AMSC/CMSC 460 Computational Methods

Exam 2, Due Tuesday April 14, 2015 **Solution**

This exam is now take-home due to power outage on April 7. Please read carefully with the instructions below.

Show all work clearly and in order, and circle your final answers. Justify your answers algebraically whenever possible. **Use no books, calculators, computers, internet, communication with others, etc, except a formula sheet (A4 one-sided) prepared by yourself. Use no more than 80 minutes to finish the exam.**

1. (20 points) Mark each of the following statements T (True) or F (False).
You will get 4 points for each correct answer, -1 points for each wrong answer, and 0 point for leaving it blank.

(a) ______ Lagrange interpolations on equally distributed nodes have the best perfomance (in the sense of minimizing L^∞ error) when the number of nodes n is large.

> **Solution:** False. Runge's phenomenon occurs for interpolant with equally distributed nodes.

(b) ______ A natural cubic spline is a $\mathcal{C}^2$ function.

> **Solution:** True. The second derivatives matches at the interface.

(c) ______ Newton-Cotes type integrations use equally spaced nodes.

> **Solution:** True.

(d) ______ Suppose $s_1(x)$ is a linear interpolating spline of $f(x)$ on equally distributed nodes in $[a, b]$. Then, $\int_a^b s_1(x)dx$ defines a composite trapezoid rule to approximate $\int_a^b f(x)dx$.

> **Solution:** True. Newton-Cotes type quadrature rule is to use the integrand of Lagrange polynomial.

(e) ______ A Gauss quadrature with n nodes has higher algebraic accuracy than a Newton-Cotes type quadrature with n nodes.

> **Solution:** True. For Gauss quadrature, the algebraic accuracy is $2n - 1$. For Newton-Cotes, the algebraic accuracy is $n - 1$ or n, which is smaller.

2. Let $f(x) = (1+x)^{-1}$, for $x \in [0,1]$.

   (a) (8 points) Find a cubic polynomial $p_3(x)$ which interpolates f such that

$$p_3(0) = f(0), \quad p_3'(0) = f'(0), \quad p_3''(0) = f''(0), \quad \text{and } p_3(1) = f(1).$$

Solution: Use Newton's representation, we get

$$\begin{array}{c|lllll}
x_0 = 0 & f_0 = 1 & & & & \\
 & & f_{01} = f'(0) = -1 & & & \\
x_1 = 0 & f_1 = 1 & & f_{012} = \frac{f''(0)}{2} = 1 & & \\
 & & f_{12} = f'(0) = -1 & & f_{0123} = \frac{f_{123}-f_{012}}{x_3-x_0} = -\frac{1}{2} & \\
x_2 = 0 & f_2 = 1 & & f_{123} = \frac{f_{23}-f_{12}}{x_3-x_1} = \frac{1}{2} & & \\
 & & f_{23} = \frac{f_3-f_2}{x_3-x_2} = -\frac{1}{2} & & & \\
x_3 = 1 & f_3 = \frac{1}{2} & & & &
\end{array}$$

Therefore, $p_3(x) = 1 - x + x^2 - \frac{1}{2}x^3$.

   (b) (8 points) Obtain an error bound uniformly in $[0,1]$. Namely, find an upper bound of $\|f - p_3\|_{L^\infty([0,1])}$.

Solution: The point-wise error formula reads

$$f(x) - p_3(x) = \frac{f''''(\xi)}{4!}\pi_4(x), \quad \pi_4(x) = x^3(x-1).$$

For uniform estimate, we get

$$\|f - p_3\|_{L^\infty([0,1])} \le \frac{\max_{\xi\in[0,1]} |f''''(\xi)|}{4!} \max_{x\in[0,1]} |\pi_4(x)|.$$

In this case, $f''''(\xi) = -\dfrac{24}{(1+\xi)^5} \quad \Rightarrow \quad \max\limits_{\xi\in[0,1]} |f''''(\xi)| \le 24.$

For $\max_{x\in[0,1]} |\pi_4(x)|$, as $\pi_4'(x) = 4x^3 - 3x^2$, the stationary points of $\pi(x)$ for $x \in [0,1]$ is $x = \frac{3}{4}$. Compare with the endpoints: $\pi_4(\frac{3}{4}) = \frac{27}{256}, \pi_4(0) = \pi_4(1) = 0$. Therefore, $\max_{x\in[0,1]} |\pi_4(x)| = \frac{27}{256}$.

We conclude that $\|f - p_3\|_{L^\infty([0,1])} \le \frac{24}{4!} \cdot \frac{27}{256} = \frac{27}{256}$.

   (c) (3 points) $s_L(x)$ is the linear interpolating spline for f, on nodes $\{x_i\}_{i=0}^5$, where $x_i = i/5$. Let $\{\varphi_i(x)\}_{i=0}^5$ be hat functions with respect to the nodes. We can express $s_L(x) = \sum_{k=0}^{m} a_k \varphi_k(x)$. Find $a_0, \cdots, a_5$.

Solution: As hat function $\phi_i(x_j) = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$, we get $a_i = f(x_i)$. Hence, it is easy to get

$$a_0 = 1, \quad a_1 = \frac{5}{6}, \quad a_2 = \frac{5}{7}, \quad a_3 = \frac{5}{8}, \quad a_4 = \frac{5}{9}, \quad a_5 = \frac{1}{2}.$$

(d) (6 points) (*) Find an error bound of $\|f - s_L\|_{L^\infty([0,1])}$.

Solution: For $x \in [x_{i-1}, x_i]$, the approximation is a linear interpolation, where error formula says

$$|f(x) - s_L(x)| \leq \frac{\max_{\xi \in [x_{i-1}, x_i]} |f''(\xi)|}{2} \max_{x \in [x_{i-1}, x_i]} |\pi_2(x)|, \quad \pi_2(x) = (x - x_{i-1})(x - x_i).$$

It is easy to obtain $\max |\pi_2(x)| = |\pi_2(\frac{x_{i-1}+x_1}{2})| = \frac{h^2}{4}$, where $h = x_i - x_{i-1} = \frac{1}{5}$. And $\max_{x \in [0,1]} |f''(x)| = 2$. Therefore,

$$\|f - s_L\|_{L^\infty([0,1])} \leq \frac{2}{2} \cdot \frac{h^2}{4} = \frac{1}{100}.$$

3. (20 points) Let $f(x) = x^4$. Find the quadratic polynomial $p_2(x)$ which minimizes the following functional

$$\int_0^\infty (f(x) - p_2(x))^2 e^{-x} dx.$$

You do not have to simplify your answer.

Hint: To ease the computational load, you can use the following identity,

$$\int_0^\infty x^k e^{-x} dx = k!, \quad \textit{for all integers} \;\; k \geq 0.$$

Solution: Denote $\langle \cdot, \cdot \rangle$ be L^2 inner product with weight e^{-x} in $[0, \infty)$, namely

$$\langle f, g \rangle = \int_0^\infty f(x) g(x) e^{-x} dx.$$

Then, the problem becomes a least square approximation with respect to the inner product $\langle \cdot, \cdot \rangle$.

Take Laguerre polynomials $\{L_n(x)\}$, and write $p_2(x) = \sum_{i=0}^2 \alpha_i L_i(x)$. The coefficients satisfy the linear system

$$\begin{pmatrix} \langle L_0, L_0 \rangle & \langle L_0, L_1 \rangle & \langle L_0, L_2 \rangle \\ \langle L_1, L_0 \rangle & \langle L_1, L_1 \rangle & \langle L_1, L_2 \rangle \\ \langle L_2, L_0 \rangle & \langle L_2, L_1 \rangle & \langle L_2, L_2 \rangle \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} \langle L_0, f \rangle \\ \langle L_1, f \rangle \\ \langle L_2, f \rangle \end{pmatrix}.$$

By orthogonality of Laguerre polynomials with respect to the inner product, we get the matrix is an identity matrix. We are left to calculate

$$\begin{aligned} \alpha_0 &= \langle L_0, f \rangle = \int_0^\infty x^4 e^{-x} dx = 4! = 24, \\ \alpha_1 &= \langle L_1, f \rangle = \int_0^\infty (1 - x) x^4 e^{-x} dx = 4! - 5! = -96, \\ \alpha_2 &= \langle L_2, f \rangle = \int_0^\infty \left(\frac{1}{2} x^2 - 2x + 1 \right) x^4 e^{-x} dx = \frac{6!}{2} - 2 \cdot 5! + 4! = 144. \end{aligned}$$

Therefore, $p_3(x) = 24 - 96(1 - x) + 144 \left(\frac{1}{2} x^2 - 2x + 1 \right)$.

4. Simpson's 3/8 rule states the following. Let $\{x_i\}_{i=0}^3$ be equally distributed nodes in $[a, b]$, namely $x_i = a + i(b-a)/3$. Then,

$$\int_a^b f(x)dx \approx I_3[f] := \frac{b-a}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right).$$

The corresponding error formula reads

$$E = \int_a^b f(x)dx - I_3[f] = -\frac{(b-a)^5}{6480} f^{(4)}(\xi), \quad \text{where } \xi \in (a, b).$$

(a) (5 points) What is the algebraic accuracy of the Simpson's 3/8 rule.

> **Solution:** From the error formula, for all $f \in \mathbb{P}_3$, $f^{(4)}(x) \equiv 0$ and therefore $E \equiv 0$. So, algebraic accuracy is 3.

(b) (5 points) Write a composite 3/8 Simpson's rule on $\int_0^1 f(x)dx$ using 7 equally distributed nodes $\{x_i\}_{i=0}^6$, where $x_i = i/6$.

> **Solution:**
>
> $$\int_0^1 f(x)dx \approx \frac{1}{16}[f(0)+3f(1/6)+3f(1/3)+2f(1/2)+3f(2/3)+2f(5/6)+f(1)].$$

(c) (10 points) Suppose $\max_{0 \le x \le 1} |f^{(4)}(x)| = 1$. Give an upper bound on the error for the composite rule in (b).

> **Solution:** The composite rule uses Simpson's 3/8 rule in $[0, 1/2]$ and $[1/2, 1]$. For each interval, we can apply the error formula and get
>
> $$|E_i| \le \frac{(1/2)^5}{6480} \cdot 1.$$
>
> Therefore, the total error is $|E_1 + E_2| \le 2 \cdot \frac{(1/2)^5}{6480} = \frac{1}{103680}$.

5. We approximate the integrand $\int_{-1}^{1} f(x)dx$ by a Gauss quadrature rule $Q[f]$:

$$\int_{-1}^{1} f(x)dx \approx Q[f] = \sum_{i=0}^{n} w_i f(x_i),$$

where the $n+1$ nodes $\{x_i\}_{i=0}^n$ and weights $\{w_i\}_{i=0}^n$ are to be determined.

(a) (5 points) What is the minimum n to guarantee $Q[f]$ is exact for all $f \in \mathbb{P}_9$.

Solution: Given n, the algebraic accuracy for Gauss quadrature rule is $2n+1$. To ensure $2n+1 \geq 9$, the minimum $n = 4$.

(b) (10 points) Take $n = 2$. Find the nodes $\{x_i\}_{i=0}^2$ and weights $\{w_i\}_{i=0}^2$ of the quadrature rule that maximizes the algebraic accuracy.

Solution: We use Legendre polynomial $\{P_i(x)\}$. From the recursive formula, we get

$$P_0(x) = 0, \quad P_1(x) = x, \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, \quad P_3(x) = \frac{1}{2}x(5x^2 - 3).$$

The nodes are roots for P_3. Hence, $x_0 = -\sqrt{\frac{3}{5}}, x_1 = 0, x_2 = \sqrt{\frac{3}{5}}$. For the weights, we solve the following linear system

$$\begin{pmatrix} P_0(x_0) & P_0(x_1) & P_0(x_2) \\ P_1(x_0) & P_1(x_1) & P_1(x_2) \\ P_2(x_0) & P_2(x_1) & P_2(x_2) \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} \langle P_0, P_0 \rangle \\ 0 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 5/9 \\ 8/9 \\ 5/9 \end{pmatrix}.$$

Therefore, the Gauss quadrature is given as

$$\int_{-1}^{1} f(x)dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right).$$

List of classical orthogonal polynomials

- Legendre polynomials $\{P_n(x)\}_{n=0}^{\infty}$: $P_0(x) = 1, P_1(x) = x$, and

$$P_{n+1}(x) = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x), \quad \text{for } n = 1, 2, \cdots.$$

  They are orthogonal in $[-1, 1]$ with respect to the standard L^2 inner product:

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \begin{cases} 0 & m \neq n \\ \frac{2}{2n+1} & m = n \end{cases}.$$

- Chebyshev polynomials $\{T_n(x)\}_{n=0}^{\infty}$: $T_0(x) = 1, T_1(x) = x$, and

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x), \quad \text{for } n = 1, 2, \cdots.$$

  They are orthogonal in $[-1, 1]$ with respect to L^2_w inner product with weight $w(x) = \frac{1}{\sqrt{1-x^2}}$:

$$\int_{-1}^{1} T_m(x) T_n(x) \frac{1}{\sqrt{1-x^2}} dx = \begin{cases} 0 & m \neq n \\ \pi & m = n = 0 \\ \frac{\pi}{2} & m = n \neq 0 \end{cases}.$$

- Laguerre polynomials $\{L_n(x)\}_{n=0}^{\infty}$: $L_0(x) = 1, L_1(x) = 1 - x$, and

$$L_{n+1}(x) = \frac{2n+1-x}{n+1} L_n(x) - \frac{n}{n+1} L_{n-1}(x), \quad \text{for } n = 1, 2, \cdots.$$

  They are orthogonal in $[0, \infty)$ with respect to L^2_w inner product with weight $w(x) = e^{-x}$:

$$\int_{-1}^{1} L_m(x) L_n(x) e^{-x} dx = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}.$$

- Hermite polynomials $\{H_n(x)\}_{n=0}^{\infty}$: $H_0(x) = 1, H_1(x) = x$, and

$$H_{n+1}(x) = x H_n(x) - n H_{n-1}(x), \quad \text{for } n = 1, 2, \cdots.$$

  They are orthogonal in $[-1, 1]$ with respect to L^2_w inner product with weight $w(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$:

$$\int_{-1}^{1} H_m(x) H_n(x) \left(\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \right) dx = \begin{cases} 0 & m \neq n \\ n! & m = n \end{cases}.$$