Numerical Methods II

SSCM 3423

Chapter 6

This chapter solves boundary value problems (BVP) using cubic spline

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June 2016

Introduction to Cubic Splines

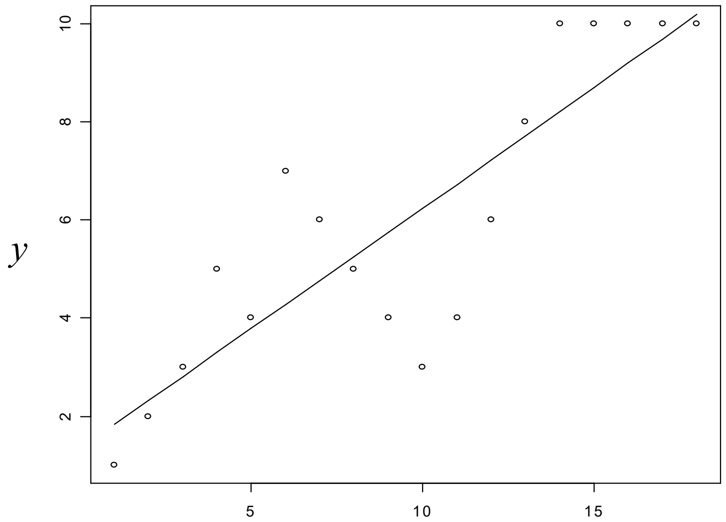


Figure (a)

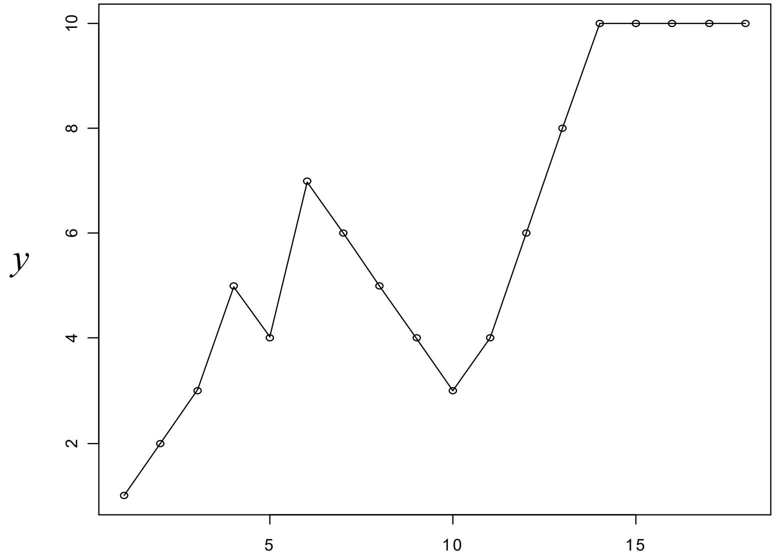


Figure (b)

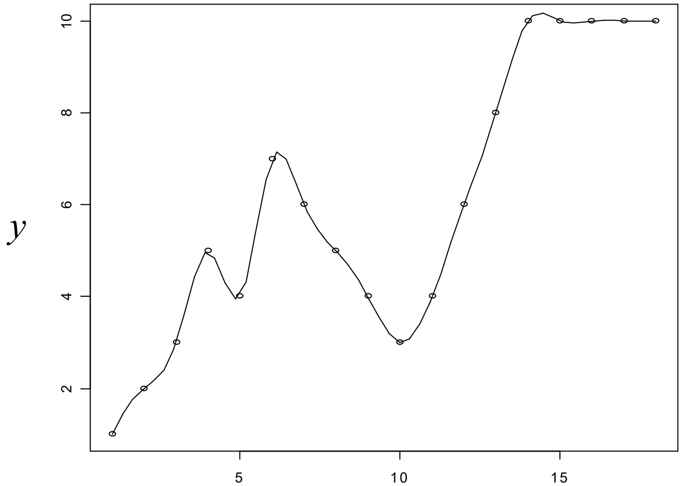


Figure (c)

Cubic spline – piecewise third order polynomial that passing all the given points (interpolation with assigned/prescribed order)

Figure (a) (linear curve fitting), Figure (b) (piecewise linear interpolation), Figure (c) (piecewise high order interpolation)

Cubic Spline Interpolation

f, function defined on interval $[a,b]$ $\qquad$ $\boldsymbol{a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b}$

Cubic Spline Interpolant : f on $a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b$

(1) On each subinterval $[x_j,x_{j+1}]$, $j=0,1,\ldots,n-1$, coincides with cubic polynomial

$$\boldsymbol{s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3}$$

(2) s interpolates f at $x_0, x_1, \ldots, x_n$.

(3) s is continuous on $[a,b]$;

(4) s' is continuous on $[a,b]$;

(5) s'' is continuous on $[a,b]$;

Function s composed of n different cubic polynomial (n intervals)
Total = $4n$ unknowns.
Interpolation provided n+1 equations.
Continuity of spline and first two derivatives contributes $3(n-1)=3n-3$ equations (continuity apply at interior points $x_1,x_2,\ldots,x_{n-1}$ only).
Definition of cubic spline provide $n+1+3(n-1)=4n-2$ equations.
– two more equations will have to be specified.

Two different types of additional constraints – boundary conditions :
Not-a-knot boundary conditions
Clamped (or complete) boundary conditions.

Cubic Spline Interpolation

Interpolation:

$s_j(x_j)=a_j=f(x_j),\ j=0,1,\ldots,n-1.$

Continuity of spline:

$a_{j+1}=a_j+b_jh_j+c_jh^2_j+d_jh^3_j, j=0,1,\ldots,n-2.$

Continuity of spline derivative:

$b_{j+1}=b_j+2c_jh_j+3d_jh^2_j, j=0,1,\ldots,n-2.$

Continuity of spline second derivative:

$c_{j+1}=c_j+3d_jh_j, j=0,1,\ldots,n-2.$

For simplicity, let $h_j=x_{j+1}-x_j$.

$a_n=f(x_n)=f(b)$.

Interpolation conditions directly provide values of a_j.

Solve for continuity of spline second derivative for d_j:

$$d_j=\frac{c_{j+1}-c_j}{3h_j} \quad (1)$$

Combine with continuity of spline and first derivative gives:

$$a_{j+1}=a_j+b_jh_j+c_jh_j^2+\frac{c_{j+1}-c_j}{3}h_j^2=a_j+b_jh_j+\frac{c_{j+1}+2c_j}{3}h_j^2 \quad (2)$$

$$b_{j+1}=b_j+2c_jh_j+\left(c_{j+1}-c_j\right)h_j=b_j+\left(c_{j+1}+c_j\right)h_j \quad (3)$$

Solve eq (2) for b_j:

$$b_j=\frac{a_{j+1}-a_j}{h_j}-\frac{2c_j+c_{j+1}}{3}h_j \quad (4)$$

Cubic Spline Interpolation

Substitute eq (4) into eq (3):

$$h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_j c_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}) \quad , j=1,2,\ldots,n-1. \qquad (5)$$

Eq (5) produce tridiagonal system of equations

Equations for $j=0$ and $j=n$ depend on type of boundary conditions.

Solve tridiagonal system in eq(5) to compute c_j.
Use eq(1) to compute d_j,
Eq(4) is used to compute b_j.
Use $a_j=f(x_j)$.

$$s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3$$

Not-a-Knot boundary conditions

When no information other than the value of f at each interpolating point is available (boundary Point), not-a-knot BC is applied.

on $a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b$

On subinterval $[x_j,x_{j+1}]$, $j=0,1,\ldots,n-1$,

$$s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3$$

→ s''' be continuous at $x=x_1$ and $x=x_{n-1}$.

$$\frac{d^3}{dx^3}s_0(x_1) = 6d_0, \quad \frac{d^3}{dx^3}s_1(x_1) = 6d_1$$

$$\frac{d^3}{dx^3}s_{n-2}(x_{n-1}) = 6d_{n-2}, \quad \frac{d^3}{dx^3}s_{n-1}(x_{n-1}) = 6d_{n-1}$$

$$\rightarrow d_0=d_1, \quad d_{n-2}=d_{n-1}.$$

Cubic Spline Interpolation

Not-a-Knot boundary conditions

$\rightarrow d_0 = d_1, \; d_{n\text{-}2} = d_{n\text{-}1}.$ Using eq (1),

$$d_j = \frac{c_{j+1} - c_j}{3h_j} \quad (1)$$

$$d_0 = \frac{c_1 - c_0}{3h_0} = d_1 = \frac{c_2 - c_1}{3h_1} \qquad d_{n-2} = \frac{c_{n-1} - c_{n-2}}{3h_{n-2}} = d_{n-1} = \frac{c_n - c_{n-1}}{3h_{n-1}}$$

Become:

$$h_1 c_0 - (h_0 + h_1) c_1 + h_0 c_2 = 0, \quad (6)$$

$$h_{n-1} c_{n-2} - (h_{n-2} + h_{n-1}) c_{n-1} + h_{n-2} c_n = 0. \quad (7)$$

Eq (6) & (7) do not preserve the tridiagonal structure.

Solve eq (6) & (7) for c_0 & c_n. →

$$c_0 = \left(1 + \frac{h_0}{h_1}\right) c_1 - \frac{h_0}{h_1} c_2, \quad (8)$$

$$c_n = -\frac{h_{n-1}}{h_{n-2}} c_{n-2} + \left(1 + \frac{h_{n-1}}{h_{n-2}}\right) c_{n-1}. \quad (9)$$

Substitute c_0 from eq (8) into (5), for j=1, we get

$$\left(3h_0 + 2h_1 + \frac{h_0^2}{h_1}\right) c_1 + \left(h_1 - \frac{h_0^2}{h_1}\right) c_2 = \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \quad (10)$$

Substitute c_n from eq (9) into (5), for j=n–1, we get

$$\left(h_{n-2} - \frac{h_{n-1}^2}{h_{n-2}}\right) c_{n-2} + \left(3h_{n-1} + 2h_{n-2} + \frac{h_{n-1}^2}{h_{n-2}}\right) c_{n-1} = \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \quad (11)$$

Cubic Spline Interpolation

Not-a-Knot boundary conditions

$$h_{j-1}c_{j-1}+2(h_{j-1}+h_j)c_j+h_jc_{j+1}=\frac{3}{h_j}(a_{j+1}-a_j)-\frac{3}{h_{j-1}}(a_j-a_{j-1}) \quad ,j=2,3,\ldots,n-2. \qquad (5.a)$$

$$\left(3h_0+2h_1+\frac{h_0^2}{h_1}\right)c_1+\left(h_1-\frac{h_0^2}{h_1}\right)c_2=\frac{3}{h_1}(a_2-a_1)-\frac{3}{h_0}(a_1-a_0) \quad (10)$$

$$\left(h_{n-2}-\frac{h_{n-1}^2}{h_{n-2}}\right)c_{n-2}+\left(3h_{n-1}+2h_{n-2}+\frac{h_{n-1}^2}{h_{n-2}}\right)c_{n-1}=\frac{3}{h_{n-1}}(a_n-a_{n-1})-\frac{3}{h_{n-2}}(a_{n-1}-a_{n-2}) \quad (11)$$

(5.a), (10), (11) produce complete tridiagonal system for c_1, c_2, …,c_{n-1}.
→ strictly diagonally dominant → nonsingular matrix → unique solution for c_j.

Example: h_j=100

$$\begin{bmatrix} 600 & 0 & & & & & \\ 100 & 400 & 100 & & & & \\ & 100 & 400 & 100 & & & \\ & & 100 & 400 & 100 & & \\ & & & 100 & 400 & 100 & \\ & & & & 100 & 400 & 100 \\ & & & & & 0 & 600 \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \end{bmatrix}=0.03\begin{bmatrix} 0 \\ 0.001 \\ -0.003 \\ 0.007 \\ -0.002 \\ 0 \\ 0 \end{bmatrix}$$

Temperature, K	Emittance, E	Temperature, K	Emittance, E
300	0.024	800	0.083
400	0.035	900	0.097
500	0.046	1000	0.111
600	0.058	1100	0.125
700	0.067		

Apply (8) & (9) to compute c_0 & c_8. $\quad a=300=x_0<x_1<x_2<\ldots<x_7<x_8=1100=b$

On each subinterval $[x_j,x_{j+1}]$, $j=0,1,\ldots,8-1$, coincides with cubic polynomial

$$s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3 \qquad a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b$$

Cubic Spline Interpolation

Not-a-Knot boundary conditions

$a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b$

$a=300=x_0<x_1<x_2<\ldots<x_7<x_8=1100=b$

On each subinterval $[x_j,x_{j+1}]$, $j=0,1,\ldots,8-1$, coincides with cubic polynomial

$s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3$

j	a_j	b_j	c_j	d_j
0	0.024	0.00012256410	-0.00000018846	0.00000000063
1	0.035	0.00010371795	0	0.00000000063
2	0.046	0.00012256410	0.00000018846	-0.00000000214
3	0.058	0.00009602564	-0.00000045385	0.00000000391
4	0.067	0.00012333333	0.00000072692	-0.00000000360
5	0.083	0.00016064103	-0.00000035385	0.00000000147
6	0.097	0.00013410256	0.00000008846	-0.00000000029
7	0.111	0.00014294872	0	-0.00000000029

Cubic Spline Interpolation

Clamped boundary conditions

If the values $f'(a)$ and $f'(b)$ are known, better apply clamped (or complete) BC:
$s'(a)=f'(a)$ and $s'(b)=f'(b)$.

$a=x_0<x_1<x_2<\ldots<x_{n-1}<x_n=b$

On each subinterval $[x_j,x_{j+1}]$, $j=0,1,\ldots,n-1$, coincides with cubic polynomial

$s(x)=s_j(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3$

$$b_j=\frac{a_{j+1}-a_j}{h_j}-\frac{2c_j+c_{j+1}}{3}h_j \quad (4)$$

Start with $x=a$, $f'(a)=s'(a)=s_0'(a)=b_0$.

Eq (4) with $j=0$, we get $f'(a)=\frac{a_1-a_0}{h_0}-\frac{2c_0+c_1}{3}h_0$ ⇒

$$2h_0c_0+h_0c_1=\frac{3}{h_0}(a_1-a_0)-3f'(a) \quad (12)$$

At $x=b$, $f'(b)=s'(b)=s_n'(b)=b_n$.

$$b_{j+1}=b_j+2c_jh_j+(c_{j+1}-c_j)h_j=b_j+(c_{j+1}+c_j)h_j \quad (3)$$

Use eq (3) and eq(4), we get

$$h_{n-1}c_{n-1}+2h_{n-1}c_n=3f'(b)-\frac{3}{h_{n-1}}(a_n-a_{n-1}) \qquad j=1,2,\ldots,n-1, \quad (13)$$

$$h_{j-1}c_{j-1}+2(h_{j-1}+h_j)c_j+h_jc_{j+1}=\frac{3}{h_j}(a_{j+1}-a_j)-\frac{3}{h_{j-1}}(a_j-a_{j-1}),\ j=2,3,\ldots,n-2. \quad (5.a)$$

(5.a), (12), (13) produce complete tridiagonal system for $c_1, c_2, \ldots, c_{n-1}$.
→ strictly diagonally dominant → nonsingular matrix → unique solution for c_j.

Cubic Spline Interpolation

Clamped boundary conditions

Example: $h_j=0.5$

Exact: $f(x)=(x+1)e^{-x}$

$$h_{j-1}c_{j-1}+2(h_{j-1}+h_j)c_j+h_jc_{j+1}=\frac{3}{h_j}(a_{j+1}-a_j)-\frac{3}{h_{j-1}}(a_j-a_{j-1})$$

$, j=2,3,\ldots,n-2.$

$$\begin{bmatrix} 1 & 0.5 & & & \\ 0.5 & 2 & 0.5 & & \\ & 0.5 & 2 & 0.5 & \\ & & 0.5 & 2 & 0.5 \\ & & & 0.5 & 1 \end{bmatrix}\begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}=\begin{bmatrix} -3.20868 \\ -3.89232 \\ -1.59504 \\ -0.50304 \\ -0.05940 \end{bmatrix}$$

x	***f*(*x*)**	***f'*(*x*)**
-1.0	0.00000	2.71828
-0.5	0.82436	
0.0	1.00000	
0.5	0.90980	
1.0	0.73576	-0.36788

Apply eq (1) &(4), we get

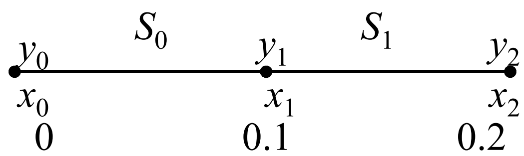
$$d_j=\frac{c_{j+1}-c_j}{3h_j} \qquad (1)$$

$$b_j=\frac{a_{j+1}-a_j}{h_j}-\frac{2c_j+c_{j+1}}{3}h_j \qquad (4)$$

j	a_j	b_j	c_j	d_j
0	0.00000	2.71828000000	-2.62214571429	0.96605142857
1	0.82436	0.82067285714	-1.17306857143	0.46856571429
2	1.00000	-0.00097142857	-0.47022000000	0.22272571429
3	0.90980	-0.30414714286	-0.13613142857	0.09653142857

Cubic Spline for Boundary value problem

E.g. $y''-2y'=e^x$, $0\le x\le 0.2$, step size (h=0.1),
Boundary condition, $y(0)=1$, $y'(0.2)=1.7622$.
Analytical solution: $y=1+e^{2x}-e^x$. $y(0.1)=1.1162$, $y(0.2)=1.2704$



$s_0(x_1)=s_1(x_1)$

$$a_0+b_0(h_0)+c_0(h_0)^2+d_0(h_0)^3=a_1 \quad (1)$$

$s'_0(x_1)=s'_1(x_1)$

$$b_0+2c_0(h_0)+3d_0(h_0)^2=b_1 \quad (2)$$

$s''_0(x_1)=s''_1(x_1)$

$$2c_0+6d_0(h_0)=2c_1 \quad (3)$$

$s''_0(x_{0.5})-2s'_0(x_{0.5})=\exp(x_{0.5})$

$$\left(2c_0+6d_0 \tfrac{h_0}{2}\right)-2\left[b_0+2c_0 \tfrac{h_0}{2}+3d_0\left(\tfrac{h_0}{2}\right)^2\right]=\exp(x_{0.5}) \quad (4)$$

BVP →Use middle point

$s''_1(x_{1.5})-2s'_1(x_{1.5})=\exp(x_{1.5})$

$$\left(2c_1+6d_1 \tfrac{h_1}{2}\right)-2\left[b_1+2c_1 \tfrac{h_1}{2}+3d_1\left(\tfrac{h_1}{2}\right)^2\right]=\exp(x_{1.5}) \quad (5)$$

BVP →Use middle point

$$s_0(x_0)=a_0=1 \quad (6)$$

B.C., $y(0)=1$

$$s'_1(x_2)=b_1+2c_1(h_1)+3d_1(h_1)^2=1.7622 \quad (7)$$

B.C. $y'(0.2)=1.7622$

$$s'''_0(x_1)=s'''_1(x_1) \rightarrow 6d_0=6d_1 \quad (8)$$

Not a knot B.C.

Cubic Spline for Boundary value problem

Let $s=[a_0\ b_0\ c_0\ d_0\ a_1\ b_1\ c_1\ d_1]^T$ Let As = B

$$\mathbf{A}=\begin{bmatrix}A_1\\ \vdots \\ A_8\end{bmatrix},\ B=\begin{bmatrix}B_1\\ \vdots \\ B_8\end{bmatrix}$$

where A_i is the i^{th} row of A

Then eq (1) can be rewritten as

$[1, (h_0), (h_0)^2{}_{,} (h_0)^3, -1, 0, 0, 0]s = 0$ (1a) $\rightarrow A_1\ s = B_1$

eq (2) $\rightarrow [0, 1, (2h_0){}_{,} 3(h_0)^2, 0, -1, 0, 0]s = 0$ (2a) $\rightarrow A_2\ s = B_2$

eq (3) $\rightarrow [0, 0, 2{}_{,} 6(h_0), 0, 0, -2, 0]s = 0$ (3a) $\rightarrow A_3\ s = B_3$

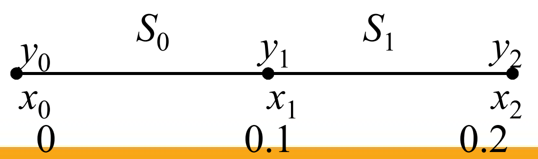
eq (4) $\rightarrow \left[0,\quad -2,\quad (2-2h_0),\quad \left(3h_0 - h_0^2\ 3/2\right),\quad 0,\quad 0,\quad 0,\quad 0\right]\mathbf{s} = \exp(0.05)$ (4a) $\rightarrow A_4\ s = B_4$

eq (5) $\rightarrow \left[0,\quad 0,\quad 0,\quad 0,\quad 0,\quad -2,\quad (2-2h_1),\quad \left(3h_1 - h_1^2\ 3/2\right)\right]\mathbf{s} = \exp(0.15)$ (5a) $\rightarrow A_5\ s = B_5$

eq (6) $\rightarrow [1, 0, 0{}_{,} 0, 0, 0, 0, 0]s = 1$ (6a) $\rightarrow A_6\ s = B_6$

eq (7) $\rightarrow [0, 0, 0, 0, 0, 1, (2h_1){}_{,} 3(h_1)^2,]s = 1.7622$ (7a) $\rightarrow A_7\ s = B_7$

eq (8) $\rightarrow [0, 0, 0{}_{,} 6, 0, 0, 0, -6]s = 1$ (8a) $\rightarrow A_8\ s = B_8$



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Cubic Spline for Boundary value problem

Let s=[a_0 b_0 c_0 d_0 a_1 b_1 c_1 d_1]^T

Let As = B $\quad \mathbf{A} = \begin{bmatrix} A_1 \\ \vdots \\ A_8 \end{bmatrix}, B = \begin{bmatrix} B_1 \\ \vdots \\ B_8 \end{bmatrix}$ where A_i is the i^{th} row of A

$$\Rightarrow \quad \begin{bmatrix} 1 & 0.1 & 0.01 & 0.001 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0.2 & 0.03 & 0 & -1 & 0 & 0 \\ 0 & 0 & 2 & 0.6 & 0 & 0 & -2 & 0 \\ 0 & -2 & 1.8 & 0.285 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 1.8 & 0.285 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0.2 & 0.03 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & -6 \end{bmatrix} \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1.051271096 \\ 1.161834243 \\ 1 \\ 1.7622 \\ 1 \end{bmatrix}$$

After solving As = B, we get

s=[1,1.001299, 1.45277, 1.53994, 1.116198, 1.338051,1.914752,1.373273]^T

$s_1(h) = 1.116198+1.338051\,h+1.914752\,h^2+1.373273\,h^3,\ h = x-0.1$

$y(0.2) = s_1(x_2) = 1.2705$

Analytical solution: $y=1+e^{2x}-e^x$. $y(0.1)=1.1162$, $y(0.2)=1.2704$

If using FDM with same grid arrangement, we will get $y_1=1.1341$, $y_2=1.3104$

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