AMSC/CMSC 460 Computational Methods

Final Exam, Thursday, December 18, 2014 **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).

   [32] This part contains 8 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 $\|\cdot\|_\infty$ be the matrix norm induced by the corresponding vector infinity norm. Then, $\|A\|_\infty = \max_{i,j} |a_{ij}|$, where a_{ij} is the $(i,j)-$entry of matrix A.

   Solution: False.

   (b) ______ Matlab script `sparse`$([1,3],[2,1],[1,2])$ generates a sparse matrix $\begin{pmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \end{pmatrix}$.

   Solution: False.

   (c) ______ The best way to solve a linear system with a tridiagonal matrix is through Gauss elimination.

   Solution: False.

   (d) ______ A Hermite cubic spline is a piecewise polynomial which is not everywhere twice differentiable.

   Solution: True.

   (e) ______ Matlab function `quad` use Gauss quadrature for numerical integration.

   Solution: False.

   (f) ______ The accuracy of a multi-step method can be affected by the scheme used to generate first few terms.

   Solution: True.

(g) ______ Backward Euler method is A-stable.

Solution: True.

(h) ______ The procedure of linear regression can be viewed as a least square approximation.

Solution: True.

[8] For the following 4 statements, choose 2 (and ONLY 2) to answer.

(i) ______ To solve an n-by-n linear system, each iteration step of Gauss-Seidel method requires a computational complexity of order $\mathcal{O}(n^2)$.

Solution: True.

(j) ______ The n-th Cheybeshev polynomial T_n has n distinct roots, and they all lie between -1 and 1.

Solution: True.

(k) ______ Performing Richardson extrapolation on Trapezoid rule once, the method is equivalent to Simpson's rule, of order $\mathcal{O}(h^4)$.

Solution: True.

(l) ______ Suppose v is an eigenvector of matrix A, then its corresponding eigenvalue can be computed by $\dfrac{v^TAv}{v^Tv}$.

Solution: True.

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

```
A = [.5 4 .5; 1 2 -1;-.2 .8 2.6];
c = norm(A,1)
[L,U,p] = lu(A,'vector')
```

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

Solution: For $c = \|A\|_1$, we have

$$\|A\|_1 = \max\{1.7, 6.8, 4.1\} = 6.8.$$

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

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

3. (25 points) Suppose $f(x) = x - e^{-x}$, in $[0, \infty)$. We use the following iterative scheme (named *relaxation method*) to find the root of f.

$$x_{k+1} = x_k - \lambda f(x_k).$$

(a) [6] Let x_* be the root, and $e_k = x_k - x_*$ be the error at k-th step. Prove the following error estimate.

$$e_{k+1} = (1 - \lambda f'(\xi_k))e_k, \quad \text{for some } \xi_k \in (x_k, x_*).$$

Solution: Compute

$$\begin{aligned} e_{k+1} &= x_{k+1} - x_* = x_k - \lambda f(x_k) - x_* \overset{(*)}{=} e_k - \lambda(f(x_k) - f(x_*)) \\ &\overset{(**)}{=} e_k - \lambda f'(\xi_k) e_k = (1 - \lambda f'(\xi_k))e_k. \end{aligned}$$

In (*), use the fact $f(x_*) = 0$. In (**), use Taylor expansion.

(b) [7] Use the estimate obtained in (a) to show that x_k converges to x_* if for all $k \geq 0$, $|1 - \lambda f'(\xi_k)| \leq L < 1$. What is the rate of convergence?

Solution: From (a) and the assumption, $|e_{k+1}| \leq L|e_k|$, for all $k \geq 0$. Hence, $|e_k| \leq L|e_{k-1}| \leq \cdots \leq L^k|e_0|$. Therefore, as $L < 1$,

$$\lim_{k\to\infty} |x_k - x_*| = \lim_{k\to\infty} |e_k| \leq |e_0| \lim_{k\to\infty} L^k = 0.$$

So x_k converges to x_*, and the convergence rate is linear.

(c) [12] Check that $f'(\xi) \in [1, 2]$ for all $\xi \in [0, \infty)$. Find the condition on λ to guarantee convergence.

Solution: $f'(\xi) = 1 + e^{-\xi}$. For $\xi \geq 0$, we get $e^{-\xi} \in [0, 1]$ and so $f'(\xi) \in [1, 2]$. To guarantee convergence, we need to find λ such that $|1 - \lambda f'(\xi)| \leq L$ for all $\xi \geq 0$. Equivalently, we need

$$\frac{1 - L}{f'(\xi)} \leq \lambda \leq \frac{1 + L}{f'(\xi)}.$$

As $f'(\xi) \in [1,2]$, a sufficient condition on λ is $1 - L \le \lambda \le \frac{1+L}{2}$.
Since the scheme converges as long as $L < 1$, we need $0 < \lambda < 1$.

4. (20 points) Let f be a smooth function with the following point values:

x_i	-1	0	1
$f(x_i)$	0	-1	0
$f'(x_i)$		0	4

(a) [10] Find a polynomial P_4 of degree 4 that interpolates f as well as its derivatives at corresponding nodes in the table. Simplify your answer in the form of $\sum_{k=0}^{4} c_k x^k$.

Solution: Use Newton's representation (the procedure is omitted here but is necessary in the exam). We obtain

$$p_4(x) = 0 + (-1)\cdot(x+1) + 1\cdot(x+1)x + 0\cdot(x+1)x^2 + 1\cdot(x+1)x^2(x-1) = x^4 - 1.$$

(b) [10] Write an estimate for the error $f(x) - P_4(x)$, and find an upper bound of the error (in L^∞ norm), assuming that $\max_{\xi\in[-1,1]} |f^{(5)}(\xi)| = 1$.

Solution: The error formula reads

$$f(x) - p_4(x) = \frac{f^{(5)}(\xi)}{5!}(x+1)x^2(x-1)^2.$$

To get an upper bound, we compute

$$\|f(x) - p_4(x)\|_{L^\infty(-1,1)} \le \frac{M_5}{5!} \max_x |(x+1)x^2(x-1)^2| \le \frac{1}{5!}2^5.$$

(The answer could be improved. But any reasonable upper bound is accepted.)

5. (20 points) Find the cubic polynomial $p_3(x)$ which minimizes $\|f - p_3\|_{L^2([-1,1])}$, for function $f(x) = x^6$.

Hint: You can make use of Legendre polynomials $\{P_n(x)\}_{n=0}^{\infty}$, which are orthogonal with respect to L^2:

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

The first 4 Legendre polynomials is given as below:

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

To save you some computational load, $\int_{-1}^{1} x^6 P_2(x)dx = \frac{4}{21}$ *and* $\int_{-1}^{1} x^6 P_3(x)dx = 0.$

Solution: Write $p_3(x) = \sum_{i=0}^{3} \alpha_i P_i(x)$. The coefficients satisfy the linear system

$$\begin{pmatrix} \langle P_0, P_0\rangle & \cdots & \langle P_0, P_3\rangle \\ \vdots & \ddots & \vdots \\ \langle P_3, P_0\rangle & \cdots & \langle P_3, P_3\rangle \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \ddots \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} \langle P_0, f\rangle \\ \vdots \\ \langle P_3, f\rangle \end{pmatrix}.$$

Make use of the orthogonality of Legendre polynomial, we get

$$\begin{pmatrix} 2 & & & \\ & 2/3 & & \\ & & 2/5 & \\ & & & 2/7 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} 2/7 \\ 0 \\ 4/21 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} 1/7 \\ 0 \\ 10/21 \\ 0 \end{pmatrix}.$$

Therefore, $p_3(x) = \frac{1}{7} + \frac{10}{21} \cdot \frac{1}{2}(3x^2 - 1) = \frac{5}{7}x^2 - \frac{2}{21}$.

6. (35 points) The goal is to numerically compute the integrand $\int_{-1}^{1} f(x)dx$.

   (a) [5] Write a composite Simpson's rule with $2m = 10$, namely, divide the domain into 5 subintervals, and apply Simpson's rule on each of them.

   Solution:

$$\int_0^1 f(x)dx \approx \frac{1}{15}[f(-1) + 4f(-.8) + 2f(-.6) + 4f(-.4) + 2f(-.2) + 4f(0) + 2f(.2) + 4f(.4) + 2f(.6) + 4f(.8) + f(1)].$$

   (b) [10] Obtain an upper bound on the error for the scheme in (a), in terms of $M_4 = \max_{x\in[-1,1]} |f''''(x)|$. You can use the following error formula on Simpson's rule without a proof.

$$\int_a^b f(x)dx - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] = -\frac{(b-a)^5}{2880} f''''(\xi), \quad \xi \in (a, b).$$

Solution: Denote E the error in (a).

$$|E| = \left|\sum_{i=1}^{5}\left[\int_{x_{2i-21}}^{x_{2i}} f(x)dx - \frac{x_{2i}-x_{2i-2}}{6}(f(x_{2i-2})+4f(x_{2i-1})+f(x_{2i}))\right]\right|$$
$$= \left|-\frac{1}{2880}\sum_{i=1}^{5}\left(\frac{2}{5}\right)^5 f''''(\xi_i)\right| \leq \frac{5}{2880}\left(\frac{2}{5}\right)^5 M_4 = \frac{1}{56250}M_4.$$

(c) [5] Take $f(x)=\sqrt{1-x^2}$. Does the bound obtained in (b) guarantee convergences of the integrand as h goes to zero? For your information, $f''''(x) = -\dfrac{12x^2+3}{(1-x^2)^{7/2}}$.

Solution: No. As in this case, f'''' blows up at ± 1, which causes $M_4=\infty$.

(d) [15] Write a Gauss quadrature rule which solves the integrand in (c) exactly. Use as few nodes as you can. *Hint: You can use Chebyshev polynomials* $\{T_n\}_{n=0}^{\infty}$ *which are orthogonal with respect to the weight* $w(x)=\frac{1}{\sqrt{1-x^2}}$ *on* $[-1,1]$. *More precisely, they satisfy the following identities.*

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

Chebyshev polynomials can be defined recursively by

$$T_0(x)=1, \quad T_1(x)=x, \quad \textit{and} \quad T_{n+1}(x)=2xT_n(x)-T_{n-1}(x), \ \textit{for } n\geq 1.$$

Solution: Rewrite the integrand as $\displaystyle\int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}\cdot(1-x^2)dx$, where $w(x)=\frac{1}{\sqrt{1-x^2}}$ is the weight and $g(x)=1-x^2$ is the function which is in $\mathbb{P}_2$. To solve it exactly, we need at least $m=2$ nodes (as $2m-1=3>2$). Therefore, the quadrature rule is given as

$$\int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}\cdot g(x)dx = w_0 g(x_0)+w_1 g(x_1).$$

The knots are roots for $T_2 = 2x^2-1$. Hence, $x_0=-\sqrt{2}/2, x_1=\sqrt{2}/2$. For the weights, we solve the following linear system

$$\begin{pmatrix} T_0(x_0) & T_0(x_1) \\ T_1(x_0) & T_1(x_1)\end{pmatrix}\begin{pmatrix} w_0 \\ w_1\end{pmatrix} = \begin{pmatrix} \int T_0(x)^2\frac{1}{\sqrt{1-x^2}}dx \\ 0\end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} w_0 \\ w_1\end{pmatrix} = \begin{pmatrix}\pi/2 \\ \pi/2\end{pmatrix}.$$

Therefore, the Gauss quadrature is given as

$$\int_{-1}^{1} g(x)\frac{1}{\sqrt{1-x^2}}dx = \frac{\pi}{2}g\left(-\frac{\sqrt{2}}{2}\right) + \frac{\pi}{2}g\left(\frac{\sqrt{2}}{2}\right).$$

In our case, $g(x) = 1 - x^2$. Therefore, the exact value of the integrand is $\pi/2$.

7. (30 points) The following Matlab code discribes the *midpoint method* which solves the ODE $y' = f(x, y)$.

```
for i = 1:N+1
    y(i+1) = y(i)+h*f(x(i)+1/2*h,y(i)+1/2*h*f(x(i),y(i)));
end
```

(a) [5] Write down the scheme. Is it explicit or implicit?

Solution: The scheme is explicit, and it reads

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

(b) [10] Express the truncation error $T_n(h)$. Prove that $T_n(h) = \mathcal{O}(h^2)$. What is the local order of accuracy?

Solution: For the exact solution, we have

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

Here we write$f = f(x_n, y_n)$ for simplicity.
For the scheme, we have

$$y_{n+1} = y_n + h\left(f + \frac{h}{2}f_x + \frac{hf}{2}f_y + \mathcal{O}(h^2)\right).$$

Therefore, the truncation error is

$$T_n = \frac{y(x_{n+1}) - y_{n+1}}{h} = \frac{y(x_{n+1}) - y_n}{h} - \frac{y_{n+1} - y_n}{h} = \mathcal{O}(h^2),$$

thanks to the cancelation. Therefore, the method has second order accuracy.

(c) [10] Obtain the region of absolute stability of the scheme. To proceed, consider the initial value problem

$$\begin{cases} y' = -\lambda y \\ y(0) = y_0. \end{cases}$$

For $\lambda > 0$, the exact solution of the initial value problem is $y(x) = y_0 e^{-\lambda x}$, which decays as x becomes larger. Find an interval of $z = \lambda h$ such that the scheme is stable, namely, $|y_{n+1}| < |y_n|$.

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

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

To ensure stability, we need $|1 - z + z^2| < 1$. It is equivalent to the condition $0 < z < 2$.

(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.

8. (20 points) (a) [10] Find a QR decomposition of the following matrix

$$A = \begin{pmatrix} 1 & 2 & 1 \\ 2 & 8 & -1 \\ 0 & 2 & 3 \\ -2 & 0 & 4 \end{pmatrix}.$$

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

$$Q = \begin{pmatrix} 1/3 & 0 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ 0 & 1/3 & 2/3 \\ -2/3 & 2/3 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} 3 & 6 & -3 \\ 0 & 6 & 3 \\ 0 & 0 & 3 \end{pmatrix}.$$

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

Solution: Solve the linear system $Rx = Q^T b$, we get $x = \begin{pmatrix} 4/9 \\ 0 \\ -1/9 \end{pmatrix}$.