

Generalizing the Condition number to Full Rank Least Squares

We were considering the perturbed full rank LS problem

$$\min_x \|(A + tE)x(t) - (b + te)\|_2,$$

where t is real, and E and e are arbitrary but fixed. The normal equations

$$(A + tE)^T(A + tE)x(t) = (A + tE)^T(b + te) \quad (1)$$

were differentiated, giving

$$\dot{x} \equiv \dot{x}(0) = (A^T A)^{-1}[A^T(e - Ex_{LS}) + E^T(b - Ax_{LS})]. \quad (2)$$

Now let's fill in some details from the previous page. Use $x \equiv x(0) \equiv x_{LS}$, and take $\|\cdot\| \equiv \|\cdot\|_2$ throughout (so in particular (i) $\|M\| = \|M^T\|$, (ii) orthogonal matrices are isometries, and (iii) for all matrix actions $\|MN\| \leq \|M\|\|N\|$).

If $A = U\Sigma V^T$ is a singular value decomposition, then $\|A\| = \|\Sigma\| = \sigma_1$, (since V and U are orthogonal matrices), and

$$\|(A^T A)^{-1}A^T\| = \|V(\Sigma^T \Sigma)^{-2}V^T V \Sigma U^T\| = \|V(\Sigma^T \Sigma)^{-2}\Sigma U^T\| = 1/\sigma_n,$$

giving the identities (you should verify)

$$\kappa_2(A) \equiv \sigma_1/\sigma_n = \|A\|\|(A^T A)^{-1}A^T\| = \sqrt{\|(A^T A)^{-1}\| \|A\|^2}.$$

The inequality we were working with (a linear Taylor approx to $\|x(t) - x\|/\|x\|$) was

$$|t| \frac{\|\dot{x}(0)\|}{\|x\|} \leq |t| \left[\frac{\|(A^T A)^{-1}A^T(e - Ex_{LS})\|}{\|x\|} + \frac{\|(A^T A)^{-1}E^T r\|}{\|x\|} \right] + O(t^2).$$

Let's break it into the 3 terms (using triangle inequality):

$$|t| \frac{\|\dot{x}(0)\|}{\|x\|} \leq |t| \frac{\|(A^T A)^{-1}A^T e\|}{\|x\|} + |t| \frac{\|(A^T A)^{-1}A^T E x\|}{\|x\|} + |t| \frac{\|(A^T A)^{-1}E^T r\|}{\|x\|} + O(t^2),$$

... and massage a bit (same 3 terms, using $\|MN\| \leq \|M\|\|N\|$ and $\|E^T\| = \|E\|$):

$$\begin{aligned} \frac{\|t\dot{x}(0)\|}{\|x\|} &\leq \frac{\|(A^T A)^{-1}A^T\| \|A\| \|te\|}{\|A\| \|x\|} + \frac{\|(A^T A)^{-1}A^T\| \|A\| \|tE\| \|x\|}{\|A\| \|x\|} + \frac{\|(A^T A)^{-1}\| \|A\|^2 \|tE\| \|r\|}{\|A\|^2 \|x\|} + O(t^2) \\ &= \frac{\kappa(A) \|te\|}{\|A\| \|x\|} + \frac{\kappa(A) \|tE\|}{\|A\|} + \frac{\|A\|^2 \|(A^T A)^{-1}\| \|tE\| \|r\|}{\|A\| \|A\| \|x\|} + O(t^2). \end{aligned}$$

If θ is the angle between b and $\text{ColSp}(A)$, then $s \equiv \sin \theta = \|r\|/\|b\|$. With $c \equiv \cos \theta$, $\|Ax\| = c \|b\| \leq \|A\| \|x\|$ (draw your projection picture), and we return to the first page (again, same 3 terms until we rearrange on the last line):

$$\begin{aligned} \frac{\|t\dot{x}(0)\|}{\|x\|} &\leq \kappa(A) \left[\frac{\|te\|}{c\|b\|} + \frac{\|tE\|}{\|A\|} \right] + \frac{\|A\|^2 \|t(A^T A)^{-1}\| \|tE\| \|r\|}{\|A\| c \|b\|} + O(t^2). \\ &= \kappa(A) \left[\frac{\|te\|}{c\|b\|} + \frac{\|tE\|}{\|A\|} \right] + \frac{\kappa^2(A) \|tE\| s}{\|A\| c} + O(t^2). \\ &= \frac{\|tE\|}{\|A\|} (\kappa(A) + \tan(\theta) \kappa^2(A)) + \frac{\|te\|}{\|b\|} \sec(\theta) \kappa(A) + O(t^2). \end{aligned}$$