6.5 Least squares problems

$\underset{m \times n}{A}\vec{x} = \vec{b}$ (possibly inconsistent)

Find $\hat{x}$ that minimizes $\|\vec{b} - A\vec{x}\|$

$\hat{x}$ a "least squares solution" to $A\vec{x} = \vec{b}$

$W = \text{Col } A$

$\hat{b} = \text{proj}_W \vec{b}$

Then $\|\vec{b} - \hat{b}\| \leq \|\vec{b} - \vec{v}\|$ for all $v \in W$

But $\vec{x} \in \mathbb{R}^n \Rightarrow \vec{v} = A\vec{x} \in \text{Col } A = W$

So $\|\vec{b} - \hat{b}\| \leq \|\vec{b} - A\vec{x}\|$ for all $x \in \mathbb{R}^n$

Can we find $\hat{x}$ such that $\hat{b} = A\hat{x}$?

YES! Because $\hat{b} \in W = \text{Col } A$.

So there does exist such an $\hat{x}$.

How do we find it?

$\vec{b} - \hat{b} \in W^\perp$

Write $A = (\vec{a}_1 \cdots \vec{a}_n)$

Each $\vec{a}_j \in W$. Therefore ...

$$\vec{a}_j \cdot (\vec{b} - \hat{b}) = 0 \quad \text{for all } j$$

$$\vec{a}_j^T (\vec{b} - A\hat{x}) = 0 \quad \text{for all } j$$

$$\begin{pmatrix} \vec{a}_1^T \\ \vdots \\ \vec{a}_n^T \end{pmatrix} (\vec{b} - A\hat{x}) = \vec{0}$$

$$A^T (\vec{b} - A\hat{x}) = \vec{0}$$

$$A^T\vec{b} - A^TA\hat{x} = \vec{0}$$

$$A^TA\hat{x} = A^T\vec{b}$$

Find $\hat{x}$ by solving

consistent

$$\boxed{A^TA\vec{x} = A^T\vec{b}}$$

called the "normal equations" for $A\vec{x} = \vec{b}$

Thm 13

The set of least-squares solns to $A\vec{x} = \vec{b}$ is the soln set to $A^TA\vec{x} = A^T\vec{b}$, which is nonempty.

Expl 1

$$A = \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 2 \\ 0 \\ 11 \end{pmatrix}$$

$A\vec{x} = \vec{b}$ is inconsistent. Find a least-squares soln to $A\vec{x} = \vec{b}$.

$$A^T A = \begin{pmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{pmatrix} \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix}$$

$$A^T \vec{b} = \begin{pmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \\ 11 \end{pmatrix} = \begin{pmatrix} 19 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix} \vec{x} = \begin{pmatrix} 19 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix}^{-1} = \frac{1}{85-1} \begin{pmatrix} 5 & -1 \\ -1 & 17 \end{pmatrix}$$

$$\vec{x} = \frac{1}{84} \begin{pmatrix} 5 & -1 \\ -1 & 17 \end{pmatrix} \begin{pmatrix} 19 \\ 11 \end{pmatrix} = \frac{1}{84} \begin{pmatrix} 95 - 11 \\ -19 + 187 \end{pmatrix}$$

$$= \frac{1}{84} \begin{pmatrix} 84 \\ 168 \end{pmatrix} = \boxed{\begin{pmatrix} 1 \\ 2 \end{pmatrix}}$$

Thm 14

Let A be $m \times n$. TFAE:

(a) $A\vec{x} = \vec{b}$ has a unique least-squares soln for each $\vec{b} \in \mathbb{R}^m$.

(b) The cols of A are lin. indep.

(c) $A^T A$ is invertible.

In these cases, $\hat{x} = (A^T A)^{-1} A^T \vec{b}$.

$\|\vec{b} - A\hat{x}\|$ is called the <u>least-squares error</u>.

Expl 3

What is the least squares error in Expl 1?

$$\vec{b} = \begin{pmatrix} 2 \\ 0 \\ 11 \end{pmatrix}, \quad \hat{x} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$A\hat{x} = \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 4 \\ 4 \\ 3 \end{pmatrix}$$

$$\|\vec{b} - A\hat{x}\|^2 = \left\| \begin{pmatrix} -2 \\ -4 \\ 8 \end{pmatrix} \right\|^2 = 4 + 16 + 64 = 84$$

$$\|\vec{b} - A\hat{x}\| = \sqrt{84} = \boxed{2\sqrt{21}}$$

Expl 4

$$A = \begin{pmatrix} 1 & -6 \\ 1 & -2 \\ 1 & 1 \\ 1 & 7 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} -1 \\ 2 \\ 1 \\ 6 \end{pmatrix}.$$

Find a least-squares soln to $A\vec{x} = \vec{b}$.

$\underbrace{\vec{a}_1 \quad \vec{a}_2}_{\text{orthogonal}}$

$$\hat{b} = \text{proj}_{\text{Col}A}\, \vec{b}$$

Span $\{\vec{a}_1, \vec{a}_2\}$

$$= \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \frac{\vec{b}\cdot\vec{a}_2}{\vec{a}_2\cdot\vec{a}_2}\vec{a}_2$$

$$= \frac{-1+2+1+6}{1+1+1+1}\vec{a}_1 + \frac{6-4+1+42}{36+4+1+49}\vec{a}_2$$

$$= 2\vec{a}_1 + \frac{45}{90}\vec{a}_2 = 2\vec{a}_1 + \frac{1}{2}\vec{a}_2$$

Solve $A\vec{x} = \hat{b}$

$$(\vec{a}_1 \ \vec{a}_2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 2\vec{a}_1 + \frac{1}{2}\vec{a}_2$$

$$x_1\vec{a}_1 + x_2\vec{a}_2 = 2\vec{a}_1 + \frac{1}{2}\vec{a}_2 \Rightarrow \begin{matrix} x_1 = 2 \\ x_2 = \frac{1}{2} \end{matrix}$$

$$\boxed{\hat{x} = \begin{pmatrix} 2 \\ 1/2 \end{pmatrix}}$$

Thm 15

A : $m \times n$, lin. indep. cols

$A = QR \longleftarrow$ QR-factorization

$m \times n$, cols are an orthonormal basis for Col A

$n \times n$, upper triangular, positive entries on the diagonal

Then $\underline{\hat{x} = R^{-1} Q^T \vec{b}}$

in practice, write $R\hat{x} = Q^T \vec{b}$ and solve by row reduction

Expl 5

$$A = \begin{pmatrix} 1 & 3 & 5 \\ 1 & 1 & 0 \\ 1 & 1 & 2 \\ 1 & 3 & 3 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 3 \\ 5 \\ 7 \\ -3 \end{pmatrix}$$

Find a least-squares soln to $A\vec{x} = \vec{b}$.

Find an orthonormal basis for Col A (use Gram-Schmidt), then make Q...

$$Q = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

$$\text{Then}\quad R = Q^T A = \overset{\text{calculate}}{\cdots} = \begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix}$$

$$Q^T \vec{b} = \overset{\text{calculate}}{\cdots} = \begin{pmatrix} 6 \\ -6 \\ 4 \end{pmatrix}$$

$$R\hat{x} = Q^T \vec{b} \Rightarrow \begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix} \hat{x} = \begin{pmatrix} 6 \\ -6 \\ 4 \end{pmatrix}$$

Solve... (easy b/c R is upper triangular)...

$$\boxed{\hat{x} = \begin{pmatrix} 10 \\ -6 \\ 2 \end{pmatrix}}$$