Linear Least Squares

Given a linear system **Ax -b = 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

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

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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 <u>orthogonal transformations</u> exist
- These methods are available in standard math libraries
- A short review follows

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Orthogonal Transformations

The key property is:

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

Some implications of this are as follows

$$\text{if} \qquad \mathbf{Q} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_n \end{bmatrix}$$

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

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

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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

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Singular Value Decomposition

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

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

or

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

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SVD Least Squares

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

$$\mathbf{U}_{m\times m}\begin{bmatrix}\mathbf{S}_{n\times n}\\ \mathbf{0}_{(m-n)\times n}\end{bmatrix}\mathbf{V}^T_{n\times n}\ \mathbf{x} = \mathbf{b}$$

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

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

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

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