Homework 9 Foundations of Computational Math 2 Spring 2012

Problem 9.1

In this problem we consider the numerical approximation of the integral

$$I = \int_{-1}^{1} f(x)dx$$

with $f(x) = e^x$. In particular, we use a priori error estimation to choose a step size h for Newton Cotes or a number of points for a Gaussian integration method.

9.1.a

Consider the use of the composite Trapezoidal rule to approximate the integral I.

- Use the fact that we have an analytical form of $f(x)$ to estimate the error using the composite trapezoidal rule and to determine a stepsize h so that the error will be less than or equal to the tolerance 10^{-2}.
- Approximately how many points does your h require?

Solution:

We must use the error expression for the composite trapezoidal rule, the expression for the appropriate derivative bound, and the required tolerance to get an a priori estimate for h.

$$f(x) = e^x = f''(x)$$
$$f''(x) \leq f''(1) \approx 2.72$$
$$E = -\frac{h^2}{12}(b-a)f''(\eta)$$
$$h^2 \leq \frac{12 \times 10^{-2}}{(b-a)f''(\eta)} = \frac{0.06}{f''(\eta)} \approx \frac{0.06}{2.72} \approx 0.02$$
$$h \approx 0.14$$
$$n = \frac{(b-a)}{h} = \frac{2}{0.14} \approx 14 \text{ steps}$$

Using the composite trapezoidal rule yields the following results:

n	I_n	$I - I_n$
2	2.5308	-0.1926
8	2.3623	-0.01223
14	2.3544	-0.00399
16	2.35346	-0.00305

9.1.b

Consider the use of the Gauss-Legendre method to approximate the integral I. Use $n = 1$, i.e., two points x_0 and x_1 with weights γ_0 and γ_1.

- Use the fact that we have an analytical form of $f(x)$ to estimate the error that will result from using the two-point Gauss-Legendre method to approximate the integral.
- How does your estimate compare to the tolerance 10^{-2} used in the first part of the question?
- Recall that for $n = 1$ we have the Gauss Legendre nodes $x_0 \approx -0.5774$ and $x_1 \approx 0.5774$. Apply the method to approximate I and compare its error to your prediction. The true value is
$$I = \int_{-1}^{1} e^x dx \approx 2.3504$$

Solution:

Recall the error formula for Gauss Legendre

$$E = \frac{2^{2n+3}\left[(n+1)!\right]^4}{(2n+3)\left[(2n+2)!\right]^3} f^{(2n+2)}(\eta)$$

We have $f^{(2n+2)}(x) = e^x \leq e^1 \approx 2.72$ and for $n = 1$

$$E = \frac{2^5\left[2!\right]^4}{5\left[4!\right]^3}(2.72)$$
$$= \frac{(512)(2.72)}{(5 \times 24 \times 24 \times 24)} \approx 0.02$$

We are given $x_0 \approx -0.5774$ and $x_1 \approx 0.5774$ and we recall that for $n = 1$ we have a symmetric formula and $\gamma_0 = \gamma_1 = 1$. This yields

$$I_1 = e^{x_0} + e^{x_1} = 1.7814 + 0.56136 = 2.34276$$

Which yields an error of $2.3504 - 2.34276 = 0.0076$ which satisfies our bound. Note the significant superiority of a two point prediction of error and the subsequent error versus the number of points predicted by a priori analysis for the composite trapezoidal rule.

Problem 9.2

Suppose $\phi_i(x)$, $i = 0, 1, \ldots$ are a set of orthonormal polynomials with respect to the inner product

$$(f, g)_\omega = \int_a^b \omega(x) f(x) g(x)\, dx$$

where $\phi_i(x)$ has degree i. Show that

$$\int_a^b \omega(\xi) G_n(x,\xi)\, d\xi = 1$$

where

$$G_n(x,\xi) = \sum_{i=0}^{n} \phi_i(x)\phi_i(\xi)$$

Solution:

$$\begin{aligned}\int_a^b \omega(\xi) G_n(x,\xi)\, d\xi &= \int_a^b \omega(\xi) \sum_{i=0}^{n} \phi_i(x)\phi_i(\xi)\, d\xi \\ &= \sum_{i=0}^{n} \int_a^b \omega(\xi)\phi_i(x)\phi_i(\xi)\, d\xi\end{aligned}$$

The value $\phi_i(x)$ is constant with respect to ξ therefore it is a polynomial of degree 0 with respect to ξ. We have

$$\int_a^b \omega(x)\phi_i(x)\phi_i(\xi)\, d\xi = \begin{cases} 0 & \text{if } i > 0 \\ 1 & \text{if } i = 0 \end{cases}$$

$$\therefore \sum_{i=0}^{n} \int_a^b \omega(\xi)\phi_i(x)\phi_i(\xi)\, d\xi = 1$$

Note this solution requires $\phi_i(x)$ is a polynomial of degree i.

Problem 9.3

Let $U(x)$ and $V(x)$ be polynomials of degree n defined on $x \in [-1,1]$. Let $x_j,\quad 0 \le j \le n$ and $\gamma_j,\quad 0 \le j \le n$ be the Gauss-Legendre quadrature points and weights. Finally, let $\ell_j(x),\quad 0 \le j \le n$ be the Lagrange characteristic interpolating polynomials defined with nodes at the Gauss-Legendre quadrature points.

Show that the following summation by parts formula holds:

$$\sum_{j=0}^{n} U'(x_j)\, V(x_j)\, \gamma_j = (U(1)V(1) - U(-1)V(-1)) - \sum_{j=0}^{n} U(x_j)\, V'(x_j)\, \gamma_j$$

Solution: Integration by parts yields

$$(U(1)V(1) - U(-1)V(-1)) = \int_{-1}^{1} U'(x)\, V(x)\, dx + \int_{-1}^{1} U(x)\, V'(x)\, dx$$

Since the products involved are polynomials of degree $2n-1$, Gauss Legendre quadrature is exact and the summation by parts follows.

Problem 9.4

For the Legendre polynomials, $P_n(x)$, we have the recurrence

$$P_0 = 1, \quad P_1 = x$$
$$P_{n+1} = \frac{2n+1}{n+1} x P_n - \frac{n}{n+1} P_{n-1}$$

This yields a form that is orthogonal but it is not monic and it is not orthonormal. For example, we have

$$P_2 = \frac{3}{2}x^2 - \frac{1}{2}$$

$$P_3 = \frac{5}{2}x^3 - \frac{3}{2}x$$

9.4.a

Let $\tilde{P}_n(x)$ be the Legendre polynomial that is normalized so that the series is orthonormal, i.e.,

$$(\tilde{P}_i,\ \tilde{P}_j) = \delta_{ij}$$

but not necessarily in monic form. Derive a recurrence that relates $\tilde{P}_{n+1}$ to $\tilde{P}_n$ and $\tilde{P}_{n-1}$.

Recall, that the class notes and the reference text by Isaacson and Keller give the following recurrence for the normalized (but not monic) Legendre polynomials

$$\tilde{P}_{n+1} = (A_n x + B_n)\tilde{P}_n - C_n \tilde{P}_{n-1}$$

where

$$\tilde{P}_n = \tilde{a}_n x^n + \tilde{b}_n x^{n-1} + q_{n-2}(x)$$

$$A_n = \frac{\tilde{a}_{n+1}}{\tilde{a}_n}$$

$$B_n = \frac{\tilde{a}_{n+1}}{\tilde{a}_n}\left(\frac{\tilde{b}_{n+1}}{\tilde{a}_{n+1}} - \frac{\tilde{b}_n}{\tilde{a}_n}\right)$$
$$C_n = \frac{\tilde{a}_{n+1}\tilde{a}_{n-1}}{\tilde{a}_n^2}$$

Show that your recurrence is equivalent to this recurrence.

Solution:

We have $(P_n, P_n) = 2/2n+1$ and therefore

$$\tilde{P}_n = \frac{\sqrt{2n+1}}{\sqrt{2}} P_n$$
$$\tilde{P}_0 = \frac{1}{\sqrt{2}}$$
$$\tilde{P}_1 = \sqrt{\frac{3}{2}}\ x$$
$$\tilde{P}_2 = \sqrt{\frac{5}{2}} \left(\frac{3}{2}x^2 - \frac{1}{2}\right)$$

It follows that

$$P_n = \frac{\sqrt{2}}{\sqrt{2n+1}} \tilde{P}_n$$

$$P_{n+1} = \frac{2n+1}{n+1} x P_n - \frac{n}{n+1} P_{n-1}$$
$$\Downarrow$$
$$\tilde{P}_{n+1} = \frac{\sqrt{(2n+1)(2n+3)}}{n+1} x \tilde{P}_n - \frac{n\sqrt{2n+3}}{(n+1)\sqrt{2n-1}} \tilde{P}_{n-1}$$

To show that this recurrence is equivalent to the Isaacson and Keller recurrence we consider B_n, A_n and C_n in turn. First note that for any $P_n(x)$ that we have alternating powers of x so the coefficient for x^{n-1} is always 0. This is true for any scaling of $P_n(x)$ so $\tilde{b}_n = 0$ and therefore $B_n = 0$ for all n and

$$\tilde{P}_{n+1} = A_n x \tilde{P}_n - C_n \tilde{P}_{n-1}$$

The leading coefficients $\tilde{a}_n$ can be deduced from the recurrence for $\tilde{P}(x)$ directly to determine A_n or it can be deduced from the original recurrence for $P_n(x)$. Let

$$P_n = a_n x^n + b_n x^{n-1} + r_{n-2}(x)$$

Since

$$P_{n+1} = \frac{2n+1}{n+1} x P_n - \frac{n}{n+1} P_{n-1}$$

if follows that

$$a_{n+1} x^{n+1} = \frac{2n+1}{n+1} x a_n x^n.$$

and

$$\tilde{a}_n = \frac{\sqrt{2n+1}}{\sqrt{2}}\ a_n$$

Therefore

$$\frac{a_{n+1}}{a_n} = \frac{2n+1}{n+1}$$

$$\frac{\tilde{a}_{n+1}}{\tilde{a}_n} = \frac{\sqrt{2n+3}}{\sqrt{2n+1}}\frac{a_{n+1}}{a_n}\frac{\sqrt{2n+3}}{\sqrt{2n+1}}\frac{2n+1}{n+1}$$

$$\therefore A_n = \frac{\sqrt{(2n+1)(2n+3)}}{n+1}$$

So the first term of the two recurrences are equivalent.

We have

$$C_n = \frac{\tilde{a}_{n+1}\tilde{a}_{n-1}}{\tilde{a}_n^2} = \frac{A_n}{A_{n-1}}$$

$$A_n = \frac{\sqrt{(2n+1)(2n+3)}}{n+1}, \quad A_{n-1} = \frac{\sqrt{(2n-1)(2n+1)}}{n}$$

$$C_n = \left(\frac{n}{n+1}\right)\left(\frac{\sqrt{(2n+1)(2n+3)}}{\sqrt{(2n-1)(2n+1)}}\right) = \frac{n\sqrt{2n+3}}{(n+1)\sqrt{2n-1}}$$

which completes the equivalence.

9.4.b

The textbook in equations (10.7) and (10.8) gives the recurrence for the monic, but not necessarily normalized, form of Legendre polynomials. The coefficients of this recurrence gives the coefficients necessary to define the Jacobi matrix whose eigendecomposition give the Gauss Legendre quadrature nodes and weights. Determine the values of α_k and β_k and show that they are consistent with the values used in the MATLAB codes for Gauss Legendre quadrature in Section 10.6 of the textbook.

Solution:

From the textbook we have

$$\hat{P}_{n+1} = (x - \alpha_n)\hat{P}_{n+1} - \beta_n \hat{P}_{n-1}$$

$$\alpha_n = \frac{(x\hat{P}_n, \hat{P}_n)}{(\hat{P}_n, \hat{P}_n)}$$

$$\beta_n = \frac{(\hat{P}_{n+1}, \hat{P}_{n+1})}{(\hat{P}_n, \hat{P}_n)}$$

where $\hat{P}_n$ is the monic but not orthonormal form of the Legendre polynomials. Since,

$$P_n = a_n x^n + b_n x^{n-1} + r_{n-2}(x)$$

the coefficient α_n can be simplified to

$$\alpha_n = \frac{(x\hat{P}_n, \hat{P}_n)}{(\hat{P}_n, \hat{P}_n)} = \frac{2n+1}{2} \ \ (xP_n,\ P_n)$$

The inner product can be determined as follows

$$P_{n+1} = \frac{2n+1}{n+1} x P_n - \frac{n}{n+1} P_{n-1}$$
$$xP_n = \frac{n+1}{2n+1} P_{n+1} + \frac{n}{2n+1} P_{n-1}$$
$$\Downarrow$$
$$(xP_n, P_n) = \frac{n+1}{2n+1}(P_{n+1},\ P_n) + \frac{n}{2n+1}(P_{n-1},\ P_n)$$

$$\therefore (xP_n, P_n) = 0 \quad \text{and} \quad \alpha_n = 0$$

The coefficient β_n can be determined as follows

$$\beta_n = \frac{(\hat{P}_{n+1}, \hat{P}_{n+1})}{(\hat{P}_n, \hat{P}_n)} = \frac{a_{n+1}^2}{a_n^2} \frac{(P_{n+1}, P_{n+1})}{(P_n, P_n)}$$

$$\frac{a_{n+1}}{a_n} = \frac{2n+1}{n+1}, \quad (P_{n+1}, P_{n+1}) = \frac{2}{2n+3}, \quad (P_n, P_n) = \frac{2}{2n+1}$$
$$\Downarrow$$
$$\beta_n = \frac{2n+1}{n+1} \times \frac{2}{2n+3} \times \frac{2n+1}{2}$$
$$= \frac{(n+1)^2}{(2n+1)^2}(2n+1)(2n+3) = \frac{(n+1)^2}{(2n+1)^2} 4(n+1)^2 - 1$$

which is consistent with the codes in Section 10.6.

These coefficients are used to determine the symmetric tridiagonal Jacobi matrix associated with the Legendre polynomials:

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & 0 & & \\ 0 & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & 0 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

The nodes for the Gauss Legendre of with n points are given by the eigenvalues of the $n \times n$ Jacobi matrix. The weights, γ_i, are given by the first component, $\phi_1^{(i)}$, of the eigenvectors, $f^{(i)}$, associated with the nodes, λ_i, using:

$$\gamma_i = \mu_0(\phi_1^{(i)})^2, \quad \mu_0 = \int_{-1}^{1} \omega(x)dx$$

where $\omega(x)$ defines the inner product associated with the polynomials (in this case 1). (See Gill, Seguro, and Tumme, Numerical methods for special functions, SIAM Publications for more details.)