Problem 1 (40%)

Consider the following four pairs of \((x, f(x)):\)

\((-2, 0), (0, 1), (1, 0), (2, 2).\)

(a) (10%) Find the Lagrange Polynomial.

(b) (15%) Find the spline by the following boundary conditions.

\[s''(x_0) = 0, \ s''(x_3) = 0.\]

(c) (10%) Draw functions obtained in (a) and (b) in the same figure. You must explain how you get the figure (e.g., by calculating certain values or checking derivatives).

(d) (5%) To verify your results in (b), directly calculate the following values:

\[s'_0(x_1), \ s'_1(x_1), \ s'_1(x_2), \ s'_2(x_2).\]

Hint: to make the solution of (a) simple, values of (b) are slightly more complicated.
Solution

(a) Lagrange polynomial:

\[ P(x) = \sum_{k=0}^{n} L_{n,k}(x) f(x_k) \]

\[ = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1) \]

\[ + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3) \]

\[ = \frac{(x)(x-1)(x-2)}{(-2)(-1)(-2)}(0) + \frac{(x+2)(x-1)(x-2)}{(0+2)(0-1)(0-2)}(1) \]

\[ + \frac{(x+2)(x)(x-2)}{(1+2)(1)(1-2)}(0) + \frac{(x+2)(x)(x-1)}{(2+2)(2)(2-1)}(2) \]

\[ = \frac{1}{4}(x^3 - x^2 - 4x + 4) + \frac{1}{4}(x^3 + x^2 - 2x) \]

\[ = \frac{1}{2}x^3 - \frac{3}{2}x + 1 \]

(b) \( a_0 = f(-2) = 0, \ a_1 = f(0) = 1, \ a_2 = f(1) = 0, \ a_3 = f(2) = 2. \)

\( h_0 = x_1 - x_0 = 2, \ h_1 = x_2 - x_1 = 1, \ h_2 = x_3 - x_2 = 1. \)

From the boundary condition,

\[ s''_0(-2) = 2c_0 = 0 \Rightarrow c_0 = 0 \]

\[ s''_2(2) = 2c_3 = 0 \Rightarrow c_3 = 0 \]

Compute \( c_1 \) and \( c_2 \) by

\[ h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_jc_{j+1} = \frac{3}{h_j} (a_{j+1} - a_j) - \frac{3}{h_{j-1}} (a_j - a_{j-1}), \quad j = 1, 2. \]

We have

\[ 2(2+1)c_1 + c_2 = \frac{3}{1} (0 - 1) - \frac{3}{2} (1 - 0) \]

\[ c_1 + 2(1+1)c_2 = \frac{3}{1} (2 - 0) - \frac{3}{1} (0 - 1) \]

The solution is

\[ c_1 = -\frac{27}{23}, \quad c_2 = \frac{117}{46}. \]
Compute $b_0$, $b_1$ and $b_2$,

\[
b_j = \frac{1}{h_j} (a_{j+1} - a_j) - \frac{h_j}{3} (2c_j + c_{j+1}), \quad j = 0, \ldots, 2.
\]

\[
b_0 = \frac{1}{2} (1 - 0) - \frac{2}{3} (2 \times 0 - \frac{27}{23}) = \frac{59}{46}
\]

\[
b_1 = \frac{1}{2} (0 - 1) - \frac{1}{3} (2 \times \left(-\frac{27}{23}\right) + \frac{117}{46}) = -\frac{49}{46}
\]

\[
b_2 = \frac{1}{2} (2 - 0) - \frac{1}{3} (2 \times \frac{117}{46} + 0) = \frac{7}{23}
\]

Compute $d_0$, $d_1$ and $d_2$,

\[
d_j = \frac{c_{j+1} - c_j}{3h_j}, \quad j = 0, \ldots, 2.
\]

\[
d_0 = -\frac{27/23 - 0}{3 \times 2} = -\frac{9}{46}
\]

\[
d_1 = \frac{117/46 + 27/23}{3 \times 1} = \frac{57}{46}
\]

\[
d_2 = 0 - \frac{117/46}{3 \times 1} = -\frac{39}{46}
\]

We get

\[
s_0(x) = \frac{59}{46} (x + 2) - \frac{9}{46} (x + 2)^3
\]

\[
s_1(x) = 1 - \frac{49}{46} x - \frac{27}{23} x^2 + \frac{57}{46} x^3
\]

\[
s_2(x) = \frac{7}{23} (x - 1) + \frac{117}{46} (x - 1)^2 - \frac{39}{46} (x - 1)^3
\]

(c) For Lagrange polynomial, we check the critical points by letting the first-order derivative to be zero and determine whether each point is a local maximum, a local minimum or a saddle point by the second-order derivative value. Let

\[
P'(x) = \frac{3}{2} x^2 - \frac{3}{2} = 0.
\]

The solution is

\[
x = \pm 1.
\]

The second-order derivative is

\[
P''(x) = 3x.
\]
Because $P''(-1) = -3 < 0$, $P''(1) = 3 > 0$ and $P''(0) = 0$, we have a local maximum at $x = -1$, a local minimum at $x = 1$ and a saddle point at $x = 0$.

For spline, we check

\[
s'_0(-2) = \frac{59}{46} \cdot \frac{27}{46} (x + 2)^2 \bigg|_{x=-2} = \frac{59}{46} < P'(-2) = \frac{9}{2},
\]
\[
s'_1(0) = -\frac{49}{46} \cdot \frac{54}{23} x + \frac{171}{46} x^2 \bigg|_{x=0} = -\frac{49}{46} > P'(0) = -\frac{3}{2},
\]
\[
s'_2(1) = \frac{7}{23} + \frac{117}{23} (x - 1) - \frac{117}{46} (x - 1)^2 \bigg|_{x=1} = \frac{7}{23} > P'(1) = 0,
\]
\[
s'_2(2) = \frac{7}{23} + \frac{117}{23} (x - 1) - \frac{117}{46} (x - 1)^2 \bigg|_{x=2} = \frac{131}{46} < P'(2) = \frac{9}{2}.
\]

By a comparison with $P'(x)$ at each given point, we can draw a figure like Figure 1.
(d) From (c), we can calculate the following values.

\[ s'_0(x_1) = \frac{59}{46} - \frac{27}{46} (x + 2)^2 \bigg|_{x=0} = -\frac{49}{46}, \]
\[ s'_1(x_1) = -\frac{49}{46} - \frac{54}{23} x + \frac{171}{46} x^2 \bigg|_{x=0} = -\frac{49}{46}, \]
\[ s'_1(x_2) = \frac{7}{23} + \frac{117}{23} (x - 1) - \frac{117}{46} (x - 1)^2 \bigg|_{x=1} = \frac{7}{23}, \]
\[ s'_2(x_2) = \frac{7}{23} + \frac{117}{23} (x - 1) - \frac{117}{46} (x - 1)^2 \bigg|_{x=1} = \frac{7}{23}. \]

Problem 2 (20%)

Consider

\[ f(x) = \log x \]

and we would like to find a solution of

\[ f(x) = 0 \]

by using the Newton method. \textbf{Here we consider natural log.}

(a) (5%) What is the formulation of a Newton iteration?

(b) (15%) Consider any point in \((0, \infty)\) as the initial point. Which leads to the convergence, while which does not? You need to theoretically prove the result. That is, you need to prove that the sequence \(\{x_n\}\) generated by the Newton method satisfies

\[ \lim_{n \to \infty} x_n = \text{the root} \]

or not.

Hint: To prove the convergent case, you might need the following properties. First,

\[ \log y < y - 1 \quad \text{if} \quad y > 1 \]

and second, an increasing sequence

\[ \{x_n\} \]

with a finite upper bound globally converges to a point \(x^*\).
Solution

(a) 
\[ x_{n+1} = x_n - \frac{\log x_n}{1/x_n} = x_n(1 - \log x_n). \]

(b) (i) If 
\[ x_1 \geq e, \]
then 
\[ x_2 = x_1(1 - \log x_1) \leq 0. \]
So Newton iterations are not well defined.

(ii) If 
\[ x_1 < 1, \]
then we prove that \( \{x_n\} \) is an increasing sequence and 
\[ x_n < 1, \quad \forall n. \]

Let 
\[ 0 < x < 1. \]
Then 
\[ y = \frac{1}{x} > 1 \quad \text{and} \quad \log y < y - 1 \]
imply that 
\[ -\log x < \frac{1}{x} - 1 \]
and 
\[ -x \log x < 1 - x. \quad (1) \]
Therefore, if 
\[ x_n < 1, \]
then from (1), 
\[ x_{n+1} = x_n(1 - \log x_n) < 1. \]
Further, 
\[ \log x_n < 0 \]
implies 
\[ x_{n+1} > x_n. \]
Thus \( \{x_n\} \) is an increasing sequence bounded by 1. Taking the limit we get

\[
x^* = x^*(1 - \log x^*).
\]

Thus

\[
\log x^* = 0 \quad \text{and} \quad x^* = 1. 
\] (2)

**Alternative solution (copied from your solutions):**

For points in \((0, 1)\), we want \( \{x_n\} \) increased and with an upper bound at 1. That is

\[
x < x(1 - \log x) < 1.
\]

L.H.S.:

\[
x < x - x \log x
\]

\[
x \log x < 0.
\]

It is true in \((0, 1)\) obviously.

R.H.S.:

\[
\frac{d}{dx}x(1 - \log x) = -\log x
\]

\[
\Rightarrow x(1 - \log x) \text{ strictly increases in } (0, 1).
\]

When \( x = 1 \),

\[
x(1 - \log x) = 1.
\]

Thus,

\[
x(1 - \log x) < 1 \quad \text{when} \quad 0 < x < 1.
\]

Therefore,

\[
x < x(1 - \log x) < 1 \quad \text{when} \quad x \in (0, 1)
\]

\[
\Rightarrow \{x_n\} \text{ is increasing, with a finite upper bound } 1.
\]

\[
\Rightarrow \text{ it converges to } x^*.
\]

(iii) If

\[
1 < x_1 < e.
\]

Because

\[
0 < \log x_1 < 1,
\]
$x_2$ is well defined. Then
\[
\frac{d}{dx}x(1 - \log x) = -\log x \in (-1, 0), \quad \text{when } 1 < x < e.
\]

We see that $x(1 - \log x)$ is a strictly decreasing function with
\[
x = 1, \ x(1 - \log x) = 1
\]
\[
x = e, \ x(1 - \log x) = 0
\]

Thus

\[
0 < x_1(1 - \log x_1) < 1.
\]

Then

\[
0 < x_2 < 1.
\]

From the case of (ii), we know that the sequence is converged.

(iv) When $x_1 = 1$,
\[
f(x_1) = 0
\]
and the procedure stops at the first iteration.

**Common mistake:**

After showing convergence you need $[2]$ to get $x^* = 1$. Otherwise you do not know what $\{x_n\}$ converges to.

**Problem 3 (10%)**

Consider
\[
f(x) = x^3 \quad \text{on} \quad [0, 1].
\]

Use continuous least square to approximate $f(x)$ by a polynomial of degree 2.

**Solution**

\[
a_0 \int_0^1 1 \, dx + a_1 \int_0^1 x \, dx + a_2 \int_0^1 x^2 \, dx = \int_0^1 x^3 \, dx
\]
\[
a_0 \int_0^1 x \, dx + a_1 \int_0^1 x^2 \, dx + a_2 \int_0^1 x^3 \, dx = \int_0^1 x^4 \, dx
\]
\[
a_0 \int_0^1 x^2 \, dx + a_1 \int_0^1 x^3 \, dx + a_2 \int_0^1 x^4 \, dx = \int_0^1 x^5 \, dx
\]
Figure 2: An approximation with polynomial of degree two.

The integral equations become

\[ a_0 \left( x^1 \right)_0 + a_1 \left( \frac{1}{2} x^2 \right)_0 + a_2 \left( \frac{1}{3} x^3 \right)_0 = \frac{1}{4} x^4 \]
\[ a_0 \left( \frac{1}{2} x^2 \right)_0 + a_1 \left( \frac{1}{3} x^3 \right)_0 + a_2 \left( \frac{1}{4} x^4 \right)_0 = \frac{1}{5} x^5 \]
\[ a_0 \left( \frac{1}{3} x^3 \right)_0 + a_1 \left( \frac{1}{4} x^4 \right)_0 + a_2 \left( \frac{1}{5} x^5 \right)_0 = \frac{1}{6} x^6 \]

After evaluating,

\[ a_0 + \frac{1}{2} a_1 + \frac{1}{3} a_2 = \frac{1}{4} \]
\[ \frac{1}{2} a_0 + \frac{1}{3} a_1 + \frac{1}{4} a_2 = \frac{1}{5} \]
\[ \frac{1}{3} a_0 + \frac{1}{4} a_1 + \frac{1}{5} a_2 = \frac{1}{6} \]
By simplifying them, we have

\[12a_0 + 6a_1 + 4a_2 = 3\]
\[30a_0 + 20a_1 + 15a_2 = 12\]
\[20a_0 + 15a_1 + 12a_2 = 10\]

and the solution is

\[a_0 = \frac{1}{20}, \quad a_1 = -\frac{3}{5}, \quad a_2 = \frac{3}{2}\]

Thus, the approximation function is

\[\frac{3}{2}x^2 - \frac{3}{5}x + \frac{1}{20}.\]

**Problem 4 (30%)**

Consider a linear system \(Ax = b\):

\[
\begin{bmatrix}
3 & 0 & 2 \\
0 & 1 & 0 \\
2 & 0 & 2
\end{bmatrix}
\begin{bmatrix}
x \\
x \\
x
\end{bmatrix}
=
\begin{bmatrix}
1 \\
1 \\
-1
\end{bmatrix}.
\]

(a) (10%)

Is the matrix \(A\) symmetric positive definite? You cannot just answer yes or no.

Assume \(x_0 = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T\). Do two CG iterations and show what \(x_1\) and \(x_2\) are? Is \(x_2\) a solution or not?

Check if \(p_1\) and \(p_2\) are \(A\)-conjugate.

(b) (10%) Let \(r_1\) and \(p_1\) be vectors from the above procedure. Solve the following optimization problem with the variable \(p\):

\[
\min_p \|p - r_1\|^2 \\
\text{subject to } p \in \text{span}\{Ap_1\}^\perp
\]

(3)

How is the solution of this problem connected to \(p_2\) obtained in the CG procedure?
(c) (5%) If we denote the solution of (3) as $\bar{p}_2$ and calculate $\bar{\alpha}_2$, $x_2$ by

$$\bar{\alpha}_2 = \frac{\bar{p}_2^T r_1}{\bar{p}_2^T A \bar{p}_2}, \quad x_2 = x_1 + \bar{\alpha}_2 \bar{p}_2,$$

what are $\bar{\alpha}_2$ and $x_2$?

(d) (5%) If we write

$$A = I + B$$

where $I$ is an identity matrix, what is $B$ and what is the rank of $B$? Can you use any theoretical results discussed in slides to double check your results?

It is true that one may make mistakes in doing the calculation. However, if you understand the concept of CG, you should be able to easily validate your results.

**Solution**

(a) Because $a_{ij} = a_{ji}$, $i \neq j$, the matrix $A$ is symmetric.

Assume $v = [v_1 \ v_2 \ v_3]^T$ is not a zero vector, it follows that

$$v^T A v = 2(v_1 + v_3)^2 + v_1^2 + v_2^2 \geq 0.$$

If it is zero, then

$$v_1 = -v_3 \quad \text{and} \quad v_1 = v_2 = 0$$

imply that $v = 0$, a contradiction. Thus $v^T A v > 0$ if $v \neq 0$, so $A$ is positive definite.

$$x_0 = [0 \ 0 \ 0]^T \Rightarrow r_0 = [1 \ 1 \ -1]^T \Rightarrow p_1 = [1 \ 1 \ -1]^T \Rightarrow \alpha_1 = r_0^T r_0 / p_1^T A p_1 = 3/2$$

$$x_1 = x_0 + \alpha_1 p_1 = [3/2 \ 3/2 \ -3/2]^T \Rightarrow r_1 = r_0 - \alpha_1 A p_1 = [-1/2 \ -1/2 \ -1]^T$$

$$\beta_2 = r_1^T r_1 / r_0^T r_0 = 1/2 \Rightarrow p_2 = r_1 + \beta_2 p_1 = [0 \ 0 \ -3/2]^T \Rightarrow \alpha_2 = r_1^T r_1 / p_2^T A p_2 = 1/3$$

$$x_2 = x_1 + \alpha_2 p_2 = [3/2 \ 3/2 \ -2]^T \Rightarrow r_2 = r_1 - \alpha_2 A p_2 = [1/2 \ -1/2 \ 0]^T$$

Because $r_2$ is not a zero vector, $x_2$ is not a solution.

$$p_2^T A p_1 = [0 \ 0 \ -3/2] \begin{bmatrix} 3 & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} = [0 \ 0 \ -3/2] \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = 0.$$
(b) The constraint in (3) is equivalent to find \( p \) such that it is linearly independent to span\( \{Ap_1\} \). Therefore, let

\[
p = \begin{bmatrix} s \\ t \\ q \end{bmatrix}, \ s, \ t, \ q \in \mathbb{R}.
\]  

(4)

Then

\[
p^\top (Ap_1) = 0
\]

\[
s + t = 0
\]

\[
t = -s
\]

(5)

Substitute (5) into (4). We have

\[
p = \begin{bmatrix} s \\ -s \\ q \end{bmatrix}, \ s, \ q \in \mathbb{R}.
\]

Then, we can derive

\[
\|p - \begin{bmatrix} -1/2 \\ -1/2 \\ -1 \end{bmatrix}\|^2 = (s + \frac{1}{2})^2 + (-s + \frac{1}{2})^2 + (q + 1)^2.
\]

Then, we can differentiate the above function with respect to \( s \) and \( t \), respectively.

\[
4s = 0
\]

\[
2q + 2 = 0
\]

And the solution of \((s, q)\) is \((0, -1)\) and the vector \( p \) is

\[
\begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}.
\]

We can see this solution \( p \) is parallel to \( p_2 \).

(c) Because

\[
\hat{\alpha}_2 = \frac{\begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} -1/2 \\ -1/2 \\ -1 \end{bmatrix} \begin{bmatrix} 3 & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix}}{2} = \frac{1}{2}.
\]
we can derive

$$x_2 = x_1 + \bar{\alpha}_2 \bar{p}_2 = \begin{bmatrix} 3/2 \\ 3/2 \\ -3/2 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix} = \begin{bmatrix} 3/2 \\ 3/2 \\ -2 \end{bmatrix}.$$ 

Finally, we have the same $x_2$ because we need to multiply $\bar{p}_2$ with $\bar{\alpha}_2$ again.

(d)

$$\begin{bmatrix} 3 & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 0 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 2 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 1 \end{bmatrix}.$$

It is clear to see that the rank of $B$ is 2 since row 1 and row 3 are linearly independent.

From Theorem 4 mentioned on page 89 in the slides, we know that

$$\text{number of CG iterations} \leq \text{rank}(B) + 1$$

$$= 3$$