

HCAI5TML01 – Mathematics of Learning. Week – 2: Lecture – 02

A Refresher on the Mathematics Behind Machine Learning. Least Squares and Fundamental Theory of Linear Algebra.

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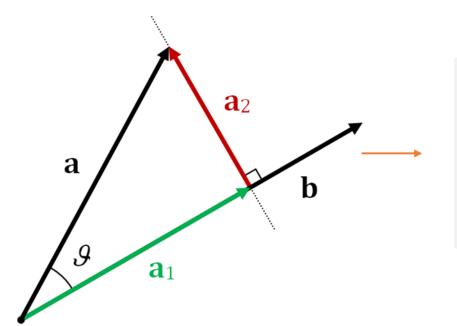
1. Some More Definitions.





1.1 Introduction: Vector projection.

- Vector projection is a fundamental concept in linear algebra that decomposes
 - a vector into components **parallel and perpendicular** to another vector or subspace.



- In this example we project vector a onto vector b,
- Then we can indeed **decompose a** into:
 - A parallel component aligned with b
 - A perpendicular component orthogonal to b.
- Mathematically, this is expressed as:
 - $\mathbf{a} = \mathbf{proj_ba} + \mathbf{perp_ba}$
 - $\mathbf{proj_ba}$ → the projection a onto b.
 - $perp_ba \rightarrow is$ the rejection of a from b (perpendicular to b)





1.2 Projection on to vector.

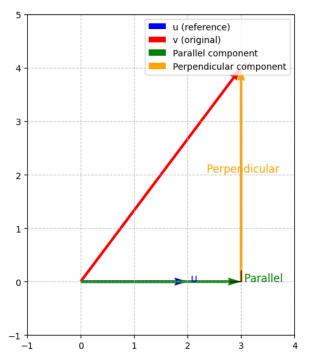
Definition:

- Given two vector **u** and **v**, the projection of **v** onto **u** (denoted proj_u**v**)
 - is a component of v that lies in the direction of u.
 - The **proj**_u**v** is commuted as:

•
$$\operatorname{proj}_{\mathbf{u}}\mathbf{v} = \left(\frac{\mathbf{u}\cdot\mathbf{v}}{\mathbf{u}\cdot\mathbf{u}}\right)\mathbf{u} = \left(\frac{\mathbf{u}\cdot\mathbf{v}}{\|\mathbf{u}\|^2}\right)\mathbf{u}$$

- Key components:
 - Dot product $(\mathbf{u} \cdot \mathbf{v})$:
 - Measures how **much v aligns with u** (the "overlap").
 - If u and v are orthogonal, $\mathbf{u} \cdot \mathbf{v} = \mathbf{0}$ (no projection).
 - Normalization $(\mathbf{u} \cdot \mathbf{u} == \|\mathbf{u}\|^2)$:
 - This is the scaled magnitude of u.
 - Purpose: scales the projection to the unit length of u,
 - ensuring the result is **proportional to u's direction** without **distorting its length**.
 - This ensures the projection depends only on the *direction* of \mathbf{u} , not its magnitude.

Vector Decomposition: Parallel and Perpendicular Components





1.2.1 Example: with and without Normalizations.

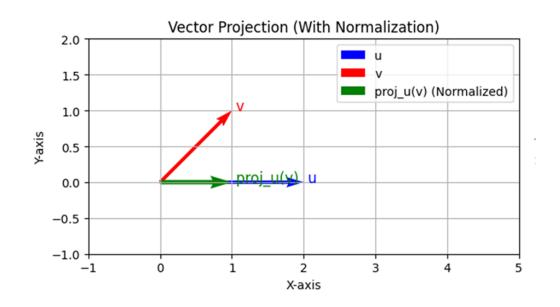
- Let's use the same vectors u and v but omit normalization to see how the projection becomes distorted.
 - Given vectors: $\mathbf{u} = \frac{2}{0}$; $\mathbf{v} = \frac{1}{1}$
 - 1. Correct Projection with Normalization:

•
$$\mathbf{u} \cdot \mathbf{v} = \begin{bmatrix} 2 & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix} = 2 \times \mathbf{1} + \mathbf{0} \times \mathbf{1} = 2$$

•
$$\mathbf{u} \cdot \mathbf{u} = 2^2 + 0^2 = 4$$

• Projection:

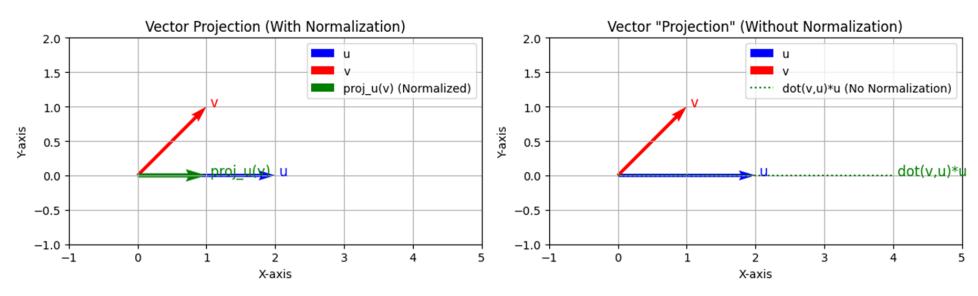
•
$$\operatorname{proj}_{\mathbf{u}}\mathbf{v} = \left(\frac{\mathbf{u}\cdot\mathbf{v}}{\mathbf{u}\cdot\mathbf{u}}\right)\mathbf{u} = \left(\frac{2}{4}\right)\begin{bmatrix}\mathbf{2}\\\mathbf{0}\end{bmatrix} = \begin{bmatrix}\mathbf{1}\\\mathbf{0}\end{bmatrix}$$



• The result is a vector in the direction of u with length scaled to match the "shadow" of v onto u.

1.2.1 Example: with and without Normalizations.

- 2. Distorted Projection (without Normalization):
 - If we **omit normalization**, the projection becomes:
 - Distored Projection = $(\mathbf{u} \cdot \mathbf{v})(\mathbf{u}) = 2 \begin{bmatrix} 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 4 \\ 0 \end{bmatrix}$
 - Without dividing by $\mathbf{u} \cdot \mathbf{u} == \|\mathbf{u}\|^2$, the result, over scales by the length of \mathbf{u} .
 - Length of **distorted projection**: 4 (2× longer than u itself!).

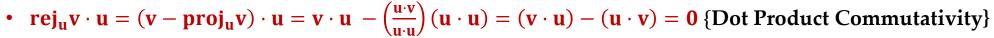




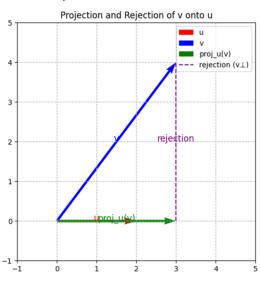


1.2.2 Orthogonal Projection (Rejection):

- When you project v onto u, you're extracting the part of v that aligns with u (the projection).
 - The **remaining part**—the **rejection**—is literally
 - "rejected" from u because it has no component in the direction of u.
- The perpendicular (rejection) component of v from u is:
 - $rej_u v = v proj_u v$
- Key Property:
 - The original vector v is the sum of its projection and rejection:
 - $\mathbf{v} = \mathbf{proj_u}\mathbf{v} + \mathbf{rej_u}\mathbf{v}$
 - The rejection component is orthogonal to u.
 - To verify orthogonality, take the dot product with u:



• This confirms $\mathbf{rej}_{\mathbf{u}}\mathbf{v}$ is orthogonal to \mathbf{u} .





1.3 Projection onto Subspace.

- Idea:
 - Instead of projecting **onto a single vector**, we can project onto a **subspace** (e.g., a plane or hyperplane).
- Using Matrix Projection {only true for $b \in C(A)$ }:
 - Given a matrix $A \in \mathbb{R}^{m \times n}$ whose columns form a basis for a subspace (full column rank matrix),
 - the projection of **b** onto **C**(**A**) (column space of **A**) is:
 - $\operatorname{proj}_{C(A)}b = A(A^{T}A)^{-1}A^{T}b.$
- Special Case: Least Square Solution,
 - If $\mathbf{b} \notin \mathbf{C}(\mathbf{A})$, this projection gives the best approximation or least square solution to $\mathbf{A}\mathbf{x} = \mathbf{b}$.

1.3.1 Derivation: $\operatorname{proj}_{C(A)}b = A(A^TA)^{-1}A^Tb$.

- Derive the projection of a vector $\mathbf{b} \in \mathbb{R}^{\mathbf{m}}$ onto the column space $\mathbf{C}(\mathbf{A}) \exists \mathbf{A} \in \mathbb{R}^{\mathbf{m} \times \mathbf{n}}$:
 - $\operatorname{proj}_{C(A)}b = A(A^{T}A)^{-1}A^{T}b$
- Step 1 Definition of Projection onto a subspace:
 - We want to find a vector $\mathbf{p} \in \mathbf{C}(\mathbf{A})$ (the projection of \mathbf{b}) such that the residual $\mathbf{b} \mathbf{p}$ is **orthogonal** to $\mathbf{C}(\mathbf{A})$.
 - Mathematically:
 - $p = A \hat{x} (since p is in C(A))$
 - And
 - $A^{T}(b A \hat{x}) = 0$ (orthogonality condition).





1.3.1 Derivation: $\operatorname{proj}_{C(A)}b = A(A^TA)^{-1}A^Tb$.

- Step 2: Solve for **x**̂:
 - From the orthogonality condition:

•
$$A^{T}(b-A\hat{x})=0$$

•
$$\mathbf{A}^{\mathsf{T}}\mathbf{b} - \mathbf{A}^{\mathsf{T}}\mathbf{A}\,\hat{\mathbf{x}} = \mathbf{0}$$

$$\bullet \quad \boxed{\mathbf{A}^{\mathsf{T}}\mathbf{A}\,\hat{\mathbf{x}} = \mathbf{A}^{\mathsf{T}}\mathbf{b}}$$

- This is called **Normal Equation**.
- Step 3: Solve the Normal Equation:
 - Assuming A has full column rank (columns are linearly independent), **A^TA is invertible**, and:

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



1.3.1 Derivation: $\operatorname{proj}_{C(A)}b = A(A^TA)^{-1}A^Tb$.

- Optional:
 - Step 4: Projection Matrix:
 - The projection p of a vector b onto the column space C(A) is:

•
$$\mathbf{p} = \mathbf{A}(\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{b} = \mathbf{P}\mathbf{b}.$$

- Here:
 - $P = A(A^TA)^{-1}A^T$ is the projection matrix, when P multiplies b, it returns the projected vector p.
- Step 4: Verification (Orthogonality Check):
 - The residual b-p must be orthogonal to C(A):

•
$$A^{T}(b-p) = A^{T}b - A^{T}A(A^{T}A)^{-1}A^{T}b = A^{T}b - IA^{T}b = A^{T}b - A^{T}b = 0.$$

•





2. Solving Linear Regression.

{ With Normal and Least Squares.}





2.1 With Normal Equation.

- The **Normal Equation** is a fundamental result in linear regression
 - that provides a **closed-form solution** for finding the optimal parameters θ
 - that minimize the **sum of squared errors** (SSE) in linear regression.

Problem Setup: For Linear Regression Problem

Given:

A design matrix

$$\mathbf{X} \in \mathbb{R}^{\mathbf{m} \times \mathbf{n}}$$

(with m examples and n features, including a bias term if applicable).

A target vector $\mathbf{y} \in \mathbb{R}^{\mathbf{m}}$.

A parameter vector $\theta \in \mathbb{R}^{\mathbf{n}}$ (the weights we want to estimate).

Model:

The linear regression model is given by:

$$\mathbf{y} = \mathbf{X}\theta + \varepsilon$$

where ε is the error term.





2.1.1 Objective.

Objective: Minimize Sum of Squared Errors (SSE)

Objective:

Minimize the sum of squared errors (SSE):

$$\mathbf{J}(\theta) = \|\mathbf{y} - \mathbf{X}\theta\|^2 = (\mathbf{y} - \mathbf{X}\theta)^{\top} (\mathbf{y} - \mathbf{X}\theta)$$





Goal: Find Optimal θ Minimizing the Cost Function

Goal: Find the optimal θ that minimizes the cost function $\mathbf{J}(\theta)$.

Start with the cost function:

$$\mathbf{J}(\theta) = \|\mathbf{y} - \mathbf{X}\theta\|^2 = (\mathbf{y} - \mathbf{X}\theta)^{\top}(\mathbf{y} - \mathbf{X}\theta)$$

Expand the expression:

$$\mathbf{J}(\theta) = \mathbf{y}^{\top} \mathbf{y} - \mathbf{y}^{\top} \mathbf{X} \theta - \theta^{\top} \mathbf{X}^{\top} \mathbf{y} + \theta^{\top} \mathbf{X}^{\top} \mathbf{X} \theta$$

Note: $\mathbf{y}^{\top}\mathbf{X}\boldsymbol{\theta}$ is a scalar, so

$$\mathbf{y}^{\top} \mathbf{X} \theta = \theta^{\top} \mathbf{X}^{\top} \mathbf{y}$$

Simplify:

$$\mathbf{J}(\theta) = \mathbf{y}^{\top} \mathbf{y} - 2\theta^{\top} \mathbf{X}^{\top} \mathbf{y} + \theta^{\top} \mathbf{X}^{\top} \mathbf{X} \theta$$

Next, take the gradient with respect to θ .





Gradient Calculation of the Least Squares Cost Function

1. Cost Function Definition

The least squares cost function is:

$$\mathbf{J}(\theta) = \mathbf{y}^{\top}\mathbf{y} - 2\theta^{\top}\mathbf{X}^{\top}\mathbf{y} + \theta^{\top}\mathbf{X}^{\top}\mathbf{X}\theta$$

2. Term-by-Term Gradient Calculation

We compute the gradient $\nabla_{\theta} J(\theta)$ by differentiating each term separately.

• Term 1: $\mathbf{y}^{\mathsf{T}}\mathbf{y}$

This term does not depend on θ .

Its gradient is zero:

$$abla_{ heta}(\mathbf{y}^{ op}\mathbf{y}) = \mathbf{0}$$

• Term 2:

$$-\mathbf{2}\theta^{\top}\mathbf{X}^{\top}\mathbf{y}$$

This is a linear term in θ .

Using the identity

$$\nabla_{\theta}(\theta^{\top}\mathbf{a}) = \mathbf{a}$$

where $a = X^{\top}y$, we get

$$abla_{ heta}(-\mathbf{2} heta^{ op}\mathbf{X}^{ op}\mathbf{y}) = -\mathbf{2}\mathbf{X}^{ op}\mathbf{y}$$





Gradient Calculation (Continued)

• Term 3:

$$\theta^{\top} \mathbf{X}^{\top} \mathbf{X} \theta$$

This is a quadratic term in θ .

Using the identity

$$\nabla_{\theta}(\theta^{\top} \mathbf{A} \theta) = (\mathbf{A} + \mathbf{A}^{\top})\theta$$

and noting that $X^{\top}X$ is symmetric (i.e., $A^{\top}=A$), we have:

$$\nabla_{\boldsymbol{\theta}}(\boldsymbol{\theta}^{\top}\mathbf{X}^{\top}\mathbf{X}\boldsymbol{\theta}) = \mathbf{2}\mathbf{X}^{\top}\mathbf{X}\boldsymbol{\theta}$$





Combined Gradient of the Cost Function

Adding the gradients of all three terms, we get:

$$\nabla_{\theta} \mathbf{J}(\theta) = \mathbf{0} - \mathbf{2} \mathbf{X}^{\top} \mathbf{y} + \mathbf{2} \mathbf{X}^{\top} \mathbf{X} \theta$$

Simplifying:

$$\nabla_{\theta} \mathbf{J}(\theta) = -2\mathbf{X}^{\top} \mathbf{y} + 2\mathbf{X}^{\top} \mathbf{X} \theta$$





Setting Gradient to Zero and Deriving Normal Equation

To find the optimal θ , set the gradient to zero:

$$-\mathbf{2}\mathbf{X}^{\top}\mathbf{y} + \mathbf{2}\mathbf{X}^{\top}\mathbf{X}\boldsymbol{\theta} = \mathbf{0}$$

Divide both sides by 2:

$$-\mathbf{X}^{\top}\mathbf{y} + \mathbf{X}^{\top}\mathbf{X}\boldsymbol{\theta} = \mathbf{0}$$

Rearranged, this gives the **Normal Equation**:

$$\mathbf{X}^{\top}\mathbf{X}\boldsymbol{\theta} = \mathbf{X}^{\top}\mathbf{y}$$

- Why this works?
 - The cost function $J(\theta)$ is convex (bowl-shaped), so the gradient zero-point gives the global minimum.
 - The solution $\theta = (X^T X)^{-1} X^T y$ is the least squares estimator.





2.1.3 Intuition Behind Normal Equation.

Geometric Intuition Behind the Normal Equation

Geometric Insight:

The normal equation arises from the fact that the optimal θ minimizes the distance between the observed vector y and the predicted vector $X\theta$, which lies in the column space of X.

This means the residual vector $r = y - X\theta$ must be **orthogonal to the column space** of X.

Mathematically, this orthogonality condition is expressed as:

$$X^{\top}(y - X\theta) = 0$$

This condition ensures that $X\theta$ is the orthogonal projection of y onto the column space of X, and the residual lies in the orthogonal complement (i.e., the left null space of X).



2.1.4 Interpretation of the Solution.

- The solution θ minimizes the least-squares error.
 - **X**^T**X** must be invertible (i.e., **X** must have full column rank).
 - If not, regularization (like Ridge Regression) can be used.
- Advantage: Direct solution (no iterative optimization needed).
- **Disadvantage:** Computationally expensive for large n (since $(X^TX)^{-1}$ is $O(n^3)$).

2.2 What is the Least Square Solution?

- The least squares method solves the overdetermined system
- $X\theta \approx y$; $X \in \mathbb{R}^{m \times n} \& m > n$ by minimizing the sum of squared residuals:
- $J(\theta) = \|y X\theta\|^2$
- The minimizer θ^* is called the least square solution and is:
- $\theta^* = (X^T X)^{-1} X^T y$
- Key Notes:
- Uniqueness: If X has full column rank (rank(X) = n), X^TX is invertible, and θ^* is unique.
- **Degenerate case:** If rank(X) < n
 - infinitely many solutions exist (use pseudoinverses or regularization).





2.2.1 Why call it Least Squares?

1. Minimizes Squared Error:

• θ^* minimizes $\|\mathbf{y} = \mathbf{X}\theta\|^2$ the sum of squared vertical distances (residuals) between data points and the model predictions.

2. Geometric Interpretation:

• Projects **y** onto the **column space of X**, giving the **closest point X0*** in the subspace.

3. Statistical Justification:

• Under Gaussian noise assumptions, θ^* is the maximum likelihood estimator.





2.2.1 Existence and Uniqueness of Least Squares Solution

Conditions for Existence and Uniqueness of Least Squares Solution

Least Squares Solution:

$$\hat{\theta}_{LS} = (X^{\top} X)^{-1} X^{\top} y$$

Condition for Existence and Uniqueness:

- $X^{\top}X$ must be **invertible**.
- This requires that X has full column rank, i.e., rank(X) = n.
- Geometrically: the columns of X must be linearly independent.
- If $X^{\top}X$ is not invertible (i.e., singular or ill-conditioned), the solution:

$$\hat{\theta}_{LS} = (X^{\top}X)^{-1}X^{\top}y$$

does not exist in the usual sense.

In such cases, we need a remedy — this is where regularization comes in.





2.2.2 Regularized Least Squares

Regularization: Ridge Regression (L2 Regularization)

Motivation: When $X^{\top}X$ is not invertible or when we want to control model complexity, we add a penalty on the size of the coefficients.

Modified Objective:

$$J_{\text{ridge}}(\theta) = \|y - X\theta\|^2 + \lambda \|\theta\|^2$$

where $\lambda > 0$ is the regularization parameter.

Ridge Solution:

$$\hat{\theta}_{\text{ridge}} = (X^{\top}X + \lambda I)^{-1}X^{\top}y$$

Why This Helps:

- $X^{\top}X + \lambda I$ is always invertible when $\lambda > 0$, even if $X^{\top}X$ is not.
- Helps prevent overfitting by penalizing large weights.
- Especially useful in high-dimensional or multicollinear data settings.





2.2.3 When Solution exist but is Not Unique.

What Does a Unique Solution Mean?

A unique solution is one where there is exactly *one* parameter vector θ that minimizes the residual error.

- No other distinct vector $\theta' \neq \theta$ achieves the same minimal error.
- Ensures stability and interpretability of the model.
- Occurs when the design matrix X has full column rank and $X^{\top}X$ is invertible.
- Geometrically, the projection of y onto the column space of X corresponds to exactly one $\hat{\theta}$.

27



2.2.3 When Solution exist but is Not Unique.

When Least Squares Solution Exists but Is Not Unique

Scenario:

A least squares solution always exists, but it may not be unique when:

$$rank(X) < n$$
 (i.e., X does not have full column rank)

Implications:

- $X^{\top}X$ is not invertible (singular matrix).
- There are infinitely many solutions θ that minimize $||y X\theta||^2$.
- The system is underdetermined: multiple θ produce the same projection $X\theta$.

Selecting a Unique Solution:

To obtain a unique solution, we can use:

 $\hat{\theta} = X^+ y$ (minimum norm solution via Moore–Penrose pseudoinverse)

or apply regularization:

$$\hat{\theta}_{\text{ridge}} = (X^{\top}X + \lambda I)^{-1}X^{\top}y$$
 (ridge regression with $\lambda > 0$)

Both methods produce a unique $\hat{\theta}$ that minimizes the residual error.

7/11/2025 Algebra.

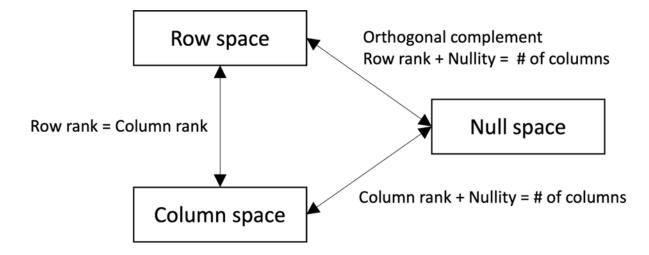




3. Fundamental Theorem of Linear Algebra. {Combining all the fundamental subspaces of Matrix.}

3.1 What is FTLA?

• The **Fundamental Theorem of Linear Algebra (FTLA)** summarizes the relationships between the four fundamental subspaces associated with a matrix.







3.2 Domain vs Range Space.

- In Linear Algebra, if $A \in \mathbb{R}^{m \times n}$, we think of A as a linear transformation:
- $A: \mathbb{R}^n \to \mathbb{R}^m$
- So:
 - Domain $\to \mathbb{R}^n$: the space where the input vectors x live.
 - Range/Co-domain $\to \mathbb{R}^m$: the space where the output vectors Ax live.
- Fundamental Subspaces in Each space:
- Domain Space \mathbb{R}^n
- This is the space of input vectors x, and it contains:
- Row space: $C(A^T) \subseteq \mathbb{R}^n$
- Null space: $\mathcal{N}(A) \subseteq \mathbb{R}^n$
- Together:
 - $\mathbb{R}^n = C(A^T) \oplus N(A)$

3.2.1 Fundamental Subspaces in Each space:

- Domain Space \mathbb{R}^n :
 - This is the space of input vectors x, and it contains:
 - Row space: $C(A^T) \subseteq \mathbb{R}^n$
 - Null space: $\mathcal{N}(A) \subseteq \mathbb{R}^n$
 - Together:
 - $\mathbb{R}^n = C(A^T) \oplus \mathcal{N}(A)$
- Range/Co-domain Space ℝ^m:
 - This is the space of **output vectors** y = Ax and it contains:
 - Column Space: $C(A) \subseteq \mathbb{R}^m$
 - Left Null Space: $\mathcal{N}(A^T) \subseteq \mathbb{R}^n$
 - Together:
 - $\mathbb{R}^{\mathbf{n}} = \mathbf{C}(A) \oplus \mathcal{N}(\mathbf{A}^{\mathsf{T}})$





3.3 The Three Standard Statements of the FTLA

Statement 1:

- The Column Space and Left Null Space Are Orthogonal Complements in \mathbb{R}^m :
 - $C(A) \perp \mathcal{N}(A^T)$ and $\mathbb{R}^n = C(A) \oplus \mathcal{N}(A^T)$

Statement 2:

- The Row Space and Null Space Are Orthogonal Complements in \mathbb{R}^n :
 - $C(A^T) \perp \mathcal{N}(A)$ and $\mathbb{R}^n = C(A) \oplus \mathcal{N}(A)$

Statement 3:

- The Dimensions of the Four Subspaces Are Related by Rank:
 - $\dim(C(A)) = \operatorname{rank}(A)$
 - $\dim (C(A^T)) = \operatorname{rank}(A)$
 - $\dim(\mathcal{N}(A)) = n \operatorname{rank}(A)$
 - $\dim \left(\mathcal{N}(\mathbf{A}^{\mathsf{T}}) \right) = \mathbf{m} \operatorname{rank}(\mathbf{A})$





Putting them Together.

Range Space and FTAL

Fundamental Theorem of Linear Algebra – Orthogonality and Decomposition (Range Space)

- 1. Orthogonality: $C(A) \perp N(A^{\top})$
 - The column space $C(A) \subseteq \mathbb{R}^m$ is orthogonal to the left null space $N(A^\top) \subseteq \mathbb{R}^m$.
 - For $y_1 = Ax \in C(A)$ and $y_2 \in N(A^\top)$:

$$y_1^{\top} y_2 = x^{\top} A^{\top} y_2 = 0 \Rightarrow y_1 \perp y_2$$

- 2. Direct Sum: $\mathbb{R}^m = C(A) \oplus N(A^\top)$
 - Every vector $y \in \mathbb{R}^m$ can be uniquely decomposed as:

$$y = y_c + y_n$$
, with $y_c \in C(A)$, $y_n \in N(A^{\top})$

• Since:

$$\dim(C(A))+\dim(N(A^\top))=\operatorname{rank}(A)+(m-\operatorname{rank}(A))=m$$
 and $C(A)\cap N(A^\top)=\{0\}$

Column Space and FTAL

Fundamental Theorem of Linear Algebra – Orthogonality and Decomposition (Domain Space)

- 3. Orthogonality: $C(A^{\top}) \perp N(A)$
 - The row space $C(A^{\top}) \subseteq \mathbb{R}^n$ is orthogonal to the null space $N(A) \subseteq \mathbb{R}^n$.
 - For $x_1 \in C(A^{\top})$ and $x_2 \in N(A)$, $Ax_2 = 0 \Rightarrow x_1^{\top} x_2 = 0$
- **4. Direct Sum:** $\mathbb{R}^n = C(A^\top) \oplus N(A)$
 - Every vector $x \in \mathbb{R}^n$ can be uniquely written as:

$$x = x_r + x_n$$
, with $x_r \in C(A^\top)$, $x_n \in N(A)$

• Since:

$$\dim(C(A^\top)) + \dim(N(A)) = \operatorname{rank}(A) + (n - \operatorname{rank}(A)) = n$$
 and $C(A^\top) \cap N(A) = \{0\}$

Thank You.