Announcements
Wednesday, November 28

► Please fill out your CIOS survey!

If 85% of the class completes the survey by 11:59pm on December 7, then we will drop two quizzes instead of one.

► Final exam time: Tuesday, December 11, 6–8:50pm.

► WeBWorK 6.6, 7.1, 7.2 are due today.

► No quiz on Friday! But this is the only recitation on chapter 7.

► My office is Skiles 244 and Rabin office hours are: Mondays, 12–1pm; Wednesdays, 1–3pm.
Section 7.5

The Method of Least Squares
Motivation

We now are in a position to solve the motivating problem of this third part of the course:

**Problem**

Suppose that $Ax = b$ does not have a solution. What is the best possible approximate solution?

To say $Ax = b$ does not have a solution means that $b$ is not in $\text{Col } A$.

The closest possible $\hat{b}$ for which $Ax = \hat{b}$ does have a solution is $\hat{b} = b_{\text{Col } A}$.

Then $A\hat{x} = \hat{b}$ is a consistent equation.

A solution $\hat{x}$ to $A\hat{x} = \hat{b}$ is a **least squares solution**.
Let $A$ be an $m \times n$ matrix.

**Definition**

A **least squares solution** of $Ax = b$ is a vector $\hat{x}$ in $\mathbb{R}^n$ such that

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

for all $x$ in $\mathbb{R}^n$.

Note that $b - A\hat{x}$ is in $(\text{Col } A)^\perp$.

In other words, a least squares solution $\hat{x}$ solves $Ax = b$ as closely as possible.

Equivalently, a least squares solution to $Ax = b$ is a vector $\hat{x}$ in $\mathbb{R}^n$ such that

$$A\hat{x} = \hat{b} = b_{\text{Col } A}.$$

This is because $\hat{b}$ is the closest vector to $b$ such that $A\hat{x} = \hat{b}$ is consistent.
Least Squares Solutions
Computation

We want to solve $A\hat{x} = \hat{b} = b_{\text{Col } A}$. Or, $A\hat{x} = b_W$ for $W = \text{Col } A$.
To compute $b_W$ we need to solve $A^T Av = A^T b$; then $b_W = Av$.

**Conclusion:** $\hat{x}$ is just a solution of $A^T Av = A^T b$!

**Theorem**
The least squares solutions of $Ax = b$ are the solutions of

$$(A^T A)\hat{x} = A^T b.$$

Note we compute $\hat{x}$ directly, without computing $\hat{b}$ first.
Find the least squares solutions of \( Ax = b \) where:

\[
A = \begin{pmatrix}
0 & 1 \\
1 & 1 \\
2 & 1
\end{pmatrix} \quad b = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.
\]

So the only least squares solution is \( \hat{x} = \begin{pmatrix} -3 \\ 5 \end{pmatrix} \).
Least Squares Solutions

Example, continued

How close did we get?

$$\hat{b} = Ax = \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} -3 \\ 5 \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix}$$

The distance from $b$ is

$$\|b - A\hat{x}\| = \left\| \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \right\| = \sqrt{1^2 + (-2)^2 + 1^2} = \sqrt{6}.$$

Note that $\begin{pmatrix} -3 \\ 5 \end{pmatrix}$ records the coefficients of $v_1$ and $v_2$ in $\hat{b}$.
Find the least squares solutions of $Ax = b$ where:

$$A = \begin{pmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{pmatrix} \quad b = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$  

So the only least squares solution is $\hat{x} = \begin{pmatrix} 1/3 \\ -1/3 \end{pmatrix}$. 

[interactive]
Least Squares Solutions
Uniqueness

When does \( Ax = b \) have a *unique* least squares solution \( \hat{x} \)?

**Theorem**
Let \( A \) be an \( m \times n \) matrix. The following are equivalent:

1. \( Ax = b \) has a *unique* least squares solution for all \( b \) in \( \mathbb{R}^n \).
2. The columns of \( A \) are linearly independent.
3. \( A^T A \) is invertible.

In this case, the least squares solution is \((A^T A)^{-1}(A^T b)\).

**Why?** If the columns of \( A \) are linearly *dependent*, then \( A\hat{x} = \hat{b} \) has many solutions:

\[
\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}
\]

\[ b = \hat{b} \]

Note: \( A^T A \) is always a square matrix, but it need not be invertible.
Find the best fit line through \((0, 6), (1, 0),\) and \((2, 0)\).
Poll

What does the best fit line minimize?

A. The sum of the squares of the distances from the data points to the line.
B. The sum of the squares of the vertical distances from the data points to the line.
C. The sum of the squares of the horizontal distances from the data points to the line.
D. The maximal distance from the data points to the line.

Poll

Answer: B. See the picture on the previous slide.
Find the best fit ellipse for the points \((0, 2), (2, 1), (1, -1), (-1, -2), (-3, 1), (-1, -1)\).

The general equation for an ellipse is

\[
x^2 + Ay^2 + Bxy + Cx + Dy + E = 0
\]

So we want to solve:

\[
(0)^2 + A(2)^2 + B(0)(2) + C(0) + D(2) + E = 0
\]

\[
(2)^2 + A(1)^2 + B(2)(1) + C(2) + D(1) + E = 0
\]

\[
(1)^2 + A(-1)^2 + B(1)(-1) + C(1) + D(-1) + E = 0
\]

\[
(-1)^2 + A(-2)^2 + B(-1)(-2) + C(-1) + D(-2) + E = 0
\]

\[
(-3)^2 + A(1)^2 + B(-3)(1) + C(-3) + D(1) + E = 0
\]

\[
(-1)^2 + A(-1)^2 + B(-1)(-1) + C(-1) + D(-1) + E = 0
\]

In matrix form:

\[
\begin{pmatrix}
4 & 0 & 0 & 2 & 1 \\
1 & 2 & 2 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
4 & 2 & -1 & -2 & 1 \\
1 & -3 & -3 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
\end{pmatrix}
\begin{pmatrix}
A \\
B \\
C \\
D \\
E
\end{pmatrix} =
\begin{pmatrix}
0 \\
-4 \\
-1 \\
-1 \\
-9 \\
-1
\end{pmatrix}.
\]
Application

Best fit ellipse, continued

\[ A = \begin{pmatrix}
4 & 0 & 0 & 2 & 1 \\
1 & 2 & 2 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
4 & 2 & -1 & -2 & 1 \\
1 & -3 & -3 & 1 & 1 \\
1 & 1 & -1 & -1 & 1
\end{pmatrix}, \quad
b = \begin{pmatrix}
0 \\
-4 \\
-1 \\
-1 \\
-9 \\
-1
\end{pmatrix}. \]

\[ A^T A = \begin{pmatrix}
36 & 7 & -5 & 0 & 12 \\
7 & 19 & 9 & -5 & 1 \\
-5 & 9 & 16 & 1 & -2 \\
0 & -5 & 1 & 12 & 0 \\
12 & 1 & -2 & 0 & 6
\end{pmatrix}, \quad
A^T b = \begin{pmatrix}
-19 \\
17 \\
20 \\
-9 \\
-16
\end{pmatrix}. \]

Row reduce:

\[
\begin{pmatrix}
36 & 7 & -5 & 0 & 12 & -19 \\
7 & 19 & 9 & -5 & 1 & 17 \\
-5 & 9 & 16 & 1 & -2 & 20 \\
0 & -5 & 1 & 12 & 0 & -9 \\
12 & 1 & -2 & 0 & 6 & -16
\end{pmatrix} \xrightarrow{\text{Row reduce}} \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 405/266 \\
0 & 1 & 0 & 0 & 0 & -89/133 \\
0 & 0 & 1 & 0 & 0 & 201/133 \\
0 & 0 & 0 & 1 & 0 & -123/266 \\
0 & 0 & 0 & 0 & 1 & -687/133
\end{pmatrix}
\]

Best fit ellipse:

\[ x^2 + \frac{405}{266} y^2 - \frac{89}{133} xy + \frac{201}{133} x - \frac{123}{266} y - \frac{687}{133} = 0 \]

or

\[ 266x^2 + 405y^2 - 178xy + 402x - 123y - 1374 = 0. \]
Application
Best fit ellipse, picture

Remark: Gauss invented the method of least squares to do exactly this: he predicted the (elliptical) orbit of the asteroid Ceres as it passed behind the sun in 1801.
Application

Best fit parabola

What least squares problem $Ax = b$ finds the best parabola through the points $(-1, 0.5), (1, -1), (2, -0.5), (3, 2)$?

Answer: $88y = 53x^2 \quad \frac{379}{5}x - 82$
Application
Best fit parabola, picture

\[ 88y = 53x^2 - \frac{379}{5}x - 82 \]

[interactive]
What least squares problem $Ax = b$ finds the best linear function $f(x, y)$ fitting the following data?

<table>
<thead>
<tr>
<th>$x$</th>
<th>$y$</th>
<th>$f(x, y)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>-1</td>
<td>4</td>
</tr>
</tbody>
</table>

Answer: $f(x, y) = -\frac{3}{2}x - \frac{3}{2}y + 2$
Application
Best fit linear function, picture

Graph of
\[ f(x, y) = -\frac{3}{2}x - \frac{3}{2}y + 2 \]
For fun: what is the best-fit function of the form

\[ y = A + B \cos(x) + C \sin(x) + D \cos(2x) + E \sin(2x) + F \cos(3x) + G \sin(3x) \]

passing through the points

\[
\begin{align*}
(-4, -1), & \quad (-3, 0), & \quad (-2, -1.5), & \quad (-1, .5), & \quad (0, 1), & \quad (1, -1), & \quad (2, -.5), & \quad (3, 2), & \quad (4, -1)
\end{align*}
\]

\[ y \approx -0.14 + 0.26 \cos(x) - 0.23 \sin(x) + 1.11 \cos(2x) - 0.60 \sin(2x) - 0.28 \cos(3x) + 0.11 \sin(3x) \]
A least squares solution of $Ax = b$ is a vector $\hat{x}$ such that $\hat{b} = A\hat{x}$ is as close to $b$ as possible.

This means that $\hat{b} = b_{\text{Col } A}$.

One way to compute a least squares solution is by solving the system of equations

$$(A^T A)\hat{x} = A^T b.$$ 

Note that $A^T A$ is a (symmetric) square matrix.

Least-squares solutions are unique when the columns of $A$ are linearly independent.

You can use least-squares to find best-fit lines, parabolas, ellipses, planes, etc.