Homework No.5, 553.481/681, Due April 5, 2024.

Problem 1. (a) Verify that the formula

$$p_n(x) = e^x \left(-\frac{d}{dx}\right)^n (x^n e^{-x}), \quad n = 0, 1, 2, ...$$

defines a monic polynomial of degree n. Derive an explicit formula for the coefficients of each polynomial.

(b) Show that these polynomials satisfy the orthogonality condition

$$\int_0^\infty p_n(x) p_m(x)\, e^{-x}\, dx = 0, \quad n \neq m.$$

Hint: You will find useful the following result:

$$\left(\frac{d}{dx}\right)^n (e^{ax} f(x)) = e^{ax} \left(a + \frac{d}{dx}\right)^n f(x),$$

called the *exponential shift property* of the derivative operator d/dx. The polynomials

$$L_n(x) = p_n(x)/n!$$

are called the *Laguerre polynomials*.

Problem 2. Continuing Problem 1, consider Gaussian quadrature for integrals of the form

$$I(f) = \int_0^\infty f(x)\, e^{-x}\, dx,$$

or so-called *Gauss-Laguerre quadrature*.

(a) Write out explicitly $p_0(x), p_1(x), p_2(x), p_3(x)$

(b) Find the two roots $x_1 < x_2$ of $p_2(x)$.

(c) Derive the weights w_1, w_2 corresponding to x_1, x_2 using the formula

$$w_i = \int_0^\infty \ell_i(x)\, e^{-x}\, dx, \quad i = 1, 2$$

where $\ell_i(x),\ i = 1, 2$ are the Lagrange interpolating polynomials for the two points.

(d) Show that the same weights as in (c) may be derived instead from the two conditions

$$w_1 x_1^i + w_2 x_2^i = \int_0^\infty x^i\, e^{-x}\, dx = i!$$

for $i = 0, 1$ using the results from (b).

(e) Use the results of (b)–(d) to calculate the $n = 2$ Gauss-Laguerre quadrature approximation $I_2(f) = w_1 f(x_1) + w_2 f(x_2)$ for

$$f(x) = \exp(-x/2).$$

Compare this simple approximation with the exact analytical result.

Problem 3. (a) Modify the MATLAB script `gaussleg.m` to define a function `gaussleg2`, as follows:

```
function [I, fnct]=gaussleg2(f,a,b,tol)
```

The function should output the Gauss-Legendre approximation I of the integral $\int_a^b f(x)\, dx$ to a tolerance *tol*, and also the number of function calls $fnct$ used in the entire calculation. Start with $n = 1$ points and increase n by 1 in each iteration, to a maximum of 400 iterations. You may use as your stopping criterion the condition on the relative error in successive quadratures, $|I_n(f) - I_{n-1}(f)|/|I_n(f)| < tol$.

(b) Use your script to calculate the following integrals to the specified tolerances:

(i) $\int_0^1 dx\, x\exp(x^2)$, $tol = 10^{-15}$ *(ii)* $\int_0^1 dx\, [x(1-x)]^{1/3}$, $tol = 10^{-7}$.

Compare your results with those of Romberg integration for the wall clock time and number of function calls required. Try to explain your results, in particular the difference in the results for these two distinct measures of computational cost. Is there a simple way to reduce the wall clock time for Gauss-Legendre?

Problem 4. This problem studies the Gauss-Kronrod pair (G_3, K_7) and compares with the Gauss method G_7 for the same number of points.

(a) The 3-point Gauss rule is given explicitly by

$$G_3(f) = w_0 f(0) + w_1[f(\xi_1) + f(-\xi_1)]$$

with $\xi_1 = \sqrt{\frac{3}{5}}$, $w_0 = \frac{8}{9}$, $w_1 = \frac{5}{9}$. The 7-point Kronrod rule adds four new points

$$K_7(f) = w_0' f(0) + w_1'[f(\xi_1) + f(-\xi_1)] + w_2'[f(\xi_2) + f(-\xi_2)] + w_3'[f(\xi_3) + f(-\xi_3)]$$

where $\pm\xi_2$, $\pm\xi_3$ are smallest and largest magnitude roots of the *Stieltjes polynomial*

$$x^4 - \frac{10}{9}x^2 + \frac{155}{891} = 0.$$

Use this information to find the modified weights w_i', $i = 0, 1, 2, 3$ by requiring that K_7 exactly integrates the even powers x^{2i}, i=0,1,2,3 and using Matlab's `mldivide` to solve the resulting linear system for the weights.

(b) Write a Matlab function code `G3K7.m` to evaluate both $G_3(f)$ and $K_7(f)$ for an input function f on the interval $[-1, 1]$. Make certain to save the three function values $f(0), f(\xi_1), f(-\xi_1)$ needed for $G_3(f)$ and reuse them in the calculation of $K_7(f)$.

(c) Use your code from (b) to compare G_3, K_7 and G_7 for the following three functions on the interval $[-1, 1]$:

$$i)\ f(x) = (x+1)^{10}, \quad (ii)\ f(x) = \cosh(x), \quad (iii)\ f(x) = \cos(\pi x^2/2).$$

You can get the nodes and weights for G_7 from the class code `glquad.m`. Compare each approximation with the exact value of the integral $I = \int_{-1}^{1} f(x)\,dx$. Which has the least/greatest relative error? What is the advantage of using K_7 rather than G_7?

Remark: The exact value of integral (iii) is given in terms of the cosine Fresnel integral which is calculated in Matlab with `fresnelc`.

Problem 5*. This problem explores the use of Gauss-Hermite quadrature to approximate improper integrals of the form

$$I(f) = \int_{-\infty}^{+\infty} f(x)w(x)\,dx, \quad w(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}.$$

(a) Show that the infinite series expansion of the *generating function*

$$e^{xt-\frac{1}{2}t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

defines a sequence $H_n(x)$ of monic polynomials of degree n. These *Hermite polynomials* are the orthogonal polynomials on $(-\infty, +\infty)$ with the Gaussian weight $w(x)$.

(b) By differentiating the expansion in (a) with respect to x and with respect to t, show both of the following:

$$H_n'(x) = nH_{n-1}(x), \quad H_{n+1}(x) = xH_n(x) - nH_{n-1}(x).$$

The second result is called a *recurrence relation* for the Hermite polynomials.

(c) Define for each n the $n \times n$ symmetric, tridiagonal matrix $\mathbf{A}_n$ with 0's along the diagonal and the vector $b(i) = \sqrt{i}$, $i = 1, ..., n-1$ along the first two off-diagonals. Show that the characteristic polynomials

$$p_n(x) = \det(x\mathbf{I}_n - \mathbf{A}_n)$$

with $\mathbf{I}_n$ the $n \times n$ identity matrix are monic polynomials which satisfy the same recurrence relation as in (b) and thus that $p_n(x) = H_n(x)$, $n = 0, 1, 2, ..$ Explain why the nodes $x_1, ..., x_n$ for n-point Gauss-Hermite quadrature are the eigenvalues of $\mathbf{A}_n$.

(d) Use the results in part (c) to write a Matlab function code `ghquad.m` which evaluates the n-point Gauss-Hermite quadrature rule for given f and n. You may take as your model the class code `glquad.m` for Gauss-Legendre quadrature. You can use the fact, without proof, that the weight $w_i = |e_1^i|^2$ where $\mathbf{e}^{(i)}$ is the normalized eigenvector of $\mathbf{A}_n$ for the eigenvalue x_i, $i = 1, ..., n$.

(e) Apply your code in (d) to evaluate the integral $I(f)$ for the function $f(x) = \cosh x$ by Gauss-Hermite quadrature with odd $n = 1, 3, 5, ..., 15$. Give the approximate value and the error for each choice of n and show by a semilog plot that the error is decreasing approximately exponentially in n.