Least Squares Review Sheet. Math 54, Fall 2012

This is a review of least squares problems.

Suppose that A is an $m \times n$ matrix with $m > n$. Thus, the matrix equation

$$A\underline{x} = \underline{b},$$

does not necessarily have a solution (ie, the choice of $\underline{b}$ may result in an inconsistent system). Suppose that this system is inconsistent. Thus, we have $\underline{b} \notin col(A)$.

Main things to know

- a *least squares solution* of $A\underline{x} = \underline{b}$ is a vector $\underline{x}_0$ such that

$$A\underline{x}_0 = \text{proj}_{col(A)}\underline{b}$$

Note: in the book a least squares solution is denoted $\hat{x}$ *and* $\text{proj}_{col(A)}\underline{b} = \hat{b}$.

- a least squares solution of $A\underline{x} = \underline{b}$ is a vector $\underline{x}_0$ such that $||A\underline{x}_0 - \underline{b}||$ is minimal, ie, the distance between $A\underline{x}_0$ and $\underline{b}$ is minimal.

- a least squares solution of $A\underline{x} = \underline{b}$ is also a solution of the matrix equation

$$A^t A\underline{x} = A^t\underline{b};$$

in particular, this previous matrix equation is consistent.

Why? Observe that $\underline{b} - \text{proj}_{col(A)}\underline{b} \in (col(A))^{\perp}$. In particular, we have

$$0 = \underline{a}_i \cdot (\underline{b} - \text{proj}_{col(A)}\underline{b}) = \underline{a}_i^t(\underline{b} - \text{proj}_{col(A)}\underline{b}), \quad \text{where } \underline{a}_i \text{ is the } i^{th} \text{ column of } A.$$

Thus, we have the n equalities

$$\begin{bmatrix} \underline{a}_1^t(\underline{b} - \text{proj}_{col(A)}\underline{b}) \\ \vdots \\ \underline{a}_n^t(\underline{b} - \text{proj}_{col(A)}\underline{b}) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \Leftrightarrow A^t(\underline{b} - \text{proj}_{col(A)}\underline{b}) = \underline{0}$$

Hence, if $\underline{x}_0$ is a least squares solution of $A\underline{x} = \underline{b}$ then we have

$$A^t\underline{b} = A^t\text{proj}_{col(A)}\underline{b} = A^t A\underline{x}_0$$

- let $\underline{x} \in \mathbb{R}^n$. Then,

$$A\underline{x} = \text{proj}_{col(A)}\underline{b} \Leftrightarrow A^t A\underline{x} = A^t\underline{b}$$

- there is a unique least squares solution of $A\underline{x} = \underline{b}$ if and only if the columns of A are linearly independent,

- there is a unique least squares solution if and only if $A^t A$ is invertible,

- the columns of A are linearly independent if and only if the square matrix $A^t A$ is invertible.

Example Consider the matrix equation

$$\begin{bmatrix}1 & -1 & 0\\ 1 & 3 & 1\\ 2 & 2 & 1\\ 0 & 2 & 1\end{bmatrix}\underline{x} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

This is an inconsistent matrix equation. Let's determine a least squares solution: we have

$$\begin{bmatrix}1 & 1 & 2 & 0\\ -1 & 3 & 2 & 2\\ 0 & 1 & 1 & 1\end{bmatrix}\begin{bmatrix}1 & -1 & 0\\ 1 & 3 & 1\\ 2 & 2 & 1\\ 0 & 2 & 1\end{bmatrix} = \begin{bmatrix}6 & 6 & 3\\ 6 & 18 & 7\\ 3 & 7 & 3\end{bmatrix}$$

and

$$\begin{bmatrix}1 & 1 & 2 & 0\\ -1 & 3 & 2 & 2\\ 0 & 1 & 1 & 1\end{bmatrix}\begin{bmatrix}0\\0\\0\\1\end{bmatrix} = \begin{bmatrix}0\\2\\1\end{bmatrix}$$

so that we need to determine solutions of the matrix equation

$$\begin{bmatrix}6 & 6 & 3\\ 6 & 18 & 7\\ 3 & 7 & 3\end{bmatrix}\underline{x} = \begin{bmatrix}0\\2\\1\end{bmatrix}$$

Since

$$\begin{bmatrix}6 & 6 & 3 & 0\\ 6 & 18 & 7 & 2\\ 3 & 7 & 3 & 1\end{bmatrix} \sim \begin{bmatrix}1 & 0 & 0 & -1/2\\ 0 & 1 & 0 & -1/2\\ 0 & 0 & 1 & 2\end{bmatrix}$$

we see that there is exactly one least squares solution

$$\begin{bmatrix}-1/2\\ -1/2\\ 2\end{bmatrix}.$$

Moreover, we see that the columns of A are linearly independent since the matrix

$$\begin{bmatrix}6 & 6 & 3\\ 6 & 18 & 7\\ 3 & 7 & 3\end{bmatrix}$$

is invertible.