Computational Physics

Lecture-20

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Contents

Approximation of a Function

Interpolation is needed when we want to infer some **local information** from a set of incomplete or discrete data.

- Lagrange Interpolation
- Spline Approximation

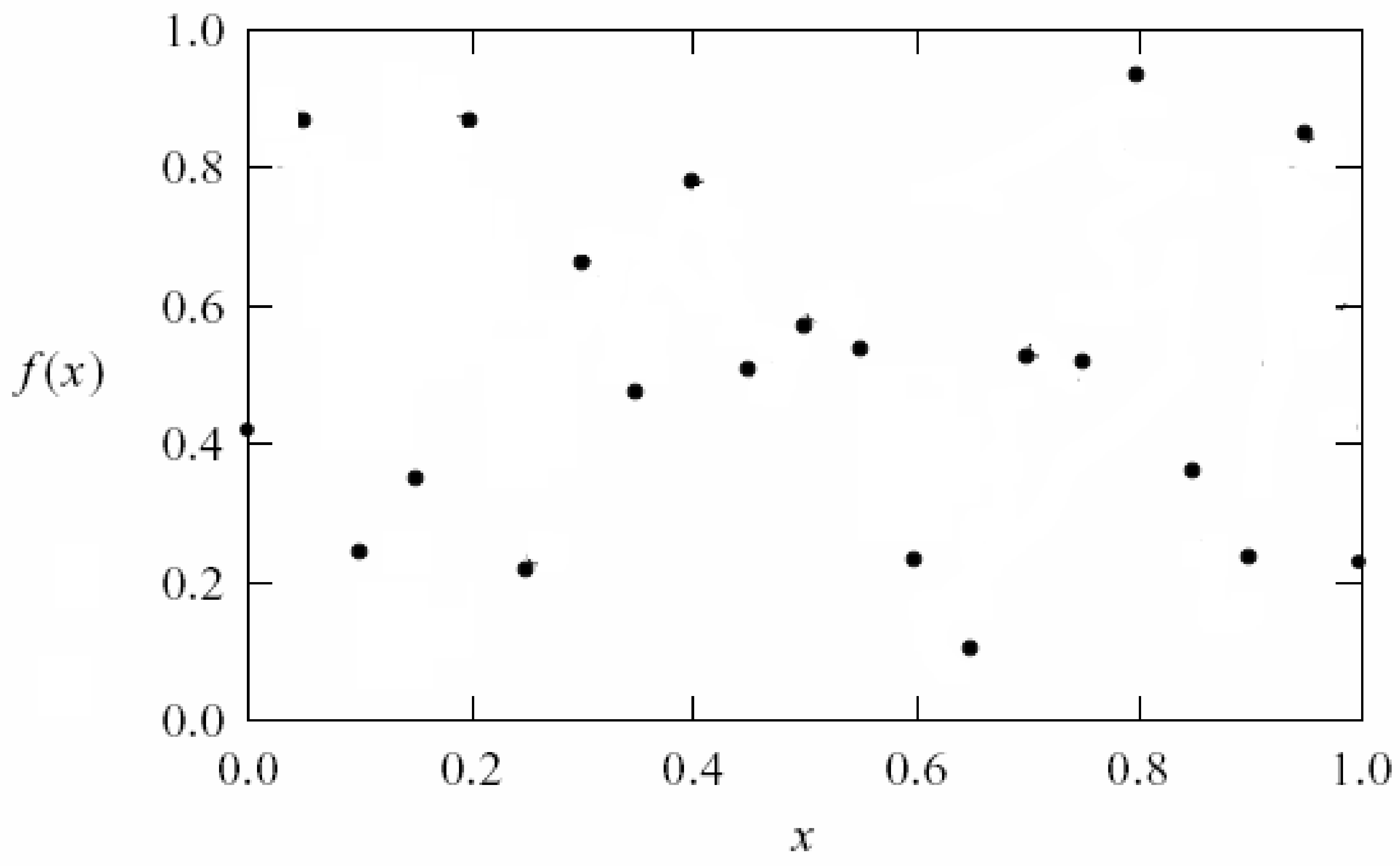
Overall approximation or fitting is needed when we want to know the **general or global behavior** of the data.

- Least Square

Approximation of a Function

- Lagrange Interpolation

x	f
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_i	f_i
$\vdots$	$\vdots$
x_n	f_n

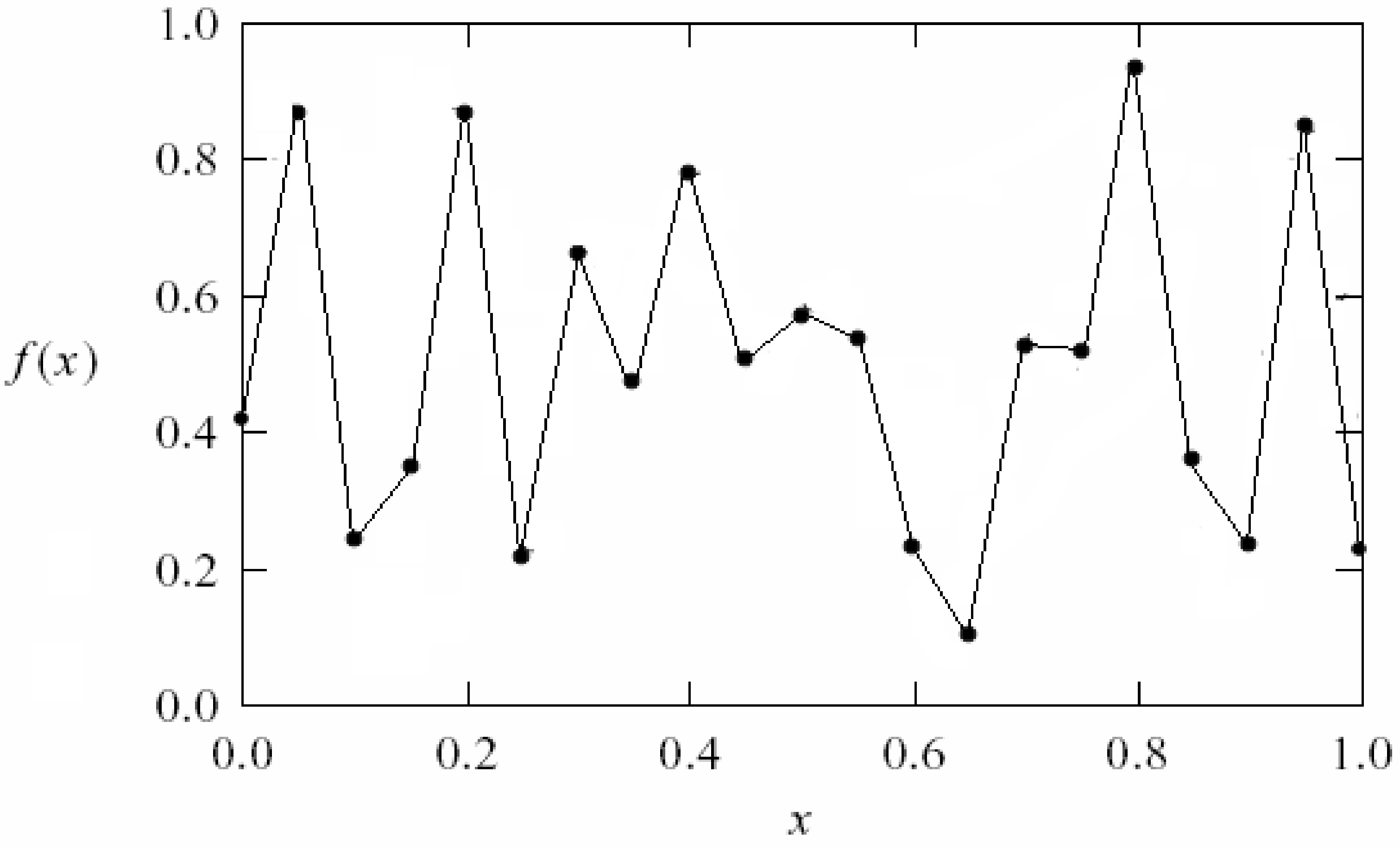


Approximation of a Function

- Lagrange Interpolation

x	f
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_i	f_i
$\vdots$	$\vdots$
x_n	f_n

Simplest way to obtain the approximation of $f(x)$

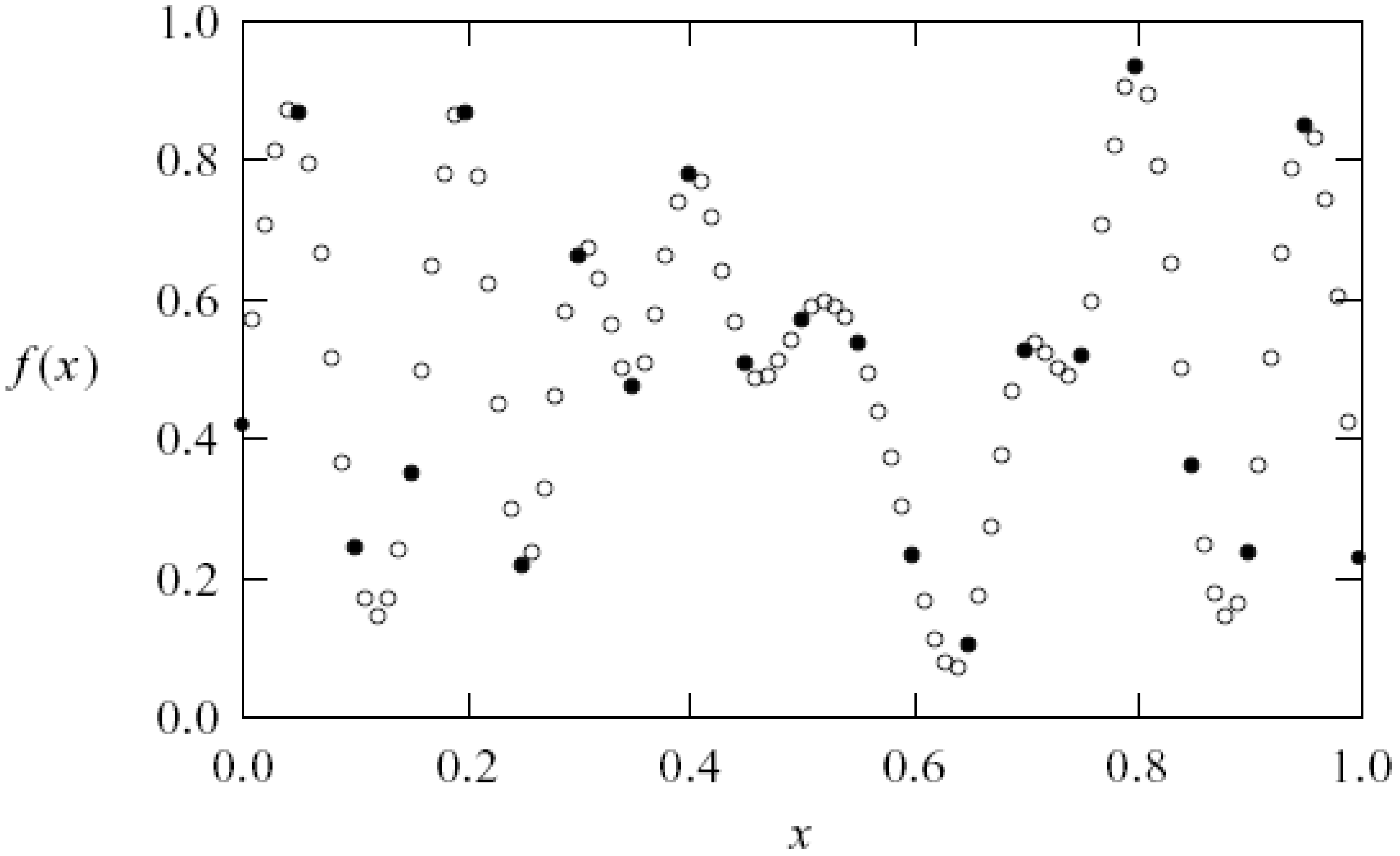


Approximation of a Function

- Lagrange Interpolation

x	f
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_i	f_i
$\vdots$	$\vdots$
x_n	f_n

More accurate approximation of $f(x)$



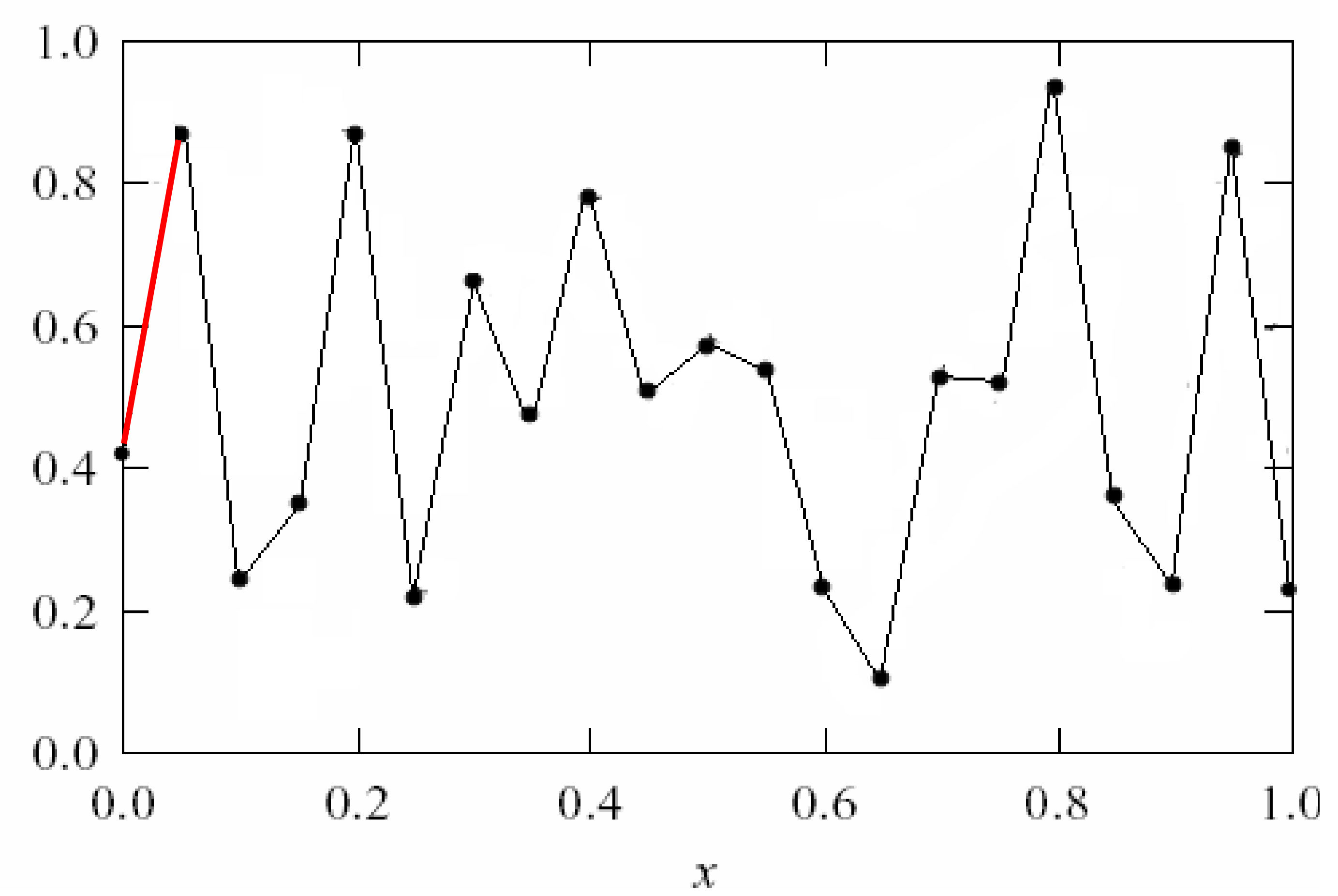
Approximation of a Function

- Lagrange Interpolation

x	x_0	x_1	x_2	$\cdots$	x_i	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	$\cdots$	f_n

$$f(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1$$

Simplest way to obtain the approximation of $f(x)$



Approximation of a Function

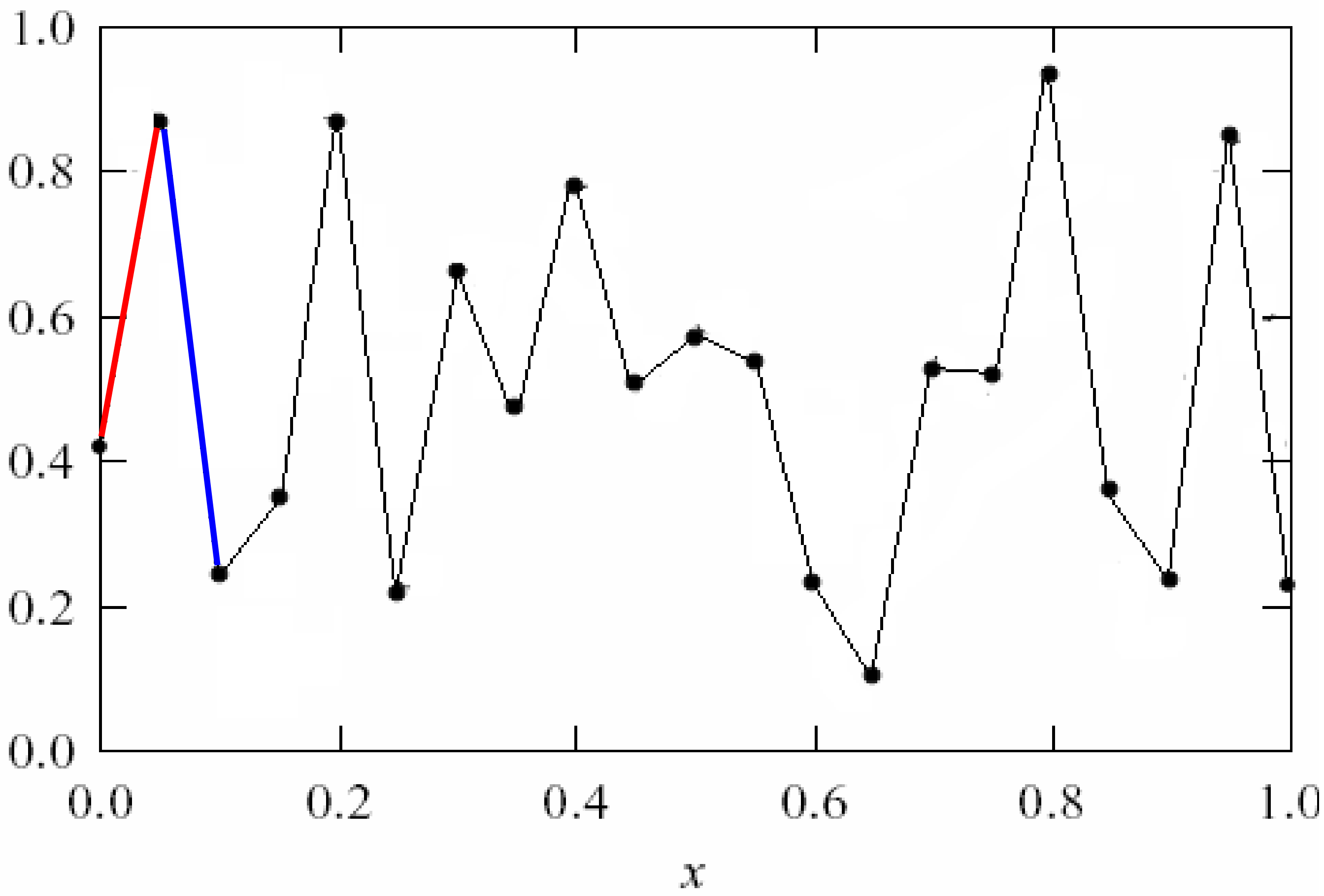
- Lagrange Interpolation

x	x_0	x_1	x_2	$\cdots$	x_i	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	$\cdots$	f_n

$$f(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1$$

$$f(x) = \frac{x - x_2}{x_1 - x_2} f_1 + \frac{x - x_1}{x_2 - x_1} f_2$$

Simplest way to obtain the approximation of $f(x)$



Approximation of a Function

- Lagrange Interpolation

Simplest way to obtain the approximation of $f(x)$

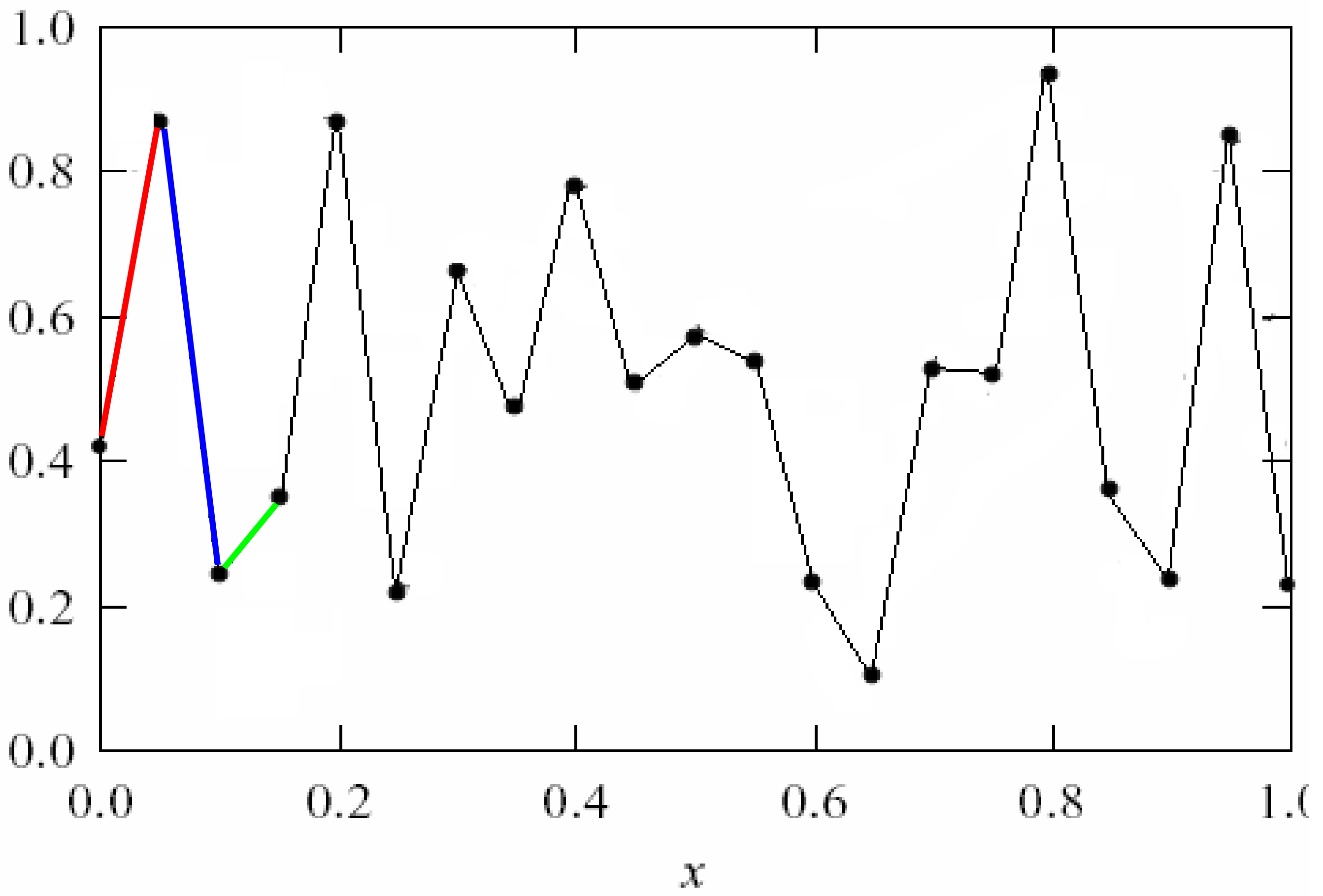
x	x_0	x_1	x_2	x_3	$\cdots$	x_i	$\cdots$	x_n
f	f_0	f_1	f_2	f_3	$\cdots$	f_i	$\cdots$	f_n

$$f(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1$$

$$f(x) = \frac{x - x_2}{x_1 - x_2} f_1 + \frac{x - x_1}{x_2 - x_1} f_2$$

$$f(x) = \frac{x - x_3}{x_2 - x_3} f_2 + \frac{x - x_2}{x_3 - x_2} f_3$$

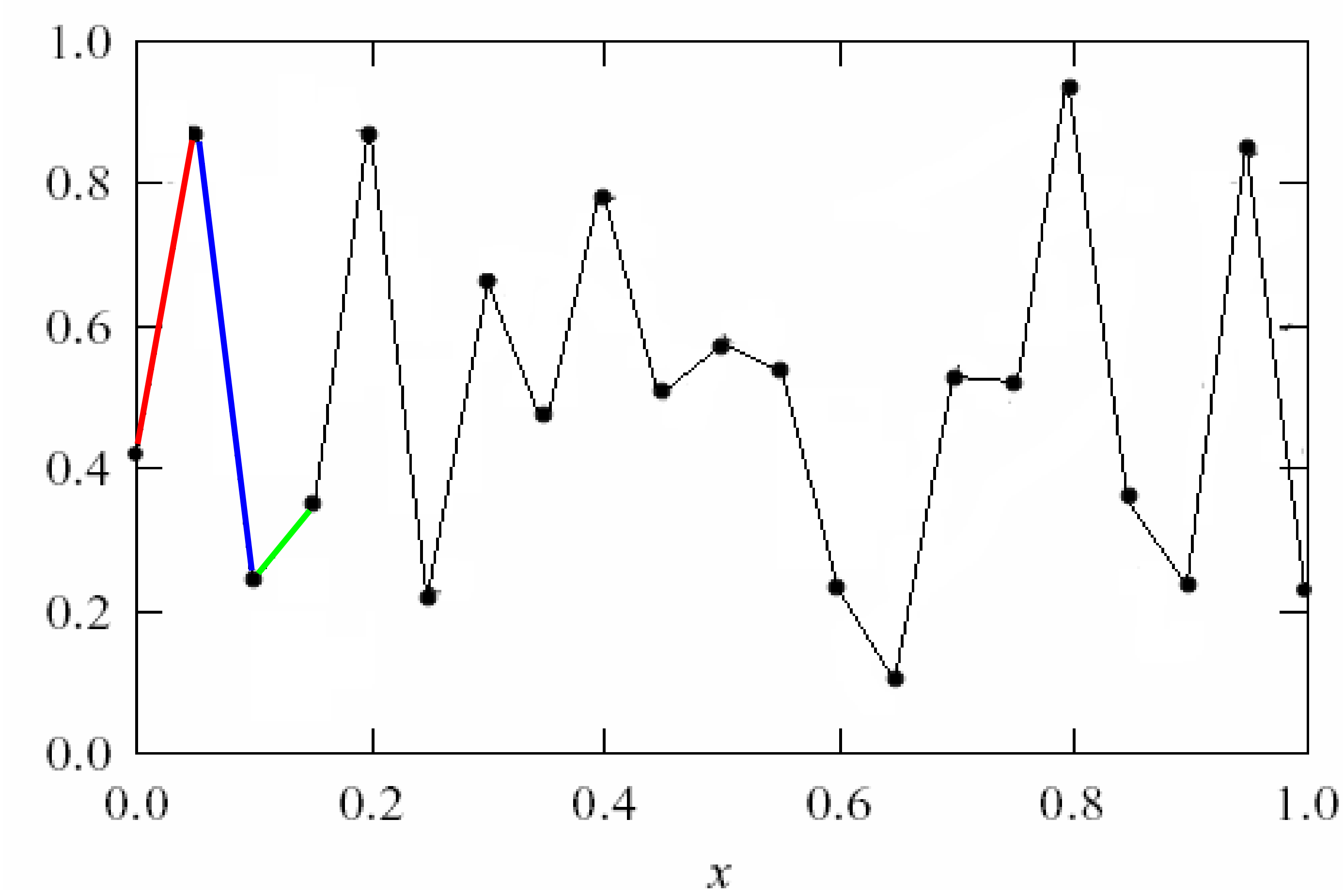
$$\vdots$$



Approximation of a Function

- Lagrange Interpolation

x	x_0	x_1	x_2	$\cdots$	x_i	x_{i+1}	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	f_{i+1}	$\cdots$	f_n



$$x \in [x_i, x_{i+1}]$$

$$f(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i + \frac{x - x_i}{x_{i+1} - x_i} f_{i+1}$$

$$f(x) = L_i(x) f_i + L_{i+1}(x) f_{i+1}$$

$$L_i(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}}$$

$$L_{i+1}(x) = \frac{x - x_i}{x_{i+1} - x_i}$$

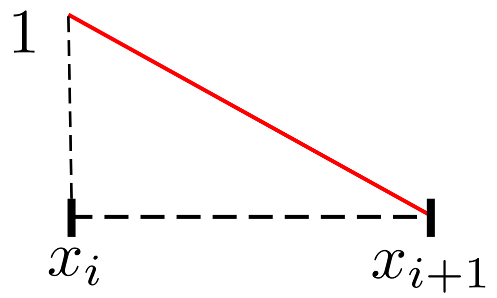
Approximation of a Function

- Lagrange Interpolation

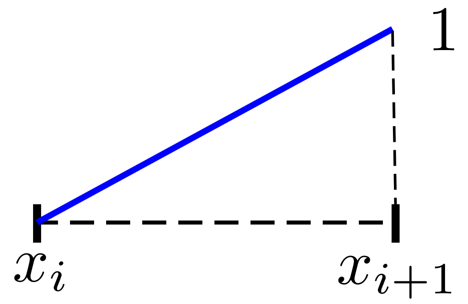
x	x_0	x_1	x_2	$\cdots$	x_i	x_{i+1}	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	f_{i+1}	$\cdots$	f_n

$x \in [x_i, x_{i+1}]$

$$f(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i + \frac{x - x_i}{x_{i+1} - x_i} f_{i+1} = L_i(x) f_i + L_{i+1}(x) f_{i+1}$$



$$L_i(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}}, \quad L_{i+1}(x) = \frac{x - x_i}{x_{i+1} - x_i}$$



$$L_i(x_i) = 1, \quad L_i(x_{i+1}) = 0$$

$$L_{i+1}(x_i) = 0, \quad L_{i+1}(x_{i+1}) = 1$$

Approximation of a Function

- Lagrange Interpolation

$$x \in [x_i, x_{i+1}]$$

Error

$$f(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i + \frac{x - x_i}{x_{i+1} - x_i} f_{i+1} + \boxed{\Delta f(x)}$$

$$\Delta f(x) = \frac{\gamma}{2}(x - x_i)(x - x_{i+1})$$

$$\gamma = \frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2}\Big|_{x=a}, \quad a \in [x_i, x_{i+1}]$$

$$\Delta f(x = x_i) = 0, \quad \Delta f(x = x_{i+1}) = 0$$

Maximum Error:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Delta f(x) = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\Delta f(x) = \frac{\gamma}{2}[2x - (x_i + x_{i+1})] = 0$$

$$x_{\max} = \frac{x_i + x_{i+1}}{2}$$

$$\Delta f(x_{\max}) = \frac{\gamma}{8}(x_{i+1} - x_i)^2$$

$$|\Delta f(x)| \leq \Delta f(x_{\max})$$

Approximation of a Function

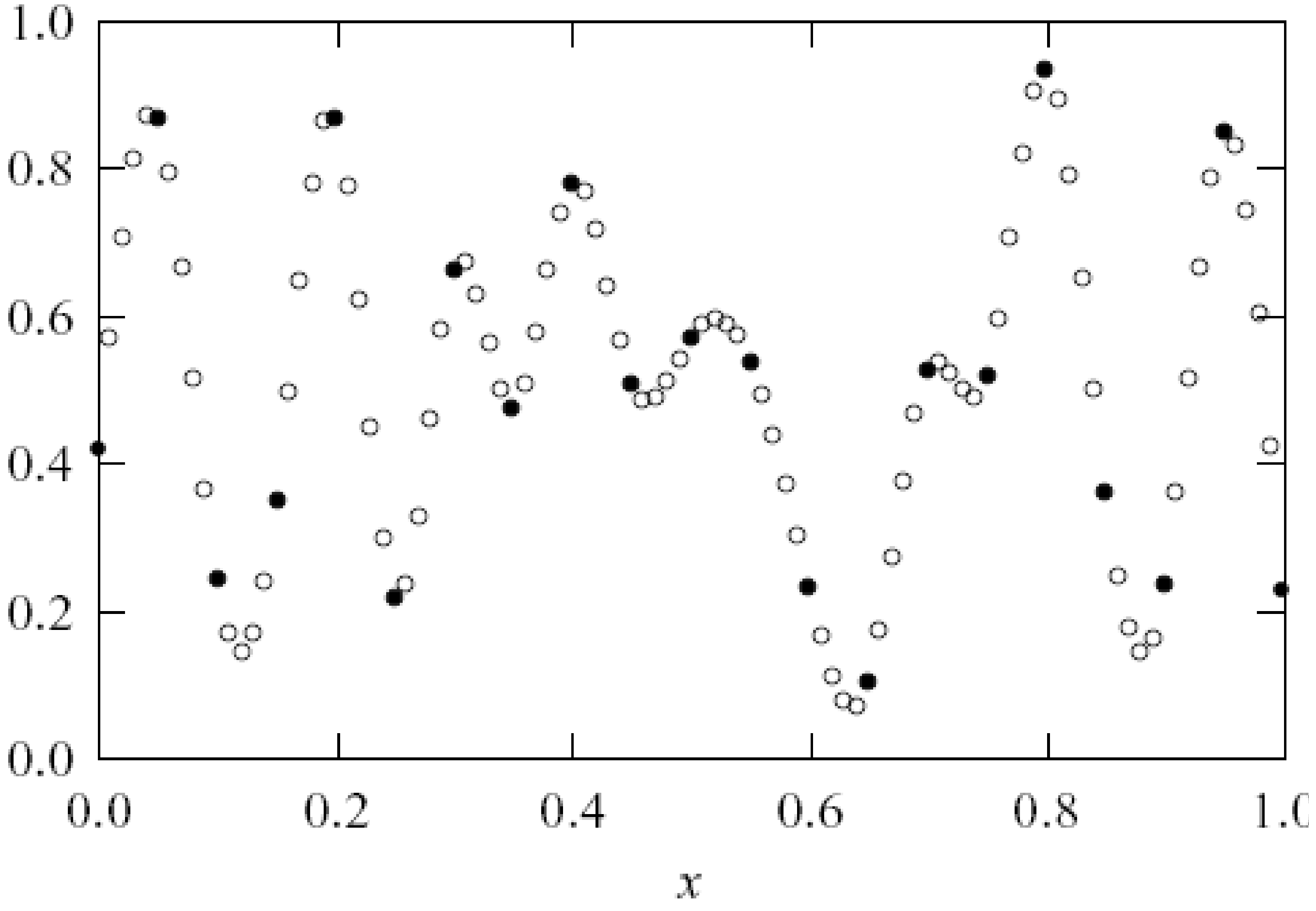
- Lagrange Interpolation

x	x_0	x_1	x_2	$\cdots$	x_i	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	$\cdots$	f_n

$$f(x) = \sum_{i}^{n} L_i(x) f_i$$

$$L_i(x) = \prod_{j \neq i}^{n} \frac{x - x_i}{x_j - x_i}$$

More accurate approximation of $f(x)$



Approximation of a Function

- Lagrange Interpolation

x	x_0	x_1	x_2	$\cdots$	x_i	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	$\cdots$	f_n

Error

$$f(x) = \sum_i^n L_i(x) f_i + \boxed{\Delta f(x)}$$

$$L_i(x) = \prod_{j \neq i}^n \frac{x - x_i}{x_j - x_i}$$

$$\Delta f(x) = \frac{\gamma}{n!}(x - x_1)(x - x_2)\cdots(x - x_n)$$

$$\gamma = \frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}\Big|_{x=a}, \quad a \in [x_1, x_n]$$

Maximum Error:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Delta f(x) = 0$$

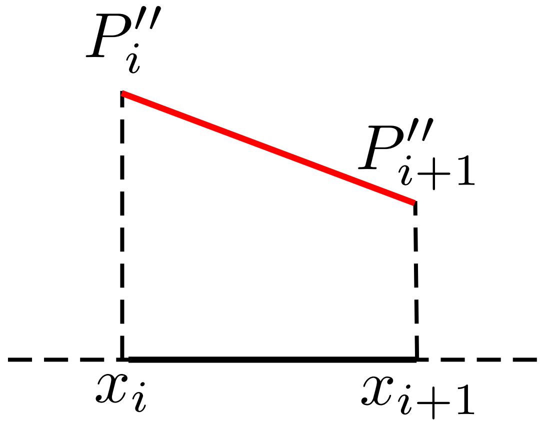
Approximation of a Function

- Spline Approximation

We want to fit the function locally and to connect each piece of the function smoothly. A spline is such a tool that interpolates the data locally through a polynomial and fits the data overall by connecting each segment of the interpolation polynomial by **matching the function and its derivatives at the data points.**

x	f
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_i	f_i
$\vdots$	$\vdots$
x_n	f_n

x	x_0	x_1	x_2	$\cdots$	x_i	x_{i+1}	$\cdots$	x_n
P''	P''_0	P''_1	P''_2	$\cdots$	P''_i	P''_{i+1}	$\cdots$	P''_n

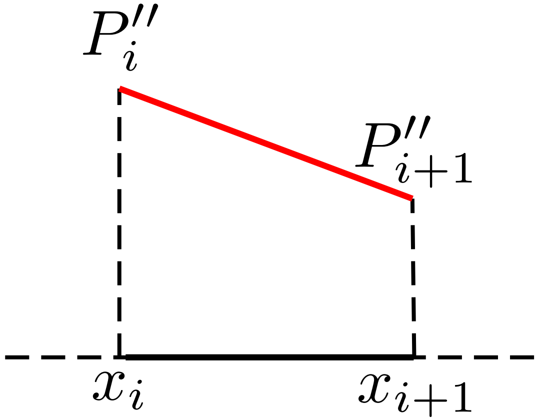


$$x \in [x_i, x_{i+1}] : \; P''_i(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} P''_i + \frac{x - x_i}{x_{i+1} - x_i} P''_{i+1}$$

Approximation of a Function

- Spline Approximation

x	x_0	x_1	x_2	$\cdots$	x_i	x_{i+1}	$\cdots$	x_n
P''	P''_0	P''_1	P''_2	$\cdots$	P''_i	P''_{i+1}	$\cdots$	P''_n



x	f
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_i	f_i
$\vdots$	$\vdots$
x_n	f_n

$$P''_i(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} P''_i + \frac{x - x_i}{x_{i+1} - x_i} P''_{i+1}, \qquad x_{i+1} = x_i + h_i$$

$$P''_i(x) = \frac{1}{h_i}\left[-(x - x_{i+1})P''_i + (x - x_i)P''_{i+1}\right]$$

$$\boxed{P_i(x) = c_0(x - x_i) + c_1(x - x_{i+1}) + \frac{1}{6h_i}\left[-(x - x_{i+1})^3 P''_i + (x - x_i)^3 P''_{i+1}\right]}$$

Approximation of a Function

- Spline Approximation

x	x_0	x_1	x_2	$\cdots$	x_i	x_{i+1}	$\cdots$	x_n
f	f_0	f_1	f_2	$\cdots$	f_i	f_{i+1}	$\cdots$	f_n
P	P_0	P_1	P_2	$\cdots$	P_i	P_{i+1}	$\cdots$	P_n

$$P_i(x) = c_0(x - x_i) + c_1(x - x_{i+1}) + \frac{1}{6h_i}[-(x - x_{i+1})^3 P_i'' + (x - x_i)^3 P_{i+1}'']$$

$$\begin{cases} P_i(x = x_i) = f_i = -h_i c_1 + \dfrac{h_i^2}{6} P_i'' \\ P_i(x = x_{i+1}) = f_{i+1} = h_i c_0 + \dfrac{h_i^2}{6} P_{i+1}'' \end{cases} \Rightarrow \begin{cases} c_1 = -\dfrac{f_i}{h_i} + \dfrac{h_i}{6} P_i'' \\ c_0 = \dfrac{f_{i+1}}{h_i} - \dfrac{h_i}{6} P_{i+1}'' \end{cases}$$

Approximation of a Function

- Spline Approximation

$$P_i(x) = c_0(x - x_i) + c_1(x - x_{i+1}) + \frac{1}{6h_i}[-(x - x_{i+1})^3 P_i'' + (x - x_i)^3 P_{i+1}'']$$

$$\begin{cases} c_1 = -\dfrac{f_i}{h_i} + \dfrac{h_i}{6} P_i'' \\ c_0 = \dfrac{f_{i+1}}{h_i} - \dfrac{h_i}{6} P_{i+1}'' \end{cases}$$

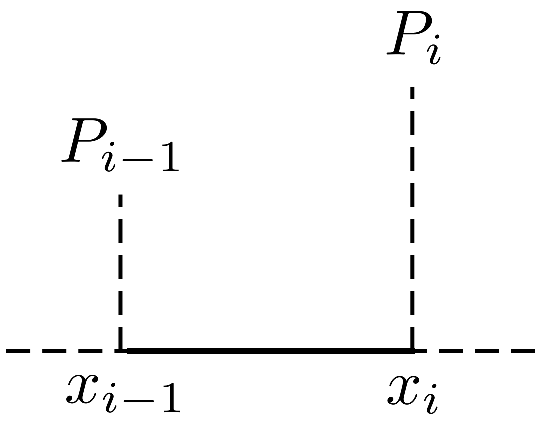
$$P_i(x) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6} P_{i+1}''\right)(x - x_i) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6} P_i''\right)(x - x_{i+1})$$

$$+\frac{1}{6h_i}[-(x - x_{i+1})^3 P_i'' + (x - x_i)^3 P_{i+1}'']$$

Approximation of a Function

- Spline Approximation

$$P_i(x) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right)(x - x_i) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right)(x - x_{i+1})$$
$$+\frac{1}{6h_i}[-(x - x_{i+1})^3 P''_i + (x - x_i)^3 P''_{i+1}]$$



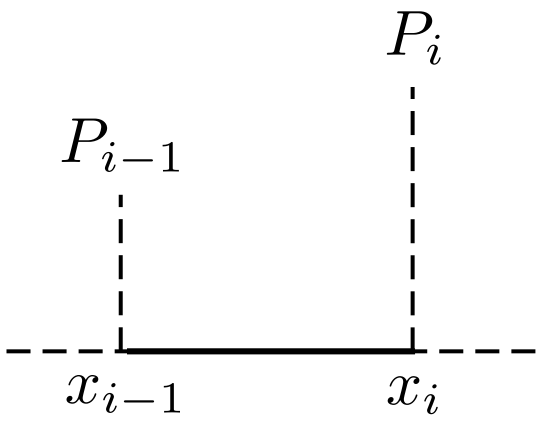
$$P'_{i-1}(x_i) = P'_i(x_i)$$

$i \to i - 1 :$

$$P_{i-1}(x) = \left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P''_i\right)(x - x_{i-1}) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P''_{i-1}\right)(x - x_i)$$
$$+\frac{1}{6h_{i-1}}[-(x - x_i)^3 P''_{i-1} + (x - x_{i-1})^3 P''_i]$$

Approximation of a Function

- Spline Approximation



$$P'_{i-1}(x_i) = P'_i(x_i)$$

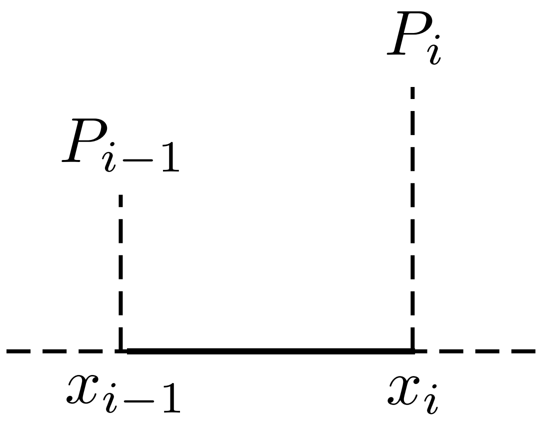
$$P'_i(x) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right) + \frac{1}{2h_i}[-(x - x_{i+1})^2 P''_i + (x - x_i)^2 P''_{i+1}]$$

$$P'_{i-1}(x) = \left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P''_i\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P''_{i-1}\right) + \frac{1}{2h_{i-1}}[-(x - x_i)^2 P''_{i-1} + (x - x_{i-1})^2 P''_i]$$

Approximation of a Function

- Spline Approximation

$$P_i'(x_i) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P_{i+1}''\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P_i''\right) + \frac{1}{2h_i}\left[-(x_i - x_{i+1})^2 P_i'' + (x_i - x_i)^2 P_{i+1}''\right]$$

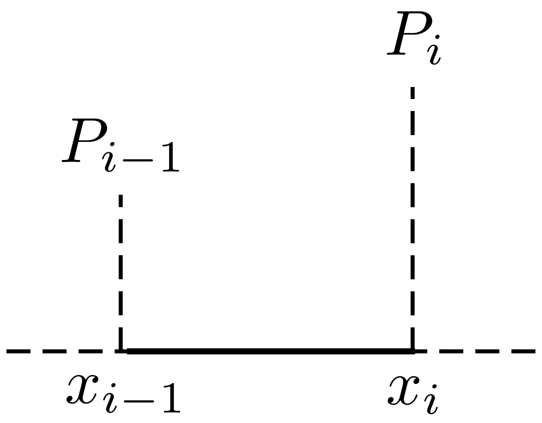


$$P_{i-1}'(x_i) = P_i'(x_i)$$

$$P_{i-1}'(x_i) = \left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P_i''\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P_{i-1}''\right) + \frac{1}{2h_{i-1}}\left[-(x_i - x_i)^2 P_{i-1}'' + (x_i - x_{i-1})^2 P_i''\right]$$

Approximation of a Function

- Spline Approximation



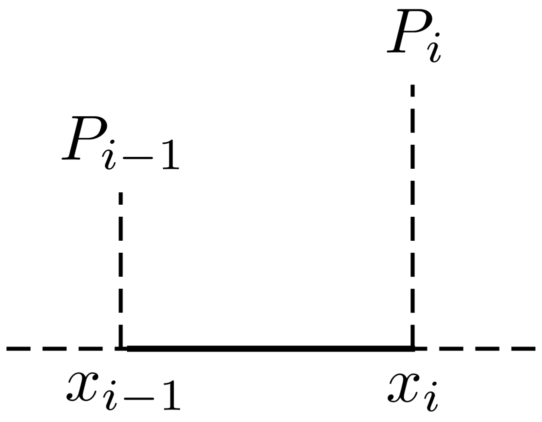
$$P'_{i-1}(x_i) = P'_i(x_i)$$

$$P'_i(x_i) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right) + \frac{1}{2h_i}\left[-\underbrace{(x_i - x_{i+1})^2}_{=h_i^2}P''_i + (x_i - x_i)^2 P''_{i+1}\right]$$

$$P'_{i-1}(x_i) = \left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P''_i\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P''_{i-1}\right) + \frac{1}{2h_{i-1}}\left[-(x_i - x_i)^2 P''_{i-1} + \underbrace{(x_i - x_{i-1})^2}_{=h_{i-1}^2}P''_i\right]$$

Approximation of a Function

- Spline Approximation



$$P'_{i-1}(x_i) = P'_i(x_i)$$

$$\begin{cases} P'_i(x_i) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right) - \frac{h_i}{2}P''_i \\ P'_{i-1}(x_i) = \left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P''_i\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P''_{i-1}\right) + \frac{h_{i-1}}{2}P''_i \end{cases}$$

$$\left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P''_i\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P''_{i-1}\right) + \frac{h_{i-1}}{2}P''_i =$$

$$\left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right) - \frac{h_i}{2}P''_i$$

Approximation of a Function

- Spline Approximation

$$\left(\frac{f_i}{h_{i-1}} - \frac{h_{i-1}}{6}P_i''\right) + \left(-\frac{f_{i-1}}{h_{i-1}} + \frac{h_{i-1}}{6}P_{i-1}''\right) + \frac{h_{i-1}}{2}P_i'' =$$

$$\left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P_{i+1}''\right) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P_i''\right) - \frac{h_i}{2}P_i''$$

$$\frac{h_{i-1}}{6}P_{i-1}'' + \frac{1}{3}(h_{i-1} + h_i)P_i'' + \frac{h_i}{6}P_{i+1}'' = -\frac{f_i - f_{i-1}}{h_{i-1}} + \frac{f_{i+1} - f_i}{h_i}$$

$$\overset{\times 6}{\Longrightarrow} h_{i-1}P_{i-1}'' + 2(h_{i-1} + h_i)P_i'' + h_i P_{i+1}'' = -6\frac{f_i - f_{i-1}}{h_{i-1}} + 6\frac{f_{i+1} - f_i}{h_i}$$

$$h_{i-1}P_{i-1}'' + 2d_i P_i'' + h_i P_{i+1}'' = b_i, \qquad d_i = h_{i-1} + h_i, \qquad b_i = -6\frac{f_i - f_{i-1}}{h_{i-1}} + 6\frac{f_{i+1} - f_i}{h_i}$$

Approximation of a Function

- Spline Approximation

$$h_{i-1}P''_{i-1} + 2d_iP''_i + h_iP''_{i+1} = b_i, \qquad d_i = h_{i-1} + h_i, \qquad b_i = -6\frac{f_i - f_{i-1}}{h_{i-1}} + 6\frac{f_{i+1} - f_i}{h_i}$$

Suppose: $P''_0 = P''_n = 0$

$$\begin{bmatrix} d_1 & h_1 & 0 & \cdots & \cdots & 0 \\ h_1 & d_2 & h_2 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & h_{n-3} & d_{n-2} & h_{n-2} \\ 0 & \cdots & \cdots & 0 & h_{n-2} & d_{n-1} \end{bmatrix} \begin{bmatrix} P''_1 \\ P''_2 \\ \vdots \\ P''_{n-2} \\ P''_{n-1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n-2} \\ b_{n-1} \end{bmatrix}$$

Approximation of a Function

- Spline Approximation

$$\begin{bmatrix} d_1 & h_1 & 0 & \cdots & \cdots & 0 \\ h_1 & d_2 & h_2 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & h_{n-3} & d_{n-2} & h_{n-2} \\ 0 & \cdots & \cdots & 0 & h_{n-2} & d_{n-1} \end{bmatrix} \begin{bmatrix} P''_1 \\ P''_2 \\ \vdots \\ P''_{n-2} \\ P''_{n-1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n-2} \\ b_{n-1} \end{bmatrix}$$

$$x \in [x_i, x_{i+1}]: \quad P_i(x) = \left(\frac{f_{i+1}}{h_i} - \frac{h_i}{6}P''_{i+1}\right)(x - x_i) + \left(-\frac{f_i}{h_i} + \frac{h_i}{6}P''_i\right)(x - x_{i+1})$$

$$+\frac{1}{6h_i}[-(x - x_{i+1})^3 P''_i + (x - x_i)^3 P''_{i+1}]$$