Section 6.5

Least Squares Problems

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

Least Squares Solutions

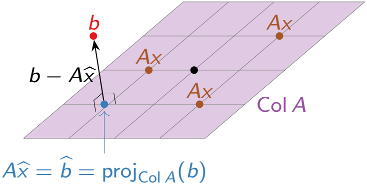
Let A be an $m \times n$ matrix.

Definition

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

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

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



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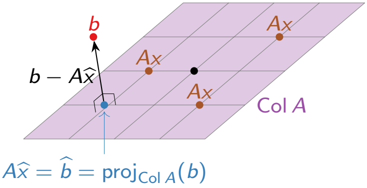

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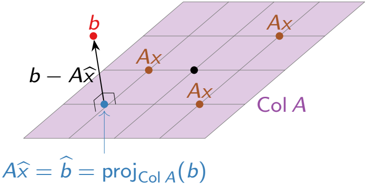

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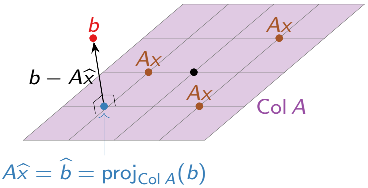

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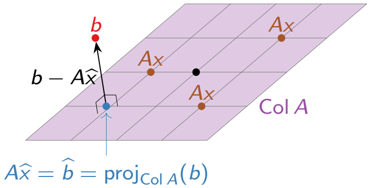

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$$A\widehat{x} = \widehat{b} = \mathrm{proj}_{\operatorname{Col} A}(b).$$

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

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

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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:

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

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

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Least Squares Solutions

Example, continued

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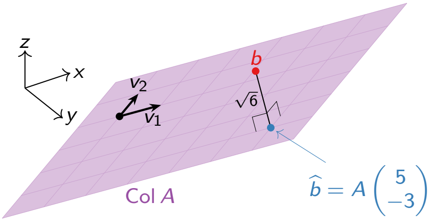

Let

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

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

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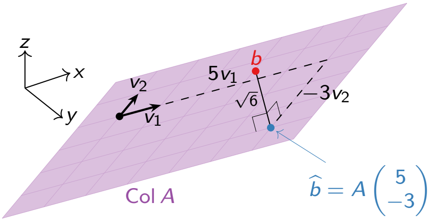

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Note $\widehat{x} = \binom{5}{-3}$ is just the $\mathcal{B}$-coordinates of $\widehat{b}$, in Col $A = \text{Span}\{v_1, v_2\}$.

Least Squares Solutions

Second example

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

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

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

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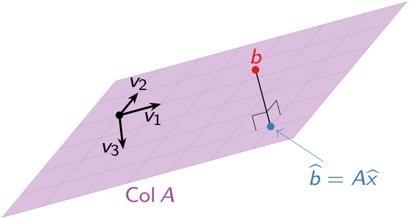
Why? If the columns of A are linearly *dependent*, then $A\widehat{x} = \widehat{b}$ has many solutions:



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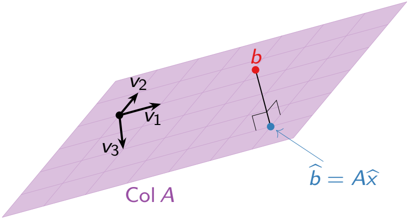
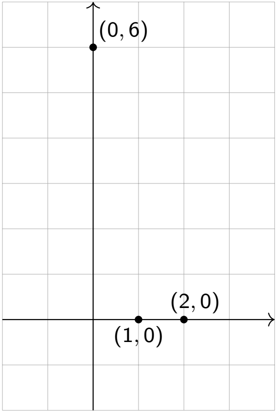


Note: $A^T A$ is always a square matrix, but it need not be invertible.

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



Application

Data modeling: best fit line

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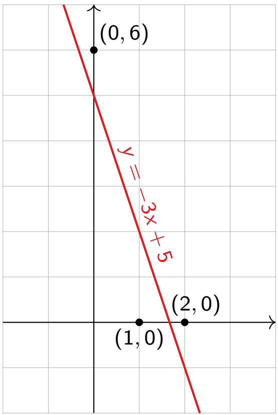

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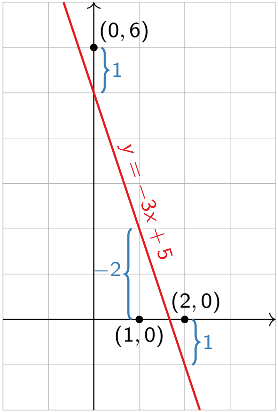

$$A\begin{pmatrix}5\\-3\end{pmatrix}-\begin{pmatrix}6\\0\\0\end{pmatrix}=\begin{pmatrix}1\\-2\\1\end{pmatrix}$$

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

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So we want to solve:

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(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
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\end{aligned}$$

In matrix form:

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

Application

Best fit ellipse, continued

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

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Row reduce:

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Best fit ellipse:

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

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Best fit ellipse:

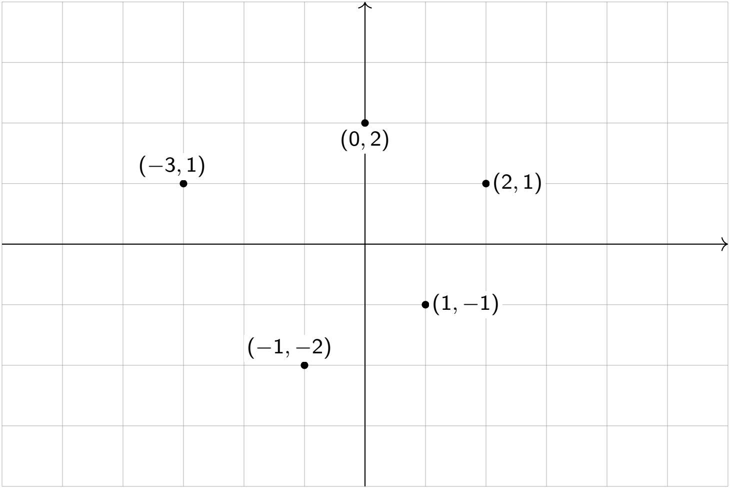
$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

or

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

Application

Best fit ellipse, picture



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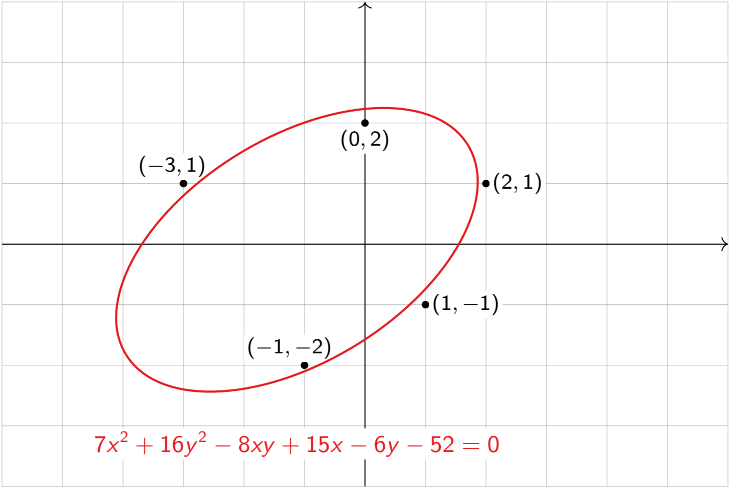
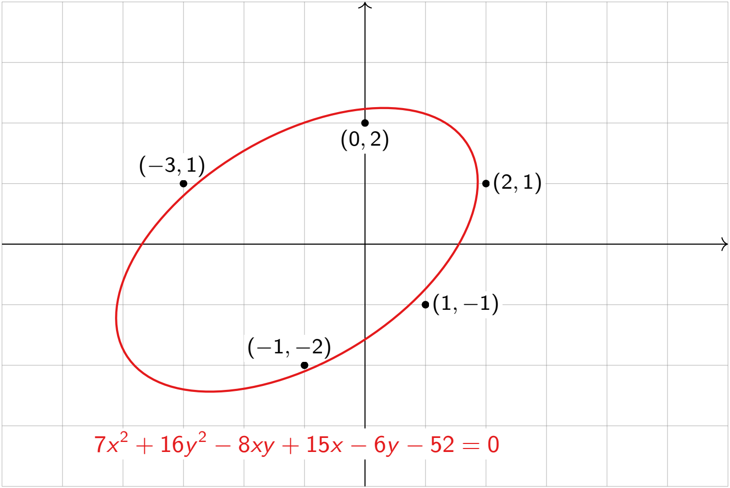




Remark: Gauss invented the method of least squares to do exactly this: he predicted the (elliptical) orbit of the asteroid Ceres as it passed behind the sun in 1801.

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

Application

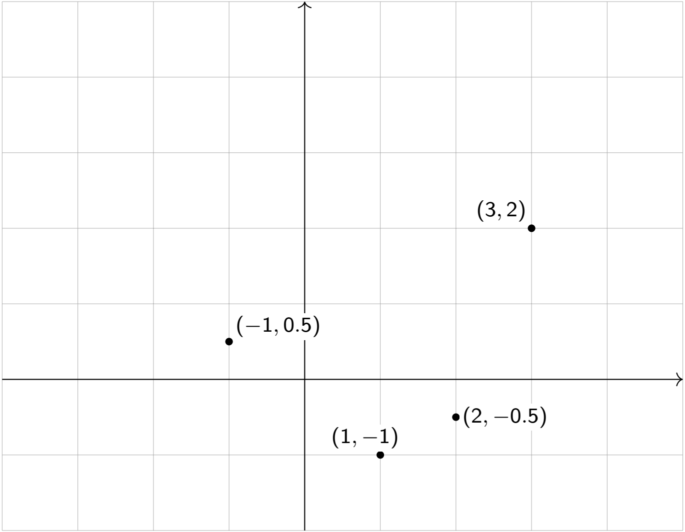
Best fit parabola

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

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

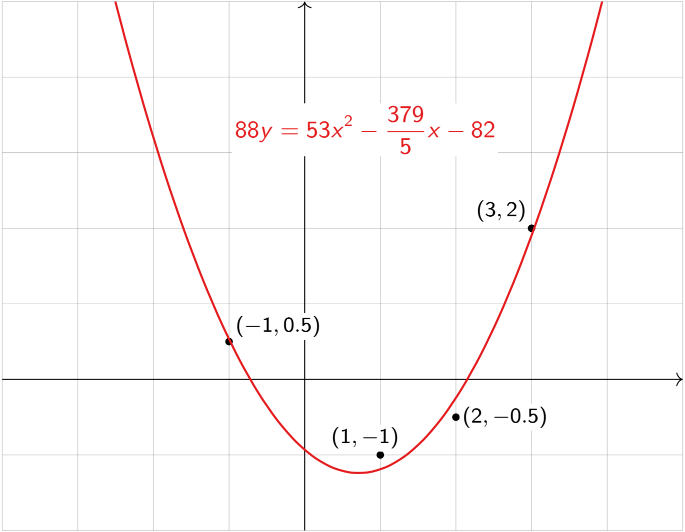
Application

Best fit parabola, picture



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?

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

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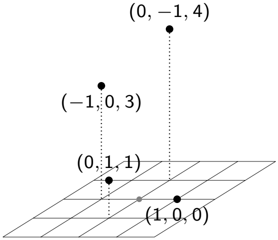
Answer:

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

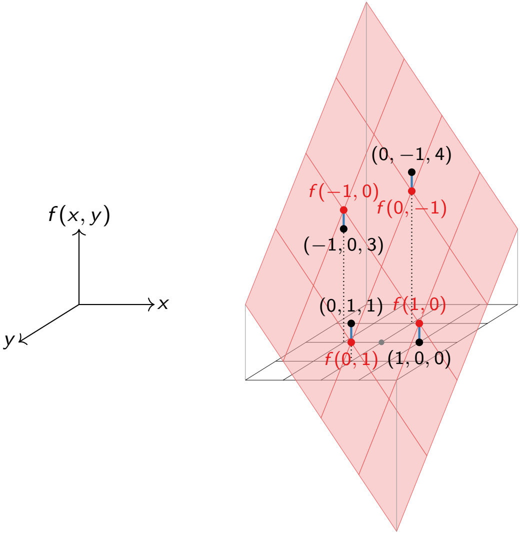
Application

Best fit linear function, picture



Application

Best fit linear function, picture



Graph of

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