

QUESTION 1 (S2-2014 - MATH 2089)

a) i) $\text{ans1} = 0$

ii) $v = [-2; 2; 2]$

$$= [-2 \ 0 \ 2]$$

$$\text{ans2} = v ./ v = [-2 \ 0 \ 2] ./ [-2 \ 0 \ 2]$$

$$= [1 \ \text{NaN} \ 1]$$

ii) $\text{ans3} = \text{Inf}$

b) i) In 1 hour, the computer can do

$$\underbrace{3600}_{\text{\#secs}} \times \underbrace{3 \times 10^9}_{3 \text{ GHz}} \times \underbrace{4}_{\text{quad core}} \times \underbrace{2}_{2 \text{ flops/core/clock cycle}} = 3600 \times 24 \times 10^9 \text{ flops.}$$

No special structure \Rightarrow use LU factorization, So

$$\frac{2n^3}{3} = 24 \times 10^9 \times 3600 = 86.4 \times 10^{12}$$

(ignoring $O(n^2)$ terms)

$$n = \left(\frac{3}{2} \times 86.4 \times 10^{12} \right)^{1/3} \approx 50252$$

= .

The largest linear system the computer can solve in 1 hour has size about 50252×50252 .

ii) $2n^3$ (matrix multiplication) flops take 1000 s

For solving a linear system via Cholesky factorization it takes about $\frac{n^3}{3}$ flops, so it takes about 166 seconds.

c) i) A is symmetric since $\|A - A^T\|$ closer to ep.

$$\text{ii) } \kappa_2(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} = \frac{100}{0.01} = 10^4$$

$$\text{iii) } \kappa_2(A^{-1}) = \kappa_2(A) = 10^4$$

$$\text{iv) } \text{rel-err}(b) \leq 0.5 \times 10^{-6}$$

$$\text{rel-err}(\underline{x}) \approx \kappa_2(A) [\text{rel-err}(A) + \text{rel-err}(\underline{b})]$$

$$\leq 10^4 (2 \times 10^{-16} + 0.5 \times 10^{-6})$$

$$\leq 0.5 \times 10^{-2}$$

v) 2 significant figures.

vi) Suppose $\text{rel-err}(\underline{x}) \approx 0.5 \times 10^{-5}$

From (*) we have

$$0.5 \times 10^{-5} \approx 10^4 (2 \times 10^{-16} + \text{rel-err}(\underline{b}))$$

$$\Rightarrow \text{rel-err}(b) \approx 0.5 \times 10^{-9}$$

\Rightarrow 9 significant figures in \underline{b} .

$$\text{d) i) } \|A\|_2 = \sqrt{\lambda_{\max}(A^T A)} \text{ true.}$$

ii) \odot orthogonal $\Rightarrow \kappa_2(Q) = 1$ true since

$$\|Q\| = \max_{x \neq 0} \frac{\|Qx\|}{\|x\|} = \max_{x \neq 0} \frac{\|x\|}{\|x\|} = 1$$

$$\text{Here, we used } \|Qx\|^2 = (Qx)^T Qx = x^T Q^T Q x = x^T x = \|x\|^2$$

$$\|Q^T\| = \|Q^{-1}\| = \|Q\| = 1.$$

a) i)
$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$= 4 - \frac{4^2 - 9}{2 \times 4} = 4 - \frac{7}{8} = 3.125$$

ii) the order of convergence is quadratic since $e(k+1)/e(k)^2$ tends to a constant.

b) The vector \underline{x} which satisfies $A^T A \underline{x} = A^T b$ will minimize $\|A \underline{x} - b\|_2^2$

c) $A = QR \quad \kappa_2(A) = 10^6$

i) $\kappa_2(A^T A) = [\kappa_2(A)]^2 = 10^{12}$

ii) $\kappa_2(R) = \kappa_2(A) = 10^6$

iii) The normal equation has ill-conditioned matrix. In this case, to solve the least squares problem, I would use the QR factorization

d) i) $A = [\text{ones}(\text{length}(\text{tdata}), 1) \quad \text{tdata}];$

ii) $x = A \setminus \text{ydata};$

iii) $r = A * x - \text{ydata};$
 $\text{ans} = \text{sum}(r.^2);$

e) i)
$$\begin{cases} \frac{dx_1}{dt} = -k x_1 x_2 \\ \frac{dx_2}{dt} = -k x_1 x_2 \\ \frac{dx_3}{dt} = k x_1 x_2 \end{cases}$$

$\Rightarrow \underline{x}' = f(t, \underline{x})$ with $f(t, \underline{x}) = \begin{bmatrix} -k x_1 x_2 \\ -k x_1 x_2 \\ k x_1 x_2 \end{bmatrix}$

ii) Initial condition

$\underline{x}_0 = \underline{x}(0) = \begin{pmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 0 \end{pmatrix} \text{ moles/m}^3$

iii) $k = 2$;

myode = @ (t, x) $\begin{bmatrix} -k * x(1) * x(2); \\ -k * x(1) * x(2); \\ k * x(1) * x(2) \end{bmatrix}$

OR function f = myode (t, x)

$k = 2$;

$f(1) = -k * x(1) * x(2);$

$f(2) = -k * x(1) * x(2);$

$f(3) = k * x(1) * x(2)$

iv)

$\underline{x}(0.1) = \underline{x}(0) + h * f(0)$

$= \begin{bmatrix} 3 \\ 4 \\ 0 \end{bmatrix} + 0.1 \begin{bmatrix} -2 \times 3 \times 4 \\ -2 \times 3 \times 4 \\ 2 \times 3 \times 4 \end{bmatrix} = \begin{bmatrix} 3 - 2.4 \\ 4 - 2.4 \\ 0 + 2.4 \end{bmatrix} = \begin{bmatrix} 0.6 \\ 1.6 \\ 2.4 \end{bmatrix}$

Question 3

(S2-2014) MATH 2089

3.1

- a) Initial condition $u(x, 0)$
Boundary conditions $u(0, t)$ and $u(L, t)$
- b) $O(h)$ order 1
- c) Implicit method, since the unknowns u^{l+1} are in both left and right hand side.
- d) Implicit method is more stable, doesn't require condition on $\Delta x / \Delta t$ or $\Delta t / (\Delta x)^2$
- e) With central difference approximation for $\frac{\partial^2 u}{\partial x^2}$, (3.2) is reduced to

$$(*) \quad \frac{u_j^{l+1} - u_j^l}{\Delta t} = \frac{u_{j+1}^{l+1} - 2u_j^{l+1} + u_{j-1}^{l+1}}{(\Delta x)^2}, \quad j=1, \dots, n.$$

when $j=0$ $u_0^l = 0$ since $u(x_0, t) = u(0, t) = 0$
 $j=n+1$ $u_{n+1}^l = 0$ since $u(x_{n+1}, t) = u(L, t) = 0$

i) For $j=1$, (*) reduces to

$$\frac{u_1^{l+1} - u_1^l}{\Delta t} = \frac{u_2^{l+1} - 2u_1^{l+1} + u_0^{l+1}}{(\Delta x)^2} = \frac{-2u_1^{l+1} + u_2^{l+1}}{(\Delta x)^2}$$

$\nearrow 0$

So the first row of A is

$$[2 \quad -1 \quad 0 \quad 0 \quad \dots \quad 0]$$

ii) For $j=2$, (*) reduces to

$$\frac{u_2^{l+1} - u_2^l}{\Delta t} = \frac{u_3^{l+1} - 2u_2^{l+1} + u_1^{l+1}}{(\Delta x)^2} = \frac{u_1^{l+1} - 2u_2^{l+1} + u_3^{l+1}}{(\Delta x)^2}$$

So the 2nd row of the matrix A is

$$[-1 \quad 2 \quad 1 \quad 0 \quad 0 \dots 0]$$

iii) For $j=n$, (*) reduces to

$$\frac{u_n^{l+1} - u_n^l}{\Delta t} = \frac{\overset{0}{u_{n+1}^{l+1}} - 2u_n^{l+1} + u_{n-1}^{l+1}}{(\Delta x)^2} = \frac{u_{n-1}^{l+1} - 2u_n^{l+1}}{(\Delta x)^2}$$

So the last row of the matrix A is

$$[0 \quad 0 \dots -1 \quad 2]$$

iv) $v.^A 0 = [1 \quad 1 \quad 1 \dots 1]$

$$w = A * (v.^A 0)$$

$$= \begin{bmatrix} 2 & -1 & 0 & 0 & \dots \\ -1 & 2 & 1 & 0 & \dots \\ 0 & -1 & 2 & -1 & \\ & & & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

So $w(j) = w(2) = 0$
ans $0 = 0$

since $j=2$.

$$v.^A 1 = [1 \quad 2 \quad 3 \quad 4 \dots]$$

$$W = A * (v.^1)$$

$$= \begin{bmatrix} +2 & -1 & 0 & 0 & \dots \\ -1 & 2 & -1 & 0 & \dots \\ 0 & -1 & 2 & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ -1 & 2 & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ \vdots \\ 20 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

$$\Rightarrow W(j) = W(2) = 0$$

ans 1 = 0

$$W = A * (v.^2)$$

$$= \begin{bmatrix} 2 & -1 & 0 & 0 & \dots \\ -1 & 2 & -1 & 0 & \dots \\ 0 & -1 & 2 & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & -1 & 2 & -1 & \dots \end{bmatrix} \begin{bmatrix} 1 \\ 4 \\ 9 \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} -2 \\ -2 \\ \vdots \end{bmatrix}$$

$-1 \times 1 + 2 \times 4$
 -1×9

$$\Rightarrow W(j) = W(2) = -2$$

ans 2 = -2.

$$v) \quad u(x, 0) = 1 - \cos\left(x \frac{2\pi}{L}\right)$$

$$(3.2) \quad \text{at } t = 0$$

$$\frac{u^1 - u^0}{\Delta t} = -A \frac{u^1}{(\Delta x)^2}$$

where

$$u^0 = \left[1 - \cos\left(x_j \frac{2\pi}{L}\right) \right]_{j=1}^n$$

$$= \left[1 - \cos\left(j \frac{L}{n+1} \frac{2\pi}{L}\right) \right]_{j=1}^n = \left[1 - \cos\left(\frac{2\pi j}{n+1}\right) \right]_{j=1}^n$$

f) For $n = 20$

3.4

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \\ & & & & -1 & 2 \end{bmatrix} \left. \vphantom{\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \\ & & & & -1 & 2 \end{bmatrix}} \right\} 20 \text{ rows.}$$

Number of non-zero elements of A

$$\text{nnz}(A) = \underset{\substack{\uparrow \\ \text{first row}}}{2} + \underbrace{3 \times 18}_{\substack{\text{middle} \\ \text{rows}}} + \underset{\substack{\uparrow \\ \text{last row}}}{2} = 58$$

$$\text{Number of elements of } A = 20^2 = 400$$

$$\text{Sparsity of } A = \frac{58}{400} = 14.5\%$$

g) No, A^{-1} is not very sparse.

$$h) A = B^T B$$

$$\underline{\underline{x}}^T A \underline{\underline{x}} = \underline{\underline{x}}^T B^T B \underline{\underline{x}} = (B \underline{\underline{x}})^T B \underline{\underline{x}} = \|B \underline{\underline{x}}\|^2 \geq 0$$

If $B \underline{\underline{x}} = 0$ then $\underline{\underline{x}} = 0$ since B
has independent columns.

So A is positive definite.

$$i) A = R^T R$$

$$\Rightarrow A \underline{\underline{x}} = \underline{\underline{b}} \Leftrightarrow R^T R \underline{\underline{x}} = \underline{\underline{b}}$$

Step 1: solve $R^T \underline{\underline{y}} = \underline{\underline{b}}$ by forward substitution

Step 2: solve $R \underline{\underline{x}} = \underline{\underline{y}}$ by back-substitution

j).

$$(\tilde{u}^{l+1} - \tilde{u}^l) / \Delta t = -A \tilde{u}^{l+1} / (\Delta x)^2$$

$$\Leftrightarrow \tilde{u}^{l+1} / \Delta t + A \tilde{u}^{l+1} / (\Delta x)^2 = \tilde{u}^l / \Delta t$$

$$\Leftrightarrow \Delta t \left(\frac{1}{\Delta t} I + \frac{1}{(\Delta x)^2} A \right) \tilde{u}^{l+1} = \tilde{u}^l$$

$$\Leftrightarrow \underbrace{\left(I + \frac{\Delta t}{(\Delta x)^2} A \right)}_K \tilde{u}^{l+1} = \tilde{u}^l$$

$$\tilde{u}^{l+1} = \tilde{u}^l$$

With $\Delta t = 0.1$, $\Delta x = 0.5$

$$K = I + \frac{1}{2.5} A$$