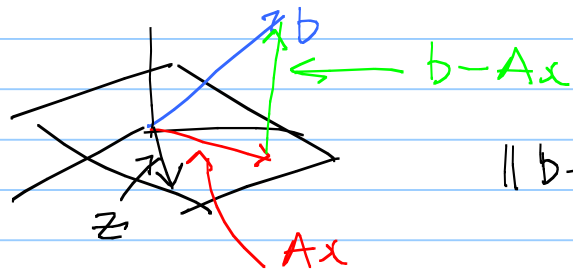
Least Squares

Let A be an $m \times n$ matrix and consider the equation $Ax = b$, which may or may not have a (unique?) solution. The method of least squares finds a "best" solution, which is the unique solution if it exists. Let $A = [A_1, \dots, A_n]$ be written as an array of column m-vectors. Let Π be the column space of A, which is the set of linear combinations of the columns of A. $y \in \Pi \Leftrightarrow y = x_1 A_1 + \cdots + x_n A_n = Ax$. The vector b may not be in Π and even if it is it may not be a unique combination of the columns. The "best" solution will be a vector x so that $\|b - Ax\|$ is least. Choose x so that $b - Ax$ is orthogonal to Π.



Let z be any vector in Π.

$$\|b - z\|^2 = \|b - Ax + Ax - z\|^2$$

$$= \|b - Ax\|^2 + \|Ax - z\|^2 \geq \|b - Ax\|^2$$

since $Ax - z \in \Pi$.

Thus $\|b - Ax\|$ is least. Is x uniquely determined?

The condition on x is $b - Ax \perp A_j$, $j = 1, \dots, n$.

This can be written as

$$(1) \qquad A^T A x = A b.$$

Suppose the columns of A are linearly independent.

$A^T A$ is square $n \times n$ and if $A^T A x = 0$, then $x^T A^T A x = \|Ax\|^2 = 0$, so $Ax = 0$ and $x = 0$. Thus in this case there is a unique solution.

How do we know that there is a vector $v \in \Pi$ so that $b - v \perp \Pi$, and is v unique? Yes. For simplicity suppose the first k columns of A: $A_1, \dots, A_k$ are a basis for Π (linearly independent spanning set).

Then $A^T A x = A^T b$ has a unique solution and $v = Ax$ satisfies $A^T(v-b) = 0$, so $v - b$ is $\perp$ to $A_1, \dots, A_k$, hence $\perp$ to any vector in the linear space spanned by $\{A_1, \dots, A_k\}$, hence $\perp$ to Π.

Let x_0 be such an x. Then let $f(x) = \|Ax - b\|^2$.

$$f(x_0+h) = \|Ax_0 - b\|^2 + 2\underbrace{(Ax_0 - b)^T A}_{=0} h + \|Ah\|^2$$

$$= f(x_0) + \|Ah\|^2, \quad (\|Ah\|^2 = h^T A^T A h)$$

$$\geq f(x_0) \quad \text{for all } h, \text{ so } f(x_0) \text{ is the minimum}$$