$$\begin{bmatrix} \times & \times & & \times \\ & \times & & \\ 0 & & \ddots & \\ & & & \times \end{bmatrix}$$

# Math 2270-6

$$\begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

# Notes of 11/12/19

- Tying up loose end from yesterday. Suppose

$$A = [\,\mathbf{a}_1 \quad \mathbf{a}_2 \quad \ldots \quad \mathbf{a}_n\,]$$

  is $m \times n$ and

$$\underset{m\times n}{A} = \underset{m\times n}{Q}\,\underset{n\times n}{R}$$

  $Q^TQ = n\times n$ identity

  where

$$Q = [\,\mathbf{q}_1 \quad \mathbf{q}_2 \quad \ldots \quad \mathbf{q}_n\,]$$

  is $m \times n$ with orthonormal columns and $R$ is $n \times n$ upper triangular.

- Then the first $k$ columns of $A$ span the same space as the first $k$ columns of $Q$.

- In principle, $Q$ can be computed by applying the Gram-Schmidt process to the columns of $A$.

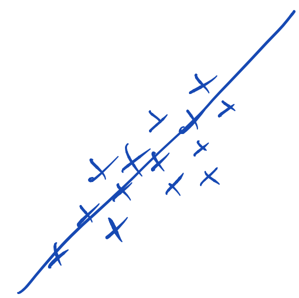
- Since

$$Q^T Q = I_n$$

  with $I_n$ being the $n \times n$ identity matrix we can compute $R$ by

$$R = Q^T A.$$

# 6.5 Least Squares Problems



- We start with a somewhat elaborate example. You may have seen it before in Calculus, and we'll use Calculus notation. Then we will generalize it, turn it into a Linear Algebra Problems, and change the notation to Linear Algebra notation.
- On your calculator there may be a "linear regression" button.
- What does it do?
- It computes a line that approximates a set of specified points in an optimal sense. The points may represent, for example, inaccurately measured values.
- Suppose we are given the points $(2, 2)$, $(5, 5)$, and $(7, 5)$. There is no line that passes through all three points, but we can represent them approximately by a line, as shown in Figure 1.
- How do we find that line?
- We use three points in this example for computational simplicity, there could be many more points!
- Lets present our line as

  $$y = L(x) = mx + b$$

  as usual.
- The key idea is to minimize the sum of squares:

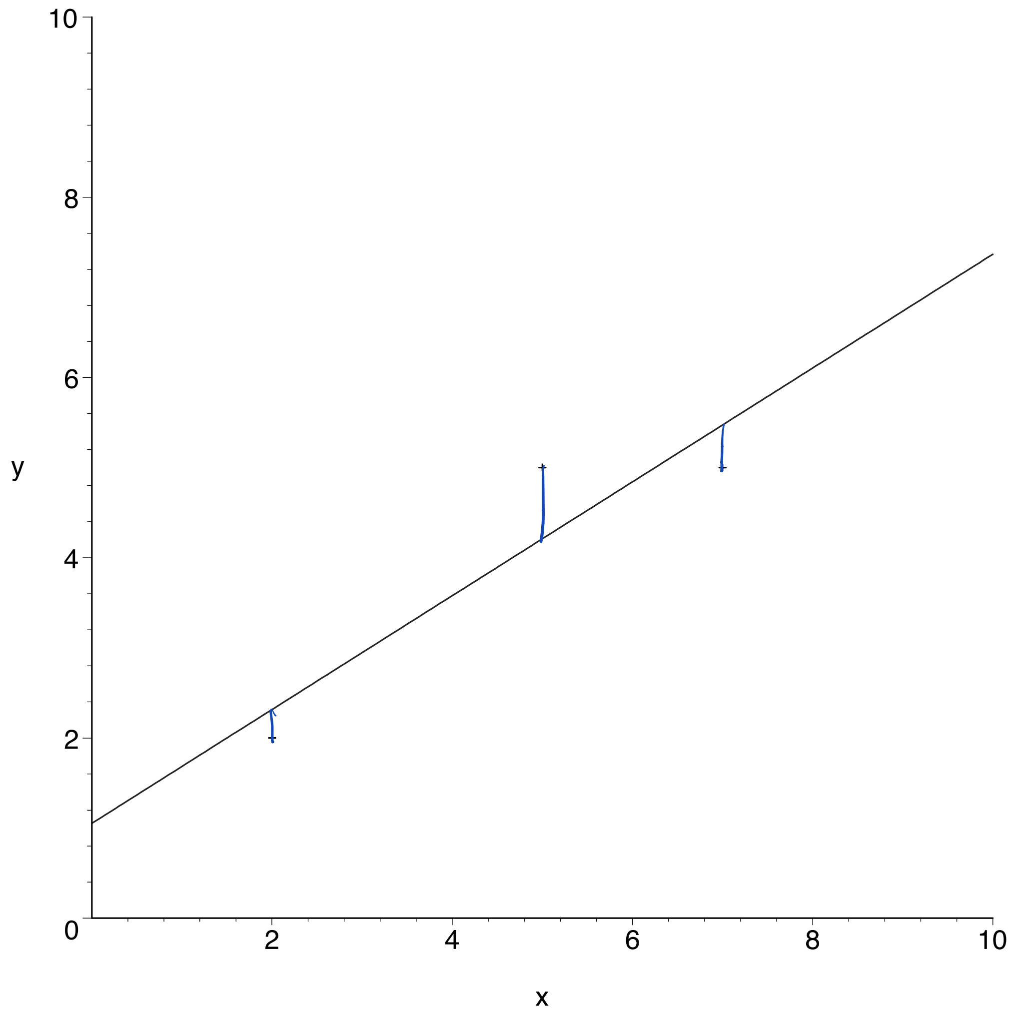



**Figure 1.** 3 points and a line.

$$
\begin{aligned}
F(m,b) &= \big(2-(2m+b)\big)^2 \\
&+ \big(5-(5m+b)\big)^2 \\
&+ \big(5-(7m+b)\big)^2 = \min
\end{aligned}
\tag{1}
$$

- Thus we want to minimize a function of two variables. In Calculus we learned that the way to do is to compute the gradient, set it to zero, and then solve the resulting system.

$$\nabla F = \begin{bmatrix} F_m(m,b) \\ F_b(m,b) \end{bmatrix} = \mathbf{0}.$$

- In our case, since we are minimizing a sum of squares, we will get a **linear system**.
- We could expand the squares in (1) and then differentiate, or differentiate first. The second approach is better. We get

$$\begin{aligned} F_m(m,b) &= -2\bigl(2-(2m+b)\bigr)\times 2 \\ &- \quad 2\bigl(5-(5m+b)\bigr)\times 5 \\ &- \quad 2\bigl(5-(7m+b)\bigr)\times 7 \qquad = \quad 0 \end{aligned}$$

i.e.,

$$-2\bigl[2\times2+5\times5+5\times7-m(2\times2+5\times5+7\times7)-b(2+5+7)\bigr]=0.$$

This becomes

$$78m + 14b = 64. \qquad (2)$$

- similarly,

$$\begin{aligned} F_b(m,b) &= -2\bigl(2-(2m+b)\bigr) \\ &- \quad 2\bigl(5-(5m+b)\bigr) \\ &- \quad 2\bigl(5-(7m+b)\bigr) \qquad = \quad 0 \end{aligned}$$

i.e.,

$$-2\bigl[2\times2+5\times5+5\times7-m(2\times2+5\times5+7\times7)-b(2+5+7)\bigr]=0.$$

This gives the equation

$$14m + 3b = 12 \tag{3}$$

- The equations (2) and (3) are two linear equations in the 2 unknowns $m$ and $b$. Solving them gives

$$m = \frac{12}{19} \quad \text{and} \quad b = \frac{20}{19}.$$

- The points and the line

$$y = \frac{12}{19}x + \frac{20}{19}$$

are shown in Figure 1.

- We might be given hundreds of points. The calculation just indicated would become quite tedious. So let's do the problem in general.
- Suppose we are given $n$ points $(x_i, y_i)$, $i = 1, \ldots, n$.
- We want to find $m$ and $b$ such that

$$y_i \approx m x_i + b, \qquad i = 1, \ldots, n \tag{4}$$

- To that end we pick $m$ and $b$ so as to minimize

$$F(m, b) = \sum_{i=1}^{n} \big(y_i - (m x_i + b)\big)^2 = \min.$$

- As usual we compute the partial derivatives and set them equal to zero:

$$\frac{\partial}{\partial m}F(m,b) = -2\sum_{i=1}^{n}\big(y_i - (mx_i + b)\big)x_i = 0$$

and

$$\frac{\partial}{\partial b}F(m,b) = -2\sum_{i=1}^{n}\big(y_i - (mx_i + b)\big) = 0$$

- Dividing by -2, distributing the sums, and collecting the $m$ and $b$ terms on one side and the constant terms on the other side gives the linear system

$$\begin{array}{ccccc} m\sum_{i=1}^{n} x_i^2 & + & b\sum_{i=1}^{n} x_i & = & \sum_{i=1}^{n} x_i y_i \\ m\sum_{i=1}^{n} x_i & + & b\sum_{i=1}^{n} 1 & = & \sum_{i=1}^{n} y_i \end{array}$$

- This is the linear system your calculator solves when you press the linear regression button.

- In our previous example we have the data

| $x_i$ | $y_i$ |
|---|---|
| 2 | 2 |
| 5 | 5 |
| 7 | 5 |

and get

$$
\begin{array}{rcccl}
\sum x_i^2 & = & 2^2+5^2+7^2 & = & 78 \\
\sum x_i & = & 2+5+7 & = & 14 \\
\sum 1 & = & 1+1+1 & = & 3 \\
\sum x_i y_i & = & 2\times 2+5\times 5+7\times 5 & = & 64 \\
\sum y_i & = & 2+5+5 & = & 12
\end{array}
$$

which leads to the same linear system

$$
\begin{array}{rcrcl}
78m & + & 14b & = & 64 \\
14m & + & 3b & = & 12
\end{array}
$$

as before.

- Of course, instead of a linear function you could use a quadratic function. You'll get 3 equations in 3 unknowns.
- The concept we discussed is much more general. You could consider polynomials of degree greater than 2 or even non-polynomial functions.
- Let's take a different tack. Suppose all the points actually are on the lines. Then we would have the equations

$$
y_i = mx_i + b, \qquad i = 1, \ldots, n \tag{5}
$$

- We can write this as the linear system

$A \quad x \quad = \quad b \qquad \longleftrightarrow \qquad \|Ax - b\|^2 = \min$

$$
\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}
$$

- However, minimizing the sum of squares of the difference between the left and right sides of the equations (5) in this case gives the **Least Squares Problem**

$$\left\| \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \right\|^2 = \min$$

- Also notice that the previously obtained linear system

$$\begin{array}{ccccc} m\sum_{i=1}^n x_i^2 & + & b\sum_{i=1}^n x_i & = & \sum_{i=1}^n x_i y_i \\ m\sum_{i=1}^n x_i & + & b\sum_{i=1}^n 1 & = & \sum_{i=1}^n y_i \end{array}$$

$\cancel{0 = 0}$

$\cancel{Ax = b}$

$\cancel{A^T A x = A^T b}$

can be rewritten in terms of our matrix notation as

$A^T A x = A^T b$

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}^T \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}^T \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

## Least Squares in General

- Let's take a fresh start (and also make a change in notation). Suppose we have an overdetermined linear system

$$A\mathbf{x} = \mathbf{b} \tag{6}$$

- Here $A$ is $m \times n$, $\mathbf{x}$ is in $\mathbb{R}^n$, $\mathbf{b}$ is in $\mathbb{R}^m$, and $m \geq n$ (and typically, $m > n$).
- Usually, the system (6) will not have a solution. In that case, the next best thing is to solve the alternative problem

$$\|A\mathbf{x} - \mathbf{b}\|^2 = \min$$

- In other words (the words of our textbook), we want to find a vector $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

  for all $\mathbf{x}$ in $\mathbb{R}^n$.
- The textbook calls such an $\hat{\mathbf{x}}$ a **Least Squares Solution** of

$$A\mathbf{x} = \mathbf{b}.$$

- I would call it a solution of

$$\|A\mathbf{x} - \mathbf{b}\| = \min.$$

We will soon see that $\hat{x}$ is unique if the columns of $A$ are linearly independent.

- First: **Theorem 13** (p. 363) The set of least square solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the **normal equations**

$$A^T A\mathbf{x} = A^T\mathbf{b}.$$

- Before seeing why this is true, let's go back to our introductory example.
- There

$$A = \begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 5 \\ 5 \end{bmatrix}.$$

- We get

$$A^T A\mathbf{x} = \begin{bmatrix} 78 & 14 \\ 14 & 3 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 64 \\ 12 \end{bmatrix}$$

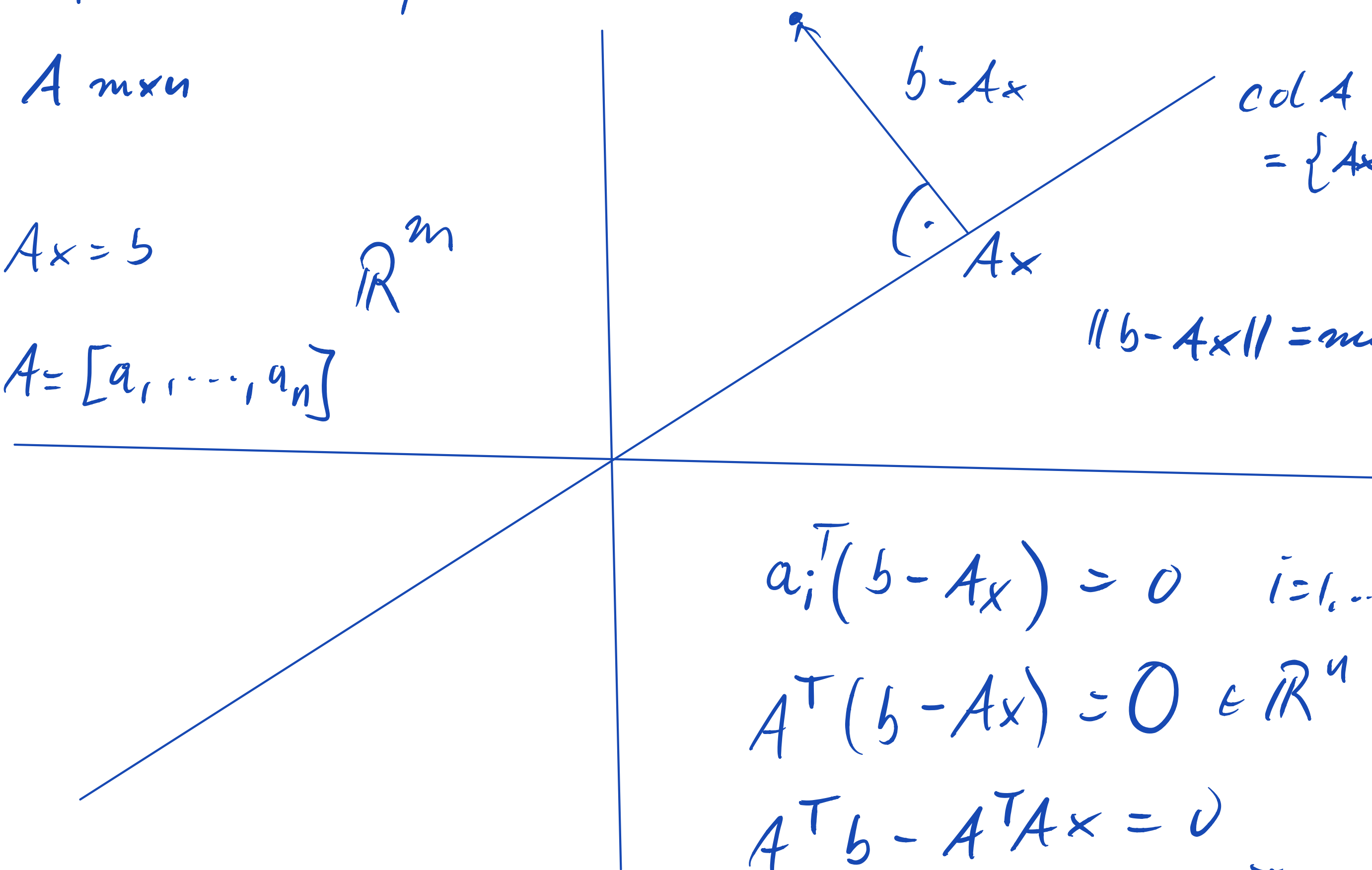
- This is the same set of equations as before, with the same solution.
- So let's see why Theorem 14 is true

1. Calculus, exercise

$A$ $m \times n$

$Ax = b$

$A = [a_1, \ldots, a_n]$




$\|b - Ax\| = \min$

$$a_i^T (b - Ax) = 0 \quad i = 1, \ldots, n$$

$$A^T (b - Ax) = 0 \in \mathbb{R}^n$$

$$A^T b - A^T A x = 0$$

$$A^T A x = A^T b$$

$$\|Ax - b\|^2 = \min$$

$$A^T A x = A^T b$$

Normal Equations

- We can tell more than Theorem 13!
- **Theorem 14** (p. 365) Let $A$ be an $m \times n$ matrix. The following statements are logically equivalent. (This means they are either all true or all false):

**a.** The equation $A\mathbf{x} = \mathbf{b}$ has a unique least square solution for each $\mathbf{b}$ in $\mathbb{R}^m$.

**b.** The columns of $A$ are linearly independent.

**c.** The matrix $A^T A$ is invertible.

## Using the $QR$ factorization

$R = Q^T A$ $\qquad$ $\underset{m\times n}{A} = \underset{m\times m}{Q}\,\underset{m\times n}{R}$ $\qquad$ $Q$ $m\times m$ orthogonal

$\|Ax - b\|^2 = \min$ $\qquad$ $R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$

$Q^T Q = I$

$Q = [\underset{m\times n}{Q_1}, Q_2]$ $\qquad$ $R_1$ $n\times n$ upper triangular

$A = [Q_1 \; Q_2]\begin{bmatrix} R_1 \\ 0 \end{bmatrix} [Q_1 R_1 + Q_2 0] = [Q_1 R_1]$

$\begin{bmatrix} x & \ddots & x \\ & & x \\ & 0 & \end{bmatrix}$

$[a_1\; a_2 \cdots a_n] = [q_1 \cdots q_n \; q_{n+1} \cdots q_m]$

$$\|Qx\|^2 = (Qx)^T(Qx) = x^T Q^T Q x = x^T x = \|x\|^2$$

$$\begin{aligned}
\min = \|Ax - b\|^2 &= \|Q^T(Ax - b)\|^2 \\
&= \|Q^T A x - Q^T b\|^2 \\
&= \|Rx - Q^T b\|^2 \\
&= \left\| \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} b \right\|^2 \\
&= \left\| \begin{bmatrix} R_1 x \\ 0 \end{bmatrix} - \begin{bmatrix} Q_1^T b \\ Q_2^T b \end{bmatrix} \right\|^2 = \min
\end{aligned}$$

$$= \|R_1 x - Q_1^T b\|^2 + \|Q_2^T b\|^2 = \min$$

solve $R_1 x = Q_1^T b$