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 $\mathrm{Col}\, A$.

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

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.**

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

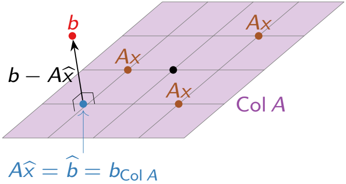
Definition

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 $(\mathrm{Col}\,A)^\perp$.



[interactive]

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

$$A\widehat{x} = \widehat{b} = b_{\mathrm{Col}\,A}.$$

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

We want to solve $A\widehat{x} = \widehat{b} = b_{\mathrm{Col}\,A}$. Or, $A\widehat{x} = b_W$ for $W = \mathrm{Col}\,A$.

To compute b_W we need to solve $A^T Av = A^T b$; then $b_W = Av$.

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

Theorem

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

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

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

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

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

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:

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

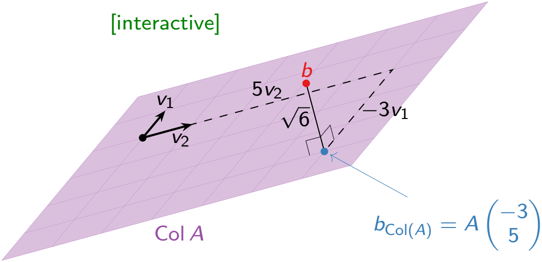
So the only least squares solution is $\widehat{x} = \begin{pmatrix} -3 \\ 5 \end{pmatrix}$.

How close did we get?

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

The distance from b is

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



Note that

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

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

Least Squares Solutions

Second example

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

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

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 $\widehat{x} = \begin{pmatrix} 1/3 \\ -1/3 \end{pmatrix}$. [interactive]

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

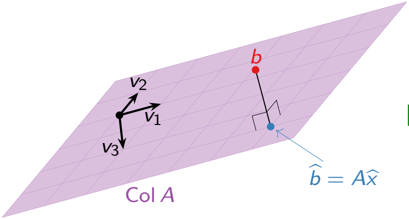
Theorem

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 *dependent*, 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.

Application

Data modeling: best fit line

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

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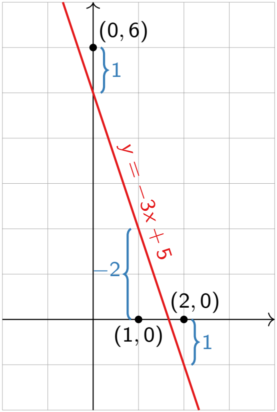


$$A\begin{pmatrix}5\\-3\end{pmatrix} - \begin{pmatrix}6\\0\\0\end{pmatrix} = \begin{pmatrix}1\\-2\\1\end{pmatrix}$$

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

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

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

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:

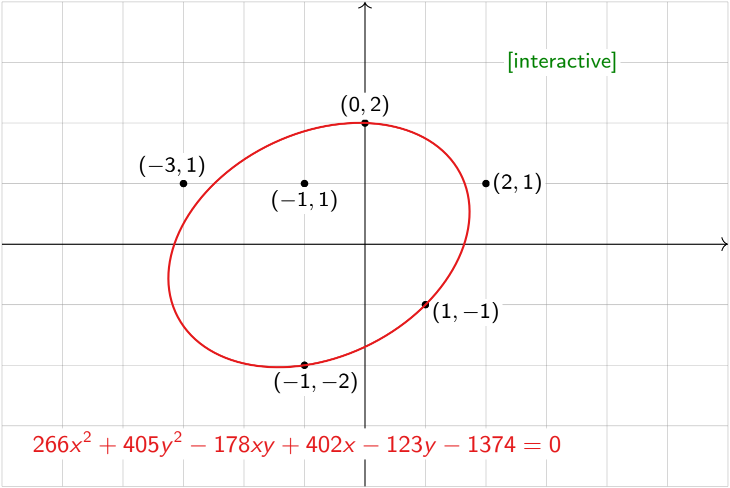
$$x^2 + \frac{405}{266}y^2 - \frac{89}{133}xy + \frac{201}{133}x - \frac{123}{266}y - \frac{687}{133} = 0$$

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

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:

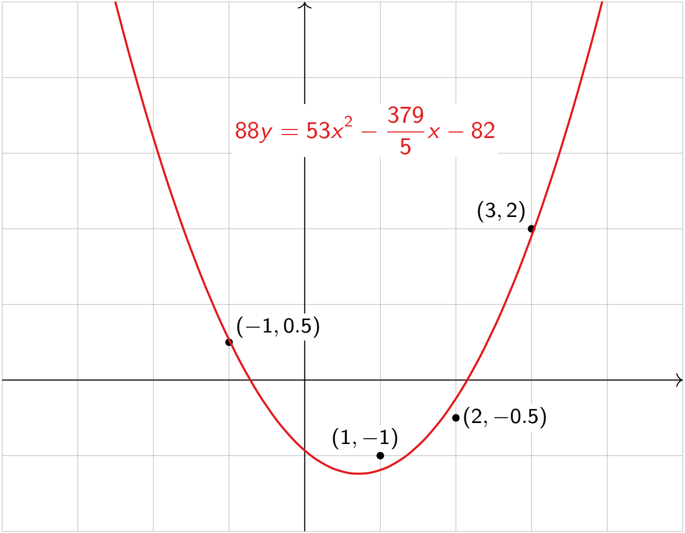
$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Answer:

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

Application

Best fit parabola, picture



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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

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

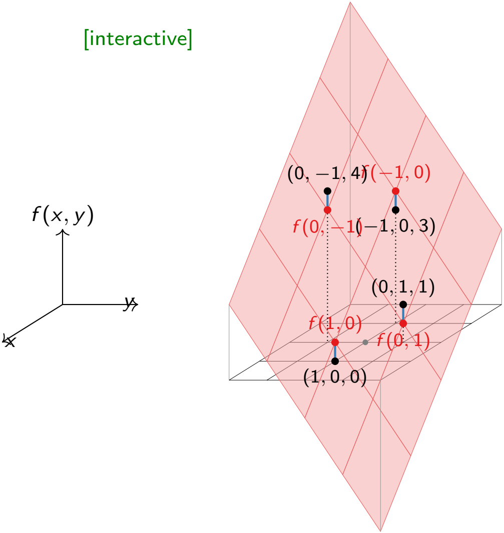
In matrix form:

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

Answer:

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

[interactive]



Graph of

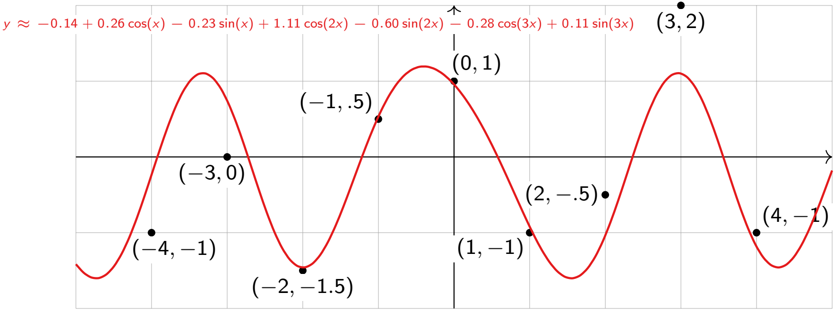
$$f(x,y) = -\frac{3}{2}x - \frac{3}{2}y + 2$$

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

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



[interactive]

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 $\widehat{b} = b_{\text{Col}\,A}$.
- 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.