(1)})\} \\ &= 1.0 + \frac{1}{2} \times 0.2 \times \{(-2.0 \times 0.0 \times 1.0) + (-2.0 \times 0.2 \times 0.96)\} \\ &= 0.9616\,. \end{aligned}$$

3. *3-Step Gear's Method*. The 3-step method of Gear for stiff problems is of the form

$$y_{n+1} = a_1y_n + a_2y_{n-1} + a_3y_{n-2} + hb_0f(t_{n+1}, y_{n+1})\,.$$

(a) Give a condition that determines the coefficients a_1, a_2, a_3, b_0. Use this condition to find a_1, a_2, a_3, b_0.

(b) Is the method implicit or explicit ? Suggest a suitable technique for implementing this method on stiff problems.

Solution.

The 3-step Gear's method for solving the initial value problem,

$$\frac{dy}{dt} = f(t, y)\,, \qquad y(t_0) = y_0\,,$$

is of the form

$$y_{n+1} = \alpha_1y_n + \alpha_2y_{n-1} + \alpha_3y_{n-2} + h\beta_0f(t_{n+1}, y_{n+1})\,.$$

The coefficients α_1, α_2, α_3 and β_0 are determined by requiring the rule to be exact for polynomial functions $y(t)$ of degree 3 or less. The last term, involving β_0, is simply $h\beta_0y'_{n+1}$, where y'_{n+1} is dy/dt evaluated at $t = t_{n+1}$. With this interpretation of the last term, the rule is linear in y(t). This means that the rule only needs to made exact for $y(t) = 1$, t, t^2 and t^3 and it will be exact for all cubic polynomials. The coefficients are independent of n, which allows us to set $t_n = 0$ in order to simplify the calculation of α_1, α_2, α_3 and β_0. Then $t_{n+1} = h$, $t_{n-1} = -h$ and $t_{n-2} = -2h$. Imposing the conditions gives the following algebraic equations.

$y(t)$	$y'(t)$	y_{n+1}	$=$	$\alpha_1 y_n$	$+$	$\alpha_2 y_{n-1}$	$+$	$\alpha_3 y_{n-2}$	$+$	$h\beta_0 y_{n+1}$
1	0	1	$=$	α_1	$+$	α_2	$+$	α_3		
t	1	h	$=$		$-$	$\alpha_2 h$	$-$	$2\alpha_3 h$	$+$	$h\beta_0$
t^2	$2t$	h^2	$=$			$\alpha_2 h^2$	$+$	$4\alpha_3 h^2$	$+$	$2\beta_0 h^2$
t^3	$3t^2$	h^3	$=$		$-$	$\alpha_2 h^3$	$-$	$8\alpha_3 h^3$	$+$	$3\beta_0 h^3$

Simplify the equations by dividing the second, third and fourth through by h, h^2 and h^3 respectively.

$$\begin{array}{rclcccccl} 1 & = & \alpha_1 & + & \alpha_2 & + & \alpha_3 & & \\ 1 & = & & - & \alpha_2 & - & 2\alpha_3 & + & \beta_0 \\ 1 & = & & & \alpha_2 & + & 4\alpha_3 & + & 2\beta_0 \\ 1 & = & & - & \alpha_2 & - & 8\alpha_3 & + & 3\beta_0 \end{array}$$

Add the second and the third equations, and the third and the fourth equations to eliminate α_2.

$$\begin{array}{rcccl} 2 & = & & 2\alpha_3 & + \; 3\beta_0 \\ 2 & = & - & 4\alpha_3 & + \; 5\beta_0 \end{array}$$

Add 2 times the first of these equations to the second to eliminate α_3, $\beta_0 = 6/11$ and $\alpha_3 = 2/11$, $\alpha_2 = -9/11$ and $\alpha_1 = 18/11$. Hence the method is

$$y_{n+1} = \frac{1}{11}\{18y_n - 9y_{n-1} + 2y_{n-2} + 6hf(t_{n+1}, y_{n+1})\}\,.$$

(c) The method is implicit, since the unknown y_{n+1} occurs on the right-hand side of the equation (unless $f(t, y)$ does not explicitly depend on y). One way to implement this method is to use the Newton-Raphson root-finding method to solve for y_{n+1}.