

Section 6.5

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**.

Least Squares Solutions

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

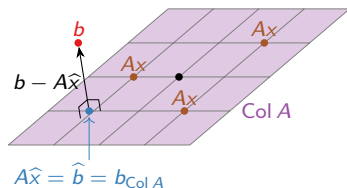
Definition

A **least squares solution** of $Ax = b$ 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 $(\text{Col } A)^\perp$.



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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

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

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 $A^T A v = A^T b$; then $b_W = Av$.

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

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.

Least Squares Solutions

Example

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

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

We have

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

and

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

Row reduce:

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

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

Least Squares Solutions

Example, continued

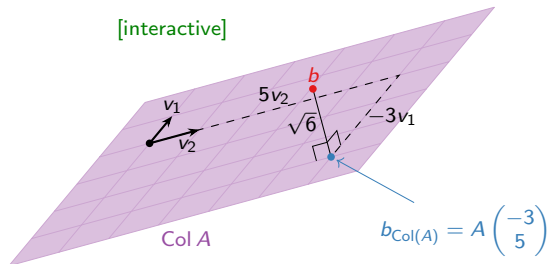
How close did we get?

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

The distance from b is

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

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Note that

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

records the coefficients of v_1 and v_2 in \hat{b} .

Least Squares Solutions

Second example

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

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

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

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Least Squares Solutions

Uniqueness

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

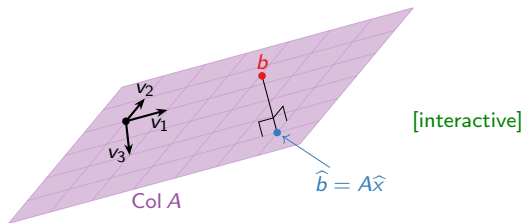
Theorem

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}^m .
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:

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

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

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

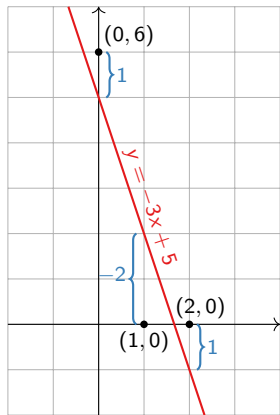
In matrix form:

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

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

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

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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

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 $(0, 2)$, $(2, 1)$, $(1, -1)$, $(-1, -2)$, $(-3, 1)$, $(-1, -1)$.

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:

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

Best fit ellipse:

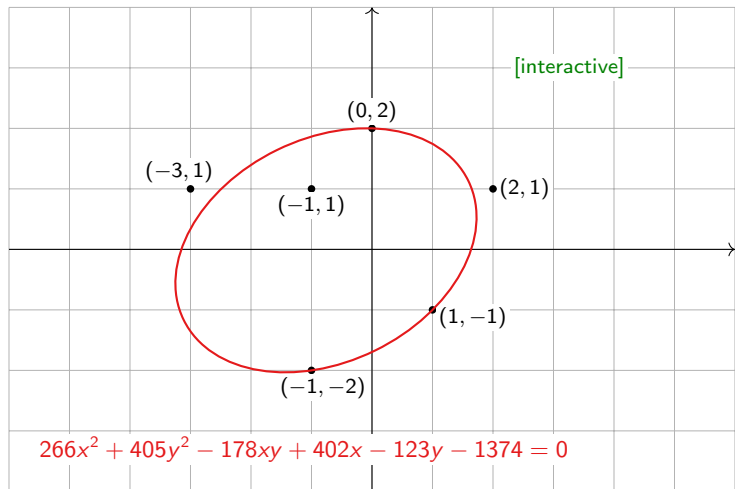
$$x^2 + \frac{405}{266}y^2 - \frac{89}{133}xy + \frac{201}{133}x - \frac{123}{266}y - \frac{687}{133} = 0$$

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.

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:

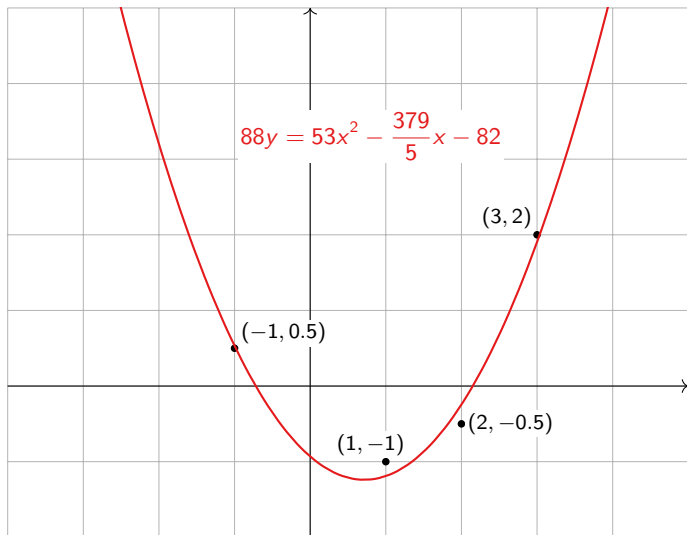
$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Answer:

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

Application

Best fit parabola, picture



[interactive]

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:

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

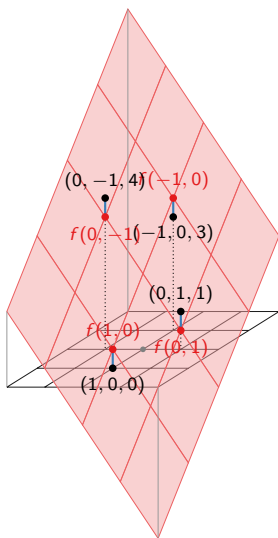
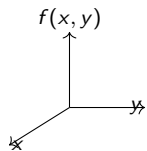
Answer:

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

Application

Best fit linear function, picture

[interactive]



Graph of

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

Application

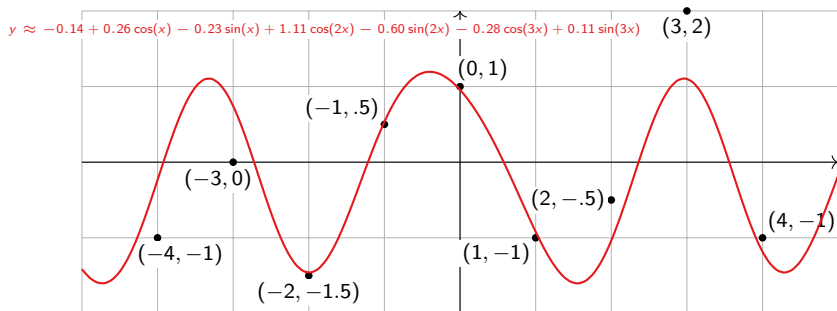
Best-fit Trigonometric Function

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

$$\begin{pmatrix} -4 \\ -1 \end{pmatrix}, \begin{pmatrix} -3 \\ 0 \end{pmatrix}, \begin{pmatrix} -2 \\ -1.5 \end{pmatrix}, \begin{pmatrix} -1 \\ .5 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 2 \\ -0.5 \end{pmatrix}, \begin{pmatrix} 3 \\ 2 \end{pmatrix}, \begin{pmatrix} 4 \\ -1 \end{pmatrix}?$$



[interactive]

Summary

- ▶ 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.