Linear Least Squares

Given a linear system $Ax - b = e$,

$$a_1 \cdot x - b_1 = e_1$$

$$\vdots$$

$$a_i \cdot x - b_i = e_i$$

$$\vdots$$

$$a_m \cdot x - b_m = e_m$$

(sometimes written $Ax \underline{\bowtie} b$)

We want to minimize the sum of squares of the errors

$$\min_x \sum_i e_i^2 = e^T e = (Ax - b)^T (Ax - b)$$
Linear Least Squares

• Many methods for $Ax \cong b$
• One simple one is to compute

$$Ax \cong b$$
$$A^T Ax \cong A^T b$$
$$x \cong (A^T A)^{-1} A^T b$$

• Better methods based on orthogonal transformations exist
• These methods are available in standard math libraries
• A short review follows
Orthogonal Transformations

The key property is:

$$Q^{-1} = Q^T$$

Some implications of this are as follows

if

$$Q = [q_1, q_2, \cdots, q_n]$$

then

$$q_i \bullet q_j = \begin{cases} 1, & \text{if } i=j \\ 0, & \text{if } i \neq j \end{cases}$$

$$\| Qx \| = \sqrt{(Qx)^T(Qx)}$$

$$= \sqrt{x^TQ^TQx} = \sqrt{x^Tx}$$

$$= \| x \|$$
Singular Value Decomposition

• Developed by Golub, et al in late 1960’s
• Commonly available in mathematical libraries
• E.g.,
  – MATLAB
  – IMSL
  – Numerical Recipes (Wm. Press, et. al., Cambridge Press)
  – CISST ERC Math Library
Singular Value Decomposition

Given an arbitrary $m \times n$ matrix $A$, there exist orthogonal matrices $U$, $V$ and a diagonal matrix $S$ that:

$$A_{m \times n} = U_{m \times m} S_{n \times n} V^T_{n \times n}$$

for $m \geq n$

or

$$A_{m \times n} = U_{m \times m} [S_{n \times n} \ 0_{(m \times (n-m))}] V^T_{n \times n}$$

for $m \leq n$
SVD Least Squares

\[ A_{m \times n} x \approx b \]

\[ U_{m \times m} S_{n \times n} Q_{(m-n) \times n}^T x = b \]

\[ y = U_{m \times m}^T b \quad \text{where} \quad y = V^T x \]

Solve this for \( y \) (trivial, since \( S \) is diagonal), then compute

\[ Vy = VV^T x = x \]