Linear Least Squares in a Nutshell

Let A denote a given real $n\times m$ matrix where the dimension $m < n$. Let vectors be columns and use the superscript notation $^{\mathrm{T}}$ to denote vector-matrix transposition. Let b denote a given real n-vector and suppose that it is desired to solve the equation

$$A\cdot x \;=\; b$$

for an unknown m-vector x. In general this may not be possible unless b satisfies a compatibility constraint to be derived below. So if the Euclidean norm $||v||$ of a vector v is defined as the positive square-root of $||v||^2 \equiv v^{\mathrm{T}}\cdot v$ then one might seek to minimize $||A\cdot x - b||^2$ to get an approximate solution. This is most concisely understood in terms of the following formalism.

Let A^+ denote the *pseudo-inverse* of A, a unique $m\times n$ matrix which always exists and satisfies the following four conditions:

$$A\cdot A^+\cdot A \;=\; A, \qquad A^+\cdot A\cdot A^+ \;=\; A^+, \qquad (A\cdot A^+)^{\mathrm{T}} \;=\; A\cdot A^+, \qquad (A^+\cdot A)^{\mathrm{T}} \;=\; A^+\cdot A.$$

Using the pseudo-inverse, one may define *symmetric* square matrices L and R, of dimensions n and m respectively, as

$$L \;=\; I_{\mathrm{n}} - A\cdot A^+ \;\equiv\; L^{\mathrm{T}}, \qquad\qquad R \;=\; I_{\mathrm{m}} - A^+\cdot A \;\equiv\; R^{\mathrm{T}},$$

where I_{k} denotes the k-dimensional identity matrix, and readily verify that

$$L\cdot A \;=\; 0, \qquad\qquad A\cdot R \;=\; 0,$$

so that L and R serve as left and right *annihilators* of A. It can be proved that

$$\min ||A\cdot x - b||^2 \;\;=\;\; ||A\cdot \hat{x} - b||^2 \;\;\equiv\;\; ||L\cdot b||^2\,,$$

where by definition

$$\hat{x} \;\;=\;\; A^+\cdot b \;\;+\;\; R\cdot c$$

and c is an arbitrary m-vector, and (because $R\cdot A^+ \equiv 0$) it is easy to verify that

$$||\hat{x}||^2 \;\;\equiv\;\; ||A^+\cdot b||^2 \;+\; ||R\cdot c||^2\,.$$

Accordingly the *shortest* least-squares solution is given by choosing

$$R\cdot c \;=\; 0,$$

in which case the solution is *exact* if and only if

$$L\cdot b \;=\; 0.$$

Reference: Problems 17-20, *pp.* 270-271, Gilbert Strang & Kai Borre, *Linear Algebra, Geodesy, and GPS*, Wellesley-Cambridge Press, 1997.