

# Linear Least Squares

Given a linear system  $\mathbf{Ax} - \mathbf{b} = \mathbf{e}$ ,

$$\mathbf{a}_1 \bullet \mathbf{x} - b_1 = e_1$$

$$\vdots$$

$$\mathbf{a}_i \bullet \mathbf{x} - b_i = e_i$$

$$\vdots$$

$$\mathbf{a}_m \bullet \mathbf{x} - b_m = e_m$$

(sometimes written  $\mathbf{Ax} \cong \mathbf{b}$ )

We want to minimize the sum of squares of the errors

$$\min_{\mathbf{x}} \sum_i e_i^2 = \mathbf{e}^T \mathbf{e} = (\mathbf{Ax} - \mathbf{b})^T (\mathbf{Ax} - \mathbf{b})$$

# Linear Least Squares

- Many methods for  $\mathbf{Ax} \cong \mathbf{b}$
- One simple one is to compute

$$\mathbf{Ax} \cong \mathbf{b}$$

$$\mathbf{A}^T \mathbf{Ax} \cong \mathbf{A}^T \mathbf{b}$$

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

- 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:

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

Some implications of this are as follows

$$\text{if } \mathbf{Q} = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_n]$$

$$\text{then } \mathbf{q}_i \bullet \mathbf{q}_j = \begin{cases} 1, & \text{if } i=j \\ 0, & \text{if } i \neq j \end{cases}$$

$$\begin{aligned} \|\mathbf{Q}\mathbf{x}\| &= \sqrt{(\mathbf{Q}\mathbf{x})^T (\mathbf{Q}\mathbf{x})} \\ &= \sqrt{\mathbf{x}^T \mathbf{Q}^T \mathbf{Q} \mathbf{x}} = \sqrt{\mathbf{x}^T \mathbf{x}} \\ &= \|\mathbf{x}\| \end{aligned}$$

# 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  $\mathbf{A}$ , there exist orthogonal matrices  $\mathbf{U}$ ,  $\mathbf{V}$  and a diagonal matrix  $\mathbf{S}$  that:

$$\mathbf{A}_{m \times n} = \mathbf{U}_{m \times m} \begin{bmatrix} \mathbf{S}_{n \times n} \\ \mathbf{0}_{(m-n) \times n} \end{bmatrix} \mathbf{V}_{n \times n}^T \quad \text{for } m \geq n$$

or

$$\mathbf{A}_{m \times n} = \mathbf{U}_{m \times m} \begin{bmatrix} \mathbf{S}_{n \times n} & \mathbf{0}_{(m \times (n-m))} \end{bmatrix} \mathbf{V}_{n \times n}^T \quad \text{for } m \leq n$$

# SVD Least Squares

$$\mathbf{A}_{m \times n} \mathbf{x} \approx \mathbf{b}$$

$$\mathbf{U}_{m \times m} \begin{matrix} \mathbf{I}_n \\ \mathbf{0}_{(m-n) \times n} \end{matrix} \mathbf{S}_{n \times n} \mathbf{V}_{n \times n}^T \mathbf{x} = \mathbf{b}$$

$$\begin{matrix} \mathbf{I}_n \\ \mathbf{0}_{(m-n) \times n} \end{matrix} \mathbf{S}_{n \times n} \mathbf{y} = \mathbf{U}_{m \times m}^T \mathbf{b} \quad \text{where } \mathbf{y} = \mathbf{V}^T \mathbf{x}$$

Solve this for  $\mathbf{y}$  (trivial, since  $\mathbf{S}$  is diagonal), then compute

$$\mathbf{V} \mathbf{y} = \mathbf{V} \mathbf{V}^T \mathbf{x} = \mathbf{x}$$