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18.085 Computational Science and Engineering I  
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## Solutions - Problem Set 1

**Section 1.1**

$$2) \quad T_3 = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \quad U = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$U^T = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$

$$U^T U = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} = T_3$$

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

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I$$

$$T_3 = U^T U$$

$$T_3^{-1} = (U^T U)^{-1}$$

$$= (U^{-1})(U^{-1})^T$$

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

$$= \begin{bmatrix} 3 & 2 & 1 \\ 2 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \#$$

$$5) \quad K_2 = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

$$K_2^{-1} = \frac{1}{4-1} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$= \frac{1}{3} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \#$$

Given that

$$K_3^{-1} = \frac{1}{4} \begin{bmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{bmatrix}$$

$$K_4^{-1} = \frac{1}{5} \begin{bmatrix} 4 & 3 & 2 & 1 \\ 3 & 6 & 4 & 2 \\ 2 & 4 & 6 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

Since  $\det(K_2) = 3$ ,  $\det(K_3) = 4$ ,  $\det(K_4) = 5$

$\therefore$  determinant of  $K_5 = 6 \#$

From MATLAB,

$$\det(K_5) = 6 \#$$

$$\text{inv}(K_5) = \frac{1}{6} \begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ 4 & 8 & 6 & 4 & 2 \\ 3 & 6 & 9 & 6 & 3 \\ 2 & 4 & 6 & 8 & 4 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} \#$$

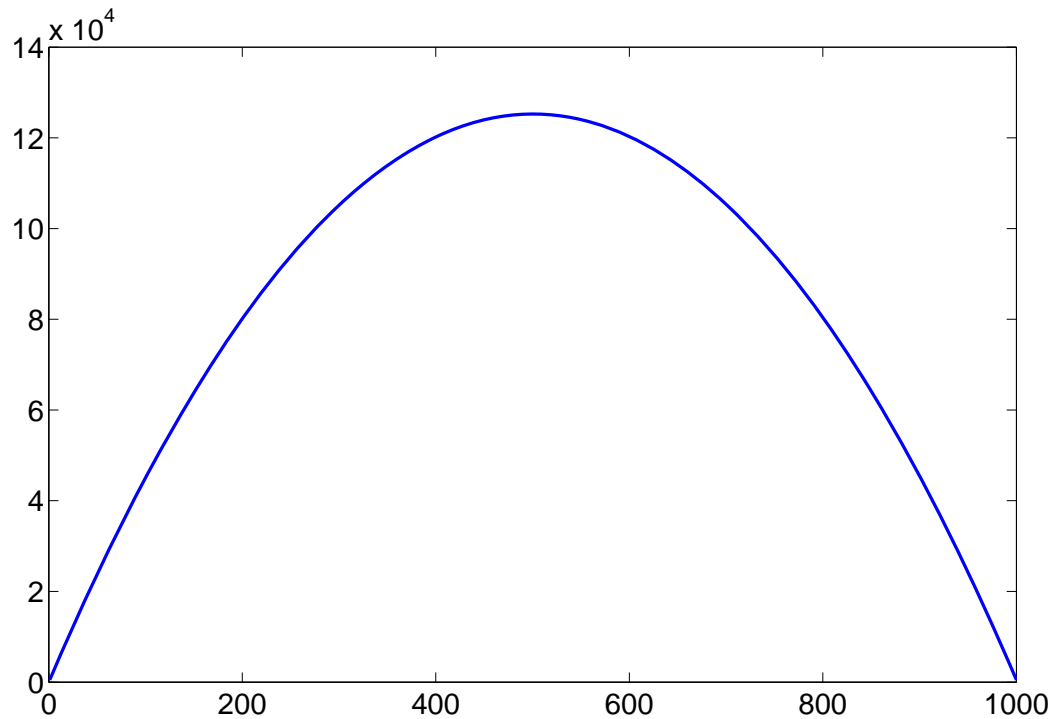
$$\det(K) * \text{inv}(K) = \begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ 4 & 8 & 6 & 4 & 2 \\ 3 & 6 & 9 & 6 & 3 \\ 2 & 4 & 6 & 8 & 4 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} \#$$

$$\begin{aligned} \mathbf{20)} \quad \begin{bmatrix} 2 & 3 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} &= \begin{bmatrix} 2 \\ 4 \end{bmatrix} \begin{bmatrix} 1 & 2 \end{bmatrix} + \begin{bmatrix} 3 \\ 5 \end{bmatrix} \begin{bmatrix} 2 & 4 \end{bmatrix} \\ &= \begin{bmatrix} 2 & 4 \\ 4 & 8 \end{bmatrix} + \begin{bmatrix} 6 & 12 \\ 10 & 20 \end{bmatrix} \\ &= \begin{bmatrix} 8 & 16 \\ 14 & 28 \end{bmatrix} \# \end{aligned}$$

For columns times row,  $n$  by  $n$  would require  $n^3$  multiplications

**22)** MATLAB's code

```
n = 1000;
e = ones(n, 1);
K = spdiags([-e, 2 * e, -e], -1:1, n, n);
u = K \ e;
plot(u);
```



**Section 1.2**

$$1) \quad u(x) = \begin{cases} Ax & \text{if } x \leq 0 \\ Bx & \text{if } x \geq 0 \end{cases}$$

$$u''(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} = \delta(x) \#$$

$$U_n = \begin{cases} A_n & \text{if } n \leq 0 \\ B_n & \text{if } n \geq 0 \end{cases} = \begin{bmatrix} -2A \\ -A \\ 0 \\ B \\ 2B \end{bmatrix}$$

$$\Delta^2 U_n = \begin{bmatrix} \ddots & & & & & & & & \\ & 1 & -2 & 1 & & & & & \\ & & 1 & -2 & 1 & & & & \\ & & & 1 & -2 & 1 & & & \\ & & & & 1 & -2 & 1 & & \\ & & & & & 1 & -2 & 1 & \\ & & & & & & \ddots & & \end{bmatrix} \begin{bmatrix} \vdots \\ -3A \\ -2A \\ -A \\ 0 \\ B \\ 2B \\ 3B \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ 0 \\ 0 \\ -A+B \\ 0 \\ \vdots \end{bmatrix} \#$$

$$\begin{aligned}
2) \quad & -u''(x) = \delta(x) \\
& u(-2) = 0, \quad u(3) = 0 \\
& -\int u''(x) = \int \delta(x) \\
& -[u'(x)]_L^R = 1 \\
& u'_R(x) - u'_L(x) = -1
\end{aligned}$$

Given that  $u = \begin{cases} A(x+2) & x \leq 0 \\ B(x-3) & x \geq 0 \end{cases}$

$$B - A = -1 \quad \text{---①}$$

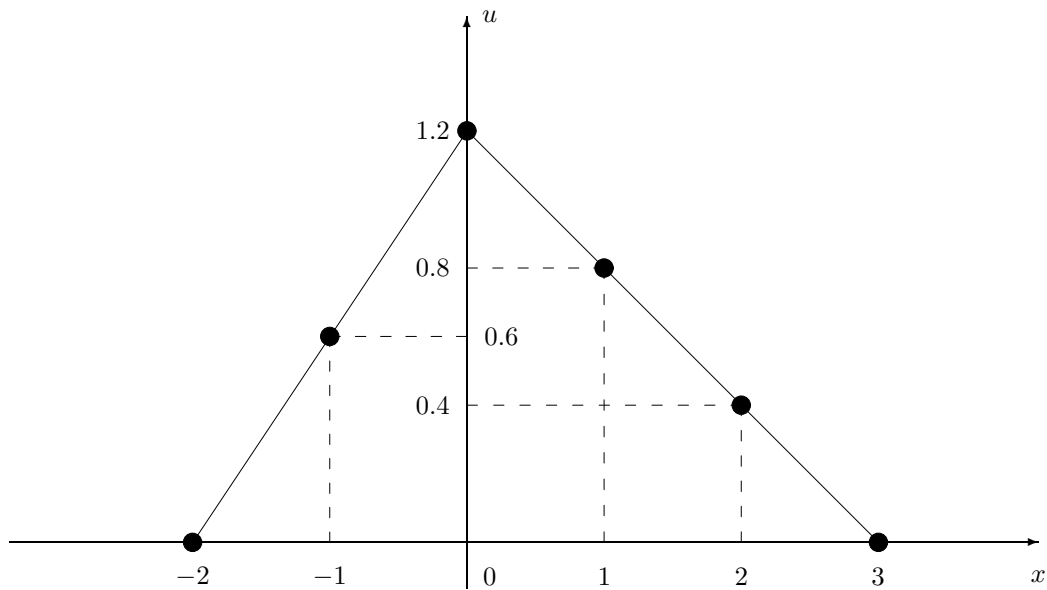
Since the pieces meet at  $x = 0$ ,

$$\begin{aligned}
A(0+2) &= B(0-3) \\
A &= -\frac{3}{2}B \quad \text{---②}
\end{aligned}$$

$$\text{②} \rightarrow \text{①}$$

$$\begin{aligned}
B - \left(-\frac{3}{2}B\right) &= -1 \\
B &= -0.4 \\
A &= 0.6
\end{aligned}$$

$$\therefore u = \begin{cases} 0.6(x+2) & x \leq 0 \\ -0.4(x-3) & x \geq 0 \end{cases}$$



$$\begin{aligned}
\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} \begin{bmatrix} u(-1) \\ u(0) \\ u(1) \\ u(2) \end{bmatrix} &= \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \\
\begin{bmatrix} u(-1) \\ u(0) \\ u(1) \\ u(2) \end{bmatrix} &= \begin{bmatrix} 4 & 3 & 2 & 1 \\ 3 & 6 & 4 & 2 \\ 2 & 4 & 6 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \frac{1}{5} \\
&= \frac{1}{5} \begin{bmatrix} 3 \\ 6 \\ 4 \\ 2 \end{bmatrix} \\
\begin{bmatrix} u(-1) \\ u(0) \\ u(1) \\ u(2) \end{bmatrix} &= \begin{bmatrix} 0.6 \\ 1.2 \\ 0.8 \\ 0.4 \end{bmatrix} \#
\end{aligned}$$

The discrete solution yields the same results as the actual solution #

$$4) \quad \Delta_- = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & & \ddots & \\ & & & -1 & 1 \end{bmatrix} \text{ Backward difference matrix}$$

$$\begin{aligned}
&\begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & & \ddots & \\ & & & -1 & 1 \end{bmatrix} \overbrace{\begin{bmatrix} 1 & & & & \\ 1 & 1 & & & \\ 1 & 1 & 1 & & \\ 1 & & & \ddots & \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix}}^{\text{sum matrix}} \\
&= \begin{bmatrix} 1 & 0 & & & \\ 0 & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ 0 & & & & 1 \end{bmatrix} \\
&= I \#
\end{aligned}$$

Verified that the inverse of backward difference matrix is the sum matrix #

$$\begin{aligned}
\Delta_0 &= \frac{1}{2}(\Delta_+ + \Delta_-) \\
&= \frac{1}{2} \left\{ \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 & \\ & & & \ddots & 1 \\ & & & & -1 \end{bmatrix} + \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & & \ddots & 1 \\ & & & & -1 & 1 \end{bmatrix} \right\} \\
&= \frac{1}{2} \begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & & \ddots & 1 \\ & & & & -1 & 0 \end{bmatrix}
\end{aligned}$$

For  $n = 3$

$$\Delta_0 u = \frac{1}{2} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} c \\ 0 \\ c \end{bmatrix}$$

For  $n = 5$

$$\Delta_0 u = \frac{1}{2} \begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} c \\ 0 \\ c \\ 0 \\ c \end{bmatrix}$$

The nullvector of  $\Delta_0 u = 0$  is not the zero vector, therefore  $\Delta_0$  is not invertible #

$$7) \quad \frac{-u_2 + 8u_1 - 8u_{-1} + u_{-2}}{12h} = \frac{du}{dx} + bh^4 \frac{d^5 u}{dx^5} + \dots$$

For  $u(x) = 1$

$$\frac{du}{dx} = \frac{-1 + 8 - 8 + 1}{12h}$$

$$= 0 \quad \# \text{ correct}$$

For  $u(x) = x^2$

$$\begin{aligned}
\frac{du}{dx} &= \frac{-(x+2h)^2 + 8(x+h)^2 - 8(x-h)^2 + (x-2h)^2}{12h} \\
&= \frac{(x-2h)^2 - (x+2h)^2 + 8\{(x+h)^2 - (x-h)^2\}}{12h} \\
&= \frac{(x-2h+x+2h)(x-2h-x-2h) + 8(x+h-x-h)(x+h-x-h)}{12h} \\
&= \frac{-4h(2x) + 8(2x)(2h)}{12h} \\
&= 2x \quad \# \text{ correct}
\end{aligned}$$

For  $u(x) = x^4$

$$\begin{aligned}
\frac{du}{dx} &= \frac{(x-2h)^4 - (x+2h)^4 + 8\{(x+h)^4 - (x-h)^4\}}{12h} \\
&= \left\{ \frac{[(x-2h)^2 + (x+2h)^2][(x-2h)^2 - (x+2h)^2]}{+ 8\{[(x+h)^2 + (x-h)^2][(x+h)^2 - (x-h)^2]\}} \right\} / 12h \\
&= \frac{1}{12h} \left\{ -8hx[(x-2h)^2 + (x+2h)^2] + 8(4xh)[(x+h)^2 + (x-h)^2] \right\} \\
&= \frac{1}{12h} \left\{ -8hx[x^2 - 4xh + 4h^2 + x^2 + 4xh + 4h^2] \right. \\
&\quad \left. + 8(4xh)[x^2 + 2xh + h^2 + x^2 - 2xh + h^2] \right\} \\
&= \frac{1}{12h} \left\{ -8hx[2x^2 + 8h^2] + 8(4xh)[2x^2 + 2h^2] \right\} \\
&= \frac{-8hx}{12h} \left\{ 2x^2 + 8h^2 - 8x^2 - 8h^2 \right\} \\
&= 4x^3 \quad \# \text{ correct}
\end{aligned}$$

$$u(x+h) = u(x) + hu'(x) + \frac{1}{2}h^2u''(x) + \frac{1}{6}h^3u'''(x) + \frac{1}{24}h^4u''''(x) + \frac{1}{120}h^5u^{(5)}(x) + \dots$$

$$u(x-h) = u(x) - hu'(x) + \frac{1}{2}h^2u''(x) - \frac{1}{6}h^3u'''(x) + \frac{1}{24}h^4u''''(x) - \frac{1}{120}h^5u^{(5)}(x) + \dots$$

$$u(x+2h) = u(x) + 2hu'(x) + \frac{1}{2}(2h)^2u''(x) + \frac{1}{6}(2h)^3u'''(x) + \frac{1}{24}(2h)^4u^{(4)}(x) + \frac{1}{120}(2h)^5u^{(5)}(x) + \dots$$

$$u(x-2h) = u(x) - 2hu'(x) + \frac{1}{2}(2h)^2u''(x) - \frac{1}{6}(2h)^3u'''(x) + \frac{1}{24}(2h)^4u^{(4)}(x) - \frac{1}{120}(2h)^5u^{(5)}(x) + \dots$$

$$\frac{-u_2 + 8u_1 - 8u_{-1} + u_{-2}}{12h}$$



$$\begin{aligned}
&= \left\{ \begin{aligned} &-4hu'(x) - \frac{2}{6}(2h)^3u'''(x) - \frac{2}{120}(2h)^5u^{(5)}(x) \\ &+ 8 \left[ 2hu'(x) + \frac{2}{6}h^3u'''(x) + \frac{2}{120}h^5u^{(5)}(x) + \dots \right] \end{aligned} \right\} / 12h \\
&= \frac{12hu'(x) - \frac{2}{5}h^5u^{(5)}(x) + \dots}{12h} \\
&= u'(x) - \frac{1}{30}h^4u^{(5)}(x) + \dots \\
\therefore \text{ the coefficient } b &= -\frac{1}{30} \#
\end{aligned}$$

$$\begin{aligned}
10) \quad \Delta_+ \Delta_- &= \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 & \\ & & & \ddots & \\ & & & & -1 \end{bmatrix} \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & & \ddots & \\ & & & & -1 & 1 \end{bmatrix} \\
&= \begin{array}{c} \boxed{\begin{array}{cc} -2 & 1 \end{array}} \longrightarrow \text{Boundary row corresponds to } u = 0_{\#} \\ \begin{array}{ccc} 1 & -2 & 1 \\ & 1 & -2 & 1 \\ & & \ddots & \\ & & & 1 & -1 \end{array} \\ \boxed{\begin{array}{cc} & 1 & -1 \end{array}} \longrightarrow \text{Approximation to } u' = 0_{\#} \end{array}
\end{aligned}$$

$$\begin{aligned}
19) \quad &-\frac{d^2u}{dx^2} + \frac{du}{dx} = 1 \\
&u(0) = 0, \quad u(1) = 0 \\
&u(x) = u_p + u_n \\
&= x + A + Be^x \\
&u(0) = 0 \\
&0 = 0 + A + Be^0
\end{aligned}$$

$$A = -B \quad \text{--- ①}$$

$$\begin{aligned}
&u(1) = 0 \\
&0 = 1 + A + Be^1 \quad \text{--- ②}
\end{aligned}$$

$$\text{①} \rightarrow \text{②}$$

$$0 = 1 + (-B) + Be^1$$

$$B(1 - e^1) = 1$$

$$B = \frac{1}{1 - e^1} \quad A = \frac{-1}{1 - e^1}$$

$$\therefore u(x) = x - \frac{1}{1 - e}(1 - e^x)_{\#} \quad \text{Actual Solution}$$

Discrete centered finite difference solution

$$\frac{1}{h^2} \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} + \frac{1}{2h} \begin{bmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ & -1 & 0 & 1 \\ & & -1 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$h = \frac{1}{5}$$

From MATLAB,

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0.0714 \\ 0.1141 \\ 0.1220 \\ 0.0871 \end{bmatrix}$$

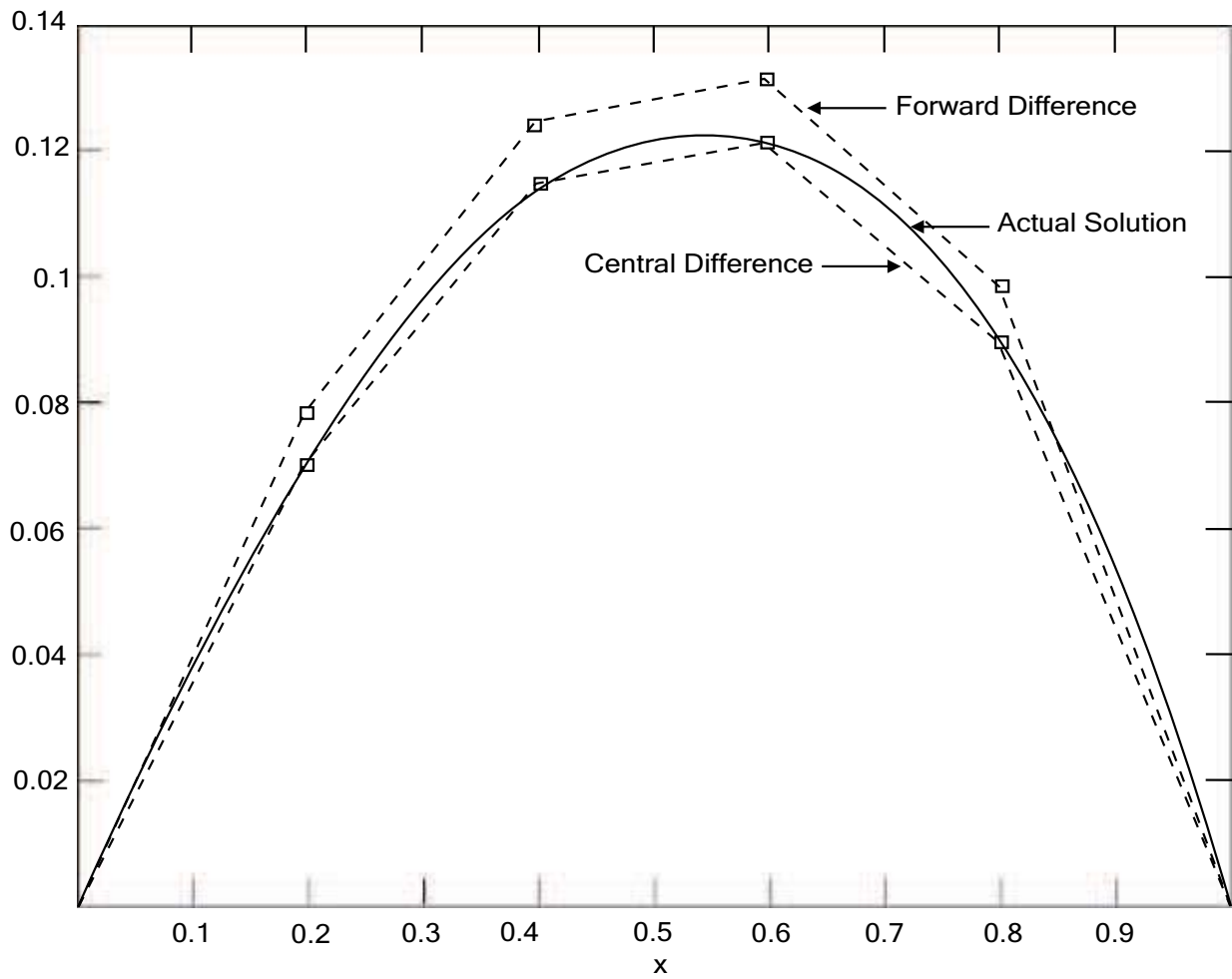
Discrete forward difference for  $u'(x)$

$$\frac{1}{h^2} \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} + \frac{1}{h} \begin{bmatrix} -1 & 1 & & \\ & -1 & 1 & \\ & & -1 & 1 \\ & & & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$h = \frac{1}{5}$$

From MATLAB,

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0.0782 \\ 0.1258 \\ 0.1355 \\ 0.0975 \end{bmatrix}$$



$$21) \quad u(h) = u(0) + hu'(0) + \frac{1}{2}h^2u''(0) + \dots$$

$$-u'' = f(x), \quad u'(0) = 0$$

$$\frac{u(h) - u(0)}{h} = \cancel{u'(0)}^0 + \frac{1}{2}hu''(0) + \dots$$

$$\therefore u(1) - u(0) = \frac{1}{2}h^2u''(0) \# \text{ (Q.E.D)}$$