Lecture 15.

- Recall from last time that we are trying to find a least squares solution to
$$A\vec{x} = \vec{b}$$
where A is $m \times n$ and $A\vec{x} = \vec{b}$ is possibly inconsistent.

- A "least squares solution" is a vector $\vec{v}$ that minimizes $\|A\vec{v} - \vec{b}\|$

- For any vector $\vec{v}$, $A\vec{v} \in col(A)$, and so from the "Best Approximation Theorem" we want to find $\vec{v}$ such that $A\vec{v} = proj_{col(A)}\vec{b}$
(such a $\vec{v}$ always exists, since $proj_{col(A)}\vec{b} \in col(A)$).

- Thus, finding a least squares solution to
$$A\vec{x} = \vec{b}$$
is equivalent to solving
$$A\vec{x} = proj_{col(A)}\vec{b}. \quad (*)$$

- We can avoid computing $proj_{col(A)}\vec{b}$ by rewriting $(*)$ as
$$\vec{b} - A\vec{x} = \vec{b} - proj_{col(A)}\vec{b}.$$

- multiplying both sides by A^T, we have

$$A^T(\vec{b} - A\vec{x}) = A^T(\vec{b} - \text{proj}_{col(A)}\vec{b}).$$

- Now, $\vec{b} - \text{proj}_{col(A)}\vec{b} \in col(A)^{\perp}$ and hence (by an earlier result: text Theorem 4.8.7(b)) $\vec{b} - \text{proj}_{col(A)}\vec{b} \in null(A^T)$ and hence

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

Equivalently

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

- the normal equation of the system.

- Note that A^TA is a symmetric, $n \times n$ matrix.

- We have shown the following:

Theorem: For any linear system $A\vec{x} = \vec{b}$, the associated normal system

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

is consistent, and all solutions are least squares solutions of $A\vec{x} = \vec{b}$. Furthermore, for any least squares solution $\bar{x}$,

$$A\vec{x} = \text{proj}_{col(A)}\vec{b}.$$

Ex: Consider the overdetermined system

$$x_1 - x_2 = 4$$
$$3x_1 + 2x_2 = 1$$
$$-2x_1 + 4x_2 = 3.$$

Then we can express the system as a matrix equation

$$\underbrace{\begin{bmatrix} 1 & -1 \\ 3 & 2 \\ -2 & 4 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} 4 \\ 1 \\ 3 \end{bmatrix}}_{\vec{b}}.$$

$$A^TA = \begin{bmatrix} 1 & 3 & -2 \\ -1 & 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 3 & 2 \\ -2 & 4 \end{bmatrix} = \begin{bmatrix} 14 & -3 \\ -3 & 21 \end{bmatrix}$$

and

$$A^T\vec{b} = \begin{bmatrix} 1 & 3 & -2 \\ -1 & 2 & 4 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ 10 \end{bmatrix}$$

So the associated normal system is

$$\begin{bmatrix} 14 & -3 \\ -3 & 21 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 10 \end{bmatrix}.$$

$\det(A^TA) = (14)(21) - 9 = 285 \neq 0$, so

there is a unique least squares solution.

$$(A^TA)^{-1} = \frac{1}{285}\begin{bmatrix} 21 & 3 \\ 3 & 14 \end{bmatrix}.$$

So $$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \frac{1}{285}\begin{bmatrix} 21 & 3 \\ 3 & 14 \end{bmatrix}\begin{bmatrix} 1 \\ 10 \end{bmatrix} = \frac{1}{285}\begin{bmatrix} 51 \\ 143 \end{bmatrix}$$

$$= \begin{bmatrix} 17/95 \\ 143/285 \end{bmatrix}$$

While there is not always a unique (see text) least squares solution, we can characterize when there is.

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

1) The columns of A
2) A^TA is invertible.

Theorem: Let A have linearly independent columns. Then $A\vec{x} = \vec{b}$ has a unique least-squares solution $\vec{x} = (A^TA)^{-1}A^T\vec{b}$.

Furthermore,

$$\text{proj}_{col(A)} \vec{b} = A(A^TA)^{-1}A^T\vec{b} = A\vec{x}.$$

Note that if A is square and invertible,
then

$$\text{proj}_{col(A)}\vec{b} = A(A^TA)^{-1}A^T\vec{b} = A\,A^{-1}A^{T^{-1}}A^T\vec{b}$$
$$= \vec{b}.$$

<u>Relation to QR decomposition</u>

In practice, one often uses QR-decomp to find least squares solutions.

<u>Theorem:</u> Let A be an $m \times n$ matrix with linearly independent columns. Suppose $A = QR$. Then the system $A\vec{x} = \vec{b}$ has a unique least squares solution given by

$$\vec{x} = R^{-1}Q^T\vec{b}.$$

<u>Pf:</u> By the previous solution, $A\vec{x} = \vec{b}$ has a unique least squares solution

$$\vec{x} = (A^TA)^{-1}A^T\vec{b}.$$

Letting $A = QR$, we have

$$\vec{x} = \left((QR)^T QR\right)^{-1} (QR)^T \vec{b}$$

$$= \left(R^T Q^T Q R\right)^{-1} R^T Q^T \vec{b}$$

Since the columns of Q are orthonormal, $Q Q^T = I$

So

$$\vec{x} = \left(R^T R\right)^{-1} R^T Q^T \vec{b}$$

$$= R^{-1} {R^T}^{-1} R^T Q^T \vec{b}$$

$$= R^{-1} Q^T \vec{b}. \qquad \square.$$