

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 $\text{Col } A$.

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

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**.

Least Squares Solutions

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

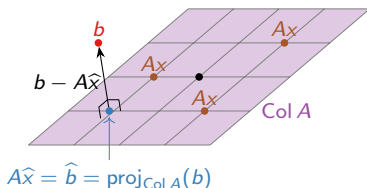
Definition

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

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

for all x in \mathbf{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 \mathbf{R}^n such that

$$A\hat{x} = \hat{b} = \text{proj}_{\text{Col } A}(b).$$

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

Least Squares Solutions

Computation

Theorem

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

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

This is just another $Ax = b$ problem, but with a *square* matrix $A^T A$!

Note we compute \hat{x} directly, without computing \hat{b} first.

Why is this true?

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

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

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

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

Least Squares Solutions

Example

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

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

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 $\hat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.

Least Squares Solutions

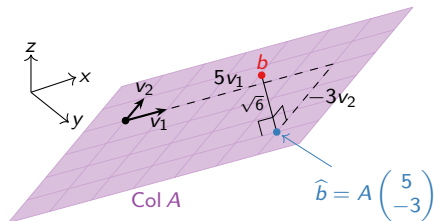
Example, continued

How close did we get?

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

The distance from b is

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



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 $\hat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$ is just the \mathcal{B} -coordinates of \hat{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:

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

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 $\hat{x} = \begin{pmatrix} 1/3 \\ -1/3 \end{pmatrix}$.

Least Squares Solutions

Uniqueness

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

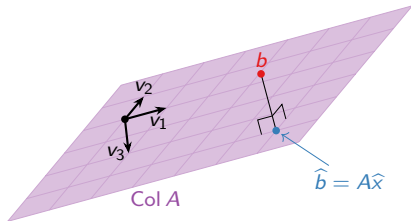
Theorem

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 \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 *dependent*, then $A\hat{x} = \hat{b}$ 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:

$$6 = C + D \cdot 0$$

$$0 = C + D \cdot 1$$

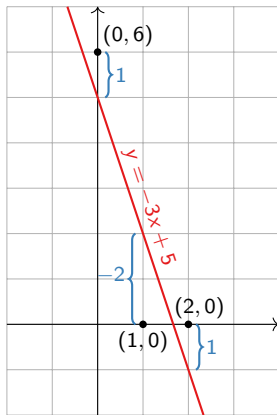
$$0 = C + D \cdot 2.$$

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 $\begin{pmatrix} 5 \\ -3 \end{pmatrix}$. 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

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.

Application

Best fit ellipse

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:

$$(0)^2 + A(2)^2 + B(0)(2) + C(0) + D(2) + E = 0$$

$$(2)^2 + A(1)^2 + B(2)(1) + C(2) + D(1) + E = 0$$

$$(1)^2 + A(-1)^2 + B(1)(-1) + C(1) + D(-1) + E = 0$$

$$(-1)^2 + A(-2)^2 + B(-1)(-2) + C(-1) + D(-2) + E = 0$$

$$(-3)^2 + A(1)^2 + B(-3)(1) + C(-3) + D(1) + E = 0$$

In matrix form:

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

Application

Best fit ellipse, continued

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

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

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:

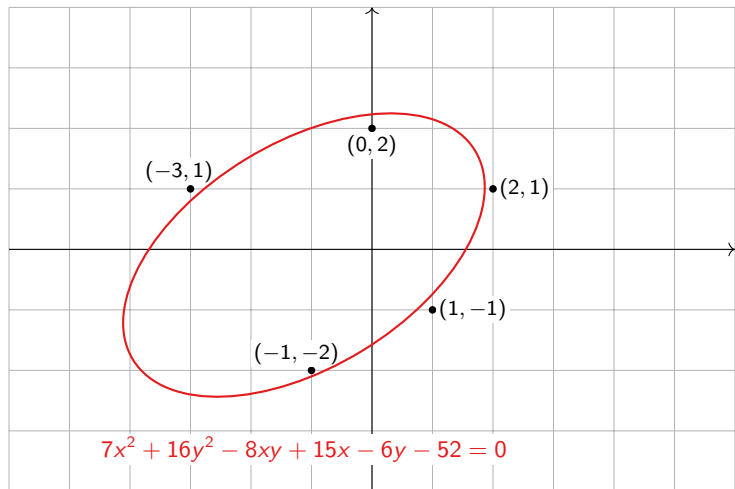
$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

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:

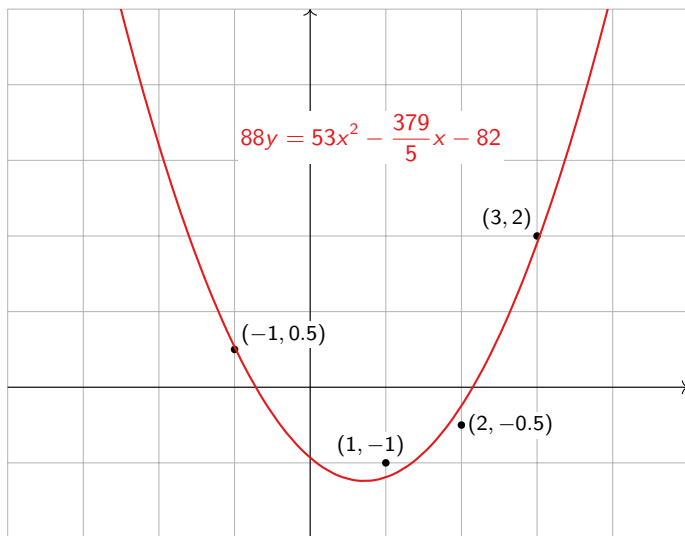
$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Answer:

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

Application

Best fit parabola, picture



Application

Best fit linear function

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

The general equation for a linear function in two variables is

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

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

So we want to solve

$$A(1) + B(0) + C = 0$$

$$A(0) + B(1) + C = 1$$

$$A(-1) + B(0) + C = 3$$

$$A(0) + B(-1) + C = 4$$

In matrix form:

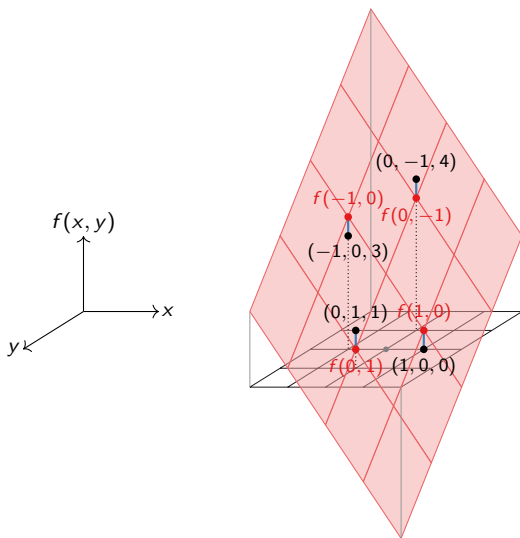
$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}.$$

Answer:

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

Application

Best fit linear function, picture



Graph of

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