MA 511, Session 16

Least Squares Approximation

Problem: Given data for the coefficients of a $m \times n$ matrix A (where $m \geq n$) and a vector $b \in \mathbb{R}^m$, find the best linear fit $\bar{x}$ for x in the model

$$Ax = b$$

when A has maximal rank. When the rank of A is not maximal, there are infinitely many solutions and we shall study later a standard way to select one of them. When $b \notin \mathcal{C}(A)$, and $\dim \mathcal{C}(A) = n$, we solve the normal system $A^T A x = A^T b$ as

$$\bar{x} = (A^T A)^{-1} A^T b.$$

Example: Consider

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 6 \\ 3 & -9 \\ 4 & -8 \end{pmatrix}, \qquad b = \begin{pmatrix} 4 \\ 10 \\ -3 \\ 0 \end{pmatrix}.$$

Then,

$$A^T A = \begin{pmatrix} 30 & -45 \\ -45 & 185 \end{pmatrix}$$

We have

$$(A^T A)^{-1} = \tfrac{1}{3525} \begin{pmatrix} 185 & 45 \\ 45 & 30 \end{pmatrix}, \qquad A^T b = \begin{pmatrix} 15 \\ 95 \end{pmatrix}$$

and

$$\bar{x} = (A^T A)^{-1} A^T b = \tfrac{1}{3525} \begin{pmatrix} 185 & 45 \\ 45 & 30 \end{pmatrix} \begin{pmatrix} 15 \\ 95 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

We can now find the projection

$$p = A\bar{x} = \begin{pmatrix} 1 & 2 \\ 2 & 6 \\ 3 & -9 \\ 4 & -8 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 4 \\ 10 \\ -3 \\ 0 \end{pmatrix} = b.$$

The reason that $p = b$ is that $b \in \mathcal{C}(A)$ (since it is twice the first column of A plus the second column) so that the closest point in $\mathcal{C}(A)$ to b is b itself.

Remark: Even though in general A is not square, $A^T A$ always is. Moreover, it has the following properties.

(i) $A^T A$ is symmetric

(ii) $\mathcal{N}(A^T A) = \mathcal{N}(A)$

(iii) rank $(A^T A) =$ rank A

Proof: (i) Note that $(A^T A)^T = A^T (A^T)^T = A^T A$.

(ii) If $x \in \mathcal{N}(A)$, then $Ax = 0 \Rightarrow A^T Ax = 0$ says that $x \in \mathcal{N}(A^T A)$. Suppose now that $A^T Ax = 0$. Then, $x^T A^T Ax = (Ax)^T Ax = \|Ax\|^2 = 0$ implies that $Ax = 0$ so that $x \in \mathcal{N}(A)$.

(iii) Follows from (ii) since on both sides the rank equals n minus the dimension of the null space.

When A^TA is invertible (A is of rank n), the matrix

$$P = A(A^TA)^{-1}A^T, \quad Pb = A\bar{x},$$

projects $\mathbb{R}^m$ onto the column space of A. In particular, since $\mathcal{C}(A)^\perp = \mathcal{N}(A^T)$, any vector $b \in \mathbb{R}^m$ can be written as the sum of its projection onto $\mathcal{C}(A)$ and a vector orthogonal to that projection: $b = Pb + (b - Pb)$ where $b - Pb \perp Pb$.

Remark: Projection matrix P has the following properties: (i) $P^2 = P$ (ii) $P^T = P$ (iii) $\mathcal{C}(P) = \mathcal{C}(A)$

<u>Proof</u>: (i) $P^2 = [A(A^TA)^{-1}A^T][A(A^TA)^{-1}A^T] =$

$[A(A^TA)^{-1}][A^TA(A^TA)^{-1}]A^T = A(A^TA)^{-1}A^T = P$

(ii) $P^T = [A(A^TA)^{-1}A^T]^T =$

$$(A^T)^T[(A^TA)^{-1}]^TA^T = A(A^TA)^{-1}A^T = P$$

(iii) $\mathcal{C}(P) \subset \mathcal{C}(A)$ since $Pb = A\bar{x}$.
If $b = Aq \in \mathcal{C}(A)$ then $Pb = A(A^TA)^{-1}(A^TA)q = Aq = b$, hence $\mathcal{C}(A) \subset \mathcal{C}(P)$.

Example: Given the data

$$
\begin{aligned}
b = 1 \quad &\text{when} \quad t = -1\\
b = 1 \quad &\text{when} \quad t = 1\\
b = 3 \quad &\text{when} \quad t = 2,
\end{aligned}
$$

find the best vector $\begin{pmatrix} C \\ D \end{pmatrix}$ to fit the model

$$C + Dt = b.$$

This is a classical "straight line" approximation. In matrix form,

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 3 \end{pmatrix}.$$

We have

$$A^T A = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \quad \text{so} \quad A^T A x = A^T b$$

becomes $\begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} \bar{C} \\ \bar{D} \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \end{pmatrix}$ and we obtain

$$\bar{C} = \frac{9}{7}, \qquad \bar{D} = \frac{4}{7}.$$

The general formula for straight line approximation of the data

$$\begin{array}{ccc} b = b_1 & \text{when} & t = t_1 \\ \dots & & \dots \\ b = b_m & \text{when} & t = t_m, \end{array}$$

using the model $C + Dt = b$, has the slope and intercept given as the unique solution of the system

$$A^T A = \begin{pmatrix} m & \sum\limits_{i=1}^{m} t_i \\ \sum\limits_{i=1}^{m} t_i & \sum\limits_{i=1}^{m} t_i^2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \sum\limits_{i=1}^{m} b_i \\ \sum\limits_{i=1}^{m} t_i b_i \end{pmatrix} = A^T b.$$