Computational Physics

Lecture-21

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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.

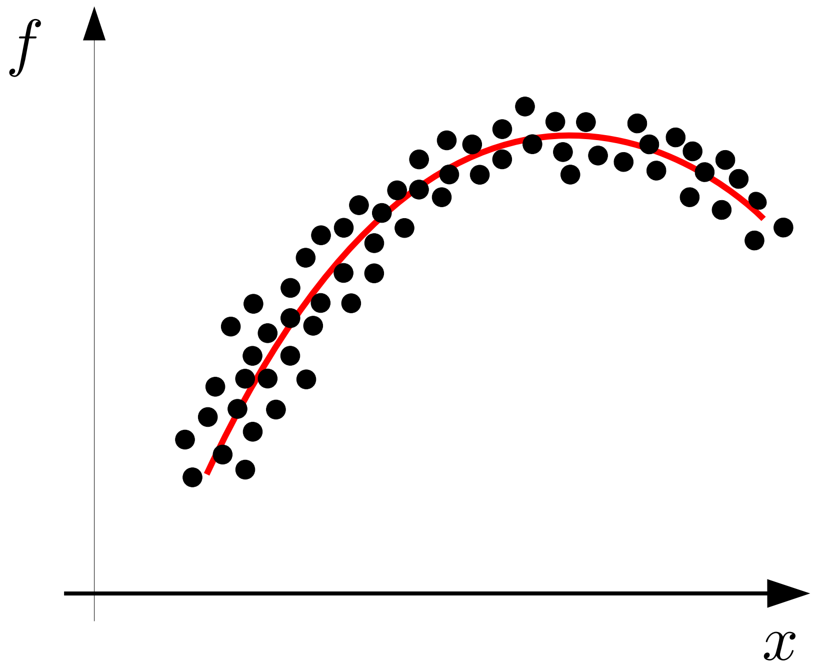
- Least Square Approximation

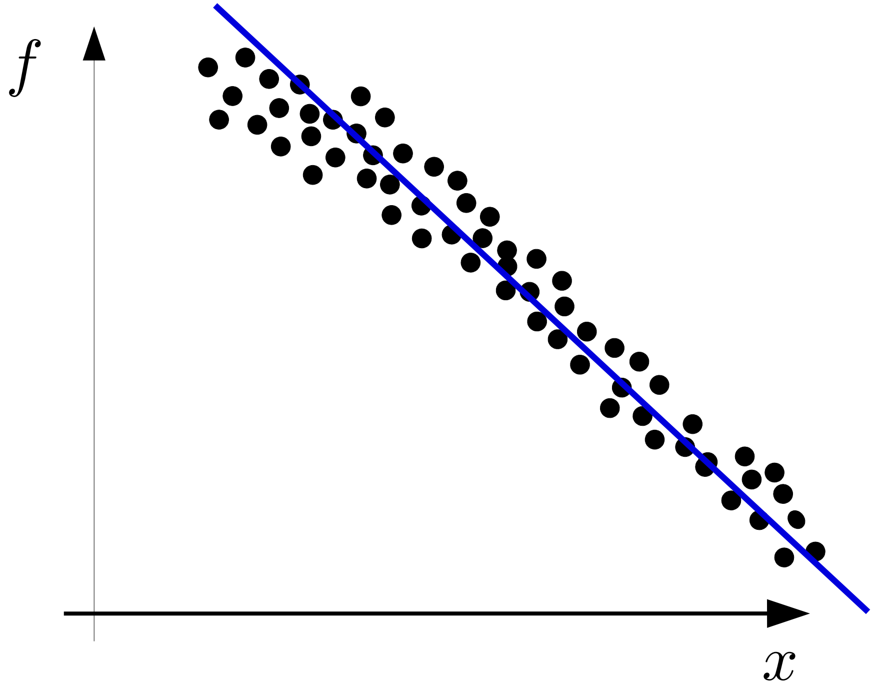
Approximation of a Function

- Least Square Approximation

  In many situations in physics we need to know the **global behavior** of a set of data in order to understand the trend in a specific measurement or observation.

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

- Least Square Approximation

$$P = P(x)$$

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

$$(P(x_0) - f_0) \to 0$$
$$(P(x_1) - f_1) \to 0$$
$$(P(x_2) - f_2) \to 0$$
$$\vdots$$
$$(P(x_i) - f_i) \to 0$$
$$\vdots$$
$$(P(x_i) - f_i) \to 0$$

$$\begin{aligned}\mathcal{L}^2 = {} & (P(x_0) - f_0)^2 \\ & + (P(x_1) - f_1)^2 \\ & + (P(x_2) - f_2)^2 \\ & \vdots \\ & + (P(x_i) - f_i)^2 \\ & \vdots \\ & + (P(x_n) - f_n)^2\end{aligned}$$

Approximation of a Function

- Least Square Approximation

$$P = P(x)$$

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

$$(P(x_0) - f_0) \to 0$$
$$(P(x_1) - f_1) \to 0$$
$$(P(x_2) - f_2) \to 0$$
$$\vdots$$
$$(P(x_i) - f_i) \to 0$$
$$\vdots$$
$$(P(x_i) - f_i) \to 0$$

$$\mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2$$

Choose the best function

$$P = P(x)$$

Approximation of a Function

- Least Square Approximation

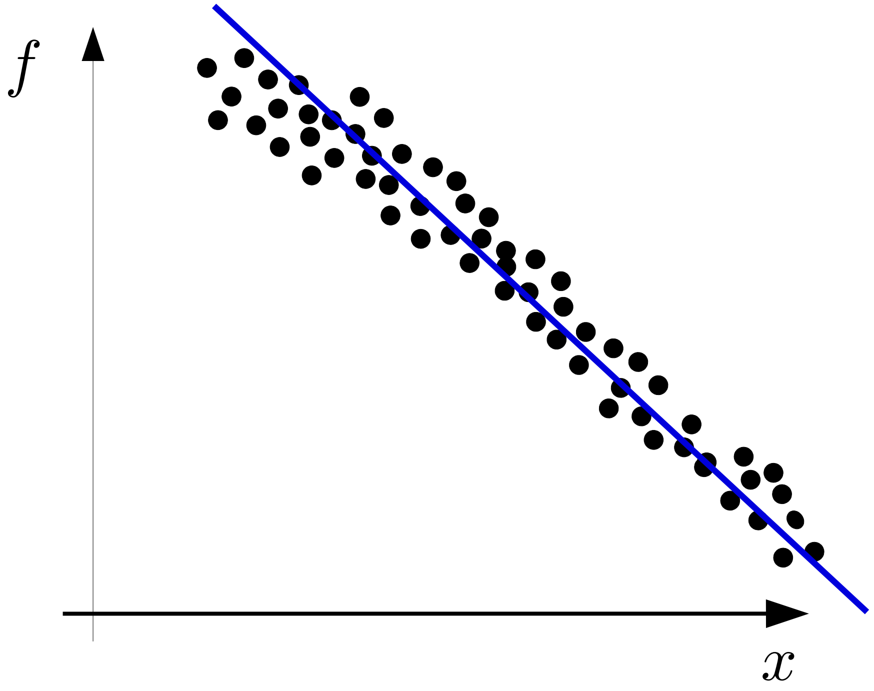
$$P = P(x)$$

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

$$\mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2$$

Choose the best function

$$P = P(x)$$



$$P(x) = c_0 + c_1 x$$

c_0 and c_1 are unknown constants.

Approximation of a Function

- Least Square Approximation

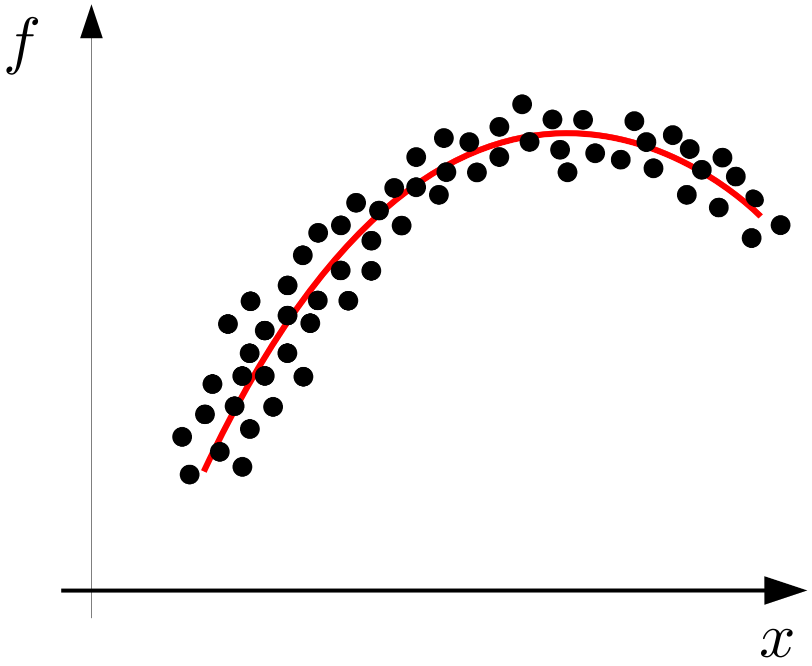
$$P = P(x)$$

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

$$\mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2$$

Choose the best function

$$P = P(x)$$



$$P(x) = c_0 + c_1 x + c_2 x^2$$

c_0, c_1 and c_2 are unknown constants.

Approximation of a Function

- Least Square Approximation

$$P = P(x)$$

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

$$\mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2$$

Choose the best function

$$P = P(x)$$

$$P(x) = \sum_{k=0}^{m} c_k x^k$$

$$P(x) = \sum_{k=0}^{m} c_k \sin kx$$

$$P(x) = \sum_{k=0}^{m} c_k J_k(x)$$

$$\vdots$$

$$P(x) = \sum_{k=0}^{m} c_k u_k(x)$$

$\{c_i\}$'s are unknown constants.

Approximation of a Function

- Least Square Approximation

$$P = P(x)$$

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

$$\boxed{\mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2}$$

Choose the best function

$$P = P(x)$$

$$\begin{cases} P(x) = \sum_{k=0}^{m} c_k u_k(x) \\ \mathcal{L}^2 = \sum_{i=0}^{n} (P(x_i) - f_i)^2 \end{cases}$$

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i \right)^2$$

Finding unknown constants.

Approximation of a Function

- Least Square Approximation

$$\frac{\delta c_l}{\delta c_j} = \delta_{lj}$$

$$\mathcal{L}^2 = \sum_{i=0}^{n}\left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i\right)^2$$

$$\frac{\delta \mathcal{L}^2}{\delta c_j} = 2\sum_{i=0}^{n}\left[\left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i\right)\left(\sum_{l=0}^{m} \delta_{lj} u_l(x_i)\right)\right]$$

Finding unknown constants.

$$\frac{\delta \mathcal{L}^2}{\delta c_j} = 0, \quad j = 0, 1, 2, \cdots, m$$

$$\frac{\delta \mathcal{L}^2}{\delta c_j} = 2\sum_{i=0}^{n}\left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i\right) u_j(x_i) = 0$$

$$\frac{\delta \mathcal{L}^2}{\delta c_j} = 2\sum_{i=0}^{n}\left[\left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i\right)\left(\sum_{l=0}^{m} \frac{\delta c_l}{\delta c_j} u_l(x_i)\right)\right]$$

$$\sum_{i=0}^{n}\left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i\right) u_j(x_i) = 0$$

Approximation of a Function

- Least Square Approximation

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i \right)^2$$

$$j: \quad \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k u_k(x_i) \right) u_j(x_i) = \sum_{i=0}^{n} f_i u_j(x_i)$$

Finding unknown constants.

$$\frac{\delta \mathcal{L}^2}{\delta c_j} = 0, \quad j = 0, 1, 2, \cdots, m$$

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} u_k(x_i) u_j(x_i) \right) = \sum_{i=0}^{n} f_i u_j(x_i)$$

$$j: \quad \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k u_k(x_i) - f_i \right) u_j(x_i) = 0$$

Approximation of a Function

- Least Square Approximation

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

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} u_k(x_i) u_j(x_i) \right) = \sum_{i=0}^{n} f_i u_j(x_i)$$

Linear polynomial interpolation: $\quad u_0(x) = 1, \quad u_1(x) = x$

$$j = 0: \quad c_0 \left(\sum_{i=0}^{n} 1 \right) + c_1 \left(\sum_{i=0}^{n} x_i \right) = \sum_{i=0}^{n} f_i$$

$$j = 1: \quad c_0 \left(\sum_{i=0}^{n} x_i \right) + c_1 \left(\sum_{i=0}^{n} x_i^2 \right) = \sum_{i=0}^{n} f_i x_i$$

Approximation of a Function

- Least Square Approximation

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

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} u_k(x_i) u_j(x_i) \right) = \sum_{i=0}^{n} f_i u_j(x_i)$$

Linear polynomial interpolation: $\quad u_0(x) = 1, \quad u_1(x) = x$

$$\begin{cases} c_0 \left(\sum_{i=0}^{n} 1 \right) + c_1 \left(\sum_{i=0}^{n} x_i \right) = \sum_{i=0}^{n} f_i \\ c_0 \left(\sum_{i=0}^{n} x_i \right) + c_1 \left(\sum_{i=0}^{n} x_i^2 \right) = \sum_{i=0}^{n} f_i x_i \end{cases}$$

Approximation of a Function

- Least Square Approximation

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} u_k(x_i) u_j(x_i) \right) = \sum_{i=0}^{n} f_i u_j(x_i)$$

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

Quadratic polynomial interpolation: $u_0(x) = 1, \quad u_1(x) = x, \quad u_2(x) = x^2$

$$j = 0: \quad c_0 \left(\sum_{i=0}^{n} 1 \right) + c_1 \left(\sum_{i=0}^{n} x_i \right) + c_2 \left(\sum_{i=0}^{n} x_i^2 \right) = \sum_{i=0}^{n} f_i$$

$$j = 1: \quad c_0 \left(\sum_{i=0}^{n} x_i \right) + c_1 \left(\sum_{i=0}^{n} x_i^2 \right) + c_2 \left(\sum_{i=0}^{n} x_i^3 \right) = \sum_{i=0}^{n} f_i x_i$$

$$j = 1: \quad c_0 \left(\sum_{i=0}^{n} x_i^2 \right) + c_1 \left(\sum_{i=0}^{n} x_i^3 \right) + c_2 \left(\sum_{i=0}^{n} x_i^4 \right) = \sum_{i=0}^{n} f_i x_i^2$$

Approximation of a Function

- Least Square Approximation

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} u_k(x_i) u_j(x_i) \right) = \sum_{i=0}^{n} f_i u_j(x_i)$$

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

Quadratic polynomial interpolation: $u_0(x) = 1, \quad u_1(x) = x, \quad u_2(x) = x^2$

$$\begin{cases} c_0 \left(\sum_{i=0}^{n} 1 \right) + c_1 \left(\sum_{i=0}^{n} x_i \right) + c_2 \left(\sum_{i=0}^{n} x_i^2 \right) = \sum_{i=0}^{n} f_i \\ c_0 \left(\sum_{i=0}^{n} x_i \right) + c_1 \left(\sum_{i=0}^{n} x_i^2 \right) + c_2 \left(\sum_{i=0}^{n} x_i^3 \right) = \sum_{i=0}^{n} f_i x_i \\ c_0 \left(\sum_{i=0}^{n} x_i^2 \right) + c_1 \left(\sum_{i=0}^{n} x_i^3 \right) + c_2 \left(\sum_{i=0}^{n} x_i^4 \right) = \sum_{i=0}^{n} f_i x_i^2 \end{cases}$$

Approximation of a Function

- Least Square Approximation

x	f	σ
x_0	f_0	σ_0
x_1	f_1	σ_1
x_2	f_2	σ_2
$\vdots$	$\vdots$	$\vdots$
x_i	f_i	σ_i
$\vdots$	$\vdots$	$\vdots$
x_n	f_n	σ_n

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\frac{P(x_i) - f_i}{\sigma_i} \right)^2 \qquad P(x) = \sum_{k=0}^{m} c_k u_k(x)$$

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k \frac{u_k(x_i)}{\sigma_i} - \frac{f_i}{\sigma_i} \right)^2$$

$$\frac{u_k(x_i)}{\sigma_i} = \hat{u}_k(x_i), \qquad \frac{f_i}{\sigma_i} = \hat{f}_i$$

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k \hat{u}_k(x_i) - \hat{f}_i \right)^2$$

Approximation of a Function

- Least Square Approximation

x	f	σ
x_0	f_0	σ_0
x_1	f_1	σ_1
x_2	f_2	σ_2
$\vdots$	$\vdots$	$\vdots$
x_i	f_i	σ_i
$\vdots$	$\vdots$	$\vdots$
x_n	f_n	σ_n

$$\mathcal{L}^2 = \sum_{i=0}^{n} \left(\sum_{k=0}^{m} c_k \hat{u}_k(x_i) - \hat{f}_i \right)^2 \qquad \frac{u_k(x_i)}{\sigma_i} = \hat{u}_k(x_i), \qquad \frac{f_i}{\sigma_i} = \hat{f}_i$$

$$j: \quad \sum_{k=0}^{m} c_k \left(\sum_{i=0}^{n} \hat{u}_k(x_i)\hat{u}_j(x_i) \right) = \sum_{i=0}^{n} \hat{f}_i \hat{u}_j(x_i)$$

Linear polynomial interpolation: $\hat{u}_0(x) = 1, \quad \hat{u}_1(x) = x$

Quadratic polynomial interpolation: $\hat{u}_0(x) = 1, \quad \hat{u}_1(x) = x, \quad \hat{u}_2(x) = x^2$