Section 6.5

Least Squares Problems

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 Col A.

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

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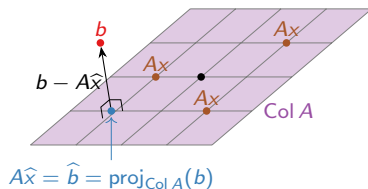
Let A be an $m \times n$ matrix.

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

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

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

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

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

[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

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

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

Theorem

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

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

This is just another $Ax = b$ problem, but with a *square* matrix $A^T A$!
Note we compute $\widehat{x}$ directly, without computing $\widehat{b}$ first.

Why is this true?

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

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

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

The right hand side equals $A\widehat{x}$, where $\widehat{x} = \left(\dfrac{b \cdot v_1}{v_1 \cdot v_1}, \ \dfrac{b \cdot v_2}{v_2 \cdot v_2}, \ \cdots, \ \dfrac{b \cdot v_n}{v_n \cdot v_n} \right)$.

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

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

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 $\widehat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.
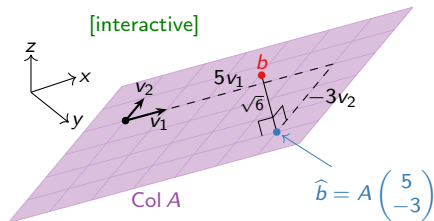
How close did we get?

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

The distance from b is

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

[interactive]

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

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

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

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 $\mathbf{R}^m$.
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 *de*pendent, then $A\widehat{x} = \widehat{b}$ has many solutions:

[interactive]

v_2
v_1
v_3

b

$\widehat{b} = A\widehat{x}$

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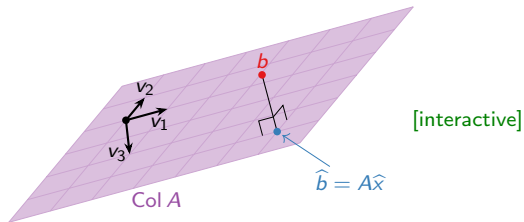
Note: $A^T A$ is always a square matrix, but it need not be invertible.

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

The general equation of a line is

$$y = C + Dx.$$

So we want to solve:

$$6 = C + D \cdot 0$$
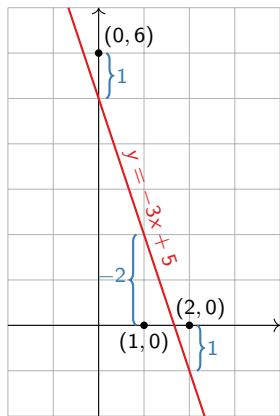$$0 = C + D \cdot 1$$
$$0 = C + D \cdot 2.$$

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

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

[interactive]

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

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.

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:

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

In matrix form:

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

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

$$A^T A = \begin{pmatrix} 36 & 7 & -5 & 0 & 12 \\ 7 & 19 & 9 & -5 & 1 \\ -5 & 9 & 16 & 1 & -2 \\ 0 & -5 & 1 & 12 & 0 \\ 12 & 1 & -2 & 0 & 6 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -19 \\ 17 \\ 20 \\ -9 \\ -16 \end{pmatrix}$$

Row reduce:

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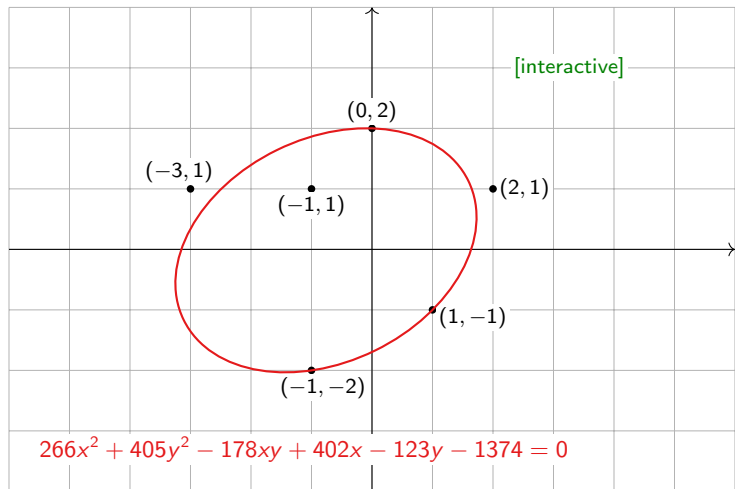
Best fit ellipse:

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

or

$$266x^2 + 405y^2 - 178xy + 402x - 123y - 1374 = 0.$$

[interactive]

$(0, 2)$

$(-3, 1)$

$(-1, 1)$

$(2, 1)$

$(1, -1)$

$(-1, -2)$

$$266x^2 + 405y^2 - 178xy + 402x - 123y - 1374 = 0$$

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:

$$
\begin{aligned}
0.5 &= A(-1)^2 + B(-1) + C \\
-1 &= A(1)^2 + B(1) + C \\
-0.5 &= A(2)^2 + B(2) + C \\
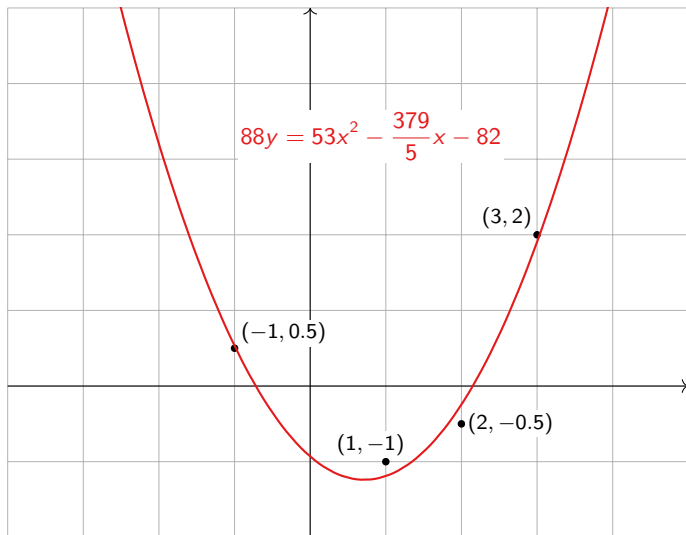2 &= A(3)^2 + B(3) + C
\end{aligned}
$$

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:

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

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

$(3, 2)$

$(-1, 0.5)$

$(2, -0.5)$

$(1, -1)$

[interactive]

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

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

In matrix form:

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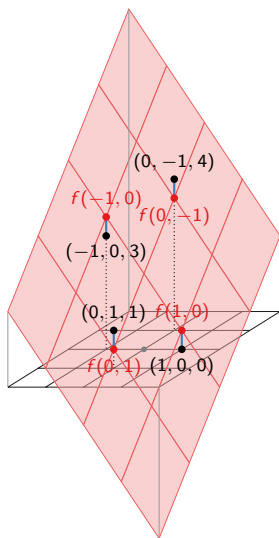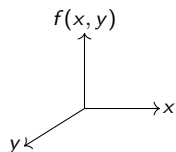=
\begin{pmatrix}
0 \\
1 \\
3 \\
4
\end{pmatrix}.
$$

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

[interactive]

$f(x, y)$

x

y

$(0, -1, 4)$

$f(-1, 0)$

$f(0, -1)$

$(-1, 0, 3)$

$(0, 1, 1)$ $f(1, 0)$

$f(0, 1)$ $(1, 0, 0)$

Graph of

$f(x, y) = -\dfrac{3}{2}x - \dfrac{3}{2}y + 2$
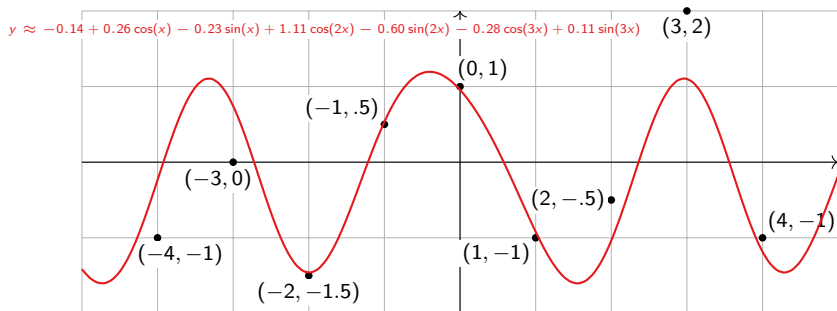
For fun: what is the best-fit function of the form

$$y = A + B\cos(x) + C\sin(x) + D\cos(2x) + E\sin(2x) + F\cos(3x) + G\sin(3x)$$

passing through the points

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

$y \approx -0.14 + 0.26\cos(x) - 0.23\sin(x) + 1.11\cos(2x) - 0.60\sin(2x) - 0.28\cos(3x) + 0.11\sin(3x)$

[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 $\widehat{b} = \text{proj}_{\text{Col } A}(b)$.
- 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.