Numerical Analysis **Sheet 7**

Orthogonal polynomials and Gaussian quadrature

Please hand in your answer to question 1 by 12 noon on Monday 17th November to the Blackboard Assessed HW2 submission point.

1. ASSESSED HW PROBLEM

   (a) (*4 marks*)
   By sketching curves $y = x$ and $y = 1/(1+x^2)$ on the same graph, show that the cubic equation $x^3 + x - 1 = 0$ has just one root, x^*, say, lying in the interval $(0, 1)$.

   (b) (*6 marks*)
   Prove that the iteration
   $$x_{n+1} = \frac{1}{1 + x_n^2}, \qquad n \geq 0$$
   converges to a unique fixed point $x^* \in (0, 1)$ for any initial guess $x_0 \in (0, 1)$, stating any theorems you rely upon. What is the order of convergence of the scheme ?

   (c) (*5 marks*)
   Show that the iteration
   $$x_{n+1} = \frac{1 - x_n}{x_n^2}, \qquad n \geq 0$$
   has the same fixed point, x^*, as in part (b) but that, for $x_0 \neq x^*$, x_n will not converge to x^* as $n \to \infty$.

   (d) (*5 marks*)
   Show that the iteration
   $$x_{n+1} = \frac{2x_n^3 + 1}{3x_n^2 + 1}, \qquad n \geq 0$$
   also has the same fixed point, x^*, as in part (b). Argue why it must converge for x_0 sufficiently close to x^* and demonstrate that convergence is faster than linear.

   (e) (*5 marks*)
   Use the approximation
   $$f(x^*) \approx f(x_n) + (x^* - x_n)f'(x_n) + \frac{1}{2}(x^* - x_n)^2 f''(x_n),$$
   which ignores terms of $O(|x^* - x_n|^3)$, as the basis of an iterative scheme for determining the roots, x^*, of the function $f(x)$. Specifically, derive the following iterative scheme
   $$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)} \left(1 - \sqrt{1 - \frac{2f(x_n)f''(x_n)}{[f'(x_n)]^2}} \right).$$
   You should give clear reasons for any choices you make in the derivation of this expression.

2. The Legendre polynomials $P_n(x)$ are orthogonal polynomials on the interval $[-1, 1]$ with weight function $w(x) = 1$ and standardisation condition $P_n(1) = 1$.

   The first three Legendre polynomials are given as $P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$.

   (a) Use the Gram-Schmidt process to derive

   $$\text{(i) } P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x, \qquad \text{and} \qquad \text{(ii) } P_4(x) = \frac{35}{8}x^4 - \frac{30}{8}x^2 + \frac{3}{8}.$$

   (b) Find the zeros, x_1 and x_2, of $P_2(x)$ and their corresponding Gauss weights, w_1 and w_2, and use them to approximate the value of the integral

   $$I = \int_0^1 \frac{1}{1+x^2}\, dx.$$

   Compare your answer to the exact value.

   (c) Why does approximating

   $$\frac{1}{2}\int_{-1}^{1} \frac{1}{1+x^2}\, dx$$

   using a two-point Gauss-Legendre quadrature lead to a worse approximation to I ?

3. Let $\phi_n(x)$, $n = 0, 1, \ldots$, be a sequence of polynomials of degree n that are orthogonal on the interval $[0, 1]$ with respect to the weight function $w(x) = x$. Hence they satisfy

   $$\int_0^1 \phi_n(x)\phi_m(x) x \,\mathrm{d}x = 0 \quad \text{if} \quad n \neq m.$$

   In addition they satisfy the standardisation condition $\phi_n(1) = 1$ for all n.

   (a) Determine the first two polynomials $\phi_0(x)$ and $\phi_1(x)$ and show that

   $$\phi_2(x) = 10x^2 - 12x + 3.$$

   (b) Determine the coefficient a_0 in the expansion

   $$x^2 = \sum_{n=0}^{2} a_n \phi_n(x).$$

   (c) Specify the points x_i and weights w_i in the 2-point Gaussian quadrature formula

   $$\int_0^1 f(x) x \,\mathrm{d}x \approx \sum_{j=1}^{2} w_j\, f(x_j).$$

   (d) Using your results, or otherwise, specify points t_i and weights v_i in terms of x_i and w_i such that the approximation

   $$\int_1^\infty \left(b_0/t^3 + b_1/t^4 + b_2/t^5 + b_3/t^6\right) \mathrm{d}t \approx \sum_{j=1}^{2} v_j \left(b_0/t_j^3 + b_1/t_j^4 + b_2/t_j^5 + b_3/t_j^6\right)$$

   is exact when b_0, b_1, b_2, b_3 are arbitrary constants.

4. The Chebyshev polynomials of the second kind U_n, $n = 0, 1, 2, \ldots$, are a sequence of polynomials of degree n that are orthogonal on the interval $[-1, 1]$ with respect to the weight function $w(x) = \sqrt{1 - x^2}$. Hence, they satisfy

$$\int_{-1}^{1} U_n(x)\, U_m(x)\, \sqrt{1 - x^2}\, dx = 0 \quad \text{if} \quad n \neq m. \tag{1}$$

In addition they satisfy the standardisation condition $U_n(1) = n + 1$ for all n.

(a) (i) Explain why

$$\int_{-1}^{1} x\sqrt{1 - x^2}\, dx \qquad \text{and} \qquad \int_{-1}^{1} x^3\sqrt{1 - x^2}\, dx$$

are both zero and calculate the values of

$$\int_{-1}^{1} \sqrt{1 - x^2}\, dx \qquad \text{and} \qquad \int_{-1}^{1} x^2\sqrt{1 - x^2}\, dx.$$

[HINT: use the substitution $x = \cos\theta$.]

(ii) Using the properties of the Chebyshev polynomials of the second kind and (i), determine the first three polynomials $U_0(x)$, $U_1(x)$ and $U_2(x)$.

(iii) Specify the sampling points x_j and weights w_j in the 2-point Gaussian quadrature formula which makes the approximation

$$\int_{-1}^{1} f(x)\, \sqrt{1 - x^2}\, dx \approx \sum_{j=1}^{2} w_j\, f(x_j)$$

exact for polynomials $f(x)$ of degree 3 or less.

(iv) Use the results of part (iii) to find an approximation for the integral

$$\int_{-1}^{1} \cos\left(\frac{\pi\, x}{2}\right)\, dx$$

and compare it to the exact value of this integral.

(b) The Chebyshev polynomials of the second kind have the explicit form

$$U_n(x) = \frac{\sin[(n + 1)\cos^{-1}(x)]}{\sin[\cos^{-1}(x)]}\,. \tag{2}$$

(i) Deduce an explicit formula for the position, x_j, of the sampling points for any n.

(ii) Show that the functions in equation (2) satisfy the recursion relation

$$U_{n+1}(x) + U_{n-1}(x) = f(x)\, U_n(x)$$

where $f(x)$ is a function that you are to determine. Use your result to argue that the functions in (2) are indeed polynomials of degree n.

Show also that the functions in (2) satisfy the standardisation condition for the Chebyshev polynomials of the second kind.

(iii) Using the formula (2) show that (1) is satisfied.

5. The Chebyshev polynomials of the first kind, $T_n(x)$, are orthogonal on $[-1, 1]$ with respect to the weight function $w(x) = 1/\sqrt{1-x^2}$ and satisfy the standardisation condition $T_n(1) = 1$ for all n.

   (a) Determine $T_0(x)$, $T_1(x)$ and show that

$$T_2(x) = 2x^2 - 1, \qquad T_3(x) = 4x^3 - 3x.$$

   [*Hint: The substitution* $x = \cos\theta$ *should prove useful when performing certain integrals.*]

   Show that these results agree with the general formula $T_n(x) = \cos(n \cos^{-1} x)$.

   (b) Calculate the sampling points, x_j, and weights, w_j, $j = 1, \ldots, n$, for the Gauss-Chebyshev quadrature formula

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx \approx \sum_{j=1}^{n} w_j\, f(x_j)$$

   for $n = 1, 2, 3$. Hence show w_j agree with the general formula π/n for $j = 1, \ldots, n$.

   (c) It is a remarkable result that

$$\int_{-1}^{1} \frac{\ln|x-t|}{\sqrt{1-x^2}}\, dx = -\pi \ln(2),$$

   a constant, for all $t \in [1, 1]$. How would you go about using Gaussian quadrature to accurately compute this integral ?

6. (a) Explain why

$$I_n = \int_{-\infty}^{\infty} x^n e^{-x^2}\, dx$$

   is zero when n is odd. You are given $I_0 = \sqrt{\pi}$. Determine that

$$I_{2n} = \frac{(2n-1)}{2} I_{2n-2}$$

   for $n \geq 1$ and hence show that

$$I_{2n} = \frac{(2n)!}{2^{2n} n!} \sqrt{\pi}.$$

   (b) The Hermite polynomials $H_n(x)$ are orthogonal on the infinite interval $(-\infty, \infty)$ with respect to the weighting function $w(x) = e^{-x^2}$. They satisfy the standardisation condition[1] that the coefficient in front of the leading power of x^n in $H_n(x)$ should be set to one.

   Calculate $H_0(x)$, $H_1(x)$ and $H_2(x)$.

[1]this is the probabilist's defnition; physicists use a different definition.

(c) Hence determine the sampling points x_1, x_2 and weights w_1, w_2 for a Gaussian quadrature formula which will evaluate

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} f(x)\, dx$$

exactly if $f(x)$ is a polynomial of degree 3 or less.

(d) Use the results of part (c) to find an approximation for the integral

$$\int_{-\infty}^{\infty} \frac{1}{1+x^2}\, dx\,.$$

What is the exact value of this integral?

(e) The Hermite polynomials $H_n(x)$ may be defined by the relation

$$f(x,t) \equiv \mathrm{e}^{2xt-t^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x)\,. \tag{3}$$

In this way they are obtained by expanding $f(x,t)$ in powers of t.

Calculate the function $g(s,t) = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} f(x,s)\, f(x,t)\, dx$ and expand the result in powers of s and t. Express $g(s,t)$ alternatively in terms of Hermite polynomials, and by comparing terms of the form $s^n t^m$ show that

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} H_n(x)\, H_m(x)\, dx = \begin{cases} 0 & \text{if} \quad n \neq m \\ 2^n n! \sqrt{\pi} & \text{if} \quad n = m \end{cases}$$

[*You may use the following identity* $\int_{-\infty}^{\infty} \mathrm{e}^{-x^2+2ax}\, dx = \sqrt{\pi}\, \mathrm{e}^{a^2}$ *for all* $a \in \mathbb{R}$.]