EECS 16A Designing Information Devices and Systems I
Summer 2020 Discussion 6D

1. Least Squares: A Toy Example

Let's start off by solving a little example of least squares.

We're given the following system of equations:

$$\begin{bmatrix} 1 & 4 \\ 3 & 8 \\ 5 & 16 \end{bmatrix} \vec{x} = \begin{bmatrix} 3 \\ 1 \\ 9 \end{bmatrix},$$

where $\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$.

(a) Why can we not solve for $\vec{x}$ exactly?

Answer:

Recall from the earlier linear algebra module that in order for there to be a solution for the matrix system $\mathbf{A}\vec{x} = \vec{b}$, we must have $\vec{b} \in \text{Col}(\mathbf{A})$.

Let us use Gaussian elimination to see if we can find $\vec{x}$.

$$\left[\begin{array}{cc|c} 1 & 4 & 3 \\ 3 & 8 & 1 \\ 5 & 16 & 9 \end{array}\right] \overbrace{\Rightarrow}^{R_3 - 2R_1 - R_2 \to R_3} \left[\begin{array}{cc|c} 1 & 4 & 3 \\ 3 & 8 & 1 \\ 0 & 0 & 2 \end{array}\right]$$

We have reached a point at which there does not exist an $\vec{x}$ that exactly solves the system of equations. Thus, in this case $\vec{b} \notin \text{Col}(\mathbf{A})$. This is because of the last row of $\mathbf{A}$ is $\begin{bmatrix} 0 & 0 \end{bmatrix} \vec{x} = 2$.

(b) Find $\vec{\hat{x}}$, the *least squares estimate* of $\vec{x}$, using the formula we derived in lecture.

Reminder: $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

Answer:

Recall the equation to find the linear least squares estimate:

$$\vec{\hat{x}} = \left(\mathbf{A}^T \mathbf{A}\right)^{-1} \mathbf{A}^T \vec{b}$$

Plugging in $\mathbf{A} = \begin{bmatrix} 1 & 4 \\ 3 & 8 \\ 5 & 16 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 3 \\ 1 \\ 9 \end{bmatrix}$, we get $\vec{\hat{x}} = \begin{bmatrix} -6 \\ 2.41\bar{6} \end{bmatrix}$.

2. Least Squares with Orthogonal Columns

(a) Consider a least squares problem of the form

$$\min_{\vec{x}} \left\| \vec{b} - \mathbf{A}\vec{x} \right\|^2 = \min_{\vec{x}} \left\| \mathbf{A}\vec{x} - \vec{b} \right\|^2 = \min_{\vec{x}} \left\| \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} - \begin{bmatrix} | & | \\ \vec{a}_1 & \vec{a}_2 \\ | & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|^2$$

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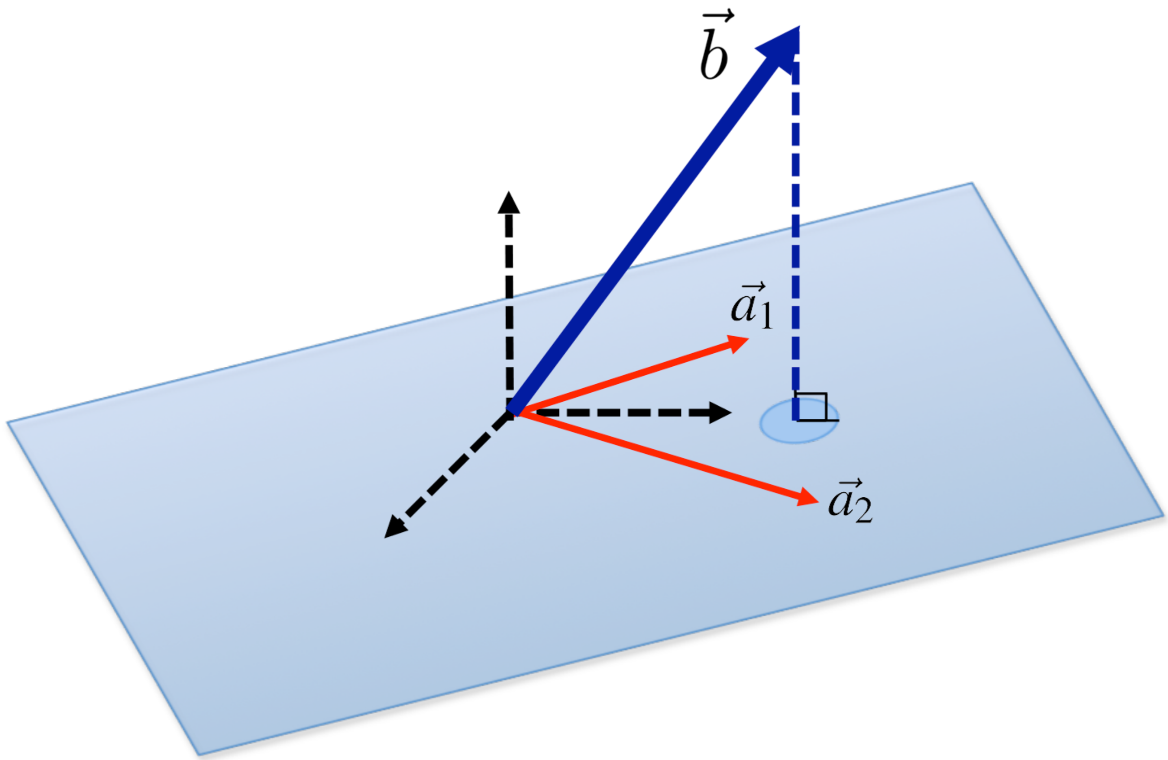
Let the solution be $\vec{\hat{x}} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix}$.

Label the following elements in the diagram below.

$$\text{span}\{\vec{a}_1, \vec{a}_2\}, \qquad \vec{e} = \vec{b} - \mathbf{A}\vec{\hat{x}}, \qquad \mathbf{A}\vec{\hat{x}}, \qquad \vec{a}_1\hat{x}_1,\ \vec{a}_2\hat{x}_2, \qquad \text{colspace}(\mathbf{A})$$



Answer:

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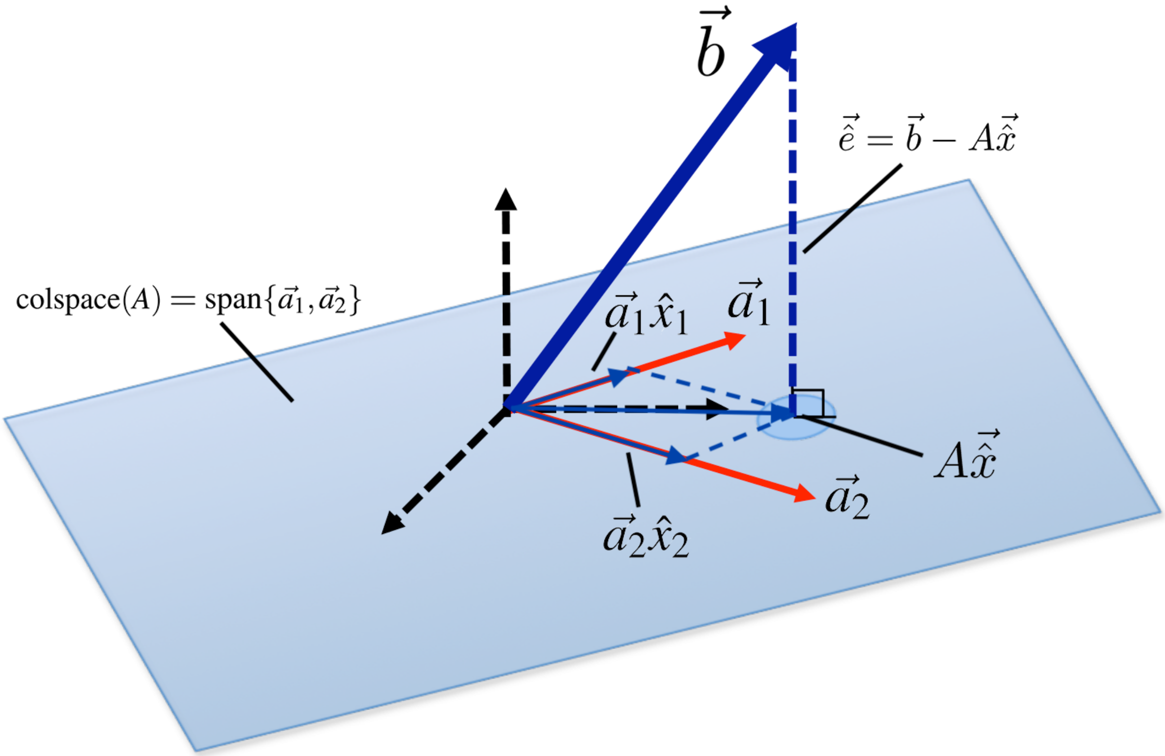
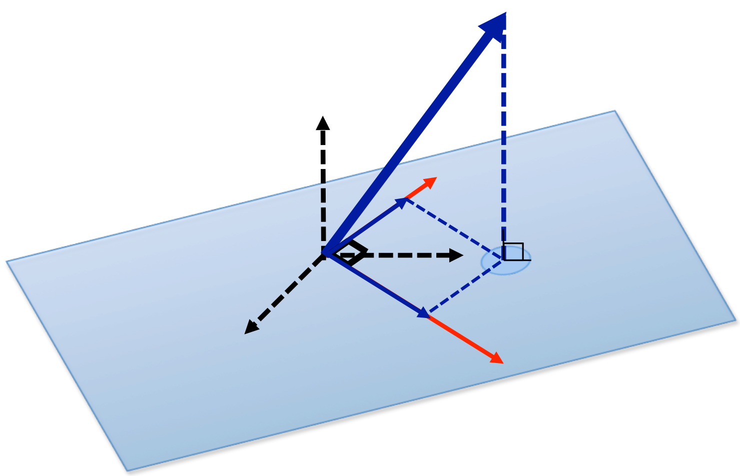


(b) We now consider the special case of least squares where the columns of $\mathbf{A}$ are orthogonal (illustrated in the figure below). Given that $\vec{\hat{x}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\vec{b}$ and $A\vec{\hat{x}} = \text{proj}_{\mathbf{A}}(\vec{b}) = \hat{x}_1\vec{a}_1 + \hat{x}_2\vec{a}_2$, show that

$$\text{proj}_{\vec{a}_1}(\vec{b}) = \hat{x}_1\vec{a}_1$$
$$\text{proj}_{\vec{a}_2}(\vec{b}) = \hat{x}_2\vec{a}_2$$



Answer:

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The projection of $\vec{b}$ onto $\vec{a}_1$ and $\vec{a}_2$ are given by:

$$\text{proj}_{\vec{a}_1}(\vec{b}) = \frac{\langle \vec{a}_1, \vec{b} \rangle}{\|\vec{a}_1\|^2} \vec{a}_1 \qquad \text{proj}_{\vec{a}_2}(\vec{b}) = \frac{\langle \vec{a}_2, \vec{b} \rangle}{\|\vec{a}_2\|^2} \vec{a}_2$$

$$\text{Length:} \quad \frac{\langle \vec{a}_1, \vec{b} \rangle}{\|\vec{a}_1\|} \qquad \frac{\langle \vec{a}_2, \vec{b} \rangle}{\|\vec{a}_2\|}$$

The least squares solution is given by:

$$\begin{aligned}
\begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} &= \left(\begin{bmatrix} - & \vec{a}_1{}^T & - \\ - & \vec{a}_2{}^T & - \end{bmatrix} \begin{bmatrix} | & | \\ \vec{a}_1 & \vec{a}_2 \\ | & | \end{bmatrix} \right)^{-1} \begin{bmatrix} - & \vec{a}_1{}^T & - \\ - & \vec{a}_2{}^T & - \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{\|\vec{a}_1\|^2} & 0 \\ 0 & \frac{1}{\|\vec{a}_2\|^2} \end{bmatrix} \begin{bmatrix} - & \vec{a}_1{}^T & - \\ - & \vec{a}_2{}^T & - \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \\
&= \begin{bmatrix} \frac{\vec{a}_1{}^T \vec{b}}{\|\vec{a}_1\|^2} \\ \frac{\vec{a}_2{}^T \vec{b}}{\|\vec{a}_2\|^2} \end{bmatrix}
\end{aligned}$$

(c) Compute the least squares solution to

$$\min_{\vec{x}} \left\| \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|^2.$$

Answer:

$$\begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

Note that the columns of $\mathbf{A}$ are orthogonal, so it is much faster to project $\vec{b}$ onto the columns of $\mathbf{A}$ than use the least squares formula to find $\vec{\hat{x}}$.

3. Polynomial Fitting

Let's try an example. Say we know that the output, y, is a quartic polynomial in x. This means that we know that y and x are related as follows:

$$y = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4$$

We're also given the following observations:

x	y
0.0	24.0
0.5	6.61
1.0	0.0
1.5	−0.95
2.0	0.07
2.5	0.73
3.0	−0.12
3.5	−0.83
4.0	−0.04
4.5	6.42

(a) What are the unknowns in this question? What are we trying to solve for?

Answer:

The unknowns are a_0, a_1, a_2, a_3, and a_4. They are also what we are trying to solve for.

(b) Can you write an equation corresponding to the first observation (x_0, y_0), in terms of a_0, a_1, a_2, a_3, and a_4? What does this equation look like? Is it linear in the unknowns?

Answer:

Plugging (x_0, y_0) into the expression for y in terms of x, we get

$$24 = a_0 + a_1 \cdot 0 + a_2 \cdot 0^2 + a_3 \cdot 0^3 + a_4 \cdot 0^4$$

You can see that this equation is linear in a_0, a_1, a_2, a_3, and a_4.

(c) Now, write a system of equations in terms of a_0, a_1, a_2, a_3, and a_4 using *all of the observations*.

Answer:

Write the next equation using the second observation. You will now get:

$$6.61 = a_0 + a_1 \cdot (0.5) + a_2 \cdot (0.5)^2 + a_3 \cdot (0.5)^3 + a_4 \cdot (0.5)^4$$

And for the third:

$$0.0 = a_0 + a_1 \cdot (1) + a_2 \cdot 1^2 + a_3 \cdot 1^3 + a_4 \cdot 1^4$$

Do you see a pattern? Let's write the entire system of equations in terms of a matrix now.

$$\begin{bmatrix} 1 & 0 & 0^2 & 0^3 & 0^4 \\ 1 & 0.5 & (0.5)^2 & (0.5)^3 & (0.5)^4 \\ 1 & 1 & 1^2 & 1^3 & 1^4 \\ 1 & 1.5 & (1.5)^2 & (1.5)^3 & (1.5)^4 \\ 1 & 2 & 2^2 & 2^3 & 2^4 \\ 1 & 2.5 & (2.5)^2 & (2.5)^3 & (2.5)^4 \\ 1 & 3 & 3^2 & 3^3 & 3^4 \\ 1 & 3.5 & (3.5)^2 & (3.5)^3 & (3.5)^4 \\ 1 & 4 & 4^2 & 4^3 & 4^4 \\ 1 & 4.5 & (4.5)^2 & (4.5)^3 & (4.5)^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} 24 \\ 6.61 \\ 0.0 \\ -0.95 \\ 0.07 \\ 0.73 \\ -0.12 \\ -0.83 \\ -0.04 \\ 6.42 \end{bmatrix}$$

(d) Finally, solve for a_0, a_1, a_2, a_3, and a_4 using IPython. You have now found the quartic polynomial that best fits the data!

Answer:

Let $\mathbf{D}$ be the big matrix from the previous part.

$$\vec{a} = (\mathbf{D}^T\mathbf{D})^{-1}\mathbf{D}^T\vec{y} = \begin{bmatrix} 24.00958042 \\ -49.99515152 \\ 35.0039627 \\ -9.99561772 \\ 0.99841492 \end{bmatrix}$$

It turns out that the actual parameters for the polynomial equation were:

$$\vec{a} = \begin{bmatrix} 24 \\ -50 \\ 35 \\ -10 \\ 1 \end{bmatrix}$$

(Remember that our observations were noisy.)

Therefore, we have actually done pretty well with the least squares estimate!