Announcements

Wednesday, November 29

- Final exam location: **Clough 152**
- Please fill out your CIOS survey!
- Post topics for Monday's review on Piazza.
- **Reading day:** Math is 1–3pm on December 6 in Clough 144 and 152. I'll be there for part of it.
- WeBWorK 6.1, 6.2, 6.3 are due today at 11:59pm.
- WeBWorK 6.4, 6.5 are posted and will be covered on the final, but they are not graded.
- No quiz on Friday! But this is the only recitation on chapter 6.
- My office is Skiles 244. Rabinoffice hours are Monday, 1–3pm and Tuesday, 9–11am.

Section 6.5

Least Squares Problems

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 $\operatorname{Col} A$.

The closest possible $\widehat{b}$ for which $Ax = \widehat{b}$ does have a solution is $\widehat{b} = \operatorname{proj}_{\operatorname{Col} A}(b)$.

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

A solution $\widehat{x}$ to $A\widehat{x} = \widehat{b}$ is a **least squares solution.**

Least Squares Solutions

Let A be an $m \times n$ matrix.

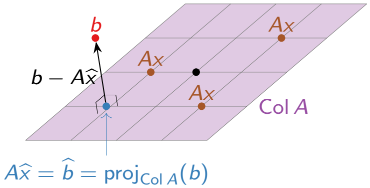
Definition

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

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

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

Note that $b - A\widehat{x}$ is in $(\mathrm{Col}\,A)^\perp$.



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

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

$$A\widehat{x} = \widehat{b} = \mathrm{proj}_{\mathrm{Col}\,A}(b).$$

This is because $\widehat{b}$ is the closest vector to b such that $A\widehat{x} = \widehat{b}$ is consistent.

Theorem

The least squares solutions to $Ax = b$ are the solutions to

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

This is just another $Ax = b$ problem, but with a *square* matrix $A^T A$!
Note we compute $\widehat{x}$ directly, without computing $\widehat{b}$ first.

Why is this true?

Alternative when A has orthogonal columns $v_1, v_2, \ldots, v_n$:

$$\widehat{b} = \mathrm{proj}_{\mathrm{Col}\,A}(b) = \sum_{i=1}^{n} \frac{b \cdot v_i}{v_i \cdot v_i}\, v_i$$

The right hand side equals $A\widehat{x}$, where $\widehat{x} = \left(\frac{b \cdot v_1}{v_1 \cdot v_1}, \ \frac{b \cdot v_2}{v_2 \cdot v_2}, \ \cdots, \ \frac{b \cdot v_n}{v_n \cdot v_n} \right).$

Least Squares Solutions

Example

Find the least squares solutions to $Ax = b$ where:

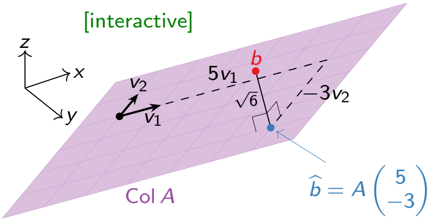
$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \qquad b = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.$$

So the only least squares solution is $\widehat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.

Least Squares Solutions

Example, continued

How close did we get?



Let

$$v_1 = \begin{pmatrix}1\\1\\1\end{pmatrix} \quad \text{and} \quad v_2 = \begin{pmatrix}0\\1\\2\end{pmatrix}$$

be the columns of A, and let $\mathcal{B} = \{v_1, v_2\}$.

Note $\widehat{x} = \binom{5}{-3}$ is just the $\mathcal{B}$-coordinates of $\widehat{b}$, in $\text{Col}\,A = \text{Span}\{v_1, v_2\}$.

Least Squares Solutions

Second example

Find the least squares solutions to $Ax = b$ where:

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

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

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When does $Ax = b$ have a *unique* least squares solution $\widehat{x}$?

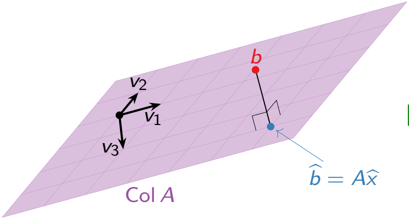
Theorem

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 $\mathbf{R}^n$.
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 *de*pendent, then $A\widehat{x} = \widehat{b}$ has many solutions:



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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 $(2,0)$.

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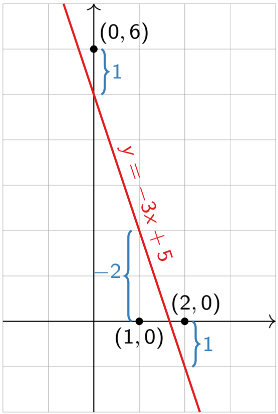


$$A\begin{pmatrix}5\\-3\end{pmatrix} - \begin{pmatrix}6\\0\\0\end{pmatrix} = \begin{pmatrix}1\\-2\\1\end{pmatrix}$$

Poll

Application

Best fit ellipse

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:

$$\begin{aligned}
(0)^2 + A(2)^2 + B(0)(2) + C(0) + D(2) + E &= 0 \\
(2)^2 + A(1)^2 + B(2)(1) + C(2) + D(1) + E &= 0 \\
(1)^2 + A(-1)^2 + B(1)(-1) + C(1) + D(-1) + E &= 0 \\
(-1)^2 + A(-2)^2 + B(-1)(-2) + C(-1) + D(-2) + E &= 0 \\
(-3)^2 + A(1)^2 + B(-3)(1) + C(-3) + D(1) + E &= 0 \\
(-1)^2 + A(-1)^2 + B(-1)(-1) + C(-1) + D(-1) + E &= 0
\end{aligned}$$

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

$$A = \begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \\ -1 \end{pmatrix}.$$

$$A^T A = \begin{pmatrix} 36 & 7 & -5 & 0 & 12 \\ 7 & 19 & 9 & -5 & 1 \\ -5 & 9 & 16 & 1 & -2 \\ 0 & -5 & 1 & 12 & 0 \\ 12 & 1 & -2 & 0 & 6 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -19 \\ 17 \\ 20 \\ -9 \\ -16 \end{pmatrix}$$

Row reduce:

$$\left(\begin{array}{ccccc|c} 36 & 7 & -5 & 0 & 12 & -19 \\ 7 & 19 & 9 & -5 & 1 & 17 \\ -5 & 9 & 16 & 1 & -2 & 20 \\ 0 & -5 & 1 & 12 & 0 & -9 \\ 12 & 1 & -2 & 0 & 6 & -16 \end{array}\right) \rightsquigarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & 405/266 \\ 0 & 1 & 0 & 0 & 0 & -89/133 \\ 0 & 0 & 1 & 0 & 0 & 201/133 \\ 0 & 0 & 0 & 1 & 0 & -123/266 \\ 0 & 0 & 0 & 0 & 1 & -687/133 \end{array}\right)$$

Best fit ellipse:

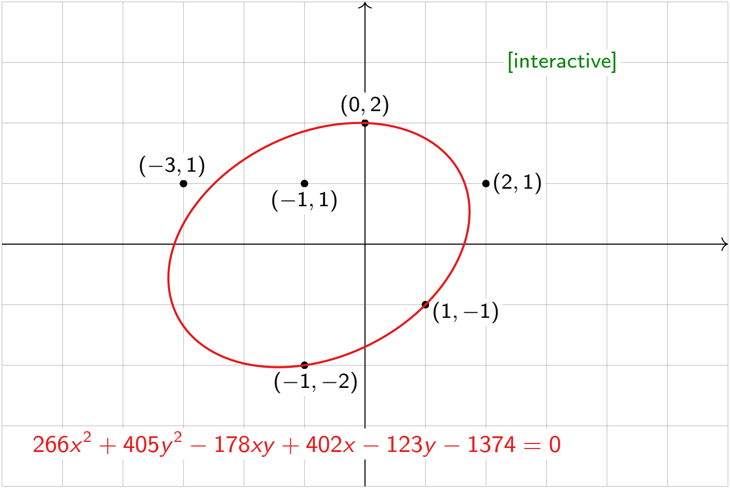
$$x^2 + \frac{405}{266}y^2 - \frac{89}{133}xy + \frac{201}{133}x - \frac{123}{266}y - \frac{687}{133} = 0$$

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.

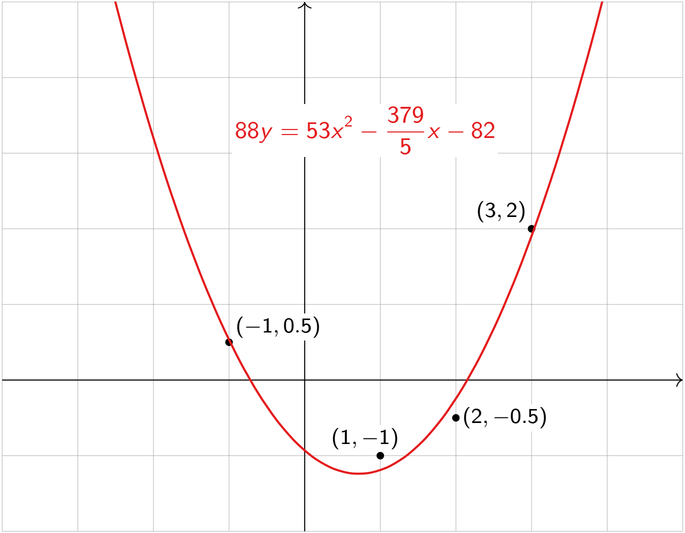
What least squares problem $Ax = b$ finds the best parabola through the points $(-1, 0.5)$, $(1, -1)$, $(2, -0.5)$, $(3, 2)$?

Answer:

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

Application

Best fit parabola, picture



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Application

Best fit linear function

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

x	y	$f(x,y)$
1	0	0
0	1	1
-1	0	3
0	-1	4

Answer: $$f(x, y) = -\frac{3}{2}x - \frac{3}{2}y + 2$$

Application

Best fit linear function, picture

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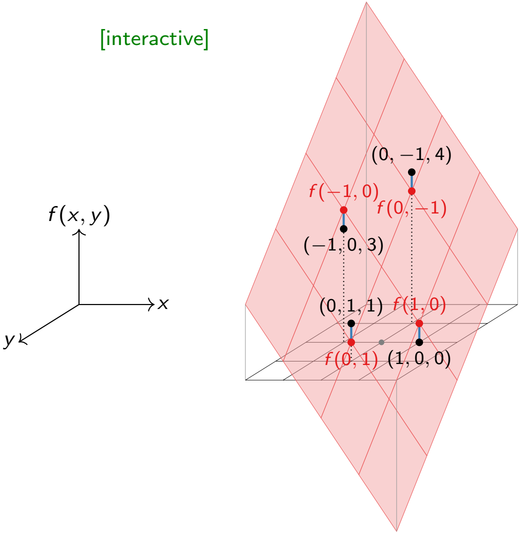


Graph of

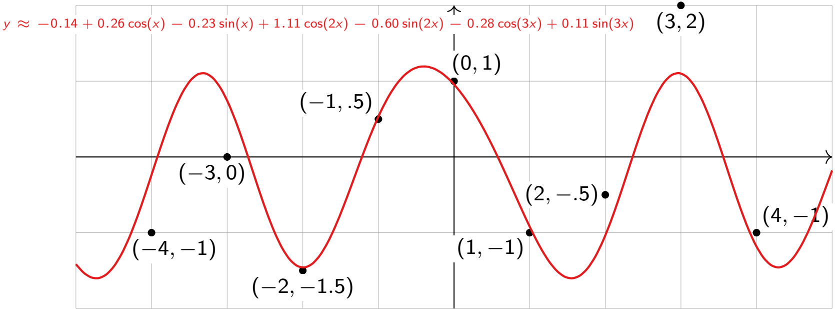
$$f(x,y) = -\frac{3}{2}x - \frac{3}{2}y + 2$$

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

$$\begin{pmatrix}-4\\-1\end{pmatrix}, \begin{pmatrix}-3\\0\end{pmatrix}, \begin{pmatrix}-2\\-1.5\end{pmatrix}, \begin{pmatrix}-1\\.5\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}, \begin{pmatrix}1\\-1\end{pmatrix}, \begin{pmatrix}2\\-.5\end{pmatrix}, \begin{pmatrix}3\\2\end{pmatrix}, \begin{pmatrix}4\\-1\end{pmatrix}?$$



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Summary

- A **least squares solution** of $Ax = b$ is a vector $\widehat{x}$ such that $\widehat{b} = A\widehat{x}$ is *as close to* b *as possible*.
- This means that $\widehat{b} = \text{proj}_{\text{Col } A}(b)$.
- One way to compute a least squares solution is by solving the system of equations
$$(A^T A)\widehat{x} = A^T b.$$
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.