# Section 6.5

## Least Squares Problems

# Motivation

**Problem**

Suppose that $Ax = b$ does not have a solution. What is the *best possible approximate* solution?

Saying $Ax = b$ **has no solution** means that $b$ is not in Col $A$.

- Using $\widehat{b} = \text{proj}_{\text{Col } A}(b)$, then $A\widehat{x} = \widehat{b}$ is a *consistent equation*.
- **Plus:** $\widehat{b}$ is the *closest vector to b* such that $A\widehat{x} = \widehat{b}$ is consistent.

**Solution**

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

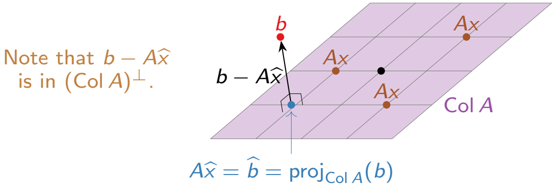
# Least Squares Solutions

## Definition

Let $A$ be an $m \times n$ matrix. A **least squares solution** to $Ax = b$ is a vector $\widehat{x}$ in $\mathbf{R}^n$ such that

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

> A least squares solution $\widehat{x}$ solves $Ax = b$ *as closely as possible*.




In *distance terms*, for all $x$ in $\mathbf{R}^n$:

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

# Least Squares Solutions: Orthogonal case

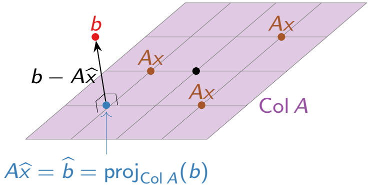
### Theorem

Let $A$ be a $m \times n$ matrix with **orthogonal columns** $v_1, v_2, \ldots, v_n$. The least squares solution to $Ax = b$ is the vector

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

This is because we have formulas for the $\mathcal{B}$**-coordinates** of orthogonal basis:

$$A\widehat{x} = \sum_{i=1}^{n} \frac{b \cdot v_i}{v_i \cdot v_i} \, v_i = \mathrm{proj}_{\mathrm{Col}\,A}(b)$$



# Least Squares Solutions: General Solution

### Theorem

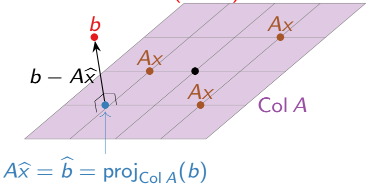
Let $A$ be a $m \times n$ **matrix**. Least squares solutions to $Ax = b$ are *any of the solutions to*

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

Now we can solve the problem without computing $\widehat{b}$ first.

> This is just another sysmtem of equations,
> but now it *is consistent* and uses *square matrix $A^T A$*!

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




Why is this true?

**Recall:** $(\text{Col } A)^\perp = \text{Nul}(A^T)$.

Now, $b - A\widehat{x}$ is in $(\text{Col } A)^\perp$ if and only if

$$A^T(b - A\widehat{x}) = 0.$$

In other words, $A^T A\widehat{x} = A^T b$.

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

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

First: Compute new matrix and vector

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

and

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

Second: Solve the new system; 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 *unique* least squares *solution is* $\widehat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.

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

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

First: Compute new matrix and vector

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

and

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

Second: Solve the new system; 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 *unique* least squares *solution is* $\widehat{x} = \begin{pmatrix} 1/3 \\ -1/3 \end{pmatrix}$.

# Least Squares Solutions: Uniqueness

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

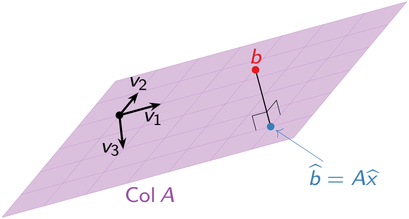
- $A^T A$ is always a square matrix, but it need not be invertible.

**Theorem**

Let $A$ be an $m \times n$ matrix. The following *are equivalent*:

1. $A^T A$ is invertible.
2. The columns of $A$ are *linearly independent*.
3. $Ax = b$ has a **unique least squares solution** for all $b$ in $\mathbf{R}^n$, which is

$$(A^T A)^{-1}(A^T b).$$




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

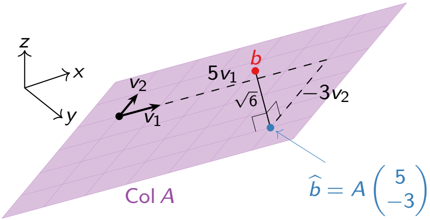
# Extra: More details

From Example 1

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

1. The solution $\widehat{x}$ makes the *distance from $b$ to its approximation:*

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




2. If $A^TA$ is invertible: Let $v_1, v_2$ be the columns of $A$, and $\mathcal{B} = \{v_1, v_2\}$, then $\widehat{x} = \binom{5}{-3}$ are the $\mathcal{B}$-coordinates of $\widehat{b}$, in Col $A = \text{Span}\{v_1, v_2\}$.

# 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

$$c + dx = y.$$

So we want to solve:

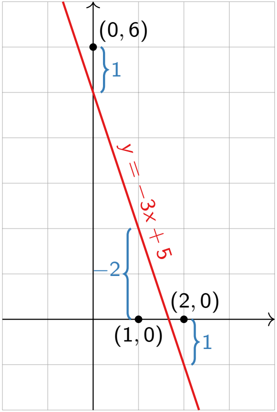
$$c + d \cdot 0 = 6$$
$$c + d \cdot 1 = 0$$
$$c + d \cdot 2 = 0.$$

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 **has $\widehat{c} = 5$ and $\widehat{d} = -3$**:

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

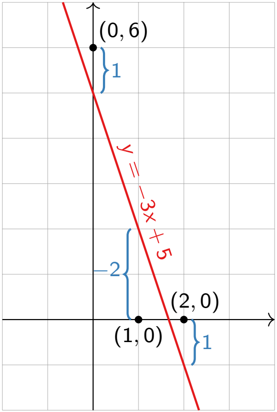



$$A\begin{pmatrix} 5 \\ -3 \end{pmatrix} - \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

# Data Modeling: Best fit line

**What does it minimize?**

**Best fit line** minimizes the **sum of the squares** of the *vertical distances from the data points* to the line.



# Data modeling: 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

$$ax^2 + bx + c = y.$$

So we want to solve:

$$\begin{aligned} a(-1)^2 + b(-1) + c &= 0.5 \\ a(1)^2 + b(1) + c &= -1 \\ a(2)^2 + b(2) + c &= -0.5 \\ a(3)^2 + b(3) + c &= 2 \end{aligned}$$

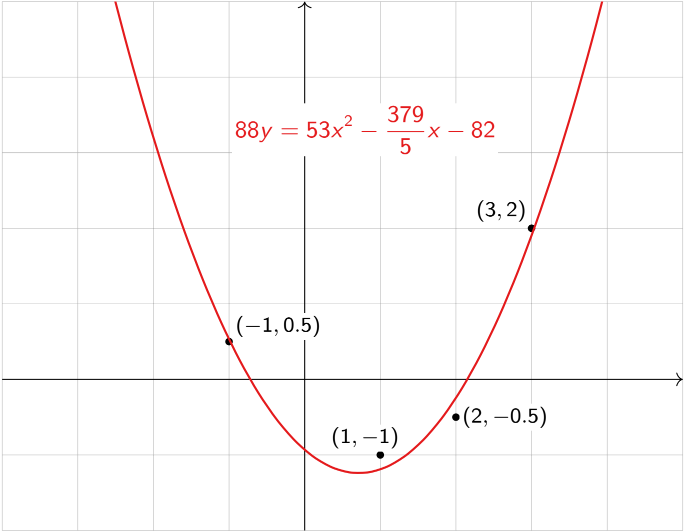
In matrix form:

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Answer: $\widehat{a} = \frac{53}{88}, \widehat{b} = \frac{379}{440}, \widehat{c} = \frac{82}{88}$ so best fit is: $53x^2 - \dfrac{379}{5}x - 82 = 88y$

# Data modeling: best fit parabola

## Picture



# Data modeling: 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:

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

In matrix form:

$$\begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \end{pmatrix}.$$

# Data modeling: best fit ellipse

## Complete procedure

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

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

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:

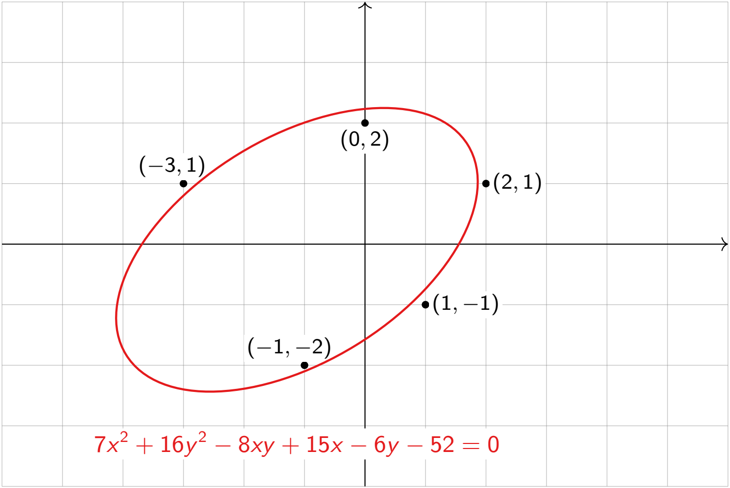
$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

or

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

# Data modeling: 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.

# Extra: 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 |

The general equation for a linear function in two variables is

$$f(x, y) = ax + by + c.$$

So we want to solve

$$\begin{aligned} a(1) + \quad b(0) + c &= 0 \\ a(0) + \quad b(1) + c &= 1 \\ a(-1) + \quad b(0) + c &= 3 \\ a(0) + b(-1) + c &= 4 \end{aligned}$$

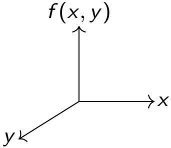
In matrix form:

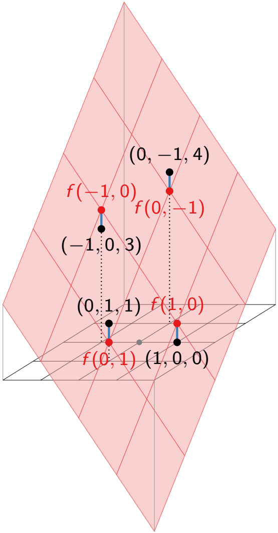
$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}.$$

Answer: $\widehat{a} = -\frac{3}{2}, \widehat{b} = -\frac{3}{2}, \widehat{c} = 2$ so best fit is: $f(x, y) = -\dfrac{3}{2}x - \dfrac{3}{2}y + 2$

# Extra: Best fit linear function

## Picture




Graph of

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