

Lecture 24: 6.5-6.6 Least-Square Problems. A standard statistical technique is to find a least square fit to data points in the by some simple curve e.g. a line. Since there might be errors in the measurements of the data we do not require the curve to pass through the points but instead be such that it is the optimal approximation to the data in the sense that the sum of squares of the error between the y values of the data points and the points on the curve should be minimized.

A least square problem may be formulated as an overdetermined linear system. A system with more equations than unknowns usually is inconsistent. Given a system $A\mathbf{x}=\mathbf{b}$, where A is an $m \times n$ matrix with $m > n$, we want to find an \mathbf{x} that makes $\|A\mathbf{x} - \mathbf{b}\|$ as small as possible. This is called the least square solution:

Def The **least square solution** $\hat{\mathbf{x}}$ of the system $A\mathbf{x} = \mathbf{b}$ is a vector such that

$$\|A\hat{\mathbf{x}} - \mathbf{b}\| \leq \|A\mathbf{x} - \mathbf{b}\|, \quad \text{for all } \mathbf{x} \in \mathbf{R}^n$$

Formulated differently, we want to find the vector $\hat{\mathbf{b}} \in W = \text{Col } A$ that is closest to \mathbf{b} . From the previous section we know that $\hat{\mathbf{b}} = \text{proj}_W \mathbf{b}$, is the orthogonal projection of \mathbf{b} onto W . Since $\hat{\mathbf{b}} \in \text{Col } A$, there is a vector $\hat{\mathbf{x}}$ such that $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$. Moreover $\mathbf{b} - \hat{\mathbf{b}}$ is orthogonal to W since $\hat{\mathbf{b}}$ is the orthogonal projection onto W . Therefore $\mathbf{b} - \hat{\mathbf{b}}$ is orthogonal to the columns of $A = [\mathbf{a}_1 \ \cdots \ \mathbf{a}_n]$, i.e.

$$0 = \mathbf{a}_i \cdot (\mathbf{b} - \hat{\mathbf{b}}) = \mathbf{a}_i^T (\mathbf{b} - \hat{\mathbf{b}}) = \mathbf{a}_i^T (\mathbf{b} - A\hat{\mathbf{x}}), \quad i = 1, \dots, m$$

which is the same as

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

Hence $\hat{\mathbf{x}}$ is a solution of

$$A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$$

This so called **normal equation** represents an $n \times n$ system. If $A^T A$ is invertible;

$$\hat{\mathbf{x}} = (A^T A)^{-1} A \mathbf{b}$$

Ex Find the least square solution to $A\mathbf{x}=\mathbf{b}$ where $A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}$, $\mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ 6 \end{bmatrix}$.

$$A^T A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix}$$

and

$$(A^T A)^{-1} = \frac{1}{6} \begin{bmatrix} 14 & -6 \\ -6 & 3 \end{bmatrix}$$

and

$$A^T \mathbf{b} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 6 \end{bmatrix} = \begin{bmatrix} 6 \\ 18 \end{bmatrix}$$

Hence

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b} = \frac{1}{6} \begin{bmatrix} 14 & -6 \\ -6 & 3 \end{bmatrix} \begin{bmatrix} 6 \\ 18 \end{bmatrix} = \begin{bmatrix} -4 \\ 3 \end{bmatrix}$$

Ex Find the least square fit by a line to the following three points in the plane:

x	1	2	3
y	0	0	6

Sol We want to find the line $y = c_0 + c_1 x$ that is closest to going through the three points, (x_i, y_i) , $i = 1, 2, 3$, i.e. such that $\Delta_1^2 + \Delta_2^2 + \Delta_3^2$ is as small as possible, where

$$\Delta_i = y_i - (c_0 + c_1 x_i), \quad i = 1, 2, 3$$

Or if we plug in the values of (x_i, y_i) and write it in matrix form we want to make the vector

$$\Delta = \begin{bmatrix} 0 \\ 0 \\ 6 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}$$

as small as possible. But this is exactly the least square problem in the previous example, and the solution is $(c_0, c_1)^T = (-4, 3)^T$.