EECS 16A Designing Information Devices and Systems I
Spring 2020 Discussion 13A

1. Least Squares with Orthogonal Columns

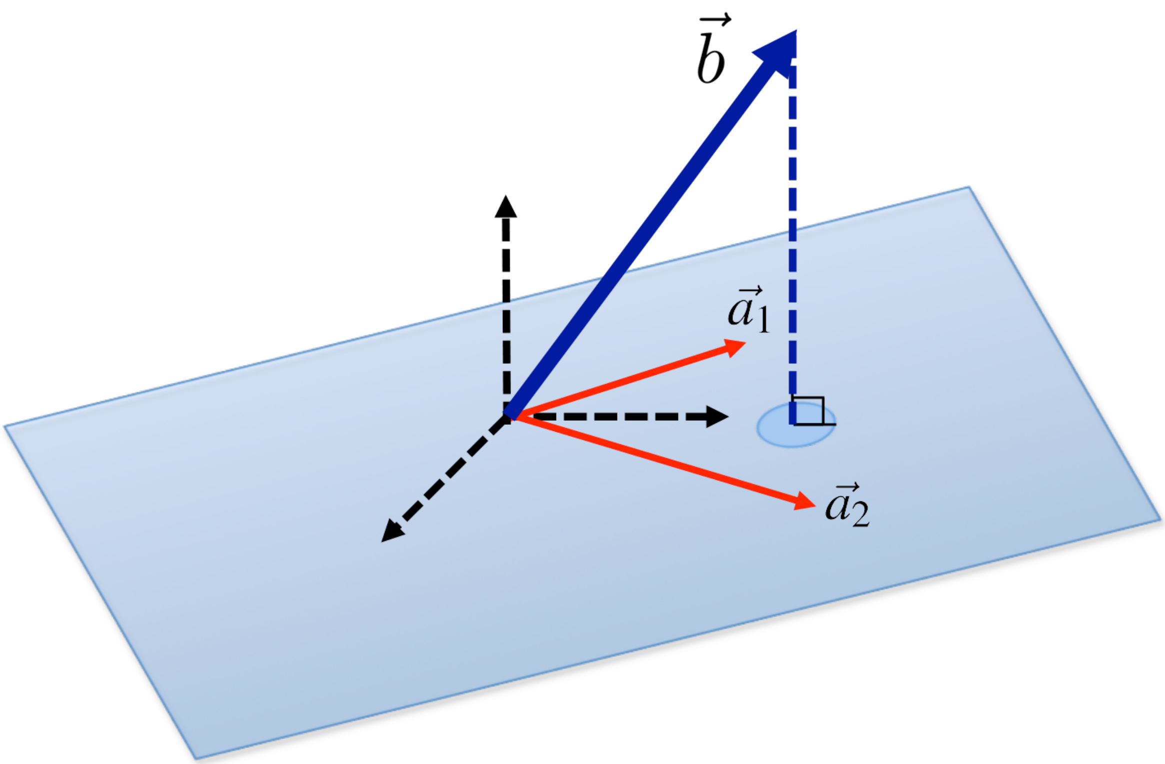
(a) Consider a least squares problem of the form

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

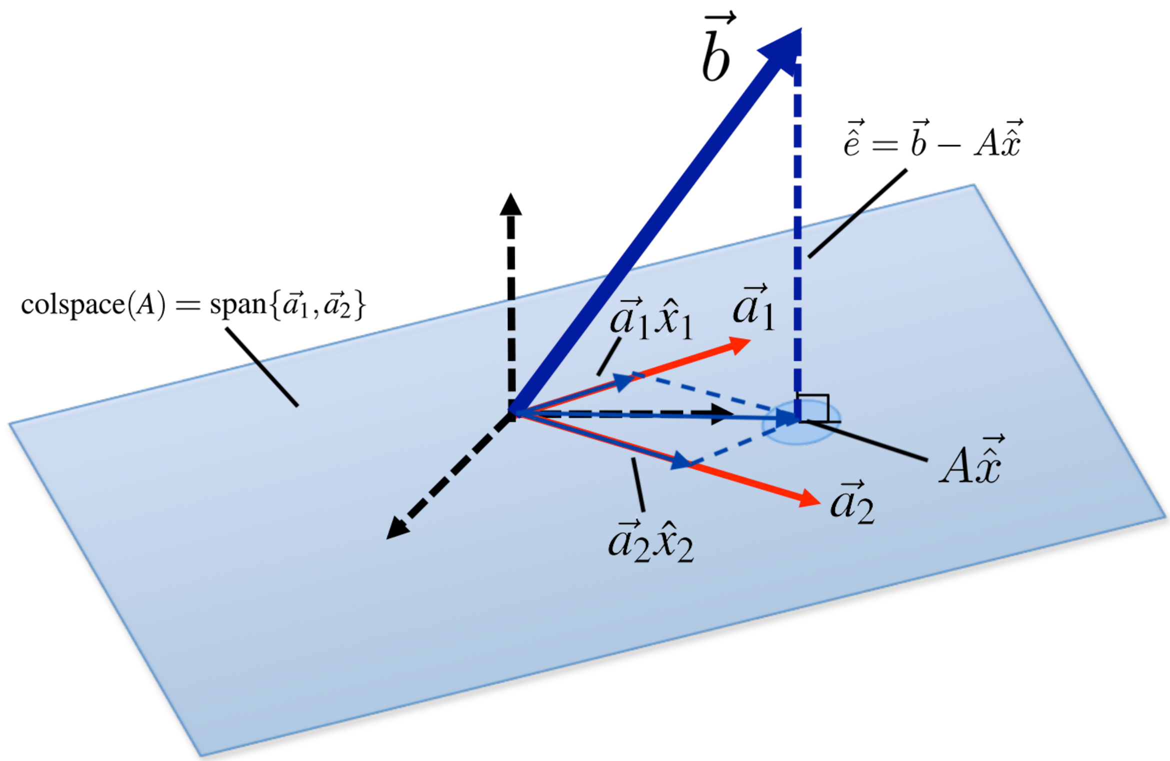
Let the solution be $\hat{\vec{x}} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix}$.

Label the following elements in the diagram below.

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

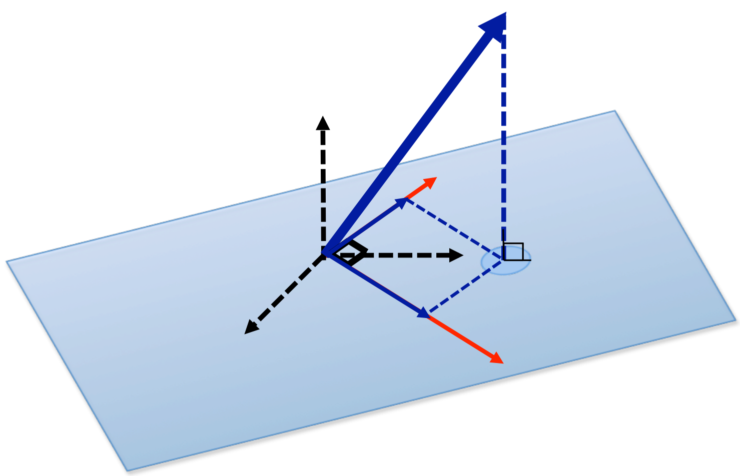


Answer:



(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:

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 $\hat{\vec{x}}$.

2. 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!

3. Vector Derivative for Least Squares

Recall that for least squares, we are trying to minimize $\|\vec{b}-\mathbf{A}\vec{x}\|^2$.

$$\begin{aligned}
\|\vec{b}-\mathbf{A}\vec{x}\|^2 &= \langle \vec{b}-\mathbf{A}\vec{x}, \vec{b}-\mathbf{A}\vec{x} \rangle \\
&= \left(\vec{b}-\mathbf{A}\vec{x}\right)^T \left(\vec{b}-\mathbf{A}\vec{x}\right) \\
&= \left(\vec{b}^T-\vec{x}^T\mathbf{A}^T\right) \left(\vec{b}-\mathbf{A}\vec{x}\right) \\
&= \vec{x}^T\mathbf{A}^T\mathbf{A}\vec{x}-\vec{b}^T\mathbf{A}\vec{x}-\vec{x}^T\mathbf{A}^T\vec{b}+\vec{b}^T\vec{b}
\end{aligned}$$

Note that $\vec{b}^T\mathbf{A}\vec{x}=\vec{x}^T\mathbf{A}^T\vec{b}$ since both sides are scalars. Therefore,

$$\|\vec{b}-\mathbf{A}\vec{x}\|^2 = \vec{x}^T\mathbf{A}^T\mathbf{A}\vec{x}-2\vec{b}^T\mathbf{A}\vec{x}+\vec{b}^T\vec{b}$$

For a column vector $\vec{x}=\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, the vector derivative of a scalar y is defined as a row vector:

$$\frac{dy}{d\vec{x}} = \begin{bmatrix} \frac{dy}{dx_1} & \frac{dy}{dx_2} & \cdots & \frac{dy}{dx_n} \end{bmatrix}$$

In this case, $y=\vec{x}^T\mathbf{A}^T\mathbf{A}\vec{x}-2\vec{b}^T\mathbf{A}\vec{x}+\vec{b}^T\vec{b}$. Evaluating $\frac{dy}{d\vec{x}}$ (out-of-scope for this class) gives:

$$\frac{dy}{d\vec{x}} = 2\vec{x}^T\mathbf{A}^T\mathbf{A}-2\vec{b}^T\mathbf{A}$$

To find the minimum, we set $\frac{dy}{d\vec{x}}=\vec{0}^T$.

$$\frac{dy}{d\vec{x}} = 2\vec{x}^T\mathbf{A}^T\mathbf{A}-2\vec{b}^T\mathbf{A}=\vec{0}^T$$

$$2\mathbf{A}^T\mathbf{A}\vec{x}-2\mathbf{A}^T\vec{b}=\vec{0}$$

$$2\mathbf{A}^T\mathbf{A}\vec{x}=2\mathbf{A}^T\vec{b}$$

$$\mathbf{A}^T\mathbf{A}\vec{x}=\mathbf{A}^T\vec{b}$$