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.

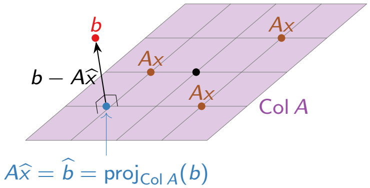
Definition

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

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

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

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



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?

- We want to find $\widehat{x}$ such that $A\widehat{x} = \mathrm{proj}_{\mathrm{Col}\,A}(b)$.
- This means $b - A\widehat{x}$ is in $(\mathrm{Col}\,A)^\perp$.
- Recall that $(\mathrm{Col}\,A)^\perp = \mathrm{Nul}(A^T)$.
- So $b - A\widehat{x}$ is in $(\mathrm{Col}\,A)^\perp$ if and only if $A^T(b - A\widehat{x}) = 0$.
- In other words, $A^T A\widehat{x} = A^T b$.

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 $\widehat{x} = \left(\frac{b \cdot v_1}{v_1 \cdot v_1}, \frac{b \cdot v_2}{v_2 \cdot v_2}, \cdots, \frac{b \cdot v_n}{v_n \cdot v_n} \right)$.

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

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

We have

$$A^T A = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 3 \\ 3 & 5 \end{pmatrix}$$

and

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

Row reduce:

$$\left(\begin{array}{cc|c} 3 & 3 & 6 \\ 3 & 5 & 0 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|c} 1 & 0 & 5 \\ 0 & 1 & -3 \end{array}\right).$$

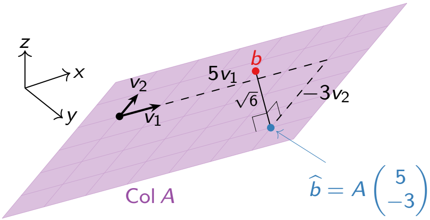
So the only least squares solution is $\widehat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.

How close did we get?

$$\widehat{b} = A\widehat{x} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 5 \\ -3 \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix}$$

The distance from b is

$$\|b - A\widehat{x}\| = \left\| \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix} \right\| = \left\| \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \right\| = \sqrt{1^2 + (-2)^2 + 1^2} = \sqrt{6}.$$



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 Col $A = \text{Span}\{v_1, v_2\}$.

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

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

We have

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

and

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

Row reduce:

$$\left(\begin{array}{cc|c} 5 & -1 & 2 \\ -1 & 5 & -2 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|c} 1 & 0 & 1/3 \\ 0 & 1 & -1/3 \end{array}\right).$$

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

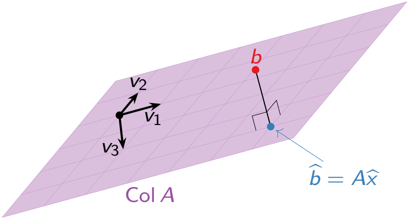
When does $Ax = b$ have a *unique* least squares solution $\widehat{x}$?

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:



Note: $A^T A$ is always a square matrix, but it need not be invertible.

Application

Data modeling: best fit line

Find the best fit line through $(0,6)$, $(1,0)$, and $(2,0)$.

The general equation of a line is

$$y = C + Dx.$$

So we want to solve:

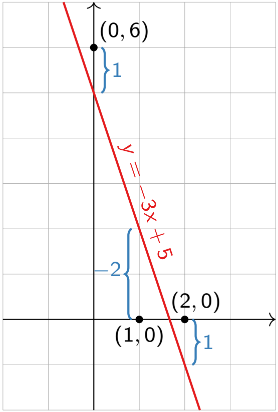
$$\begin{aligned} 6 &= C + D\cdot 0 \\ 0 &= C + D\cdot 1 \\ 0 &= C + D\cdot 2. \end{aligned}$$

In matrix form:

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.$$

We already saw: the least squares solution is $\binom{5}{-3}$. So the best fit line is

$$y = -3x + 5.$$



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

Poll

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.

Answer: B. See the picture on the previous slide.

Find the best fit ellipse for the points $(0, 2)$, $(2, 1)$, $(1, -1)$, $(-1, -2)$, $(-3, 1)$.

The general equation for an ellipse is

$$x^2 + Ay^2 + Bxy + Cx + Dy + E = 0$$

So we want to solve:

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

In matrix form:

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

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

$$A^T A = \begin{pmatrix} 35 & 6 & -4 & 1 & 11 \\ 6 & 18 & 10 & -4 & 0 \\ -4 & 10 & 15 & 0 & -1 \\ 1 & -4 & 0 & 11 & 1 \\ 11 & 0 & -1 & 1 & 5 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -18 \\ 18 \\ 19 \\ -10 \\ -15 \end{pmatrix}$$

Row reduce:

$$\left(\begin{array}{ccccc|c} 35 & 6 & -4 & 1 & 11 & -18 \\ 6 & 18 & 10 & -4 & 0 & 18 \\ -4 & 10 & 15 & 0 & -1 & 19 \\ 1 & -4 & 0 & 11 & 1 & -10 \\ 11 & 0 & -1 & 1 & 5 & -15 \end{array}\right) \rightsquigarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & 16/7 \\ 0 & 1 & 0 & 0 & 0 & -8/7 \\ 0 & 0 & 1 & 0 & 0 & 15/7 \\ 0 & 0 & 0 & 1 & 0 & -6/7 \\ 0 & 0 & 0 & 0 & 1 & -52/7 \end{array}\right)$$

Best fit ellipse:

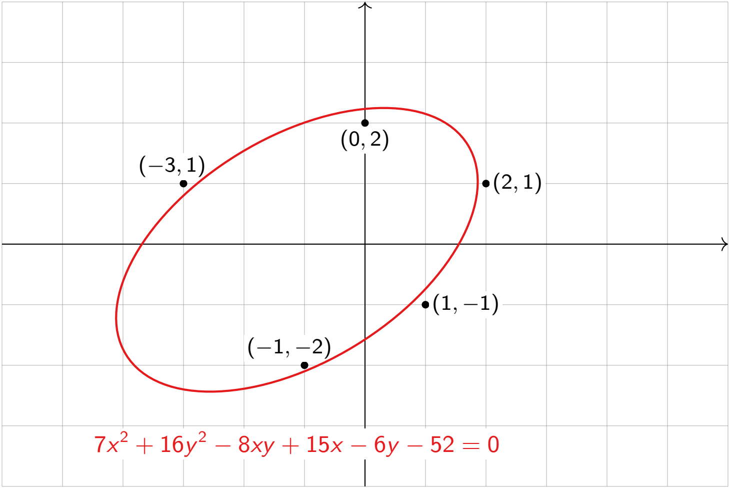
$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

or

$$7x^2 + 16y^2 - 8xy + 15x - 6y - 52 = 0.$$

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 $(-1, 0.5)$, $(1, -1)$, $(2, -0.5)$, $(3, 2)$?

The general equation for a parabola is

$$y = Ax^2 + Bx + C.$$

So we want to solve:

$$\begin{aligned}
0.5 &= A(-1)^2 + B(-1) + C \\
-1 &= A(1)^2 + B(1) + C \\
-0.5 &= A(2)^2 + B(2) + C \\
2 &= A(3)^2 + B(3) + C
\end{aligned}$$

In matrix form:

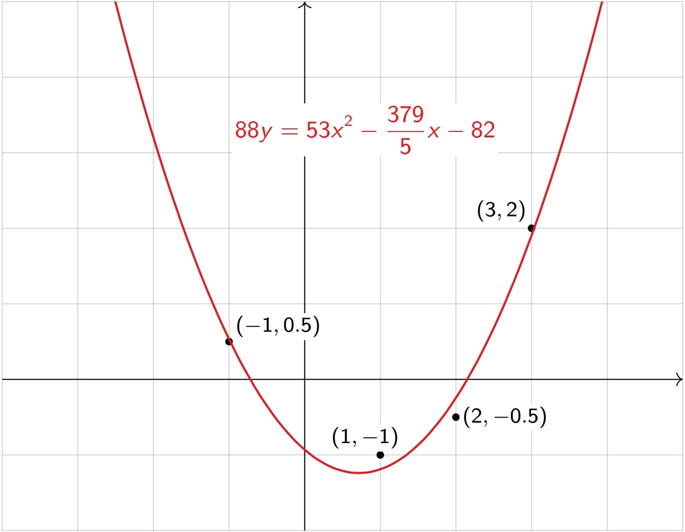
$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Answer:

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

Application

Best fit parabola, picture



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

The general equation for a linear function in two variables is

$$f(x, y) = Ax + By + C.$$

So we want to solve

$$\begin{aligned} A(1) + \quad B(0) + C &= 0 \\ A(0) + \quad B(1) + C &= 1 \\ A(-1) + \quad B(0) + C &= 3 \\ A(0) + B(-1) + C &= 4 \end{aligned}$$

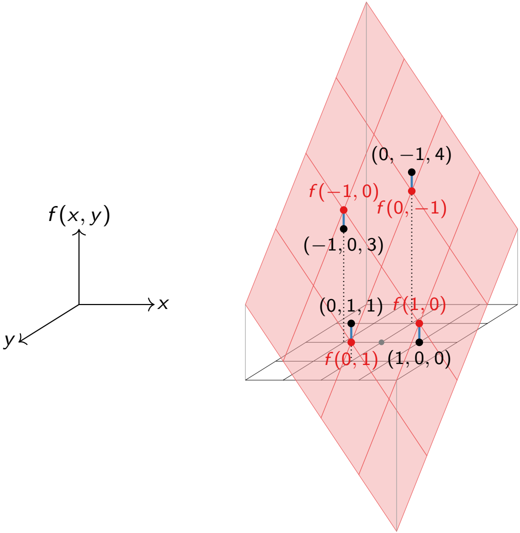
In matrix form:

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}.$$

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

Application

Best fit linear function, picture



Graph of

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