UNIVERSITY OF NEW SOUTH WALES
School of Mathematics and Statistics

MATH2089 Numerical Methods and Statistics
Term 2, 2019

Numerical Methods Laboratory – Week 9

1 Quadrature

1. It is known that
$$\int_1^2 \frac{dx}{x} = \ln 2.$$
   (a) Write an MATLAB anonymous function to calculate the integrand $f(x) = 1/x$. Your function should accept a vector of inputs, producing a vector of function values.
   (b) Find an approximate value to the above integral by using the composite trapezoidal rule and Simpson's rule with $h = 1/8$.
   (c) Estimate the integral using Gauss-Legendre quadrature with $N = 4$ where the nodes and weights for the standard interval $[-1, 1]$ are (using the MATLAB function `gauleg.m`)

z	−0.861136311594053	−0.339981043584856	0.339981043584856	0.861136311594053
w	0.347854845137454	0.652145154862546	0.652145154862546	0.347854845137454

   (d) Which rule gives a better result?
   (e) The error estimates for $E_N(f) = I(f) - Q_N(f)$ given in lectures are
   - Trapezoidal rule: $E_N(f) = -\frac{(b-a)h^2}{12} f''(\eta_1)$
   - Simpson's rule: $E_N(f) = -\frac{(b-a)h^4}{180} f^{(4)}(\eta_2)$
   - Gauss-Legendre rule: $E_N(f) = \frac{e_N}{(2N)!} f^{(2N)}(\eta_3)$

   Find upper bounds for the errors in each method. Compare these bounds with the actual error.

2. Identify feature(s) of the following integrals which will make them difficult for numerical integration, and suggest remedies.
   - $\displaystyle\int_0^2 \sin(x)^{\frac{1}{3}}\, dx$
   - $\displaystyle\int_0^\pi |\cos(x)|\, dx$

3. From the simple trapezoidal rule
$$\int_c^d f(x)\, dx \approx \left(\frac{d-c}{2}\right)[f(c) + f(d)],$$
derive the composite rule (as given in the lecture notes)
$$\int_a^b f(x)\, dx \approx h\left(\frac{1}{2}f_0 + \sum_{j=1}^{N-1} f_j + \frac{1}{2}f_N\right)$$
where N is a given integer, $h = (b-a)/N$, $x_j = a + hj$, and $f_j = f(x_j)$ for $j = 0, \ldots, N$.

4. Consider the integral
$$I(f) = \int_{\bar{x}-h}^{\bar{x}+h} f(x)\, dx.$$
   (a) Find the polynomial that interpolates f at $\bar{x} - h$, $\bar{x}$, and $\bar{x} + h$.
   (b) Hence derive Simpson's rule
$$I(f) \approx \frac{h}{3}[f(\bar{x} - h) + 4f(\bar{x}) + f(\bar{x} + h)].$$
   (c) Hence deduce the composite Simpson rule introduced in lectures:
$$\int_a^b f(x)\, dx \approx \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots 2f_{N-2} + 4f_{N-1} + f_N\right)$$
   where N is an even integer, $h = (b-a)/N$, $x_j = a + jh$ and $f_j = f(x_j)$ for $j = 0, \ldots, N$.

2 Initial value problems

A model of a stirred tank chemical reactor in which two chemicals react under controlled conditions to produce a certain product involves the problem data

- V = volume of the tank (m^3)
- q = constant flow rate into and out of the tank (m^3/min)
- u_1 = concentration (moles/m^3) of chemical 1 in the input stream
- u_2 = concentration (moles/m^3) of chemical 2 in the input stream
- r = reaction rate (moles/m^3-min)

The state variables are

- x_1 = concentration of chemical 1 (moles/m^3)
- x_2 = concentration of chemical 2 (moles/m^3)
- x_3 = concentration of product (moles/m^3)

The governing system of ordinary differential equations (ODEs) is
$$\begin{aligned} V\frac{dx_1}{dt} - qu_1 + qx_1 + Vr &= 0 \\ V\frac{dx_2}{dt} - qu_2 + qx_2 + Vr &= 0 \\ V\frac{dx_3}{dt} + qx_3 - Vr &= 0 \end{aligned}$$
and the reaction rate r is assumed to satisfy
$$r = \alpha x_1 x_2$$
where $\alpha > 0$ is constant.

The concentrations of the the two reactants in the constant feed stream is $u(t) = (3.2,\ 4.8)^T$, the flow rate is $q = 10$ m^3/min, the volume of the tank is $V = 2$ m^3 and the reaction rate constant is $\alpha = 2.6$ m^3/moles-min.

Initially the mixture in the tank has 5 moles/m^3 of chemical 1 and 3 moles/m^3 of chemical 2, and no product is initially present.

We want to find the concentrations of the chemicals and product over a period of 72 seconds.

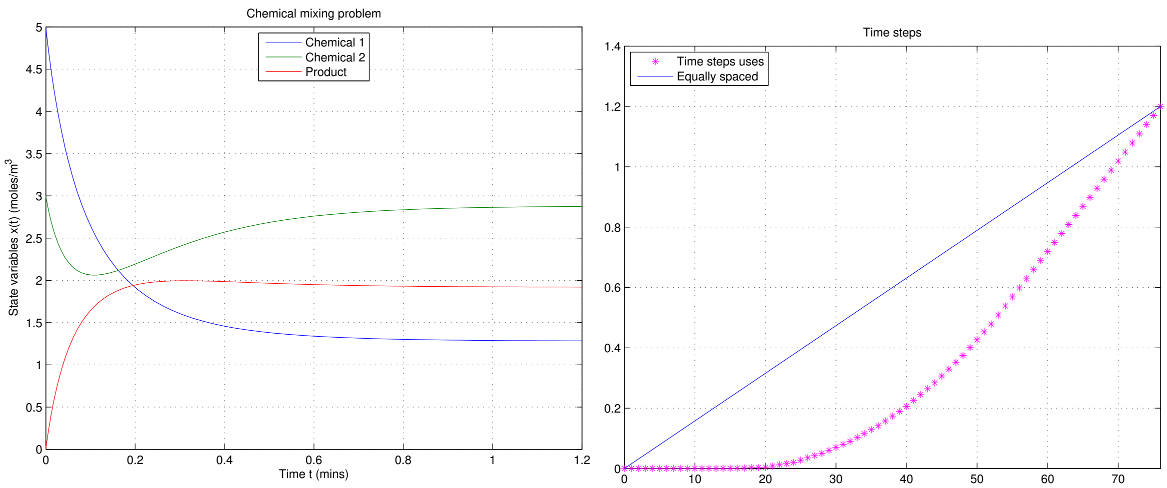

Figure 1: Concentration of chemicals and step-sizes

1. Write this as an IVP in the standard form

$$\mathbf{x}' = \mathbf{f}(t, \mathbf{x}) \quad t \in [t_0, t_{\max}], \qquad \mathbf{x}(t_0) = \mathbf{y}_0$$

2. Write a MATLAB function M-file

```
function f = mixf(t, x)
```

to specify the system of ODEs to be solved. Initially define any problem data required in this function.

3. Write a MATLAB script to
   (a) Define the time interval and initial conditions.
   (b) Call the MATLAB solver `ode45`.
   (c) Calculate the number of time intervals used.
   (d) Plot the solution as in the first plot in Figure 1.
   (e) In another figure window, plot the steps used against a constant step size (see second plot in Figure 1).

4. Try some of the following solvers using $N = 100$ intervals. They are available from the course web page.
   (a) Explicit Euler
   (b) Heun
   (c) RK4

5. Modify your script and function so that the problem data is defined in the main M-file and not in the function M-file. This will involve passing the problem data to `ode45`.