AMSC/CMSC 460 Computational Methods

Final Exam, Monday, May 18, 2015 **Solution**

Show all work clearly and in order, and circle your final answers. Justify your answers algebraically whenever possible. Use no books, calculators, cellphones, communication with others, etc, except two formula sheets (A4 one-sided) prepared by yourself. You have 120 minutes to take this 210 point exam. If you get more than 200 points, your grade will be 200.

1. (40 points) Mark each of the following statements T (True) or F (False).

   [28] This part contains 7 statements. You will get 4 points for each correct answer, -1 points for each wrong answer, and 0 point for leaving it blank.

   (a) ______ Let $\|\cdot\|_p$ be the matrix norm induced by the corresponding vector p-norm. Then the three norms $\|\cdot\|_1, \|\cdot\|_2$ and $\|\cdot\|_\infty$ are equivalent.

   Solution: True.

   (b) ______ QR factorization of a matrix is unique, namely, for any matrix A, there exists only one pair of orthonormal matrix Q and upper triangular matrix R such that $A = QR$.

   Solution: False.

   (c) ______ Bisection method has a linear convergence rate.

   Solution: True.

   (d) ______ Natural cubic spline is smoother than Hermite cubic spline.

   Solution: True.

   (e) ______ Gauss quadrature uses equally distributed nodes.

   Solution: False.

   (f) ______ Explicit schemes for initial value problems of first order ODE can never be A-stable.

   Solution: True.

   (g) ______ The best way to solve a stiff ODE system is to use higher order explicit Runge-Kutta methods.

Solution: False.

[12] For the following 5 statements, choose 3 (and ONLY 3) to answer.

(h) ______ Iterative methods are more efficient than Gauss elimination when the linear system is large and sparse.

Solution: True.

(i) ______ A similar transform does not change the eigenvalues and the corresponding eigenvectors of the matrix.

Solution: False.

(j) ______ Normalized Chebyshev polynomial of degree n (namely T_n divided by its leading coefficient 2^{n-1}) minimizes the L^∞-norm in $[-1, 1]$, among all the monic polynomials of degree n.

Solution: True.

(k) ______ Richardson extrapolation is used to improve the rate of convergence of a sequence.

Solution: True.

(l) ______ The shooting method can be used to solve second order ODE with Neumann or Robin boundary condition.

Solution: False.

2. (20 points) Consider the following Matlab code.

```
A = [1 2 2; 1 3 3;2 4 0];
c = cond(A(1:2,1:2),1)
[L,U,P] = lu(A)
```

Find the output `c`, `L`, `U`, `P` by hand.

Solution: `A(1 : 2, 1 : 2)` represents the submatrix $\begin{pmatrix} 1 & 2 \\ 1 & 3 \end{pmatrix}$, we donote it with B. Clearly, $B^{-1} = \begin{pmatrix} 3 & -2 \\ -1 & 1 \end{pmatrix}$. Therefore,

$$\kappa_1(B) = \|B\|_1 \cdot \|B^{-1}\|_1 = 5 \cdot 4 = 20.$$

For L, U, P, Gauss elimination procedure is omitted here. The result is:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ .5 & 1 & 0 \\ .5 & 0 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 2 & 4 & 0 \\ 0 & 1 & 3 \\ 0 & 0 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

3. (20 points) (a) [10] Complete the following QR decomposition

$$A = \begin{pmatrix} -1 & -3 & 0 & 0 \\ -1 & 1 & 4 & 4 \\ 1 & 3 & -2 & -2 \\ 1 & -1 & -2 & 2 \end{pmatrix} = \begin{pmatrix} * & -.5 & * & .5 \\ * & .5 & * & .5 \\ * & .5 & * & .5 \\ * & -.5 & * & .5 \end{pmatrix} \begin{pmatrix} -2 & * & * & * \\ * & 4 & * & * \\ * & * & -2 & * \\ * & * & * & 2 \end{pmatrix}.$$

Solution: Use Gram-Schmidt (omit the details) and get

$$Q = \begin{pmatrix} .5 & -.5 & .5 & .5 \\ .5 & .5 & -.5 & .5 \\ -.5 & .5 & .5 & .5 \\ -.5 & -.5 & -.5 & .5 \end{pmatrix}, \quad R = \begin{pmatrix} -2 & -2 & 4 & 2 \\ 0 & 4 & 2 & 0 \\ 0 & 0 & -2 & -4 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

(b) [10] Use the decomposition in (a) to find a vector $x \in \mathbb{R}^3$ which minimize $\|Ax - b\|_2$ where $b = [1, 0, -1, 0]^T$.

Solution: Solve the linear system $Rx = Q^T b$, we get $x = \begin{pmatrix} -.25 \\ -.25 \\ 0 \\ 0 \end{pmatrix}$.

4. (20 points) Suppose $f(x) = (x^2 - 187)^2$, in $(0, \infty)$. The goal is to use iterative scheme to approximate the root of f, which is $x_* = \sqrt{187}$.

(a) [5] Write the Newton's iteration for this specific f.

Solution: The Newton's iteration reads $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$. For the particular f, the scheme is

$$x_{k+1} = x_k - \frac{(x_k^2 - 187)^2}{2(x_k^2 - 187) \cdot (2x_k)} = x_k - \frac{x_k^2 - 187}{4x_k} = \frac{3}{4}x_k + \frac{187}{4x_k}.$$

(b) [5] Check the consistency condition: if x_k converges, then the limit must be a root of f.

Solution: Write the scheme as $x_{k+1} = g(x_k)$, with $g(x) = \frac{3}{4}x + \frac{187}{4x}$. We check the consistency condition

$$g(x_*) = \frac{3}{4}\sqrt{187} + \frac{187}{4\sqrt{187}} = \sqrt{187} = x_*.$$

(c) [10] What is the convergence rate of the scheme? Verify your statement rigorously.

Solution: We start to check on $g'(x_*)$.

$$g'(x) = \frac{3}{4} - \frac{187}{4x^2}, \quad \Rightarrow \quad g'(\sqrt{187}) = \frac{3}{4} - \frac{187}{4(\sqrt{187})^2} = \frac{1}{2}.$$

So $|g'(x_*)| = \frac{1}{2} < 1$, and the scheme has a linear rate of convergence.
Remark: It is accepted if one use the general setup to prove linear convergence.

5. (20 points) Let $f(x) = \dfrac{2}{1+x^2}$.

(a) [10] Find a polynomial p_3 of degree 3 which is a Hermite interpolation of f (namely it interpolates both f and f') at nodes -1 and 1. Simplify your answer in the form of $\sum_{k=0}^{3} c_k x^k$.

Solution: Polynomial p_3 satisfies $p_3(-1) = p_3(1) = 1, p_3'(-1) = 1,\ p_3'(1) = -1$. Use any of the three procedures (consult Note #2), we obtain

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

(b) [10] Find an upper bound of the error $\|f(x) - p_3(x)\|_{L^\infty([-1,1])}$.

For your convenience, $\max_{x\in[-1,1]}|f^{(n)}(x)| = |f^{(n)}(0)| = 2\cdot n!$, for all integers $n \geq 0$.

Solution: The error formula reads

$$f(x) - p_3(x) = \frac{f^{(4)}(\xi)}{4!}[(x+1)(x-1)]^2.$$

To get an upper bound, we compute

$$\|f(x) - p_3(x)\|_{L^\infty(-1,1)} \leq \frac{M_4}{4!}\left[\max_{x\in[-1,1]}(1-x^2)\right]^2 \leq \frac{2\cdot 4!}{4!}\cdot 1 = 2.$$

(Any reasonable upper bound is accepted.)

6. (20 points) Let $f(x) = x^5 - 2x^4$. Find the quadratic polynomial $p_2(x)$ which minimizes

$$\int_{-\infty}^{\infty}\left(f(x) - p_2(x)\right)^2 e^{-\frac{x^2}{2}}\,dx.$$

Hint: Hermite polynomials $\{H_n(x)\}_{n=0}^{\infty}$ *are orthogonal with respect to:*

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

They can be defined recursively as $H_{n+1}(x) = xH_n(x) - H_n'(x)$, *with* $H_0(x) = 1$.
The following decomposition on f *could save your computational load significantly:*

$$f(x) = H_5(x) - 2H_4(x) + 10H_3(x) - 12H_2(x) + 15H_1(x) - 6H_0(x).$$

Solution: Write $p_2(x) = \sum_{i=0}^{3}\alpha_i H_i(x)$. The coefficients satisfy the linear system

$$\begin{pmatrix} \langle H_0, H_0\rangle & \langle H_0, H_1\rangle & \langle H_0, H_2\rangle \\ \langle H_1, H_0\rangle & \langle H_1, H_1\rangle & \langle H_1, H_2\rangle \\ \langle H_2, H_0\rangle & \langle H_2, H_1\rangle & \langle H_2, H_2\rangle \end{pmatrix}\begin{pmatrix}\alpha_0 \\ \alpha_1 \\ \alpha_2\end{pmatrix} = \begin{pmatrix}\langle H_0, f\rangle \\ \langle H_1, f\rangle \\ \langle H_2, f\rangle\end{pmatrix}.$$

The matrix is diagonal due to orthogonality. We calculate the right hand side

$$\begin{aligned} \langle H_0, f\rangle &= -6\langle H_0, H_0\rangle = -6\sqrt{2\pi}, \\ \langle H_1, f\rangle &= 15\langle H_1, H_1\rangle = 15\sqrt{2\pi}, \\ \langle H_2, f\rangle &= -12\langle H_2, H_2\rangle = -24\sqrt{2\pi}. \end{aligned}$$

Here, we again use orthogonality, as well as the decomposition on f. We can now solve the linear system

$$\begin{pmatrix} \sqrt{2\pi} & & \\ & \sqrt{2\pi} & \\ & & 2\sqrt{2\pi} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} -6\sqrt{2\pi} \\ 15\sqrt{2\pi} \\ -24\sqrt{2\pi} \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} -6 \\ 15 \\ -12 \end{pmatrix}.$$

The first 3 Hermite polynomials are given as $H_0(x) = 1, H_1(x) = x, H_2(x) = x^2 - 1$. Therefore, $p_2(x) = -6 + 15x - 12(x^2 - 1) = -12x^2 + 15x + 6$.

7. (15 points) Suppose a quadrature rule $I[f]$ has the following error bound

$$E = \left| \int_a^b f(x)dx - I[f] \right| \le C(b-a)^7,$$

where C is a constant which depends on f. Consider the following composite rule: let $\{x_i\}_{i=0}^N$ be equally distributed nodes in $[a, b]$, namely $x_i = a + ih$ where $h = (b-a)/N$. Apply quadrature rule $I[f]$ on each interval $[x_{i-1}, x_i]$, for $i = 1, \cdots, N$. Then, sum up the integrands on all intervals.

- *Derive* an error bound E_N for the composite quadrature rule $I_N[f]$.
- What is the rate of convergence for the composite rule?

Solution:

$$E_N = \left| \int_a^b f(x)dx - I_N[f] \right| \le \sum_{i=1}^N E_i,$$

where E_i is the error by applying the quadrature rule $I[f]$ on interval $[x_{i-1}, x_i]$. From the error bound on $I[f]$, we get

$$E_i \le C(x_i - x_{i-1})^7 = Ch^7 \quad \text{or} \quad \frac{C(b-a)^7}{N^7}.$$

Therefore, we obtain

$$E_N \le N \cdot Ch^7 = C(b-a)h^6 \quad \text{or} \quad \frac{C(b-a)^7}{N^6}.$$

As $E_N = \mathcal{O}(N^{-6})$, the rate of convergence is 6.

8. (20 points) 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] 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) [15] 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.

Hint: You can make use of Legendre polynomials $\{P_i\}_{i=0}^\infty$, which are orthogonal with respect to standard L^2 inner product:

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

They can be constructed recursively as $P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x)$, for $n = 1, 2, \cdots$, with $P_0(x) = 1$ and $P_1(x) = x$.

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

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

9. (35 points) Consider the following scheme which solves the ODE $y' = f(x, y)$.

$$y_{n+1} = y_n + \frac{h}{2}\left[f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}f(x_n, y_n)\right) + f\left(x_n + \frac{h}{2}, y_{n+1} - \frac{h}{2}f(x_{n+1}, y_{n+1})\right)\right].$$

(a) [5] Is the scheme explicit or implicit?

Solution: The scheme is implicit.

(b) [15] Express the truncation error $T_n(h)$, and find the local order of accuracy.

Solution: The truncation error $T_n(h)$ can be expressed as

$$T_n(h) = \frac{y(x_{n+1}) - y(x_n)}{h} - \frac{1}{2} f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n)\right)$$
$$-\frac{1}{2} f\left(x_n + \frac{1}{2}h\ ,\ y(x_{n+1}) - \frac{h}{2} f(x_{n+1}, y(x_{n+1}))\right).$$

For the exact solution, we have

$$y(x_{n+1}) = y_n + hf + \frac{h^2}{2}(f_x + f f_y) + \mathcal{O}(h^3).$$

Here we write$f = f(x_n, y_n)$ for simplicity.
From the scheme, we calculate term by term. For the first (explicit) part,

$$f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n)\right) = f + \frac{h}{2} f_x + \frac{hf}{2} f_y + \mathcal{O}(h^2).$$

For the second (implicit) part,

$$\begin{aligned} & f\left(x_n + \frac{h}{2}, y(x_{n+1}) - \frac{h}{2} f(x_n, y(x_{n+1}))\right) \\ = \ & f + \frac{h}{2} f_x + f_y \cdot \left[y(x_{n+1}) - \frac{h}{2} f(x_n, y(x_{n+1})) - y_n\right] + \mathcal{O}(h^2) \\ = \ & f + \frac{h}{2} f_x + f_y \cdot \left[hf + \mathcal{O}(h^2) - \frac{h}{2}\left(f + \mathcal{O}(h)\right)\right] + \mathcal{O}(h^2) \\ = \ & f + \frac{h}{2} f_x + f_y \cdot \frac{h}{2} f + \mathcal{O}(h^2). \end{aligned}$$

In the second equality, we again use the fact that $y(x_{n+1}) = y_n + hf + \mathcal{O}(h^2)$.
To put everyting together, the truncation error is

$$T_n = f + \frac{h^2}{2}(f_x + f f y) - \frac{1}{2}\left(f + \frac{h}{2} f_x + \frac{hf}{2} f_y\right) - \frac{1}{2}\left(f + \frac{h}{2} f_x + f_y \cdot \frac{h}{2} f\right) \mathcal{O}(h^2).$$

Therefore, the method has second order accuracy.

(c) [10] Obtain the region of absolute stability of the scheme. Is the scheme A-stable?

Solution: Plug in $f(x,y) = \lambda y$ to the scheme, we get

$$y_{n+1} = y_n + \frac{h}{2}\lambda\left(y_n + \frac{h}{2}\lambda y_n + y_{n+1} - \frac{h}{2}\lambda y_{n+1}\right).$$

Denote $z = \lambda h$. Reorganize the scheme in the explicit way:

$$\left(1 - \frac{z}{2} + \frac{z^2}{4}\right) y_{n+1} = \left(1 + \frac{z}{2} + \frac{z^2}{4}\right) y_n, \quad \Rightarrow \quad y_{n+1} = \frac{z^2+2z+4}{z^2-2z+4} y_n.$$

The region of absolute stability is given by

$$\left|\frac{z^2+2z+4}{z^2-2z+4}\right| < 1, \quad \text{i.e.} \quad \left|1 + \frac{4z}{z^2-2z+4}\right| < 1.$$

For $z \in \mathbb{R}$, the condition is equivalent to $z \in (-\infty, 0)$. As $\mathbb{R}^-$ lies inside the region of absolute stability, the method is A-stable.

(d) [5] Does the method converge? What is the rate of convergence? (Just state the result. No need to prove.)

Solution: The method has second order convergence, as it is accurate with order 2 and stable.