Linear Algebra
Lecture 4 (Chap. 4)
Least Squares Fit (LSF)

Approximate Solution of A**x**=**b** (A_{mxn} with m>n)

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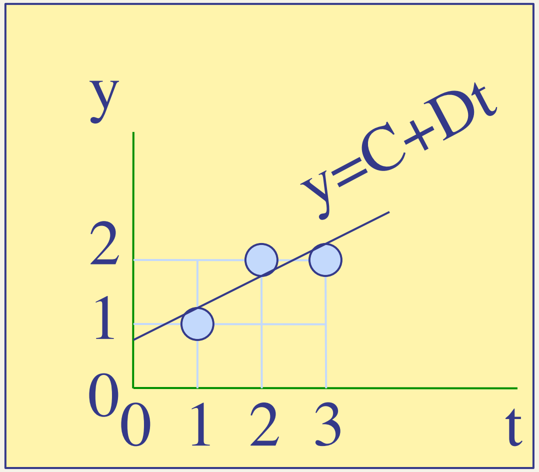
Least Squares Fitting for Approximate Solutions

- Solve A**x**=**b**
  - If A is an mxn matrix with m > n then we have more equations than unknowns.
  - When the number of equations is greater than the number of unknowns, we have one solution or no solution at all.
  - In most cases, we have no solution at all, we can only find an approximate solution!

Solving $A_{mxn}x_{nx1}=b_{mx1}$
with m > n (No. of eqn. > No. of unknown)

- Consider a set of data

i	t_i	y_i
1	1	1
2	2	2
3	3	2



If $y = C + Dt \Rightarrow$

$$\begin{matrix} C + Dt_1 = y_1 \\ C + Dt_2 = y_2 \\ C + Dt_3 = y_3 \end{matrix} \Rightarrow \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ 1 & t_3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \Rightarrow A\mathbf{x} = \mathbf{b}$$

no solution!

Best-Fit Approximate Solution $\hat{\mathbf{x}}$

$$A\mathbf{x} \approx \mathbf{b} \quad \Rightarrow \quad A\hat{\mathbf{x}} = \mathbf{p}$$

If $\quad y = C + Dt \quad \Rightarrow$

$$\begin{matrix} C + Dt_1 = y_1 \\ C + Dt_2 = y_2 \\ C + Dt_3 = y_3 \end{matrix} \Rightarrow \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ 1 & t_3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \Rightarrow \quad A\mathbf{x} = \mathbf{b}$$

no solution!

$A\hat{\mathbf{x}} = \mathbf{p}$ is the best-fit approximate solution

$$A^T\mathbf{e} = 0 = A^T(\mathbf{b} - \mathbf{p}) = A^T(\mathbf{b} - A\hat{\mathbf{x}}) \Rightarrow$$

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b} = \left(\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} 14 & -6 \\ -6 & 3 \end{bmatrix} \begin{bmatrix} 5 \\ 11 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 1/2 \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

General Forms of the Least Squares Fit

Find the approximate solution $\hat{\mathbf{x}}$ of $\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \end{bmatrix}$ $(A\hat{\mathbf{x}} = \mathbf{p})$

$$A^T \mathbf{e} = 0 = A^T(\mathbf{p} - \mathbf{b}) = A^T(A\hat{\mathbf{x}} - \mathbf{b}) \Rightarrow$$

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b} = \left(\begin{bmatrix} 1 & 1 & 1 & \dots \\ x_1 & x_2 & x_3 & \dots \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 & \dots \\ x_1 & x_2 & x_3 & \dots \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum f_i \\ \sum f_i x_i \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

General form of the least square fit :

$$f = C + Dx$$

$$\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum f_i \\ \sum f_i x_i \end{bmatrix}$$

$$f = C + Dx + Ey$$

$$\begin{bmatrix} n & \sum x_i & \sum y_i \\ \sum x_i & \sum x_i^2 & \sum x_i y_i \\ \sum y_i & \sum x_i y_i & \sum y_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} \sum f_i \\ \sum f_i x_i \\ \sum f_i y_i \end{bmatrix}$$

and so on.

Least Squares Fit: Minimize the Error

Error: $\mathbf{e} = \mathbf{b} - \mathbf{p} = \mathbf{b} - A\hat{\mathbf{x}}$

$$\Rightarrow \|\mathbf{e}\|^2 = \|\mathbf{b} - A\hat{\mathbf{x}}\|^2 = \|A\hat{\mathbf{x}} - \mathbf{b}\|^2 = \sum (C + Dx_i - f_i)^2$$

Least suqares fit (LFS) minimize the error $\|\mathbf{e}\|^2$

i.e., Find solution (C, D) such that $\partial\|\mathbf{e}\|^2 / \partial C = \partial\|\mathbf{e}\|^2 / \partial D = 0$

$$\frac{\partial\|\mathbf{e}\|^2}{\partial C} = 0 = 2(Cn + D\sum x_i - \sum f_i) = 0$$

$$\frac{\partial\|\mathbf{e}\|^2}{\partial D} = 0 = 2(C\sum x_i + D\sum x_i^2 - \sum f_i x_i) = 0$$

$$\Rightarrow \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum f_i \\ \sum f_i x_i \end{bmatrix}$$