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18.085 Computational Science and Engineering I  
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## Solutions - Problem Set 3

Section 1.6

$$1) \quad T = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}$$

$$\begin{aligned} u^T T u &= [u_1 \quad u_2] \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ &= [u_1 \quad u_2] \begin{bmatrix} u_1 - u_2 \\ -u_1 + 2u_2 \end{bmatrix} \\ &= u_1^2 - u_1 u_2 + (-u_1 u_2 + 2u_2^2) \\ &= u_1^2 - 2u_1 u_2 + 2u_2^2 \\ &= (u_1 - u_2)^2 + u_2^2 > 0 \# \end{aligned}$$

$u^T T u$  is positive definite as it is the sum of 2 squares

$$3) \quad A = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{bmatrix} \quad A^T A = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

$$A u = 0 \quad A^T A u = 0$$

$A$  is a singular matrix as it has only 2 linearly independent columns. Since  $A$  does not have full rank,  $A^T A$  will have a zero pivot

$$\begin{aligned} A^T A &= \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \\ &= \begin{bmatrix} 2 & -1 & -1 \\ 0 & 3/2 & -3/2 \\ 0 & -3/2 & 3/2 \end{bmatrix} \quad \begin{array}{l} \text{row 2} \equiv \text{row 2} + \frac{1}{2} \text{row 1} \\ \text{row 3} \equiv \text{row 3} + \frac{1}{2} \text{row 1} \end{array} \\ &= \begin{bmatrix} 2 & -1 & -1 \\ 0 & 3/2 & -3/2 \\ 0 & 0 & \boxed{0} \end{bmatrix} \quad \text{row 3} \equiv \text{row 3} + \text{row 2} \end{aligned}$$

$\therefore A^T A$  is only semidefinite #

$$A u = 0, \quad A^T A u = 0$$

The nullvector of  $A$  and  $A^T A$  would be a constant vector

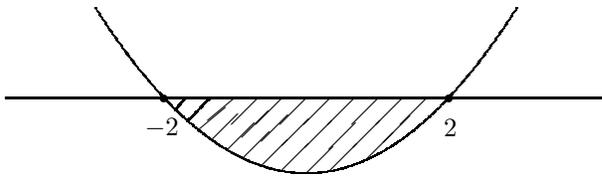
$$\begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} c \\ c \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

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

$$\therefore u = \begin{bmatrix} c \\ c \\ c \end{bmatrix} \quad \text{where } c \text{ is a constant } \neq$$

$$6) \quad K = \begin{bmatrix} 1 & b \\ b & 4 \end{bmatrix}$$

$$\begin{aligned} u^T K u &= [u_1 \quad u_2] \begin{bmatrix} 1 & b \\ b & 4 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ &= [u_1 \quad u_2] \begin{bmatrix} u_1 + bu_2 \\ bu_1 + 4u_2 \end{bmatrix} \\ &= u_1^2 + bu_1u_2 + bu_1u_2 + 4u_2^2 \\ &= u_1^2 + 2bu_1u_2 + 4u_2^2 \\ &= (u_1 + bu_2)^2 + (4 - b^2)u_2^2 > 0 \\ &\quad 4 - b^2 > 0 \\ &\quad (b + 2)(b - 2) < 0 \end{aligned}$$



$$-2 < b < 2 \neq$$

For semidefinite case, the borderline value of  $b$  is  $-2$  and  $2$

$$u^T K u = (u_1 + bu_2)^2 \quad (\text{only one square})$$

$$\text{If } b = 5, \quad K = \begin{bmatrix} 1 & 5 \\ 5 & 4 \end{bmatrix}$$

By Gaussian Elimination

$$\begin{aligned} &\begin{bmatrix} 1 & 5 \\ 5 & 4 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 5 \\ 0 & -21 \end{bmatrix} \quad \text{row 2} \equiv \text{row 2} - 5 \times \text{row 1} \end{aligned}$$

The pivots are  $1$  and  $-21$

The matrix is indefinite if  $b = 5 \neq$

$$11) \quad f(x, y) = 2xy$$

$$\frac{\partial f}{\partial x} = 2y \quad \frac{\partial f}{\partial y} = 2x$$

$$\frac{\partial^2 f}{\partial x \partial y} = 2 \quad , \quad \frac{\partial^2 f}{\partial x^2} = 0 \quad , \quad \frac{\partial^2 f}{\partial y^2} = 0$$

Hessian matrix,  $H = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$

$$\begin{aligned} \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &\equiv 2xy \\ &= \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} ax + by \\ bx + cy \end{bmatrix} \\ &= ax^2 + bxy + bxy + cy^2 \\ &= ax^2 + 2bxy + cy^2 \end{aligned}$$

By comparing coefficients,  $a = 0, \quad c = 0$   
 $b = 1$

$\therefore$  The symmetric matrix that produces  $f(x, y) = 2xy$  is  $S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

$$\begin{aligned} \det(S - \lambda I) &= 0 \\ \det \begin{bmatrix} -\lambda & 1 \\ 1 & -\lambda \end{bmatrix} &= 0 \end{aligned}$$

$$\begin{aligned} \lambda^2 - 1 &= 0 \\ (\lambda - 1)(\lambda + 1) &= 0 \\ \lambda &= 1 \text{ or } -1 \end{aligned}$$

$\therefore$  The eigenvalues for matrix  $S$  are  $-1$  and  $1$  #

**16)** Since  $A$  is positive definite,  $A$  can be diagonalized to

$$A = S\Lambda S^{-1} \quad \text{where } S = \text{eigenvector} \\ \Lambda = \text{eigenvalues}$$

$$\begin{aligned} AA^{-1} &= I \\ (S\Lambda S^{-1})A^{-1} &= I \\ A^{-1} &= S\Lambda^{-1}S^{-1} \end{aligned}$$

The eigenvalues  $\Lambda$  of  $A$  are all positives as  $A$  is positive definite matrix.

Therefore the diagonal entries of  $\Lambda^{-1}$  (reciprocal of diagonal entries of  $\Lambda$ ) is also positive.

Hence  $A^{-1}$  is also positive definite #

**Second proof**

$$\begin{aligned} A &= \begin{bmatrix} a & b \\ b & c \end{bmatrix} \\ A^{-1} &= \frac{1}{ac - b^2} \begin{bmatrix} c & -b \\ -b & a \end{bmatrix} \end{aligned}$$

Since  $A$  is positive definite, the upper left determinants are positive

$$\begin{aligned} \therefore a > 0 \text{ and } ac - b^2 > 0 \\ \text{Also implied that } c > 0 \text{ so that } ac - b^2 > 0 \end{aligned}$$

$\therefore$  The upper left determinants of  $A^{-1}$ ,  $c$  and  $ac - b^2$ , are positive, and we can conclude that  $A^{-1}$  is also positive definite #

19) If  $\lambda > 0$  and  $K$  is symmetric,  $K$  can be decomposed to

$$\begin{aligned} K &= Q\Lambda Q^T \\ u^T K u &= u^T (Q\Lambda Q^T) u \\ &= (Q^T u)^T \Lambda (Q^T u) > 0 \text{ \#(proven) for } u \neq 0 \end{aligned}$$

$$Q = \begin{bmatrix} \vdots & \vdots & & \vdots \\ x_1 & x_2 & \dots & x_n \\ \vdots & \vdots & & \vdots \end{bmatrix}$$

$$u = c_1 x_1 + c_2 x_2 + \dots + c_n x_n$$

The cross term  $x_i^T x_j = 0$  for  $i \neq j$  is because the eigenvectors are orthogonal to each other #

$$\begin{aligned} u^T K u &= (c_1 x_1 + \dots + c_n x_n)^T \Lambda u \\ &= (c_1 x_1 + \dots + c_n x_n)^T (c_1 \lambda_1 x_1 + \dots + c_n \lambda_n x_n) \\ &= c_1^2 \lambda_1 x_1^T x_1 + \dots + c_n^2 \lambda_n x_n^T x_n > 0 \quad (\because \lambda > 0, x^T x > 0) \end{aligned}$$

$$\begin{aligned} 24) \quad & \frac{1}{2} (u - K^{-1}f)^T K (u - K^{-1}f) - \frac{1}{2} f^T K^{-1} f \\ &= \frac{1}{2} [u^T - (K^{-1}f)^T] [Ku - f] - \frac{1}{2} f^T K^{-1} f \\ &= \frac{1}{2} [u^T Ku - u^T f - (K^{-1}f)^T Ku + (K^{-1}f)^T f] - \frac{1}{2} f^T K^{-1} f \\ &= \frac{1}{2} [u^T Ku - u^T f - [(Ku)^T (K^{-1}f)]^T + f^T K^{-1T} f - f^T K^{-1} f] \\ &= \frac{1}{2} [u^T Ku - u^T f - (u^T K^T K^{-1} f)^T + f^T \cancel{K^{-1}} f - f^T \cancel{K^{-1}} f] \\ &= \frac{1}{2} [u^T Ku - u^T f - u^T f] \quad \text{since } K^T = K \\ &= \frac{1}{2} u^T Ku - u^T f \\ &= P(u) \text{ \#(verified)} \end{aligned}$$

The long term  $\frac{1}{2} (u - K^{-1}f)^T K (u - K^{-1}f)$  on the right hand side is always positive except when  $u = K^{-1}f$  #

27)  $H$  and  $K$  are positive definite

$$M = \begin{bmatrix} H & 0 \\ 0 & K \end{bmatrix}$$

$$\text{Let } H = Q_H \Lambda_H Q_H^T, K = Q_K \Lambda_K Q_K^T$$

$$\therefore M = \begin{bmatrix} Q_H & 0 \\ 0 & Q_K \end{bmatrix} \begin{bmatrix} \Lambda_H & O \\ 0 & \Lambda_K \end{bmatrix} \begin{bmatrix} Q_H^T & 0 \\ 0 & Q_K^T \end{bmatrix}$$

Since  $\Lambda_H$  and  $\Lambda_K$  are positive as  $H$  and  $K$  are both positive definite.

Eigenvalues of  $M$ ,  $\Lambda_M = \Lambda_H \cup \Lambda_K > 0$

$\therefore$  We can conclude that  $M$  is positive definite #

Another way to look at the problem is to examine the determinant of upper left matrix

$$M = \left[ \begin{array}{c|c} H & 0 \\ \hline 0 & K \end{array} \right]$$

$$\det(H) > 0 \quad \text{and} \quad \det(M) = \det(H) \det(K) > 0$$

$\therefore M$  is positive definite

$$\text{Now, let's examine } N = \begin{bmatrix} K & K \\ K & K \end{bmatrix}$$

Columns of  $N$  are not linearly independent, therefore matrix  $N$  is singular and will have 0 pivot. Therefore  $N$  matrix is not positive definite #

Pivots of  $M$ ,

$$D_M = D_H \cup D_K \#$$

Eigenvalues of  $M$ ,

$$\Lambda_M = \Lambda_H \cup \Lambda_K \#$$

Pivots of  $N$ ,

$$D_N = D_K \cup 0 \#$$

Eigenvalues of  $N$ ,

$$\Lambda_N = 2\Lambda_K \cup 0 \#$$

$$\text{chol}(M) = \left[ \begin{array}{cc} \text{chol}(H) & 0 \\ 0 & \text{chol}(K) \end{array} \right] \#$$

## Section 1.7

12) "Spectral Radius"

$$\rho(A) = |\lambda_{\max}|$$

$$\text{Let} \quad A = \begin{bmatrix} 1 & 1000 \\ 100 & 1 \end{bmatrix} \quad B = \begin{bmatrix} 1 & 100 \\ 1000 & 1 \end{bmatrix}$$

$$\rho(A) = 317.2278 \quad \rho(B) = 317.2278$$

$$\rho(A+B) = 1102 \quad \rho(AB) = 1 \times 10^6$$

$$\begin{aligned}\rho(A) + \rho(B) &= 317.2278 + 317.2278 \\ &= 634.4556\end{aligned}$$

$$\rho(A + B) = 1102$$

$\therefore \rho(A + B) \leq \rho(A) + \rho(B)$  is false #

$$\begin{aligned}\rho(A)\rho(B) &= 317.2278 \times 317.2278 \\ &= 0.1006 \times 10^6\end{aligned}$$

$$\rho(AB) = 1.000 \times 10^6$$

$\therefore \rho(AB) \leq \rho(A)\rho(B)$  is false #

$\therefore \left. \begin{array}{l} \rho(A + B) \leq \rho(A) + \rho(B) \\ \rho(AB) \leq \rho(A)\rho(B) \end{array} \right\}$  can be both false #

The spectral radius is not acceptable as norm

## Solutions - MATLAB 3

Observations:

**For the case of  $d = 1/25$ ,**

It is observed that the large imaginary part of eigenvalue ( $-1.32 + 10.4782i$ ) for forward difference caused the discrete solution to be oscillatory. Correspondingly the singular value of the forward difference method is also relatively higher than the center and backward difference method (refer to the variation of singular value for  $d = 1/25$  attached). Singular value measure how close the matrix is to singular. The smaller the singular value the closer it is to singular.

From the condition number point of view, the larger the conditional number, the closer the matrix is to singular. Pseudo inverse may be required and thus higher round of errors. The condition number is the highest for the center difference ( $2.70e5$ ) as compared to the forward and backward difference (2.96 and 217.7 respectively).

**For the case of  $d = 1/100$ ,**

When the  $d$  value in the partial differential equation  $-du'' + u'$  become smaller and smaller, the second order  $u''$  term is as good as non existence. This is the case of singular perturbation where discretization near one side of the boundary become not accurate.

The center difference eigenvalue has the largest imaginary part ( $2.42 + 10.2958i$ ) and it is observed from the plot of  $u(x)$  vs  $x$  graph, the discrete solution for the center difference is oscillatory. From the variation of singular value for  $d = 1/100$  attached, the singular value for center difference is higher than that of forward and backward difference methods.

In addition, the condition number for forward and backward difference are higher than the center difference method.

$$d = 1/25$$

Eigenvalues

Forward	Center	
$-1.3200 + 10.4782i$	$9.6800 + 5.0131i$	37.48
$-1.3200 - 10.4782i$	$9.6800 - 5.0131i$	35.41
$-1.3200 + 9.1869i$	$9.6800 + 4.3953i$	32.15
$-1.3200 - 9.1869i$	$9.6800 - 4.3953i$	27.95
$-1.3200 + 7.1514i$	$9.6800 + 3.4215i$	23.17
$-1.3200 - 7.1514i$	$9.6800 - 3.4215i$	18.19
$-1.3200 + 1.5542i$	$9.6800 + 0.7436i$	3.88
$-1.3200 - 1.5542i$	$9.6800 - 0.7436i$	5.95
$-1.3200 + 4.5365i$	$9.6800 + 2.1704i$	9.21
$-1.3200 - 4.5365i$	$9.6800 - 2.1704i$	13.41

Singular Value

Forward	Center	Backward
0.51	0	0.01
0.58	0	0.02
0.66	0	0.04
0.75	0	0.08
0.85	0	0.15
0.96	0.02	0.28
1.08	0.06	0.51
1.21	0.25	0.92
1.36	0.98	1.6
1.51	2.99	2.49

Condition Number

Forward	Center	Backward
2.96	$2.70E + 005$	217.7

$$d = 1/100$$

Eigenvalues

Forward	Center	Backward
$-8.5800 + 6.6047i$	$2.4200 + 10.2958i$	20.8
$-8.5800 - 6.6047i$	$2.4200 - 10.2958i$	19.89
$-8.5800 + 5.7908i$	$2.4200 + 9.0271i$	18.45
$-8.5800 - 5.7908i$	$2.4200 - 9.0271i$	16.61
$-8.5800 + 4.5078i$	$2.4200 + 7.0270i$	14.51
$-8.5800 - 4.5078i$	$2.4200 - 7.0270i$	12.33
$-8.5800 + 2.8595i$	$2.4200 + 1.5271i$	6.04
$-8.5800 - 2.8595i$	$2.4200 - 1.5271i$	6.95
$-8.5800 + 0.9796i$	$2.4200 + 4.4576i$	8.39
$-8.5800 - 0.9796i$	$2.4200 - 4.4576i$	10.23

Singular Value

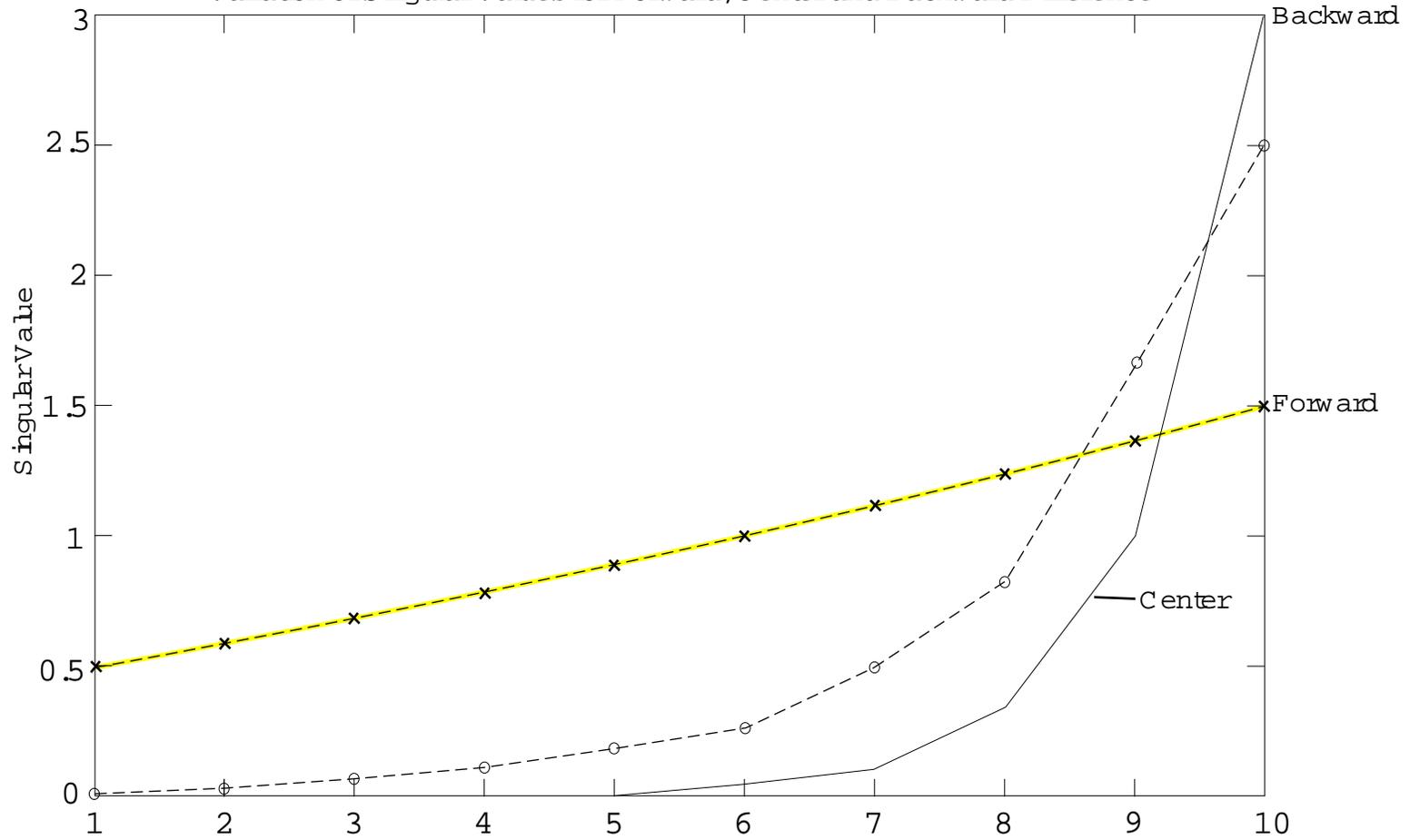
Forward	Center	Backward
0	0.25	0
0	0.32	0
0	0.4	0
0.01	0.51	0
0.02	0.64	0.01
0.06	0.81	0.04
0.16	1.01	0.12
0.46	1.25	0.38
1.27	1.53	1.17
2.86	1.85	2.91

Condition Number

Forward	Center	Backward
$1.35E + 004$	7.53	$3.67E + 004$

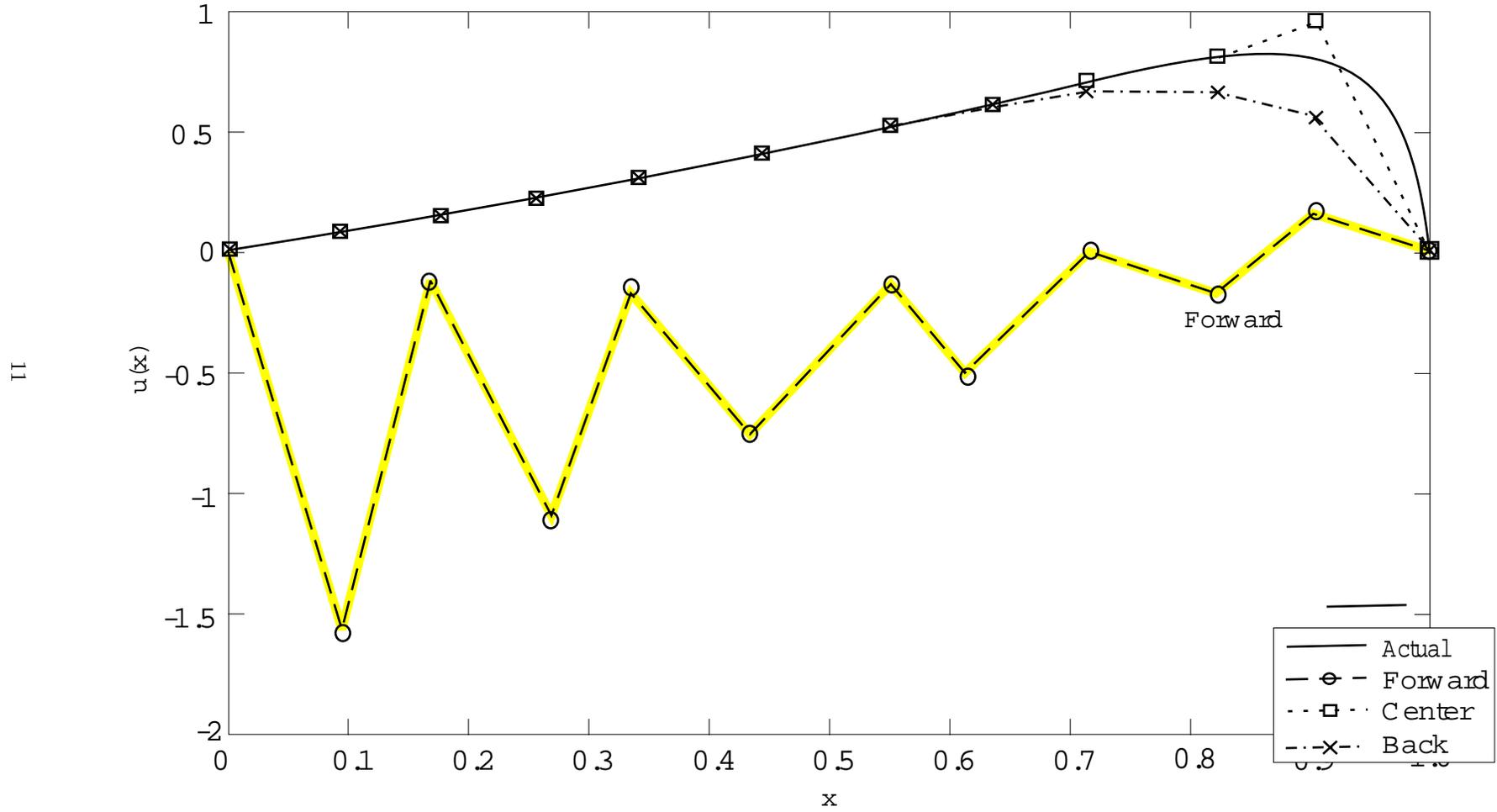
d = 1/25

Variation of Singular Values for Forward, Center and Backward Difference



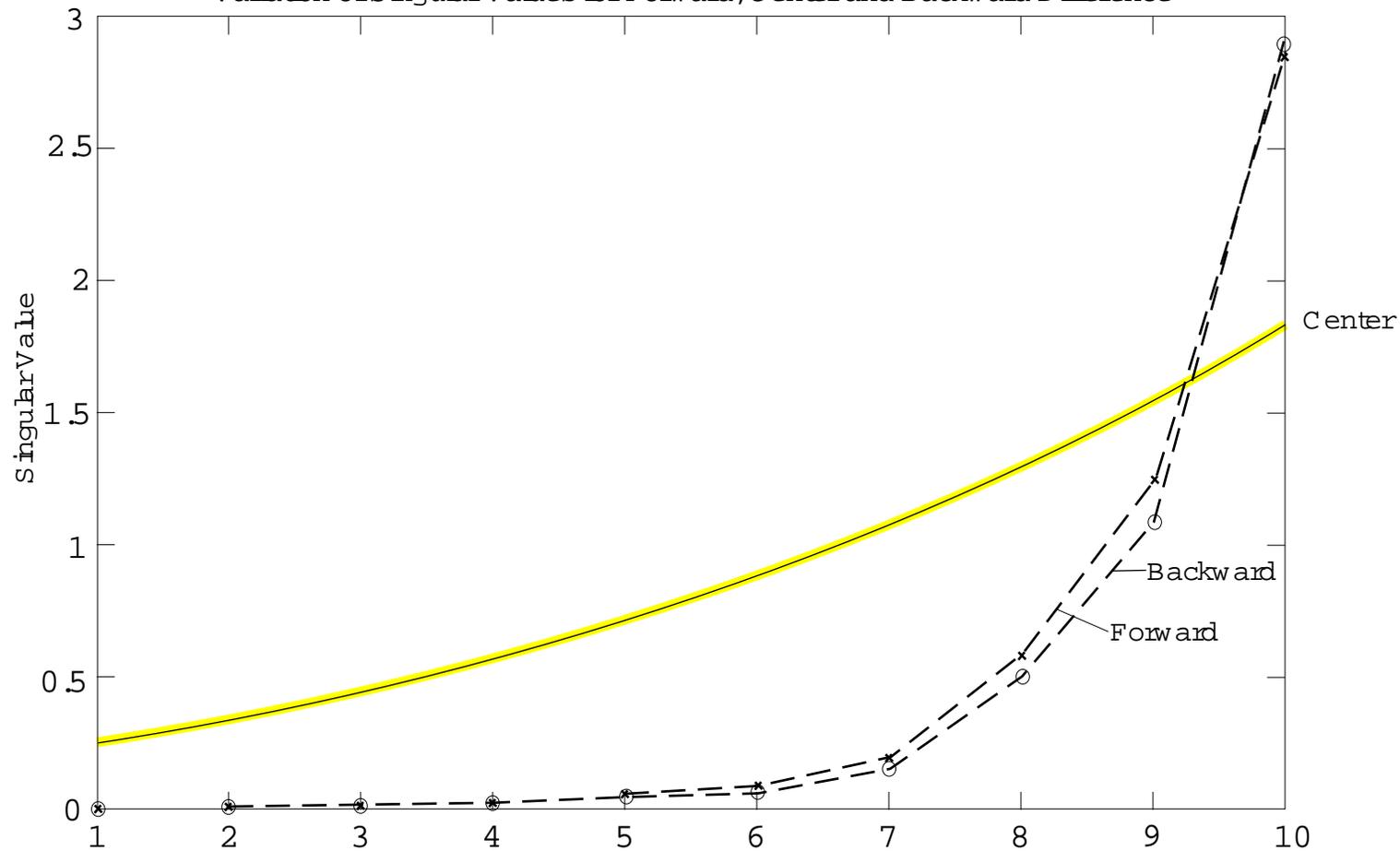
d = 1/25

Discrete Solution form = 10



d = 1/100

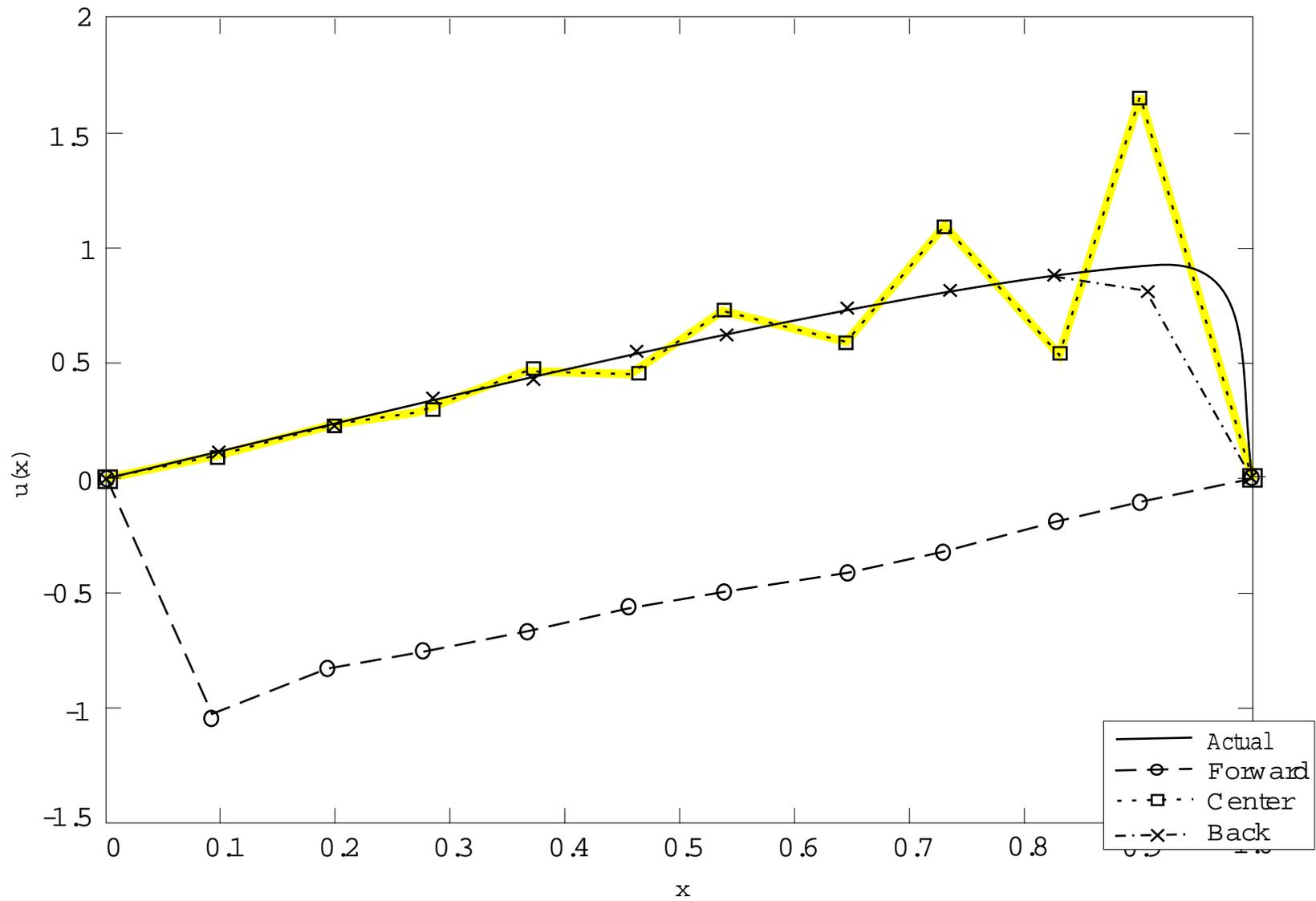
Variation of Singular Values for Forward, Center and Backward Difference



d = 1/100

Discrete Solution for n = 10

13



```

function conditionNumber(d)

n = 10;
h = 1/(n+1);

K = toeplitz([2 -1 zeros(1, n-2)]);
K = K * d;
K = K/h^2;

F = diag(-1 * ones(n, 1), 0) + diag(ones(n-1, 1), 1);
F = F/h;

C = diag(ones(n-1, 1), 1) - diag(ones(n-1, 1), -1);
C = C/(2*h);

B = diag(ones(n, 1), 0) + diag(-1*ones(n-1, 1), -1);
B = B/h;

[ForwardV, ForwardE]= eig(K + F)
[CenterV, CenterE]= eig(K + C)
[BackwardV, BackwardE]= eig(K + B)

eig(K + F)
eig(K + C)
eig(K + B)

ForwardSingular = sqrt(eig(ForwardV' * ForwardV))
CenterSingular = sqrt(eig(CenterV' * CenterV))
BackwardSingular = sqrt(eig(BackwardV' * BackwardV))

plot(ForwardSingular, '--rx')
hold
plot(CenterSingular)
plot(BackwardSingular, '--go')

Forward = max(ForwardSingular)/min(ForwardSingular)
Center = max(CenterSingular)/min(CenterSingular)
Backward = max(BackwardSingular)/min(BackwardSingular)

```