**Math 552** **Scientific Computing II** **Spring 2020**

**SOLUTIONS:** Homework Set 2

1. (Integral Mean Value Theorem) Assume the $g \in C[a,b]$ and that $f$ is an integrable function that is either nonnegative or nonpositive throughout the interval $[a,b]$. Then there exists a point $\eta \in [a,b]$ such that

$$\int_a^b g(x)f(x)\,dx = g(\eta)\int_a^b f(x)\,dx\,.$$

**ANS:** Assume $f \geq 0$. The proof for $f \leq 0$ is similar. Since $[a,b]$ is a closed and bounded subset of $\mathbb{R}$ – hence compact – and $g(x)$ is continuous, there exists constants $m, M$ such that $m \leq g(x) \leq M$ for all $x \in [a,b]$ and

$$mI \leq \int_a^b g(x)f(x) \leq MI\,.$$

where $I = \int_a^b f(x)\,dx$. If $I = 0$ then $f \equiv 0$ and the result is true for any $\xi \in [a,b]$. Otherwise, $I > 0$ and

$$m \leq \frac{\int_a^b g(x)f(x)\,dx}{I} \leq M\,.$$

Since $g(x)$ is continuous it attains all values in $[m,M]$ for some $x \in [a,b]$. Then there must be at least one point in $[a,b]$, call it $\xi$, where

$$g(\xi) = \frac{\int_a^b g(x)f(x)\,dx}{I}\,,$$

or $\int_a^b g(x)f(x)\,dx = g(\xi)I = g(\xi)\int_a^b f(x)\,dx$. #

2. Suppose that $A$ is $n \times n$ symmetric matrix, i.e. $A^T = A$. $A$ is called *positive definite* if $x^T A\, x > 0$ for all $x \neq 0$ in $\mathbb{R}^n$. Show that the following matrices are positive definite:

(a) $\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ (b) $\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$ (b) $\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$

**ANS:** It is clear that each of the matrices above is symmetric. We are left to show that $x^T Ax > 0$ for all $x \neq 0$.

(a) $x^T Ax = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2x_1 + x_2 \\ x_1 + 2x_2 \end{bmatrix} = 2x_1^2 + 2x_1x_2 + 2x_2^2.$
Rewriting this, we have $x_1^2 + x_2^2 + x_1^2 + 2x_1x_2 + x_2^2 = x_1^2 + x_2^2 + (x_1 + x_2)^2 > 0$ since $x \neq 0$.

(b) $x^T Ax = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 \end{bmatrix} = 2x_1^2 - 2x_1x_2 + 2x_2^2.$
Rewriting this, we have $x_1^2 + x_2^2 + x_1^2 - 2x_1x_2 + x_2^2 = x_1^2 + x_2^2 + (x_1 - x_2)^2 > 0$ since $x \neq 0$.

(c) $x^T Ax = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 \end{bmatrix} =$
$2x_1^2 - 2x_1x_2 + 2x_2^2 - 2x_2x_3 + 2x_3^2 = x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 > 0$ since $x \neq 0$.

3. Given a function $f(x)$, use Taylor approximations to show that a $2^{nd}$ order one-sided approximation to $f'(x_j)$ is given by

$$f'(x_j) \approx \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h} .$$

Here $f_j = f(x_j)$, $f_{j+1} = f(x_j + h)$, and $f_{j+2} = f(x_j + 2h)$. What is the precise form of the error term? Using the formula approximate $f'(0)$ where $f(x) = e^x$ for $h = 2^{-N}$ for $N = 1:12$. Form a table with columns giving $h$, the approximation, absolute error and absolute error divided by $h^2$. For each indicate to which values they are converging. Finally, verify that the last column appears to be converging to a value derived using the error term.

**<u>ANS</u>:** Expanding each term at $x = x_j$ gives

$$\begin{aligned}
\frac{-3}{2h} f_j &= \frac{-3}{2h}[f_j] \\
\frac{4}{2h} f_{j+1} &= \frac{4}{2h}[f_j + hf_j' + \frac{h^2}{2} f_j'' + \frac{h^3}{6} f'''(\xi_1)] \\
\frac{-1}{2h} f_{j+2} &= \frac{-1}{2h}[f_j + 2hf_j' + \frac{(2h)^2}{2} f_j'' + \frac{(2h)^3}{6} f'''(\xi_2)] ,
\end{aligned}$$

where $\xi_1 \in (x_j, x_{j+1})$ and $\xi_2 \in (x_j, x_{j+2})$. Summing each column gives

$$\frac{-3+4-1}{2h} f_j = 0 , \quad (\frac{4}{2h} h - \frac{1}{2h} 2h) f_j' = f_j' , \quad (\frac{4}{2h}\frac{h^2}{2} - \frac{1}{2h}\frac{(2h)^2}{2}) f_j'' = 0 .$$

So we indeed have an approximation to $f'(x_j)$. What is the error term? Well,

$$\frac{4}{2h}\frac{h^3}{6} f'''(\xi_1) - \frac{1}{2h}\frac{(2h)^3}{6} f'''(\xi_2) = \frac{h^2}{3} f'''(\xi_1) - \frac{2h^2}{3} f'''(\xi_2) = -\frac{h^2}{3} f'''(\eta) ,$$

where $\eta \in (x_j, x_{j+2})$, so we have

$$f'(x_j) \approx \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h} + O(h^2) .$$

To approximate $f'(0)$ where $f(x) = e^x$ use the following MATLAB code

```
h=[1/2 1/8 1/32 1/128 1/512]';
fp= (-3*exp(0)+4*exp(0+h)-exp(0+2*h))./ (2*h);
err=abs(fp-1);
errdh2 = err ./ (h.^2);
format short e

disp(' ')
disp('      h             fp           err         err/h^2    ')
disp('  ---------------------------------------------------')

disp([h fp err errdh2])
```

The result is

```
      h             fp            err          err/h^2
-------------------------------------------------------
 5.0000e-01   8.7660e-01   1.2340e-01   4.9359e-01
 1.2500e-01   9.9427e-01   5.7264e-03   3.6649e-01
 3.1250e-02   9.9967e-01   3.3326e-04   3.4126e-01
 7.8125e-03   9.9998e-01   2.0465e-05   3.3529e-01
 1.9531e-03   1.0000e+00   1.2734e-06   3.3382e-01
```

We see that column 1 is converging to 0, column 2 to $1 = f'(0)$, column 3 to 0, and column 4 to 1/3. The last result follows from the error term above:

$$\frac{1}{3} f'''(0) = \frac{1}{3} e^0 = \frac{1}{3} \,.$$

4. The method of undetermined coefficients was used to derived the $2^{nd}$ order centered finite difference approximation to both $f'(x_j)$ and $f''(x_j)$, given respectively by

$$(Df)(x_j) = \frac{f_{j+1} - f_{j-1}}{2h}, \quad (D^2 f)(x_j) = D_-(D_+ f)(x_j) = D_+(D_- f)(x_j) = \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$$

Here $f_j = f(x_j)$ and $f_{j\pm1} = f(x_j \pm h)$ where $x_{j\pm1} = x \pm h$. Derive the same approximations as follows:

(a) Find the Lagrange form of the polynomial $P_2(x)$ of degree $\leq 2$ such that $P_2(x_j) = f_j$ and $P_2(x_{j\pm1}) = f_{j\pm1}$.

(b) Compute $P_2'(x)$ and show that $P_2'(x_j) = (Df)(x_j)$.

(c) Compute $P_2''(x)$ and show that $P_2''(x_j) = (D^2 f)(x_j)$.

**ANS:** (a) $P_2(x)$ is given by

$$\begin{aligned}
P_2(x) &= \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f_{j-1} + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} f_j \\
&\quad + \frac{(x - x_{j-1})(x - x_j)}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f_{j+1} \\
&= \frac{(x - x_j)(x - x_{j+1})}{2h^2} f_{j-1} - \frac{(x - x_{j-1})(x - x_{j+1})}{h^2} f_j + \frac{(x - x_{j-1})(x - x_j)}{2h^2} f_{j+1}
\end{aligned}$$

(b) $P_2'(x) = \dfrac{2x - (x_j + x_{j+1})}{2h^2} f_{j-1} - \dfrac{2x - (x_{j-1} + x_{j+1})}{h^2} f_j + \dfrac{2x - (x_{j-1} + x_j)}{2h^2} f_{j+1}.$

Then

$$\begin{aligned}
P_2'(x_j) &= \frac{x_j - x_{j+1}}{2h^2} f_{j-1} - \frac{2x_j - (x_{j-1} + x_{j+1})}{h^2} f_j + \frac{x_j - x_{j-1}}{2h^2} f_{j+1} \\
&= \frac{-h}{2h^2} f_{j-1} - \frac{(x_j - x_{j-1}) - (x_j - x_{j+1})}{h^2} f_j + \frac{h}{2h^2} f_{j+1} \\
&= -\frac{1}{2h} f_{j-1} - \frac{h - h}{h^2} f_j + \frac{1}{2h} f_{j+1} = \frac{f_{j+1} - f_{j-1}}{2h} = (Df)(x_j)
\end{aligned}$$

(c) $P_2''(x) = \dfrac{1}{h^2} f_{j-1} - \dfrac{2}{h^2} f_j + \dfrac{1}{h^2} f_{j+1} = \dfrac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$, a constant, independent of $x$. So we see that $P_2''(x_j) = (D^2 f)(x_j)$.

5. (*Method of Undetermined Coefficients*) We derived Simpson's rule to approximate $I(f) = \int_a^b f(x)\, dx$,

$$S = \frac{h}{3}(f(a) + 4f(\frac{a+b}{2}) + f(b)), \qquad h = (b-a)/2\,,$$

by interpolating $f(x)$ at the points $x = a, \frac{(a+b)}{2}, b$, then integrating the interpolant over $[a, b]$. The approximation satisfies

$$I(f) = S - \frac{1}{90}h^5 f^{(4)}(\eta)\,, \quad \text{where } \eta \in (a, b)\,.$$

Note that the term $f^{(4)}(\eta)$ implies Simpson's rule is *exact* if $f(x)$ is a polynomial of degree $<= 3$, i.e., $P_n(x)$ for $0 \le n \le 3$.

(a) Use the method of undetermined coefficients to derive $S$. Assume that

$$S = c_1 f(a) + c_2 f(\frac{a+b}{2}) + c_3 f(b)\,,$$

where the coefficients $c_1, c_2$, and $c_3$ are to be determined. Evaluate the expression using the *three* functions $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$, and for each compute the exact answer. Then derive and solve a $3 \times 3$ linear system for the coefficients.

(b) Now use $S$ to approximate $I(f)$ with $f(x) = x^3$. Is the answer exact? Discuss.

**<u>ANS</u>:** (a) First, applying $I_s(f)$ to each of the three functions gives

$$\begin{aligned} I(1) &= I_s(1) &= b - a &= c_1 * 1 + c_2 * 1 + c_3 * 1\,, \\ I(x) &= I_s(x) &= (b^2 - a^2)/2 &= c_1 * a + c_2 * \tfrac{a+b}{2} + c_3 * b\,, \\ I(x^2) &= I_s(x^2) &= (b^3 - a^3)/3 &= c_1 * a^2 + c_2 * \left(\tfrac{a+b}{2}\right)^2 + c_3 * b^2\,. \end{aligned}$$

In matrix form we have

$$\begin{bmatrix} 1 & 1 & 1 \\ a & \frac{a+b}{2} & b \\ a^2 & (\frac{a+b}{2})^2 & b^2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} b-a \\ (b^2-a^2)/2 \\ (b^3-a^3)/3 \end{bmatrix}.$$

The determinant of the coefficient matrix is

$$\left(\frac{(a+b)}{2}b^2 - \left(\frac{a+b}{2}\right)^2 b\right) - (ab^2 - a^2 b) + \left(a\left(\frac{a+b}{2}\right)^2 - a^2\frac{(a+b)}{2}\right) = (b-a)^3/4\,,$$

so if $a \neq b$ then the matrix is invertible, and there is a unique solution to the system. A simple check shows that indeed $[c_1\ c_2\ c_3]^T = [h/3\ 4h/3\ h/3]^T$ is the solution!

(b) For $f(x) = x^3$ we have (check)

$$I_s(x^3) = \frac{h}{3}\left(a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right) = \frac{(b-a)}{6}\left(a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right) = (b^4 - a^4)/4\,,$$

which is exact! This is expected since the error term for $I_s(f)$ involves the fourth derivative of $f(x)$, which for $x^3$ is identically zero.

6. Write a MATLAB function M-file **trilu** to find the $LU$ decomposition as discussed in class, $A = LU$, for the tridiagonal $n \times n$ matrix $A$,

$$A = \begin{pmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ & & & b_n & a_n \end{pmatrix} = \begin{pmatrix} 1 & & & & \\ \beta_2 & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & \beta_n & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 & c_1 & & & \\ & \alpha_2 & c_2 & & \\ & & \ddots & \ddots & \\ & & & \ddots & c_{n-1} \\ & & & & \alpha_n \end{pmatrix} = LU.$$

The function should output the two $n$-vectors $\alpha$ and $\beta$, and its first line should read:

```
function [alpha,beta] = trilu(a,b,c)
```

Next, write an M-file function **trilu_solve** to solve $Ax = f$, which takes the vectors $\alpha$, $\beta$, $c$ and $f$ and returns $x$. Its first line should read:

```
function x = trilu_solve(alpha,beta,c,f)
```

Test your code with the $5\times5$ system with $a_i = 2$, $b_i = -1$, $c_i = -1$, and RHS $f = [1, 0, 0, 0, 1]^T$. The exact solution is clearly $x = [1, 1, 1, 1, 1]^T$. Use MATLAB's **diary** command to save your MATLAB session output showing that your code works properly. Include a copy of both codes.

**<u>ANS</u>**: First, let's test the code:

```
>> a=2*ones(5,1);
>> b=-ones(5,1); b(1)=0;
>> c=-ones(5,1); c(5)=0;
>> f=[1 0 0 0 1]';
>> [alpha,beta]=trilu(a,b,c);

      alpha     beta
    ----------------
    2.0000         0
    1.5000   -0.5000
    1.3333   -0.6667
    1.2500   -0.7500
    1.2000   -0.8000

>> x=trilu_solve(alpha,beta,c,f);
>> x

x =

    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
```

Here are the codes:

```
function [alpha,beta] = trilu(a,b,c)
%
%TRILU - Reduced LU decomposition of tridiagonal matrix.
%
n = length(a);  alpha = zeros(n,1);   beta = zeros(n,1);

alpha(1) = a(1);
for k = 2:n
    beta(k) = b(k)/alpha(k-1);
    alpha(k) = a(k)-beta(k)*c(k-1);
end
```

```
function x = trilu_solve(alpha,beta,c,f)
%
%TRILU_SOLVE - solve tridiagonal system using decompostion
%              produced by TRILU.
%
n = length(c);  x = zeros(n,1);  z = zeros(n,1);

% solve Lz=f by forward substitution
z(1) = f(1);
for k = 2:n
    z(k) = f(k)-beta(k)*z(k-1);
end

% solve Ux=z by backward substitution
x(n) = z(n)/alpha(n);
for k = n-1:-1:1
    x(k) = (z(k)-c(k)*x(k+1))/alpha(k);
end
```