# Numerical Methods in Engineering <br>  <br> 2- INTERPOLATION <br> AND CURVE FITTING 

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## Interpolation



- Consider a table of values $(x i, f i), i=1,2,3, \ldots$.

| $x_{0}$ | $x_{1}$ | $x_{2}$ | $x_{3}$ | $\ldots$ | $\ldots$ | $\ldots$ | $x_{n}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $f_{0}$ | $f_{1}$ | $f_{2}$ | $f_{3}$ | $\ldots$ | $\ldots$ | $\ldots$ | $f n$ |

The process of estimating $\boldsymbol{f}$ for any intermediate value of $\boldsymbol{x}$ is called interpolation.

- $\operatorname{Pn}(x) \cong f(x)$

Polynomial $\boldsymbol{P} n(x)$ is used as an estimation for the unknown function $\boldsymbol{f}(x)$ $\boldsymbol{n}$ refers to the order of polynomial $\boldsymbol{P}$

## Interpolation

- Pn descibes a curve that passes through the points of the table:

| $x 0$ | $x 1$ | $x_{2}$ | $x_{3}$ | $\ldots$ | $\ldots$ | $\ldots$ | $x_{n}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| fo | $f_{1}$ | $f 2$ | $f 3$ | $\ldots$ | $\ldots$ | $\ldots$ | $f n$ |



## Interpolation Methods (4)

- Newton method
o Newton forward formula
o Newton backward formula
o Forward difference method
o Backward difference method
- Lagrange's formula
- Spline interpolation


## Linear Interpolation (5)

- Linear estimation (a line) between every adjacent points

$$
\begin{aligned}
& \left(x_{k+1}, y_{k+1}\right) \\
& f_{k}(x)=y_{k}+\frac{x-x_{k}}{x_{k+1}-x_{k}}\left(y_{k+1}, y_{k}\right) \\
& x_{k} \leq x \leq x_{k+1}
\end{aligned}
$$

- The result is a function:
- Continuous
- Not differentiable


## Linear Interpolation (Example)

(6)

- Horizontal axis: $t$ $t=[0,1,2,3,4,5], x=[0,2,-2,3,1,4]$
- Vertical Axis: x



## Polynomial Interpolation

General Form

- A set of $n+\mathbb{1}$ points $\rightarrow$ Order $n$ Polynomial

$$
\begin{aligned}
& \left\{\left(x_{i}, y_{i}\right)\right\}_{i=0}^{n} \\
& f(x)=\sum_{k=0}^{n} a_{k} x^{k} \Rightarrow y_{i}=f\left(x_{i}\right)=\sum_{k=0}^{n} a_{k} x_{i}^{k}, \quad k=0, \cdots, n
\end{aligned}
$$

## Polynomial Interpolation

General Form
(8)

$$
\begin{aligned}
& \left\{\left(x_{i}, y_{i}\right)\right\}_{i=0}^{n} \\
& f(x)=\sum_{k=0}^{n} a_{k} x^{k} \Rightarrow y_{i}=f\left(x_{i}\right)=\sum_{k=0}^{n} a_{k} x_{i}^{k}, \quad k=0, \cdots, n \\
& y_{0}=a_{0}+a_{1} x_{0}^{1}+\cdots+a_{n} x_{0}^{n} \\
& y_{1}=a_{0}+a_{1} x_{1}^{1}+\cdots+a_{n} x_{1}^{n} \\
& y_{n}=a_{0}+a_{1} x_{n}^{1}+\cdots+a_{n} x_{n}^{n} \\
& \Rightarrow\left[\begin{array}{cccc}
1 & x_{0} & \cdots & x_{0}^{n} \\
1 & x_{1} & \cdots & x_{1}^{n} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_{n} & \cdots & x_{n}^{n}
\end{array}\right]\left[\begin{array}{c}
a_{0} \\
a_{1} \\
\vdots \\
a_{n}
\end{array}\right]=\left[\begin{array}{c}
y_{0} \\
y_{1} \\
\vdots \\
y_{n}
\end{array}\right] \\
& \therefore a=x^{-1} y
\end{aligned}
$$

## Polynomial Interpolation (Example 1)

General Form


- Determine interpolating polynomial: $\{(0,6),(1,0),(2,2)\}$
$\left[\begin{array}{lll}1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4\end{array}\right]\left[\begin{array}{l}a_{0} \\ a_{1} \\ a_{2}\end{array}\right]=\left[\begin{array}{l}6 \\ 0 \\ 2\end{array}\right]$

$$
\Rightarrow \quad f(x)=4 x^{2}-10 x+6
$$



## Polynomial Interpolation (Example 2)

General Form

1. Linear Interpolation
2. polynomial of order 5

$$
\begin{gathered}
x=[0,1,2,3,4,5], \\
y=[0,2,-2,3,1,4]
\end{gathered}
$$


$f(x)=0.4917 x^{5}-6.2083 x^{4}+27.4583 x^{3}-49.2917 x^{2}+29.55 x$

## Polynomial Interpolation



- Disadvantages:
- By increasing number of points, order of the polynomial grows
- Solving the set of linear equations might be not very easy.


## Lagrange's Interpolation Formula

 (12)- A unique polynomial that passes through all points.

$$
\begin{array}{cc}
\left\{\left(x_{i}, y_{i}\right)\right\}_{i=0}^{n} & f(x)=\sum_{k=0}^{n} L_{k}(x) y_{k} \\
L_{k}(x)=\left\{\begin{array}{ll}
1 & x=x_{k} \\
0 & x \neq x_{k}
\end{array}\right\} \Rightarrow f\left(x_{k}\right)=y_{k}
\end{array}
$$

$$
L_{k}(x)=\frac{\left(x-x_{0}\right) \cdots\left(x-x_{k-1}\right)\left(x-x_{k+1}\right) \cdots\left(x-x_{n}\right)}{\left(x_{k}-x_{0}\right) \cdots\left(x_{k}-x_{k-1}\right)\left(x_{k}-x_{k+1}\right) \cdots\left(x_{k}-x_{n}\right)}=\prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x-x_{i}}{x_{k}-x_{i}},
$$

$$
L_{k}\left(x_{k}\right)=1, \quad L_{k}\left(x_{i}\right)=0, x_{i} \neq x_{k}
$$

$$
k=0,1, \cdots, n
$$

## Lagrange's Interpolation (Example)

- Data: $\{(0,6),(1,0),(2,2)\}$

$$
L_{0}(x)=\frac{(x-1)(x-2)}{(0-1)(0-2)}=\frac{x^{2}-3 x+2}{2}
$$

$$
\begin{aligned}
& L_{1}(x)=\frac{(x-0)(x-2)}{(1-0)(1-2)}=\frac{x^{2}-2 x}{-1} \\
& L_{2}(x)=\frac{(x-0)(x-1)}{(2-0)(2-1)}=\frac{x^{2}-x}{2}
\end{aligned}
$$

$$
f(x)=\sum_{k=0}^{2} L_{k}(x) y_{k}=L_{0}(x) y_{0}+L_{1}(x) y_{1}+L_{2}(x) y_{2}
$$

$$
f(x)=\sum_{k=0}^{2} L_{k}(x) y_{k}=6 L_{0}(x)+0 L_{1}(x)+2 L_{2}(x)=4 x^{2}-10 x+6
$$

## Lagrange's Interpolation (Example)



## Newton's Interpolation Formula

 (15)$\left\{\left(x_{i}, y_{i}\right)\right\}_{i=0}^{n}$
$n_{n}(x)=a_{0}+a_{1}\left(x-x_{0}\right)+a_{2}\left(x-x_{0}\right)\left(x-x_{1}\right)+\cdots$
$+a_{n}\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)$
$n_{0}\left(x_{0}\right)=a_{0}=y_{0}$

$$
\begin{aligned}
& n_{1}\left(x_{1}\right)=a_{0}+a_{1}\left(x_{1}-x_{0}\right)=y_{1} \rightarrow a_{1}=\frac{y_{1}-y_{0}}{x_{1}-x_{0}}=D f_{0} \\
& n_{2}\left(x_{2}\right)=a_{0}+a_{1}\left(x_{2}-x_{0}\right)+a_{2}\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right) \rightarrow \\
& y_{2}-\frac{y_{2}-y_{1}-\frac{y_{1}-y_{0}}{x_{2}-x_{1}} x_{1}-x_{0}}{x_{2}-x_{0}}=\frac{D f_{1}-D f_{0}}{x_{2}-x_{0}}
\end{aligned}
$$

## Newton's Interpolation Formula

 (16)$$
\begin{aligned}
n_{n}(x)=a_{0}+a_{1}\left(x-x_{0}\right) & +a_{2}\left(x-x_{0}\right)\left(x-x_{1}\right)+\cdots \\
& +a_{n}\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)
\end{aligned}
$$

$$
a_{n}=\frac{D^{n-1} f_{1}-D^{n-1} f_{0}}{x_{n}-x_{0}} \equiv D^{n} f_{0}
$$



## Newton's Interpolation Formula (Example)


$n_{4}(x)=-5+2 x-4 x(x-1)+8 x(x-1)(x+1)+3 x(x-1)(x+1)(x-2)$

## Newton's Interpolation Formula (Example)



## Newton or Lagrange

## 19

- Disadvantage of Lagrange's method of interpolation: To add new data, new set of lagrangian multipliers must be calculated
- Advantage of Newton method:

By introducing new terms, new data can be added to the existing polynomial.

## Newton's Interpolation Formula $2^{\text {nd }}$ Method

(20)

| $x$ | 0 | 1 | -1 | 2 | -2 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $y$ | -5 | -3 | -15 | 39 | -9 |

$n_{0}(x)=a_{0} \rightarrow n_{0}(x)=-5$
$n_{1}(x)=n_{0}(x)+a_{1}\left(x-x_{0}\right)=-5+a_{1}(x-0) \quad \xrightarrow{n_{1}\left(x_{1}\right)=y_{1}} \quad n_{1}(x)=-5+2 x$
$n_{2}(x)=n_{1}(x)+a_{2}\left(x-x_{0}\right)\left(x-x_{1}\right) \xrightarrow{n_{2}\left(x_{2}\right)=y_{2}} n_{2}(x)=-5+2 x-4 x(x-1)$

$$
\begin{aligned}
n_{3}(x)=n_{2}(x)+a_{3}\left(x-x_{0}\right)\left(x-x_{1}\right)\left(x-x_{2}\right) \xrightarrow{n_{3}\left(x_{3}\right)=y_{3}} \\
\\
n_{3}(x)=-5+2 x-4 x(x-1)+8 x(x-1)(x+1)
\end{aligned}
$$

$$
n_{4}(x)=n_{3}(x)+a_{4}\left(x-x_{0}\right)\left(x-x_{1}\right)\left(x-x_{2}\right)\left(x-x_{3}\right) \xrightarrow{n_{4}\left(x_{4}\right)=y_{4}}
$$

$$
n_{4}(x)=-5+2 x-4 x(x-1)+8 x(x-1)(x+1)+3 x(x-1)(x+1)(x-2)
$$

## Equally spaced Interpolation Newton's Forward Difference Method

- If the points of interpolation are equally spaced:

$$
x_{j}=x_{0}+j h ; \quad j=0, \pm 1, \pm 2, \ldots
$$

- Assume forward difference operator as:



## HomeWork

 (22)- Do some research and find the Newton's forward difference formula for equidistance data.
- Then solve the problem of finding the interpolation polynomial by Newton's forward difference formula for the following data:

| $x$ | 0 | 1 | -1 | 2 | -2 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $y$ | -5 | -3 | -15 | 39 | -9 |

## Spline Interpolation

- Fit a single polynomial between every pair of adjacent points.
- Composition of these polynomials are called Spline
- They all form a continuous composite curve.



## Spline Interpolation

- Linear spline: $1^{\text {st-order }}$ lines between adjacent points - Continuous but not differentiable
- Cubic spline:

$3^{\text {rd }}$-order curves in each subinterval
○ $f$ is Continuous at $x i$
- $f^{*}$ is Continuous at $x i$
- $f$ " is Continuous at $x i$



## Why Spline?

(25)

- Too many data point $\rightarrow$ high order interpolating polynomial
- Cubic spline : just $3^{\text {rd }}$ order polynomials
- Spline is computationally more economic for heavy problems


## Spline Interpolation

## (26)

- The spline is defined by a set of equations each defining a $3^{\text {rd }}$-order curve for a subinterval

$$
\begin{aligned}
& \begin{cases}f_{1}(x) & x_{0} \leq x \leq x_{1} \\
f_{2}(x) & x_{1} \leq x \leq x_{2} \\
\vdots & \vdots \\
f_{i}(x) & x_{i-1} \leq x \leq x_{i} \\
\vdots & \vdots \\
f_{n}(x) & x_{n-1} \leq x \leq x_{n}\end{cases} \\
& \text { Continuouity f‘Continuouity } \\
& f_{1}(x 1)=f 2(x 1) \quad f^{\prime} 1(x 1)=f^{\prime} 2(x 1) \\
& f_{2}\left(x_{2}\right)=f 3\left(x^{2}\right) \quad f^{\prime} 2\left(x^{2}\right)=f^{\prime} 3\left(x^{2}\right) \\
& f_{3}\left(x_{3}\right)=f_{4}\left(x_{3}\right) \quad f^{\prime} 3\left(x_{3}\right)=f^{\prime} 4\left(x_{3}\right) \\
& \text { Continuouity } \\
& f^{\prime \prime}(x 1)=f " 2(x 1) \\
& f^{\prime \prime} 2(x 2)=f^{\prime \prime} 3(x 2)
\end{aligned}
$$

## Spline Curve

## (27)

- Number of data $n \rightarrow$ Number of spline curves $n-1$
- $f^{6 /}$ is continuous at each point: $f_{i-1, i}^{\prime \prime}\left(x_{i}\right)=f_{i, i+1}^{\prime \prime}\left(x_{i}\right)=k_{i}$
- Cubic spline $\rightarrow$ curvature is linear

$$
f_{i, i+1}^{\prime \prime}(x)=k_{i} l_{i}(x)+k_{i+1} l_{i+1}(x)
$$

- From Lagrange's method


$$
\begin{aligned}
& l_{i}(x)=\frac{x-x_{i+1}}{x_{i}-x_{i+1}} \quad l_{i+1}(x)=\frac{x-x_{i}}{x_{i+1}-x_{i}} \\
& f_{i, i+1}^{\prime \prime}(x)=\frac{k_{i}\left(x-x_{i+1}\right)-k_{i+1}\left(x-x_{i}\right)}{x_{i}-x_{i+1}}
\end{aligned}
$$

## Spline Curve

## (28)

- Integration of curvature:

$$
f_{i, i+1}^{\prime \prime}(x)=\frac{k_{i}\left(x-x_{i+1}\right)-k_{i+1}\left(x-x_{i}\right)}{x_{i}-x_{i+1}}
$$

$$
f_{i, i+1}(x)=\frac{k_{i}\left(x-x_{i+1}\right)^{3}-k_{i+1}\left(x-x_{i}\right)^{3}}{6\left(x_{i}-x_{i+1}\right)}+A\left(x-x_{i+1}\right)-B\left(x-x_{i}\right)
$$

- Using boundary values leads to:

$$
\begin{aligned}
f_{i, i+1}(x) & =\frac{k_{i}}{6}\left[\frac{\left(x-x_{i+1}\right)^{3}}{x_{i}-x_{i+1}}-\left(x-x_{i+1}\right)\left(x_{i}-x_{i+1}\right)\right] \\
& -\frac{k_{i+1}}{6}\left[\frac{\left(x-x_{i}\right)^{3}}{x_{i}-x_{i+1}}-\left(x-x_{i}\right)\left(x_{i}-x_{i+1}\right)\right]+\frac{y_{i}\left(x-x_{i+1}\right)-y_{i+1}\left(x-x_{i}\right)}{x_{i}-x_{i+1}}
\end{aligned}
$$

## Spline Curve 1

- Calculating intermediate curvatures $\mathbb{k} i, i=2,3,4, \ldots, n-1$. Use slope continuity at each point:
$f_{i=1, i}^{\prime}\left(x_{i}\right)=f_{i, i+1}^{\prime}\left(x_{i}\right)$
$k_{i-1}\left(x_{i-1}-x_{i}\right)+2 k_{i}\left(x_{i-1}-x_{i+1}\right)+k_{i+1}\left(x_{i}-x_{i+1}\right)=6\left(\frac{y_{i-1}-y_{i}}{x_{i-1}-x_{i}}-\frac{y_{i}-y_{i+1}}{x_{i}-x_{i+1}}\right)$
Note that $\mathbf{k} O=\mathbf{k} n=0$
- Initial and final curvatures of the composite curve is set to zero


## Spline Curve 1

- Special case:

For equidistant points: $h=x i+1-x i$

$$
\begin{cases}k_{i-1}+4 k_{i}+k_{i+1}=\frac{6}{h^{2}}\left(y_{i-1}-2 y_{i}+y_{i+1}\right), & i=2,3, \cdots, n-1 \\ k_{i}=0 & i=0, n\end{cases}
$$

## Spline Interpolation (Example)

| $i$ | $x$ | $f(x)$ | $f^{\prime \prime}(x)$ |
| :---: | :---: | :---: | :---: |
| 1 | -0.50 | 0.731 | 0.0 |
| 2 | 0.00 | 1.000 |  |
| 3 | 0.25 | 1.268 |  |
| 4 | 1.00 | 1.718 | 0.0 |

$$
\begin{gathered}
1.50 f_{2}^{\prime \prime}+0.25 f_{3}^{\prime \prime}=3.21997 \\
0.25 f_{2}^{\prime \prime}+2.0 f_{3}^{\prime \prime}=-2.8425
\end{gathered} \rightarrow\left\{\begin{array}{l}
f_{2}^{\prime \prime}=2.4342 \\
f_{3}^{\prime \prime}=-1.7255
\end{array}\right\} \begin{aligned}
& f_{1}(x)=0.81141 x^{3}+1.21712 x^{2}+0.94264 x+1 \\
& f_{2}(x)=-2.77319 x^{3}+1.21712 x^{2}+0.94164 x+1 \\
& f_{3}(x)=0.38346 x^{3}-1.15037 x^{2}+1.53452 x+0.95068
\end{aligned}
$$

## Spline Interpolation (Example)



## Spline Interpolation 2

- Instead of initial and final curvature, initial and final slopes, So and $\boldsymbol{S 1}$ are controlled
- For equidistant points: $x_{i+1}-x_{i}=h, i=n-1, \ldots, 0$

$$
x_{i} \leq x \leq x_{i+1}
$$

$$
\begin{aligned}
& f_{i, i+1}(x)=\left[\frac{\left(x-x_{i+1}\right)^{2}}{h^{2}}+2 \frac{\left(x-x_{i}\right)\left(x-x_{i+1}\right)}{h^{3}}\right] y_{i} \\
& \quad+\left[\frac{\left(x-x_{i}\right)^{2}}{h^{2}}-2 \frac{\left(x-x_{i}\right)^{2}\left(x-x_{i+1}\right)}{h^{3}}\right] y_{i+1} \\
& \quad \\
& \quad+\frac{\left(x-x_{i}\right)\left(x-x_{i+1}\right)^{2}}{h^{2}} S_{i}+\frac{\left(x-x_{i}\right)^{2}\left(x-x_{i+1}\right)}{h^{3}} S_{i+1}
\end{aligned}
$$

$$
S_{i}+4 S_{i+1}+S_{i+2}=\frac{3}{h}\left(f_{i+2}-f_{i}\right), \quad i=0,1, \cdots, n-1
$$

## Spline Interpolation 2 (Example)

(34)

$$
\begin{aligned}
& x=[3,3.5,4] ; \quad y=[1.098,1.253,1.386] ; n=3 \\
& S_{0}=S_{2}=0
\end{aligned}
$$

- Solution:

$$
S_{i}+4 S_{w, 1}+S_{n 2}=\frac{3}{h}\left(f_{n, 2}-f_{i}\right), \quad i=0,1, \cdots, n-1
$$

$$
4 S_{1}=\frac{3}{0.5}(1.386-1.098) \Rightarrow S_{1}=0.432
$$



$$
\left\{\begin{array}{r}
\left\{\begin{array}{r}
f_{1,2}(x)=-0.752 x^{3}+7.764 x^{2}-26.28 x+30.366 \\
f_{2,3}(x)=-0.416 x^{3}+4.248 x^{2}-14.016 x+16.107 \\
\\
f(3.541)=? \rightarrow
\end{array} \rightarrow f(3.541)=1.232\right.
\end{array}\right.
$$

## Spline Interpolation (Example)

(35)

- Compare Lagrange's interpolation curve with spline

$$
x=[0,1,2,3,4,5], \quad y=[0,2,-2,3,1,4]
$$



## Homework

## (36)

- Use a computer program to determine cubic curves of a spline for tabulated points

| x | 0 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 1.0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| y | 0.302 | 0.185 | 0.106 | 0.093 | 0.240 | 0.579 | 0.561 | 0.468 | 0.302 |

- Solve the problem for these conditions:

1. $k o=k n=0$
2. $S O=0$ and $S n=\pi / 2$

Deliver the solution on paper with details and attach a copy of computer program.

## 2D Interpolation (Lagrange method)

 (37)- Function $z=f(x, y)$ is evaluated in several points

$$
z i=f(x i, y i)
$$

- Goal is to calculate a function to estimate $z$ for any arbitrary value of $x$ and $y$.
- Lagrange method


## 2D Lagrangian Interpolation

## (38)

$$
\begin{aligned}
& f(x, y)=\sum_{i=1}^{M} \sum_{j=1}^{N} L_{i j}(x, y) z_{i j} \\
& L_{i j}(x, y)=\left\{\begin{array}{ll}
1, & x=x_{i} \text { and } y=y_{i} \\
0, & \text { otherwise. }
\end{array}\right\} \Rightarrow f\left(x_{i}, y_{j}\right)=z_{i j} \\
& L_{i j}(x, y)=L_{i}(x) L_{j}(y) \quad L_{k}\left(x_{k}\right)=1, \quad L_{k}\left(x_{i}\right)=0, x_{i} \neq x_{k} \\
& \begin{array}{r}
L_{k}(x)=\frac{\left(x-x_{0}\right) \cdots\left(x-x_{k-1}\right)\left(x-x_{k+1}\right) \cdots\left(x-x_{n}\right)}{\left(x_{k}-x_{0}\right) \cdots\left(x_{k}-x_{k-1}\right)\left(x_{k}-x_{k+1}\right) \cdots\left(x_{k}-x_{n}\right)} \\
=\prod_{\substack{i=0 \\
i \neq k}}^{n} \frac{x-x_{i}}{x_{k}-x_{i}}, \quad k=0,1, \cdots, n
\end{array}
\end{aligned}
$$

## Curve Fitting

## (39)

- A smooth curve passing not necessarily through the given points but with minimum distance from them.
- Polynomial interpolation passes through all points and yields an oscillatory curve.



## Least Squares Method

- Given data

$$
\left(x_{i}, y_{i}\right), i=1,2, \cdots, n
$$

- Approximating Function

$$
f(x)=f\left(x ; a_{1}, a_{2}, \cdots, a_{m}\right)
$$

$$
\mathrm{m}<\mathrm{n}
$$

- Difference between every point and its_approximated velue:

$$
r_{i}=y_{i}-f\left(x_{i}\right) \equiv \text { residual }
$$

- Sum of squares of residuals:

$$
S\left(a_{1}, a_{2}, \cdots, a_{m}\right)=\sum_{i=1}^{n}\left[y_{i}-f\left(x_{i}\right)\right]^{2}
$$

- To have the best approximation, $S$ must be minimized wrt ak:

$$
\frac{\partial S}{\partial a_{k}}=0, k=1,2, \cdots, m
$$

## Least Squares Method (Line Fitting)

- For a table of data (xi, yi), $i=1,2,3, \ldots, n$ the approximating function is a line: $f(x)=a+b x$
- To solve the problem parameters $q$ and $b$ must be evaluated:

1. Construct the error function: $\quad S(a, b)=\sum_{i=1}^{n}\left[y_{i}-a-b x_{i}\right]^{2}$
2. Minimize $S$ wrt $a$ and $b$ :

$$
\begin{aligned}
& \frac{\partial S}{\partial a}=\sum_{i=1}^{n}-2\left(y_{i}-a-b x_{i}\right)=2\left(-\sum_{i=1}^{n} y_{i}+n a+b \sum_{i=1}^{n} x_{i}\right)=0 \\
& \frac{\partial S}{\partial b}=\sum_{i=1}^{n}-2\left(y_{i}-a-b x_{i}\right) x_{i}=2\left(-\sum_{i=1}^{n} x_{i} y_{i}+a \sum_{i=1}^{n} x_{i}+b \sum_{i=1}^{n} x_{i}^{2}\right)=0
\end{aligned}
$$

## Least Squares Method (Line Fitting)

## (42)

- (xi, yi), $i=1,2,3, \ldots, n \rightarrow f(x)=a+b x$

$$
\left\{\begin{array}{l}
a=\frac{\bar{y} \sum x_{i}^{2}-\bar{x} \sum x_{i} y_{i}}{\sum x_{i}^{2}-n \bar{x}^{2}} \\
b=\frac{\sum x_{i} y_{i}-n \overline{x y}}{\sum x_{i}^{2}-n \bar{x}^{2}}
\end{array}\right.
$$

$$
\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \quad \bar{y}=\frac{1}{n} \sum_{i=1}^{n} y_{i}
$$

- Alternative formula

$$
b=\frac{\sum y_{i}\left(x_{i}-\bar{x}\right)}{\sum x_{i}\left(x_{i}-\bar{x}\right)} \quad a=\bar{y}-\bar{x} b
$$

## Least Squares Method (Line Fitting)

- Example

| x | 0.0 | 1.0 | 2.0 | 2.5 | 3.0 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| y | 2.9 | 3.7 | 4.1 | 4.4 | 5.0 |

$$
\begin{aligned}
& \bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i}=\frac{0.0+1.0+2.0+2.5+3.0}{5}=1.7 \\
& \bar{y}=\frac{1}{n} \sum_{i=1}^{n} y_{i}=\frac{2.9+3.7+4.1+4.4+5.0}{5}=4.02 \\
& b=\frac{\sum y_{i}\left(x_{i}-\bar{x}\right)}{\sum x_{i}\left(x_{i}-\bar{x}\right)} \\
& =\frac{2.9(-1.7)+3.7(-0.7)+4.1(0.3)+4.4}{0.0(-1.7)+1.0(-0.7)+2.0(0.3)+2.5} \\
& a=\bar{y}-\bar{x} b=4.02-1.7(0.6431)=2.927 \\
& f(x)=2.927+0.6431 x
\end{aligned}
$$

## Least Squares Method (Polynomial Fitting)

- Fitting a polynomial of order $m-1$ :

$$
f(x)=\sum_{j=1}^{m} a_{x^{j} x^{j-1}}
$$

$A=\left[\begin{array}{ccccc}n & \sum x_{i} & \sum x_{i}^{2} & \cdots & \sum x_{i}^{m} \\ \sum x_{i} & \sum x_{i}^{2} & \sum x_{i}^{3} & \cdots & \sum x_{i}^{m+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum x_{i}^{m-1} & \sum x_{i}^{m} & \sum x_{i}^{m+1} & \cdots & \sum x_{i}^{2 m-2}\end{array}\right] \quad b=\left[\begin{array}{c}\sum y_{i} \\ \sum x_{i} y_{i} \\ \vdots \\ \sum x_{i}^{m-1} y_{i}\end{array}\right]$

- $[a 1, a 2, a 3, \ldots, a m]=\mathrm{A}^{\wedge}(-1)^{*} \mathrm{~b}$


## Least Squares Method (Polynomial Fitting)

- Note that:
- Increasing the order does not necessarily lead to more accuracy.
- Use standard deviation to find the best curve, n: number of data
m: curve's polynomial order



## Homework

- Use a computer program and find the best curve to be fitted on the tabulated data(Check $m=2,3, \ldots, 10$ )

| $x$ Data | 1.2 | 2.8 | 4.3 | 5.4 | 6.8 | 7.0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $y$ Data | 7.5 | 16.1 | 38.9 | 67.0 | 146.6 | 266.2 |



