Linear Algebra

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Back to Over-Determined System

- Let's start with the original problem:

Person ID	Weight	Height	Is_smoking	Life-span
1	60kg	5.5ft	Yes (=1)	66
2	65kg	5.0ft	No (=0)	74
3	55kg	6.0ft	Yes (=1)	78

$$\underbrace{\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 66 \\ 74 \\ 78 \end{bmatrix}}_{\mathbf{b}}$$

- Using the inverse matrix, the solution is $\mathbf{x} = \begin{bmatrix} -0.4 \\ 20 \\ -20 \end{bmatrix}$

Back to Over-Determined System

- Let's add one more example:

Person ID	Weight	Height	Is_smoking	Life-span
1	60kg	5.5ft	Yes (=1)	66
2	65kg	5.0ft	No (=0)	74
3	55kg	6.0ft	Yes (=1)	78
4	50kg	5.0ft	Yes (=1)	72

$$\underbrace{\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 0 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix}}_{\mathbf{b}}$$

- Now, let's use the previous solution $\mathbf{x} = \begin{bmatrix} -0.4 \\ 20 \\ -20 \end{bmatrix}$

Errors

$$\underbrace{\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} -0.4 \\ 20 \\ -20 \end{bmatrix}}_{\mathbf{x}} = \begin{bmatrix} 66 \\ 74 \\ 78 \\ 60 \end{bmatrix} \neq \underbrace{\begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix}}_{\neq\ \mathbf{b}} \quad \left| \quad \begin{array}{c} (\mathbf{b} - A\mathbf{x}) \\ 0 \\ 0 \\ 0 \\ -12 \end{array} \right.$$

Back to Over-Determined System

- How about using slightly different solution $\mathbf{x} = \begin{bmatrix} -0.12 \\ 16 \\ -9.5 \end{bmatrix}$?

Errors

$$\begin{array}{ccccccc} A & \mathbf{x} & & & \neq & \mathbf{b} & (\mathbf{b} - A\mathbf{x}) \\ \begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix} & \begin{bmatrix} -0.12 \\ 16 \\ -9.5 \end{bmatrix} & = & \begin{bmatrix} 71.3 \\ 72.2 \\ 79.9 \\ 64.5 \end{bmatrix} & \neq & \begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix} & \begin{matrix} -5.3 \\ 1.8 \\ -1.9 \\ 7.5 \end{matrix} \end{array}$$

Which One is Better Solution?

$$\begin{array}{ccccc} A & \mathbf{x} & \neq & \mathbf{b} & (\mathbf{b} - A\mathbf{x}) \end{array}$$

Errors

$$\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix} \begin{bmatrix} -0.12 \\ 16 \\ -9.5 \end{bmatrix} = \begin{bmatrix} 71.3 \\ 72.2 \\ 79.9 \\ 64.5 \end{bmatrix} \neq \begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix} \quad \begin{matrix} -5.3 \\ 1.8 \\ -1.9 \\ 7.5 \end{matrix}$$

$$\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix} \begin{bmatrix} -0.4 \\ 20 \\ -20 \end{bmatrix} = \begin{bmatrix} 66 \\ 74 \\ 78 \\ 60 \end{bmatrix} \neq \begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix} \quad \begin{matrix} 0 \\ 0 \\ 0 \\ -12 \end{matrix}$$

Least Squares: Best Approximation Criterion

- Let's use the squared sum of errors:

Errors **Sum of squared errors**

$$\underset{A}{\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix}} \underset{\mathbf{x}}{\begin{bmatrix} -0.12 \\ 16 \\ -9.5 \end{bmatrix}} = \begin{bmatrix} 71.3 \\ 69 \\ 79.9 \\ 64.5 \end{bmatrix} \neq \underset{\mathbf{b}}{\begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix}} \quad \underset{(\mathbf{b} - A\mathbf{x})}{\begin{matrix} -5.3 \\ 1.8 \\ -1.9 \\ 7.5 \end{matrix}} \quad \left((-5.3)^2 + 1.8^2 + (-1.9)^2 + 7.5^2\right)^{0.5} = 9.55$$

Better solution

$$\begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix} \begin{bmatrix} -0.4 \\ 20 \\ -20 \end{bmatrix} = \begin{bmatrix} 66 \\ 74 \\ 78 \\ 60 \end{bmatrix} \neq \begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix} \quad \begin{matrix} 0 \\ 0 \\ 0 \\ -12 \end{matrix} \quad \left(0^2 + 0^2 + 0^2 + (-12)^2\right)^{0.5} = 12$$

Least Squares Problem

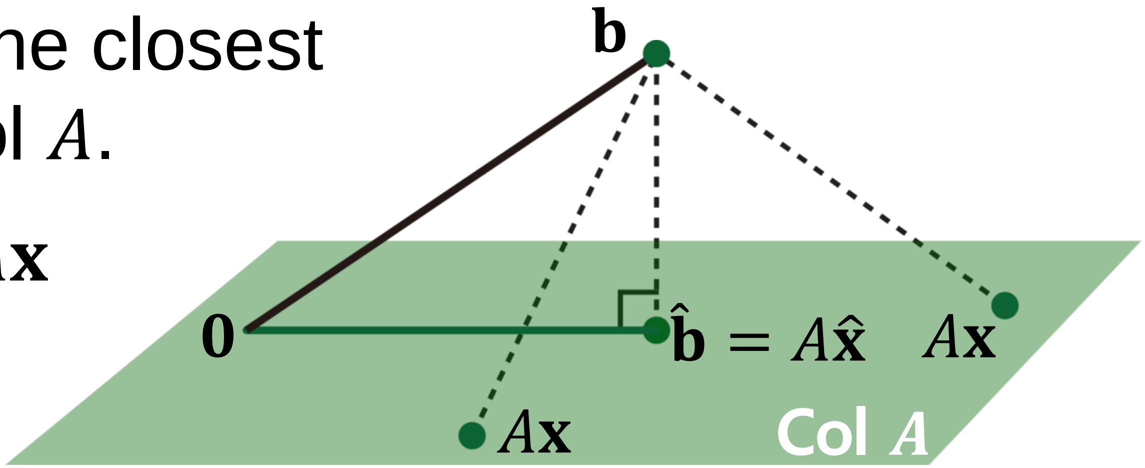
- Now, the sum of squared errors can be represented as $||\mathbf{b} - A\mathbf{x}||$.
- **Definition**: Given an overdetermined system $A\mathbf{x} \simeq \mathbf{b}$ where $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^{n}$, and $m \gg n$, a least squares solution $\hat{\mathbf{x}}$ is defined as

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} ||\mathbf{b} - A\mathbf{x}||$$

- The most important aspect of the least-squares problem is that no matter what $\mathbf{x}$ we select, the vector $A\mathbf{x}$ will necessarily be in the column space Col A.
- Thus, we seek for $\mathbf{x}$ that makes $A\mathbf{x}$ as the closest point in Col A to $\mathbf{b}$.

Geometric Interpretation of Least Squares

- Consider $\hat{\mathbf{x}}$ such that $\hat{\mathbf{b}} = A\hat{\mathbf{x}}$ is the closest point to $\mathbf{b}$ among all points in Col A.



- That is, $\mathbf{b}$ is closer to $\hat{\mathbf{b}}$ than to $A\mathbf{x}$ for any other $\mathbf{x}$.

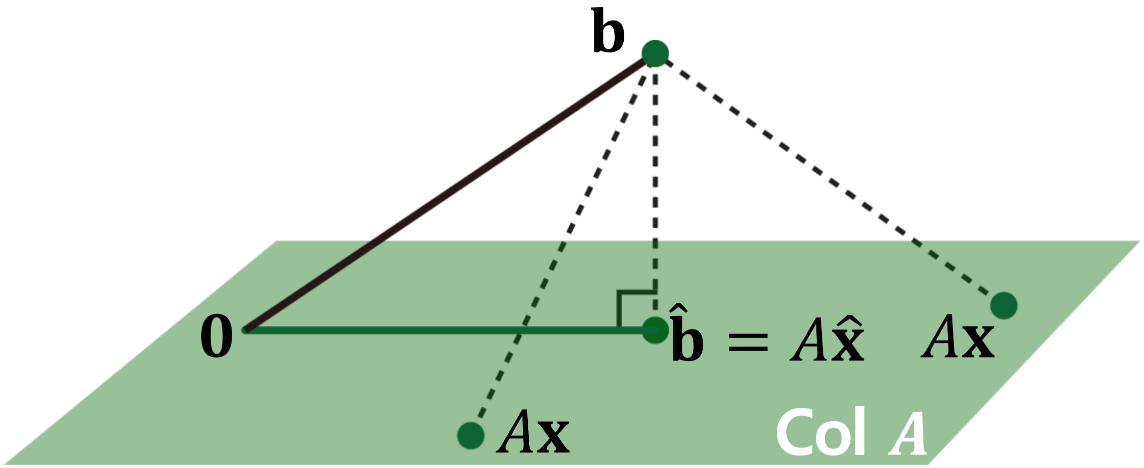
- To satisfy this, the vector $\mathbf{b} - A\hat{\mathbf{x}}$ should be orthogonal to Col A.

- This means $\mathbf{b} - A\hat{\mathbf{x}}$ should be orthogonal to any vector in Col A:

$$\mathbf{b} - A\hat{\mathbf{x}} \perp \left(x_1\mathbf{a}_1 + x_2\mathbf{a}_2 \cdots + x_p\mathbf{a}_n\right) \text{ for any vector } \mathbf{x}$$

Geometric Interpretation of Least Squares

- $\mathbf{b} - A\hat{\mathbf{x}} \perp \left(x_1\mathbf{a}_1 + x_2\mathbf{a}_2 \cdots + x_p\mathbf{a}_n\right)$ for any vector $\mathbf{x}$



- Or equivalently,

$$\begin{aligned}(\mathbf{b} - A\hat{\mathbf{x}}) &\perp \mathbf{a}_1 \\ (\mathbf{b} - A\hat{\mathbf{x}}) &\perp \mathbf{a}_2 \\ &\vdots \\ (\mathbf{b} - A\hat{\mathbf{x}}) &\perp \mathbf{a}_m\end{aligned} \Rightarrow \begin{aligned}\mathbf{a}_1^T(\mathbf{b} - A\hat{\mathbf{x}}) &= 0 \\ \mathbf{a}_2^T(\mathbf{b} - A\hat{\mathbf{x}}) &= 0 \\ &\vdots \\ \mathbf{a}_m^T(\mathbf{b} - A\hat{\mathbf{x}}) &= 0\end{aligned} \Rightarrow A^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0$$

Normal Equation

- Finally, given a least squares problem, $A\mathbf{x} \simeq \mathbf{b}$, we obtain

$$A^T A\hat{\mathbf{x}} = A^T\mathbf{b},$$

which is called a normal equation.

- This can be viewed as a new linear system, $C\mathbf{x} = \mathbf{d}$, where a square matrix $C = A^T A \in \mathbb{R}^{n\times n}$, and $\mathbf{d} = A^T\mathbf{b} \in \mathbb{R}^n$.

- If $C = A^T A$ is invertible, then the solution is computed as

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

Another Derivation of Normal Equation

- $\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\| = \arg\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|^2$

  $= \arg\min_{\mathbf{x}} (\mathbf{b} - A\mathbf{x})^{\mathrm{T}}(\mathbf{b} - A\mathbf{x}) = \mathbf{b}^{\mathrm{T}}\mathbf{b} - \mathbf{x}^{\mathrm{T}}A^{\mathrm{T}}\mathbf{b} - \mathbf{b}^{\mathrm{T}}A\mathbf{x} + \mathbf{x}^{\mathrm{T}}A^{\mathrm{T}}A\mathbf{x}$

- Computing derivatives w.r.t. $\mathbf{x}$, we obtain

$$-A^{\mathrm{T}}\mathbf{b} - A^{\mathrm{T}}\mathbf{b} + 2A^{\mathrm{T}}A\mathbf{x} = \mathbf{0} \quad \Leftrightarrow \quad A^{\mathrm{T}}A\mathbf{x} = A^{\mathrm{T}}\mathbf{b}$$

- Thus, if $C = A^T A$ is invertible, then the solution is computed as

$$\mathbf{x} = (A^T A)^{-1} A^T \mathbf{b}$$

Life-Span Example

Person ID	Weight	Height	Is_smoking	Life-span
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- The normal equation $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$ is

$$\begin{bmatrix} 60 & 65 & 55 & 50 \\ 5.5 & 5.0 & 6.0 & 5.0 \\ 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 60 & 5.5 & 1 \\ 65 & 5.0 & 0 \\ 55 & 6.0 & 1 \\ 50 & 5.0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 60 & 65 & 55 & 50 \\ 5.5 & 5.0 & 6.0 & 5.0 \\ 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 66 \\ 74 \\ 78 \\ 72 \end{bmatrix}$$

$$\begin{bmatrix} 13350 & 1235 & 165 \\ 1235 & 116.25 & 16.5 \\ 165 & 16.5 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 16600 \\ 1561 \\ 216 \end{bmatrix}$$

What If $C = A^T A$ is NOT Invertible?

- Given $A^{\mathrm{T}}A\mathbf{x} = A^{\mathrm{T}}\mathbf{b}$, what if $C = A^T A$ is NOT invertible?
- Remember that in this case, the system has either no solution or infinitely many solutions.
- However, the solution always exist for this “normal” equation, and thus infinitely many solutions exist.
- When $C = A^T A$ is NOT invertible?
  If and only if the columns of A are linearly dependent. Why?
- However, $C = A^T A$ is usually invertible. Why?