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 $\operatorname{Col} A$.

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

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.

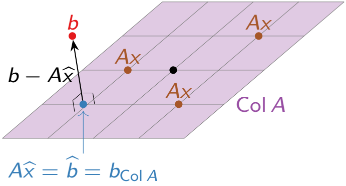
Definition

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

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

Theorem

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

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

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

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

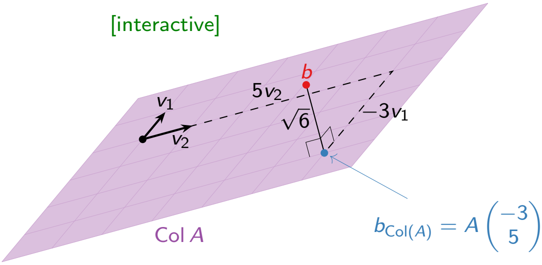
$$A = \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.$$

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

Least Squares Solutions

Example, continued

How close did we get?



Note that

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

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

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

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

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 $\widehat{x}$?

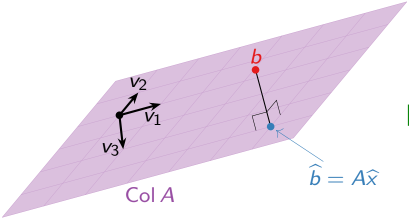
Theorem

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:

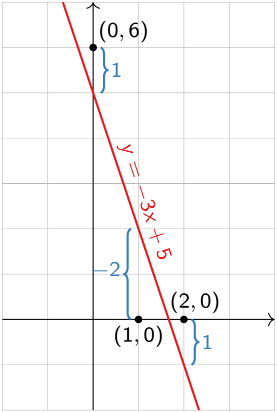


[interactive]

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 $(2,0)$.

[interactive]



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

Poll

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:

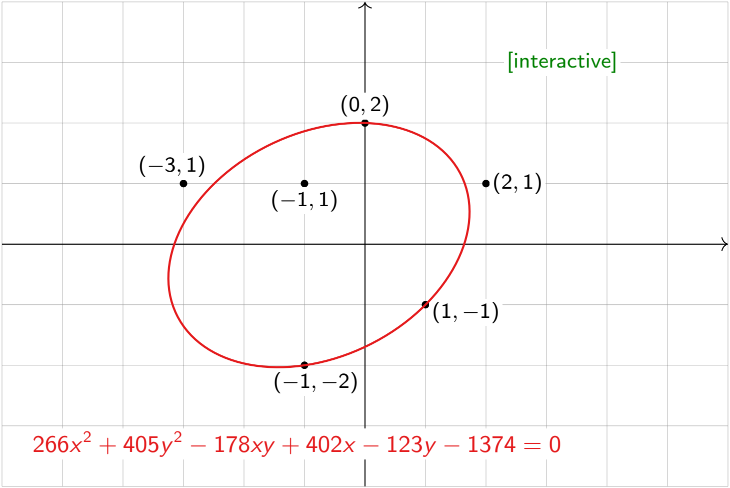
$$x^2 + \frac{405}{266}y^2 - \frac{89}{133}xy + \frac{201}{133}x - \frac{123}{266}y - \frac{687}{133} = 0$$

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.

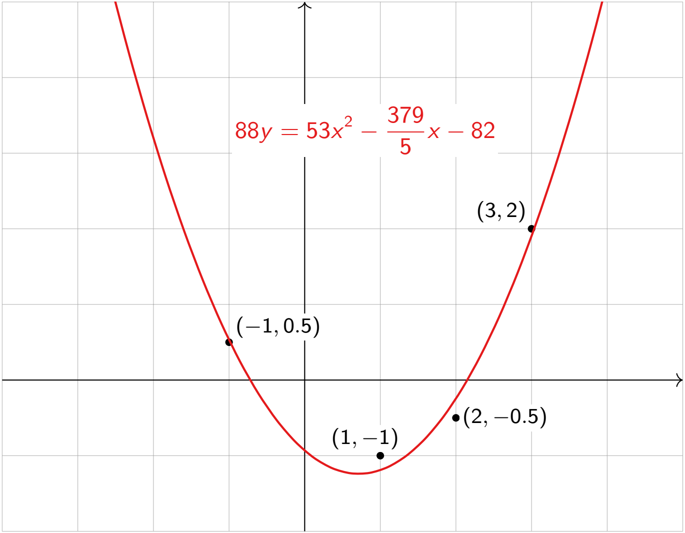
What least squares problem $Ax = b$ finds the best parabola through the points $(-1, 0.5)$, $(1, -1)$, $(2, -0.5)$, $(3, 2)$?

Answer:

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

Application

Best fit parabola, picture



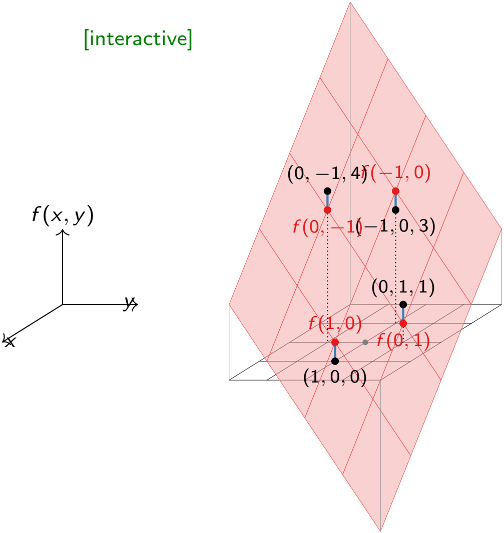
[interactive]

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

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

[interactive]



Graph of

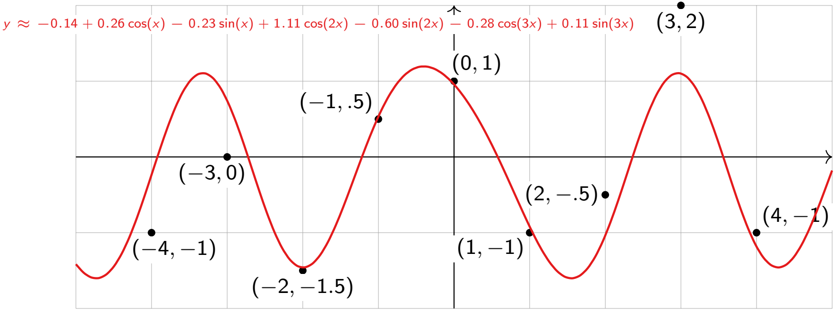
$$f(x,y) = -\frac{3}{2}x - \frac{3}{2}y + 2$$

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.