All questions may be attempted by all students. Questions tagged by * are harder. Questions tagged by A are advanced only.

1. (a) What are the UFL, OFL and $\epsilon_{\text{mach}}$ of the floating point number system with rounding,

$$\{\pm d_1.d_2d_3 \times 10^{\pm p} \mid d_2, d_3, p = 0, \ldots, 9; d_1 = 1, \ldots, 9, \text{unless } d_1 = d_2 = d_3 = 0\}.$$ 

(b) Give an example of an ill-conditioned problem.

(c) By expanding $f(x - h)$ in a Taylor series in $h$ to three terms including a remainder, find an expression for the truncation error $e^T$ in the formula

$$f'(x) = \frac{f(x) - f(x - h)}{h} + e^T.$$ 

2. (a) Consider the roots of the equation $f(x) = 0$. Using the first two terms of the Taylor expansion of $f(x)$ about $x_i$ derive the Newton-Raphson iteration formula. Give one advantage and one disadvantage of the Newton-Raphson method over the secant method.

Write down the Newton-Raphson iteration formula for $n$ nonlinear equations in $n$ variables, carefully explaining any notation you use.

(b) Show that the Newton-Raphson iteration scheme for the function

$$f(x) = \frac{1}{x} - a,$$

where $a$ is a constant, is given by

$$x_{n+1} = x_n(2 - ax_n).$$

What is the root of $f$? Do two iterations of the Newton-Raphson scheme for $a = 3$ and starting with $x_0 = 0.3$ to find $x_1$ and $x_2$. Estimate how many iterations would be needed to determine the root to 16 decimal places?
3. (a) Solve the system of equations

\[ \begin{align*}
2x + 4y - z &= 1 \\
4x + \ y + \ z &= -2 \\
2x - 3y + 6z &= 1
\end{align*} \]

using the Doolittle form of Gaussian elimination with back-substitution and without row interchanges. Write down the \( LU \)-factorisation of the coefficient matrix \( A \).

Given that the inverse of \( A \) is

\[ A^{-1} = \frac{1}{56} \begin{pmatrix}
-9 & 21 & -5 \\
22 & -14 & 6 \\
14 & -14 & 14
\end{pmatrix} \]

determine the condition number of \( A \) using the norm \( \| \cdot \|_1 \). Suppose the above system is solved by Gaussian elimination with back-substitution on a computer with \( \epsilon_{\text{mach}} = 10^{-7} \), what is the worst relative error \( \| x - \hat{x} \| / \| x \| \) you would expect in the computed solution \( \hat{x} \)?

(b) Apply a convergent Gauss-Seidel iteration scheme to the system of equations in Part (a). Start with \( x^{(0)} = y^{(0)} = z^{(0)} = 0 \), and do one iteration to find \( x^{(1)} \), \( y^{(1)} \), \( z^{(1)} \).

(c) The Gauss-Seidel iteration scheme can be written in the form

\[ x^{(k+1)} = c + Sx^{(k)}, \]

where

\[ c = \frac{1}{12} \begin{pmatrix}
-6 \\
6 \\
7
\end{pmatrix}, \quad S = \frac{1}{48} \begin{pmatrix}
0 & -12 & -12 \\
0 & 6 & 18 \\
0 & 7 & 13
\end{pmatrix}. \]

Show that the error \( e^{(k)} = x^* - x^{(k)} \), where \( x^* \) is the exact solution of the iteration scheme, satisfies

\[ e^{(k+1)} = Se^{(k)}. \]

Hence by evaluating \( \| S \|_\infty \) prove that the iteration scheme converges.
4. (a) A 2-point Gauss rule for integrals with weight function $x^{-1/3}$ has the form
\[ \int_0^1 f(x)x^{-1/3} \, dx = w_1 f(x_1) + w_2 f(x_2). \]

State the conditions which determine the weights $w_1$, $w_2$ and the nodes $x_1$, $x_2$ and hence derive the equations which determine them. Given the weights and nodes,
\[ w_1 = \frac{3(25 + \sqrt{20})}{100} \approx 0.884164, \quad w_2 = \frac{3(25 - \sqrt{20})}{100} \approx 0.615836, \]
\[ x_1 = \frac{5(1 - 3\sqrt{20})}{11} \approx 0.149627, \quad x_2 = \frac{5(1 + 3\sqrt{20})}{11} \approx 0.759464, \]
use the method to evaluate
\[ \int_0^1 x^{-1/3} \cos x \, dx. \]

(b) For the weight function in Part (a), the orthogonal polynomials on $[0, 1]$ of degree $\leq 2$ are
\[ \phi_0(x) = 1, \quad \phi_1(x) = x - \frac{2}{5}, \quad \phi_2(x) = x^2 - \frac{40}{44} x + \frac{5}{44}. \]

Give the Gram-Schmidt formula for constructing the orthogonal polynomial $\phi_n(x)$ of degree $n$, if $\phi_0(x), \ldots, \phi_{n-1}(x)$ have already been constructed. Deduce the nodes of the 1-point Gauss rule and the 2-point Gauss rule for the weight function $x^{-1/3}$ on $[0, 1]$.

5. Consider the initial value problem, $dy/dt = f(t, y)$, $y(t_0) = y_0$, $t_0 \leq t \leq T$.

(a) Second-order two-stage Runge-Kutta methods are of the form
\[ k_1 = hf(t_n, y_n) \quad (1) \]
\[ k_2 = hf(t_n + \alpha h, y_n + \beta k_1) \quad (2) \]
\[ y_{n+1} = y_n + ak_1 + bk_2 \quad (3) \]
\[ a + b = 1, \quad ab = 1/2, \quad \beta b = 1/2. \]

Do one step of the second-order Runge-Kutta method with $b = 1$ to approximate $y(1.2)$, where $y(t)$ is the solution of
\[ \frac{dy}{dt} = t - y^3, \quad y(1) = 1. \]

Is this problem well-conditioned?

(b) The Taylor expansion of the exact solution $Y(t)$ about $t_k$ is
\[ Y_{k+1} = Y_k + hY'_k + \frac{1}{2}h^2Y''_k + \frac{1}{6}h^3Y'''(\xi_k), \]
where $\xi_k$ lies between $t_k$ and $t_{k+1}$. By comparing this expansion with the solution of the two-stage Runge-Kutta method given by equations (1)–(3) in Part (a) above, assuming the propagated error at $t_k$ is zero, i.e. $y_k = Y_k$, show that the error $e_{k+1} = Y_{k+1} - y_{k+1}$ in $y_{k+1}$ is given by
\[ e_{k+1} = (1 - a - b)hf(t_k, Y_k) + (\frac{1}{2} - ab)h^2f_t(t_k, Y_k)
\]
\[ + (\frac{1}{2} - \beta b)h^2f_y(t_k, Y_k)f(t_k, Y_k) + O(h^3). \]

Hence deduce the conditions on $a$, $b$, $\alpha$, $\beta$ for the two-stage Runge-Kutta to be second order.