Numerical Methods 2021 — Final Exam

Solutions

Problem 1 (20 pts). Consider the following four pairs of $(x, f(x))$:

$$(0,3),(1,0),(2,3),(3,0).$$

(a) (5 pts) Find the Lagrange Polynomial. You must do the calculation to obtain a final form of

$$a_3x^3 + a_2x^2 + a_1x + a_0.$$

(b) (15 pts) Find the spline by the following boundary conditions

$$s_0''(x_0) = 0, s_2''(x_3) = 0.$$

You must show details of every step in calculating a_j, b_j, c_j and d_j.

Solution.

(a) Lagrange polynomial:

$$\begin{aligned}
P(x) &= \sum_{k=0}^{3} L_{n,k}(x) f(x_k) \\
&= \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1) \\
&+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3) \\
&= \frac{(x-1)(x-2)(x-3)}{(-1)(-2)(-3)} 3 + \frac{(x-0)(x-1)(x-3)}{(2)(1)(-1)} 3 \\
&= \frac{-(x-1)(x-2)(x-3) - 3(x-0)(x-1)(x-3)}{2} \\
&= \frac{-4x^3 + 18x^2 - 20x + 6}{2} \\
&= -2x^3 + 9x^2 - 10x + 3
\end{aligned}$$

(b) We have to determine a_j, b_j, c_j and d_j of

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

where $j = 0, 1, 2$.

- Define h_j

$$h_0 = x_1 - x_0 = 1, \quad h_1 = x_2 - x_1 = 1, \quad h_2 = x_3 - x_2 = 1.$$

- Compute a_j

$$a_0 = f(0) = 3, \quad a_1 = f(1) = 0, \quad a_2 = f(2) = 3, \quad a_3 \equiv f(3) = 0.$$

- Compute c_j From the boundary condition,

$$s_0''(0) = 2c_0 = 0 \Rightarrow c_0 = 0$$

and

$$c_3 \equiv \frac{s_2''(3)}{2} = 0.$$

Compute c_1 and c_2 by

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

where $j = 1, 2$. We have

$$h_0c_0 + 2(h_0 + h_1)c_1 + h_1c_2 = \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0)$$
$$h_1c_1 + 2(h_1 + h_2)c_2 + h_2c_3 = \frac{3}{h_2}(a_3 - a_2) - \frac{3}{h_1}(a_2 - a_1).$$

That is,

$$4c_1 + c_2 = 3(a_2 - a_1) - 3(a_1 - a_0) = 3 \times 3 - 3 \times (-3) = 18$$
$$c_1 + 4c_2 = 3(a_3 - a_2) - 3(a_2 - a_1) = 3 \times (-3) - 3 \times 3 = -18.$$

We have

$$c_1 = 6, c_2 = -6.$$

- Compute b_j

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

where $j = 0, 1, 2$. We have

$$b_0 = \frac{1}{h_0}(a_1 - a_0) - \frac{h_0}{3}(2c_0 + c_1) = -3 - \frac{1}{3}(6) = -5$$
$$b_1 = \frac{1}{h_1}(a_2 - a_1) - \frac{h_1}{3}(2c_1 + c_2) = 3 - \frac{1}{3}(6) = 1$$
$$b_2 = \frac{1}{h_2}(a_3 - a_2) - \frac{h_2}{3}(2c_2 + c_3) = -3 - \frac{1}{3}(-12) = 1.$$

- Compute d_j

$$d_j = \frac{c_{j+1} - c_j}{3h_j},$$

where $j = 0, 1, 2$. We have

$$d_0 = \frac{c_1 - c_0}{3h_0} = \frac{6}{3} = 2$$
$$d_1 = \frac{c_2 - c_1}{3h_1} = \frac{-12}{3} = -4$$
$$d_2 = \frac{c_3 - c_2}{3h_2} = \frac{6}{3} = 2$$

- Finally, we have

$$
\begin{aligned}
&s_0(x) = a_0 + b_0(x - x_0) + c_0(x - x_0)^2 + d_0(x - x_0)^3 \\
&= 3 + -5(x - 0) + 0(x - 0)^2 + 2(x - 0)^3 \\
&= 2x^3 - 5x + 3 \\
&s_1(x) = a_1 + b_1(x - x_1) + c_1(x - x_1)^2 + d_1(x - x_1)^3 \\
&= 0 + 1(x - 1) + 6(x - 1)^2 + -4(x - 1)^3 \\
&= (x - 1) + 6(x - 1)^2 - 4(x - 1)^3 \\
&= -4x^3 + 18x^2 - 23x + 9 \\
&s_2(x) = a_2 + b_2(x - x_2) + c_2(x - x_2)^2 + d_2(x - x_2)^3 \\
&= 3 + 1(x - 2) + -6(x - 2)^2 + 2(x - 2)^3 \\
&= 3 + (x - 2) - 6(x - 2)^2 + 2(x - 2)^3 \\
&= 2x^3 - 18x^2 + 49x - 39
\end{aligned}
$$

Problem 2 (10 pts). Consider the following linear regression

$$\min_{\boldsymbol{a}} F(\boldsymbol{a}) = \sum_{i=1}^{4} (a_0 + a_1 x_{i1} + a_2 x_{i2} - y_i)^2$$

Give an example with

$$\boldsymbol{x}_i = \begin{bmatrix} x_{i1} \\ x_{i2} \end{bmatrix} \neq \boldsymbol{x}_j = \begin{bmatrix} x_{j1} \\ x_{j2} \end{bmatrix}, \ \forall i, j$$

such that the resulting matrix in the linear system is positive semi-definite but not positive definite. You must also show the linear system and explain that it is only positive semi-definite.

Solution. Let us calculate the gradient as

$$\nabla_{\boldsymbol{a}} F = \sum_{i=1}^{4} \begin{bmatrix} 2(a_0 + a_1 + x_{i1} + a_2 x_{i2} - y_i) \\ 2(a_0 + a_1 + x_{i1} + a_2 x_{i2} - y_i) x_{i1} \\ 2(a_0 + a_1 + x_{i1} + a_2 x_{i2} - y_i) x_{i2} \end{bmatrix}$$

and the Hessian matrix can be calculated as

$$\nabla^2_{\boldsymbol{a}} F = \sum_{i=1}^{4} \begin{bmatrix} 2 & 2x_{i1} & 2x_{i2} \\ 2x_{i1} & 2x_{i1}^2 & 2x_{i1}x_{i2} \\ 2x_{i2} & 2x_{i1}x_{i2} & 2x_{i2}^2 \end{bmatrix}$$

The determinant of $\nabla^2_{\boldsymbol{a}} F$ is

$$\frac{1}{8} \left(4S_{x\cdot 1 x\cdot 1} S_{x\cdot 2 x\cdot 2} + 2S_{x\cdot 1} S_{x\cdot 2} S_{x\cdot 1 x\cdot 2} - S_{x\cdot 2} S_{x\cdot 2} S_{x\cdot 1 x\cdot 1} - S_{x\cdot 1} S_{x\cdot 1} S_{x\cdot 2 x\cdot 2} - 4S_{x\cdot 1 x\cdot 2} S_{x\cdot 1 x\cdot 2}, \right) \tag{1}$$

where

$$S_{x\cdot s} = \sum_{i=1}^{4} x_{is}$$

$$S_{x\cdot s x\cdot t} = \sum_{i=1}^{4} x_{is} x_{it}$$

for all $s, t \in \{1, 2\}$. We can take

$$\begin{aligned} \boldsymbol{x}_1 &= (1, 1) \\ \boldsymbol{x}_2 &= (1, -1) \\ \boldsymbol{x}_3 &= (1, 2) \\ \boldsymbol{x}_4 &= (1, -2) \end{aligned}$$

such that

$$S_{x \cdot 2} = S_{x \cdot 1 x \cdot 2} = 0,$$

and (1) is equal to

$$\frac{1}{8} \left(4 S_{x \cdot 1 x \cdot 1} S_{x \cdot 2 x \cdot 2} - S_{x \cdot 1} S_{x \cdot 1} S_{x \cdot 2 x \cdot 2} \right) = \frac{1}{8} \left(4 \cdot 4 \cdot 10 - 4 \cdot 4 \cdot 10 \right) = 0.$$

Furthermore, since

$$\nabla^2_{\boldsymbol{a}} F = 2 \cdot \begin{bmatrix} 4 & S_{x \cdot 1} & S_{x \cdot 2} \\ S_{x \cdot 1} & S_{x \cdot 1 x \cdot 1} & S_{x \cdot 1 x \cdot 2} \\ S_{x \cdot 2} & S_{x \cdot 1 x \cdot 2} & S_{x \cdot 2 x \cdot 2} \end{bmatrix} = 2 \cdot \begin{bmatrix} 4 & 4 & 0 \\ 4 & 4 & 0 \\ 0 & 0 & 10 \end{bmatrix},$$

we have

$$\boldsymbol{a}^T \nabla^2_{\boldsymbol{a}} F \boldsymbol{a} = 2 \left(4 (a_0 + a_1)^2 + 10 a_2^2 \right) \geq 0.$$

Therefore, we can say that $\nabla^2_{\boldsymbol{a}} F$ is positive semi-definite but not positive definite.

Problem 3 (30 pts). We mention that the most commonly used setting of spline is by piece-wise degree-3 polynomials, but now we are interested in using degree-4 polynomials. Naturally, we additionally consider

$$s'''_{j+1}(x_{j+1}) = s'''_j(x_{j+1}), \; j = 0, \cdots, n-2.$$

(a) (5 pts) Without considering boundary conditions, what are number of equations and number of variables? You need to list those equations with the functions s_j, for $j = 0, \ldots, n-1$.

(b) (10 pts) Consider the definition of $s_j(x)$

$$s_j(x) = a_j + b_j (x - x_j) + c_j (x - x_j)^2 + d_j (x - x_j)^3 + e_j (x - x_j)^4.$$

Please list the equations in (a) with the variables a_j, b_j, c_j, d_j and e_j. You can define

$$h_j = x_{j+1} - x_j$$

to simplify these equations.

(c) (15 pts) Please simplify from your equations in (b) by

i) Represent and subsitute e_j with d_j and h_j, for $j = 0, \ldots, n-1$. Please show the equations after this simplification.

ii) Represent and subsitute b_j with a_j, c_j, d_j and h_j, for $j = 0, \ldots, n-1$. Please show the equations after this simplification.

Solution.

(a) We have the following equations

$$
\begin{aligned}
s_j(x_j) =& f(x_j),\ j = 0, \dots, n-1 && (2)\\
s_{n-1}(x_n) =& f(x_n), && (3)\\
s_j(x_{j+1}) =& s_{j+1}(x_{j+1}),\ j = 0, \dots, n-2 && (4)\\
s'_j(x_{j+1}) =& s'_{j+1}(x_{j+1}),\ j = 0, \dots, n-2 && (5)\\
s''_j(x_{j+1}) =& s''_{j+1}(x_{j+1}),\ j = 0, \dots, n-2 && (6)\\
s'''_j(x_{j+1}) =& s'''_{j+1}(x_{j+1}),\ j = 0, \dots, n-2, && (7)
\end{aligned}
$$

so we have $5n-3$ equations. For the variables, our $s_j(x)$ can be defined by

$$a_j + b_j(x-x_j) + c_j(x-x_j)^2 + d_j(x-x_j)^3 + e_j(x-x_j)^4.$$

Thus, we have $5n$ variables.

(b) Case 1: The equations (2) becomes

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

Case 2: The equation (3) becomes

$$a_{n-1} + b_{n-1}h_{n-1} + c_{n-1}h_{n-1}^2 + d_{n-1}h_{n-1}^3 + e_{n-1}h_{n-1}^4 = f(x_n)$$

Case 3: The equations (4) becomes

$$a_{j+1} = a_j + b_jh_j + c_jh_j^2 + d_jh_j^3 + e_jh_j^4,\ j = 0, \dots, n-2.$$

Case 4: The equations (5) becomes

$$b_{j+1} = b_j + 2c_jh_j + 3d_jh_j^2 + 4e_jh_j^3,\ j = 0, \dots, n-2.$$

Case 5: The equations (6) becomes

$$2c_{j+1} = 2c_j + 6d_jh_j + 12e_jh_j^2,\ j = 0, \dots, n-2.$$

Case 6: The equations (7) becomes

$$6d_{j+1} = 6d_j + 24e_jh_j,\ j = 0, \dots, n-2.$$

(c) From (b)'s Case 6, we can find that

$$e_j = \frac{d_{j+1} - d_j}{4h_j},\ j = 0, \dots, n-2.$$

Therefore, we can subsitute the variable e_j in the other equations with d_j and d_{j+1}. That is, we have

$$
\begin{aligned}
a_{j+1} =& a_j + b_jh_j + c_jh_j^2 + d_jh_j^3 + \frac{d_{j+1} - d_j}{4}h_j^3,\ j = 0, \dots, n-2 && (8)\\
b_{j+1} =& b_j + 2c_jh_j + 3d_jh_j^2 + (d_{j+1} - d_j)h_j^2,\ j = 0, \dots, n-2\\
2c_{j+1} =& 2c_j + 6d_jh_j + 3(d_{j+1} - d_j)h_j,\ j = 0, \dots, n-2
\end{aligned}
$$

Next, we make (8) be

$$b_j = \frac{a_{j+1} - a_j}{h_j} - c_j h_j - \frac{d_{j+1} + 3d_j}{4} h_j^2,\ j = 0, \dots, n-2$$

Thereby, we can subsitute b_j in the equations with c_j and d_j. That is, we have

$$\begin{aligned}
&\frac{a_{j+2} - a_{j+1}}{h_{j+1}} - c_{j+1} h_{j+1} - \frac{d_{j+2} + 3d_{j+1}}{4} h_{j+1}^2 \\
=&\frac{a_{j+1} - a_j}{h_j} - c_j h_j - \frac{d_{j+1} + 3d_j}{4} h_j^2 + 2c_j h_j + 3d_j h_j^2 + (d_{j+1} - d_j) h_j^2,\ j = 0, \dots, n-2 \\
2c_{j+1} =&2c_j + 6d_j h_j + 3(d_{j+1} - d_j) h_j,\ j = 0, \dots, n-2
\end{aligned}$$

Problem 4 (10 pts). Consider continuous least square. The function

$$f(x) = x^2$$

is approximated by

$$P_1(x) = a_1 x + a_0$$

over

$$x \in [0, 1].$$

Solve the linear system to get P_1.

Solution.
Our minimization problem is

$$\begin{aligned}
&\min_{\boldsymbol{a}} \int_0^1 [P_1(x) - f(x)]^2 dx \\
=&\min_{\boldsymbol{a}} \int_0^1 [a_1 x + a_0 - x^2]^2 dx \\
=&\min_{\boldsymbol{a}} \int_0^1 (x^4 + a_0^2 + a_1^2 x^2 - 2a_1 x^3 + 2a_1 a_0 x - 2a_0 x^2) dx \\
=&\min_{\boldsymbol{a}} \int_0^1 x^4 dx + \int_0^1 a_0^2 dx + \int_0^1 a_1^2 x^2 dx - \int_0^1 2a_1 x^3 dx + \int_0^1 2a_1 a_0 x dx - \int_0^1 2a_0 x^2 dx \\
=&\min_{\boldsymbol{a}} \left(\frac{1}{5} + a_0^2 + \frac{1}{3} a_1^2 - \frac{1}{2} a_1 + a_1 a_0 - \frac{2}{3} a_0 \right)
\end{aligned}$$

Let us take

$$g(\boldsymbol{a}) = \left(\frac{1}{5} + a_0^2 + \frac{1}{3} a_1^2 - \frac{1}{2} a_1 + a_1 a_0 - \frac{2}{3} a_0 \right)$$

and utilize

$$\nabla_{\boldsymbol{a}} g = 0 \tag{9}$$

to get the solution. The linear system (9) is

$$\begin{bmatrix} 2a_0 + a_1 - 2/3 \\ 2/3 \cdot a_1 - 1/2 + a_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

After we solving it, we can get the solution

$$\boldsymbol{a} = (\frac{-1}{6}, 1).$$

Problem 5 (30 pts). Given a function

$$f(x) = \frac{2}{\pi}x,$$

approximate $f(x)$ with a Fourier series with n term

$$s_n(x) = \frac{a_0 + a_n \cos nx}{2} + \sum_{k=1}^{n-1} \left(a_k \cos kx + b_k \sin kx\right)$$

and $2m$ points

$$(x_0, f(x_0)), \cdots, (x_{2m-1}, f(x_{2m-1}))$$

where

$$x_k = -\pi + \frac{k}{m}\pi.$$

(a) (15 pt) Given $m = n = 2$, in fast Fourier transform (FFT), we show that we can calculate

$$\boldsymbol{c} = F\boldsymbol{y}.$$

Show F and corresponding $\boldsymbol{c}$. (Hint: Euler's formula: $e^{ix} = \cos x + i \sin x$)

(b) (5 pt) Calculate

$$a_0, a_1, a_2$$

and

$$b_1$$

from $\boldsymbol{c}$.

(c) (10 pt) Decompose F to a sequence of matrix products,

$$F = A_t \cdots A_1 P$$

Solution.

(a) Let

$$\delta = e^{\frac{-i\pi}{m}} = e^{\frac{-i\pi}{2}} = \cos(-\frac{\pi}{2}) + i \sin(-\frac{\pi}{2}) = -i.$$

The F is

$$F = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \delta^1 & \delta^2 & \delta^3 \\ 1 & \delta^2 & \delta^4 & \delta^6 \\ 1 & \delta^3 & \delta^6 & \delta^9 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \delta & -1 & -\delta \\ 1 & -1 & 1 & -1 \\ 1 & -\delta & -1 & \delta \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix},$$

because $\delta = -i$.

The $2m$ points are

$$(-\pi, -2), (-\frac{1}{2}\pi, -1), (0, 0), (\frac{1}{2}\pi, 1).$$

Then, we have

$$\boldsymbol{y} = \begin{bmatrix} -2 \\ -1 \\ 0 \\ 1 \end{bmatrix}$$

and

$$\boldsymbol{c} = F\boldsymbol{y} = \begin{bmatrix} -2 \\ -2+2i \\ -2 \\ -2-2i \end{bmatrix} = \begin{bmatrix} -2 \\ -2 \\ -2 \\ -2 \end{bmatrix} + \begin{bmatrix} 0 \\ 2 \\ 0 \\ -2 \end{bmatrix} i$$

(b) From

$$a_k = \mathrm{Re}(\frac{c_k(-1)^k}{m}) = \mathrm{Re}(\frac{c_k(-1)^k}{2})$$

and

$$b_k = -\,\mathrm{Im}(\frac{c_k(-1)^k}{m}) = -\,\mathrm{Im}(\frac{c_k(-1)^k}{2}).$$

We have

$$a_0 = \frac{-2(-1)^0}{2} = -1,$$
$$a_1 = \frac{-2(-1)^1}{2} = 1,$$
$$a_2 = \frac{-2(-1)^2}{2} = -1,$$

and

$$b_1 = -\frac{2(-1)^1}{2} = -(-1) = 1.$$

(c) From

$$t = \log 2m = \log 4 = 2,$$

we know that

$$F = A_2 A_1 P.$$

Now, we derive A_k. When $k = 2$, we have

$$L = 2^2 = 4, \quad r = \frac{2m}{L} = \frac{4}{4} = 1.$$

and

$$\begin{aligned} A_2 &= I_r \otimes B_L \\ &= I_1 \otimes B_4 \\ &= \begin{bmatrix} 1 \end{bmatrix} \otimes \begin{bmatrix} I_2 & \Omega_2 \\ I_2 & -\Omega_2 \end{bmatrix}, \quad \text{where } \Omega_2 = \begin{bmatrix} 1 & 0 \\ 0 & \delta \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \delta \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -\delta \end{bmatrix} \end{aligned}$$

When k = 1, we have

$$L = 2^1 = 2, \quad r = \frac{2m}{L} = 2.$$

and

$$
\begin{aligned}
A_1 &= I_r \otimes B_L \\
&= I_2 \otimes B_2 \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} I_1 & \Omega_1 \\ I_1 & -\Omega_1 \end{bmatrix}, \quad \text{where}\, \Omega_1 = \begin{bmatrix} 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}
\end{aligned}
$$

The permutation is the reverse of each column binary representation.

$$
\begin{aligned}
00 &\rightarrow 00 \quad \text{column 0 swap to column 0} \\
01 &\rightarrow 10 \quad \text{column 1 swap to column 2} \\
10 &\rightarrow 01 \quad \text{column 2 swap to column 1} \\
11 &\rightarrow 11 \quad \text{column 3 swap to column 3}
\end{aligned}
$$

Therefore, we have

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

$$
\begin{aligned}
F &= A_2 A_1 P \\
&= \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \delta \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -\delta \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} P \\
&= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & \delta & -\delta \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -\delta & \delta \end{bmatrix} P \\
&= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & \delta & -\delta \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -\delta & \delta \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \delta & -1 & -\delta \\ 1 & -1 & 1 & -1 \\ 1 & -\delta & -1 & \delta \end{bmatrix}
\end{aligned}
$$