# Introduction to Machine Learning - CS725 Instructor: Prof. Ganesh Ramakrishnan

Overview of Linear Algebra

## Solving Linear Equation: Geometric View

- Simple example of two equations and two unknowns x and y to be found: 2x y = 0 and -x + 2y = 3, and in general, Ax = b
- One view: Each equation is a straight line in the *xy* plane, and we seek the point of intersection of the two lines (Fig. 2)



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• Challenging in Higher Dimensions!

- Linear algebra, shows us three different ways of view solutions if they exist):
  - A direct solution to Ax = b, using techniques called  $\frac{2}{3}$  for codural elimination and back substitution.
  - 2 A solution by "inverting" the matrix A, to give the solution  $\mathbf{x} = A^{-1}\mathbf{b}$ .

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A vector space solution, by looking at notions called the column space and nullspace of A.

#### Vectors and Matrices

A pair of numbers represented by a *two-dimensional column vector*:

$$\mathbf{u} = \left[ \begin{array}{c} 2\\ -1 \end{array} \right]$$

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Vector operations: scalar multiplication and vector addition: If  $\mathbf{v} = (-1, 2)$ , then what is  $\mathbf{u} + \mathbf{v}$ ?

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## Vectors and Matrices (contd)

- Can be visualised as the diagonal of the parallelogram formed by **u** and **v**
- Any point on the plane containing the vectors u and v is some linear combination au + bv,
- Space of all linear combinations is simply the full two-dimensional plane ( $\Re^2$ ) containing **u** and **v**
- Similarly, vectors generated by linear combinations of 2 points in a three-dimensional space form some "subspace" of the vector space  $\Re^3$
- The space of linear combinations  $a\mathbf{u} + b\mathbf{v} + c\mathbf{w}$  could fill the entire three-dimensional space.

#### Solving Linear Systems: Linear Algebra View

Recap the two equations:

$$2x - y = 0$$

$$-x+2y=3$$

And now see their "vector" form:

$$x\begin{bmatrix}2\\-1\end{bmatrix}+y\begin{bmatrix}-1\\2\end{bmatrix}=\begin{bmatrix}0\\3\end{bmatrix}$$
 (1)

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**Solutions as linear combinations of vectors:** That is, is there some linear combination of the column vectors [2, -1] and [-1, 2] that gives the column vector [0, 3]?

#### Solving Linear Systems: Linear Algebra View

$$A = \left[ egin{array}{cc} 2 & -1 \ -1 & 2 \end{array} 
ight]$$

is a  $2\times 2$  (Coefficient) Matrix' - a rectangular array of numbers. Further, if

$$\mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}$$
 and  $\mathbf{b} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$ 

Then, the matrix equation representing the same linear combination is:

$$A\mathbf{x} = \mathbf{b} \tag{2}$$

## A 3 $\times$ 3 Case

$$2x - y = 0$$
$$-x + 2y - z = -1$$
$$-3y + 4z = 4$$

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -3 & 4 \end{bmatrix}$$
$$\mathbf{b} = \begin{bmatrix} 0 \\ -1 \\ 4 \end{bmatrix}$$

Find values of x, y and z such that:

$$x(\text{column 1 of } A) + y(\text{column 2 of } A) + z(\text{column 3 of } A) = \begin{bmatrix} 0 \\ -1 \\ 4 \end{bmatrix}$$

It is easy to see now that the solution we are after is the solution to the matrix equation  $A\mathbf{x} = b$ :

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

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It may be the case that for some values of A and b, no values of x, y and z would solve  $A\mathbf{x} = b$ :

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \mathbf{?}$$

#### Solution of Linear Equations by (Gauss) Elimination

Progressively *eliminate* variables from equations: First multiply both sides of the second equation by 2 (leaving it unchanged): back substitution

$$-2x + 4y = 6$$

2x - y = 0 f 2(-x + 2y = 3)

Adding LHS of the first equation to the LHS of this new equation, and RHS of the first equation to the RHS of this new equation (does not alter anything):

$$(-2x+4y) + (2x-y) = 6 + 0$$
 or  $3y = 6$ 

You can see that x has been "eliminated" from the second equation and the set of equations have been said to be transformed into an *upper triangular* form.

$$2x - y = 0$$
  

$$3y = 6$$

$$\begin{bmatrix} 2 & -1 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 4 \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \end{bmatrix}$$

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 $\Rightarrow$  y = 6/3 = 2. And substituting back y into the first equation, 2x - 2 = 0 or x = 1.

## Row Elimination: More illustration



- The (2,1) step: First eliminate x from the second equation  $\Rightarrow$  multiply the first equation by a multiplier  $(a_{21}/a_{11})$  and subtract it from the second equation.
- a<sub>11</sub> is called the *pivot*: Goal is to eliminate x coefficient in the second equation.

RHS, after the first elimination step, is:

$$\mathbf{b}_1 = \left[ \begin{array}{c} 2\\ 6\\ 2 \end{array} \right]$$

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#### Row Elimination: More illustration

$$A_{1} = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ \hline 0 & 4 & 1 \\ (3,1) & (3,2) \end{bmatrix}$$

- The (3,1) step for eliminating  $a_{31}$ : Nothing to do, so  $A_2 = A_1$
- The (3,2) step for eliminating  $a_{32}$ :  $a_{22}$  is the next pivot...

$$A_{3} = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & 5 \end{bmatrix}$$

$$e^{1} e^{1} e^{$$

- Sequence of operations on Ax to get A<sub>3</sub>x ⇒ multiplying by a sequence of "elimination matrices"
- Eg: A<sub>1</sub> and **b**<sub>1</sub> can be obtained by pre-multiplying A and **b** respectively by the matrix E<sub>21</sub>:

$$E_{21} = \left[ \begin{array}{rrrr} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right]$$

- This also holds for  $E_{32}$  and so on. Make sure and **verify** that you understand Matrix multiplication!
- Multiplying matrices A and B is only meaningful if the number of columns of A is the same as the number of rows of B. That is, if A is an m × n matrix, and B is an n × k matrix, then AB is an m × k matrix.

## More on Matrix Multiplication

- Matrix multiplication is "associative"; that is, (AB)C = A(BC)
- But, unlike ordinary numbers, matrix multiplication is not "commutative". That is  $AB \neq BA$
- Associativity of matrix multiplication allows us to build up a sequence of matrix operations representing elimination.

$$E_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad E_{32} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix}$$

• General rule: If we are looking at *n* equations in *m* unknowns, and an elimination step involves multiplying equation *j* by a number *q* and subtracting it from equation *i*, then the elimination matrix  $E_{ij}$  is simply the  $n \times m$  "identity matrix" *I*, with  $a_{ij} = 0$  in *I* replaced by -q.

## Elimination as Matrix Multiplication

• For example, with 3 equations in 3 unknowns, and an elimination step that "multiplies equation 2 by 2 and subtracts from equation 3":

$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad E_{32} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix}$$

• The three elimination steps give:

$$E_{32}E_{31}E_{21}(A\mathbf{x}) = E_{32}E_{31}E_{21}\mathbf{b}$$

which, using associativity is:

$$U\mathbf{x} = (E_{32}E_{31}E_{21})\mathbf{b} = \mathbf{c} \tag{3}$$

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with U be the obvious upper triangular matrix

#### Elimination as Matrix Multiplication

$$U = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & 5 \end{bmatrix} \quad \mathbf{c} = \begin{bmatrix} 2 \\ 6 \\ -10 \end{bmatrix}$$
(4)

Just as a single elimination step can be expressed as multiplication by an elimination matrix, exchange of a pair of equations can be expressed by multiplication by a *permutation* matrix. Consider...
4y + z = 2
4y + z = 2
3x + 8y + z = 12
The coefficient matrix A can benefit from permutation! Why?

## Elimination as Matrix Multiplication

- No solution exists, if, in spite of all exchanges, elimination results in a 0 in any one of the pivot positions
- Else, we will reach a point where the original equation  $A\mathbf{x} = \mathbf{b}$  is transformed into  $U\mathbf{x} = \mathbf{c}$
- Final step is *back-substitution*, in which variables are progressively assigned values using the right-hand side of this transformed equation

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• Eg: z = -2, back-substituted to give y = 1, which finally yields x = 2.

## Matrix Inversion for Solving Linear Equations

#### J mx n

- Given  $A\mathbf{x} = \mathbf{b}$ , we find  $\mathbf{x} = A^{-1}\mathbf{b}$ , where  $A^{-1}$  is called the *inverse* of the matrix.
- $A^{-1}$  is such that  $AA^{-1} = I$  where I is the identity matrix.
- Since matrix multiplication does not necessarily commute: If for an m×n matrix A, there exists a matrix A<sub>L</sub><sup>-1</sup> such that A<sub>L</sub><sup>-1</sup>A = I, (n×n), then A<sub>L</sub><sup>-1</sup> is called the left inverse of A.
  Similarly, if there exists a matrix A<sub>R</sub><sup>-1</sup> such that AA<sub>R</sub><sup>-1</sup> = I (m×m), then A<sub>R</sub><sup>-1</sup> is called the right inverse of A.
  - For square matrices, the left and right inverses are the same:

$$A_L^{-1}(AA_R^{-1}) = (AA_L^{-1})A_R^{-1}$$

- For square matrices, we can simply talk about "the inverse"  $A^{-1}$ .
- Do all square matrices have an inverse?

• Here is a matrix that is not invertible:

$$A = \begin{bmatrix} 1 & 3 \\ 2 & 6 \end{bmatrix}$$
(5)

- If  $A^{-1}$  exists, the solution will be  $\mathbf{x} = A^{-1}\mathbf{b}$  and elimination must also produce an upper triangular matrix with non-zero pivots.
- Thus, the condition works both ways: if elimination produces non-zero pivots then the inverse exists and otherwise, the matrix is not invertible or singular (verify for (5))

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- ⇔ Matrix will be singular iff its "determinant" is 0 and is related to the elimination producing non-zero pivots.

- If a set of vectors V is to qualify as a "vector space" it should be "closed" under the operations of addition and scalar multiplication.
- Thus, given vectors u and v in a vector space, all scalar multiples of vectors au and bv are in the space, as is their linear combination au + bv.
- If a subset  $(V_S)$  of any such space is itself a vector space (that is,  $(V_S)$  is also closed under linear combination) then  $(V_S)$  is called a subspace of (V).
- Eg: Set of vectors  $\Re^2$ ,  $\mathcal{M}$  consisting of all  $2 \times 2$  matrices
- Set  $(\Re^2)^+$  (2-D vectors in the positive quadrant is *not* a vector space.

## Column Space and Solution to Linear System

- Column space of A, or C(A): All possible linear combinations of the columns of A, that produce in effect, all possible **b**'s
- Is there a solution to  $A\mathbf{x} = \mathbf{b} \Leftrightarrow \mathbf{b} \in C(A)$ :
- In the example below, is C(A) the entire 4-dimensional space  $\Re^4$ ? If not, how much smaller is C(A) compared to  $\Re^4$ ?

$$A = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 3 \\ 3 & 1 & 4 \\ 4 & 1 & 5 \end{bmatrix} \xrightarrow{\text{stanks2}} Aim(C(A)) \in 2$$

- Equivalently, with Ax = b, for which right hand sides b does a solution x always exist?
- Definitely does not exist for every right hand side **b**, (4 equations in 3 unknowns)

## More on Column Space

• Which right hand side **b** allows the equation to be solved

$$A\mathbf{x} = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 3 \\ 3 & 1 & 4 \\ 4 & 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$
(6)

 Eg: If b = 0, the corresponding solution is x = 0. Or whenever b ∈ C(A) (such as b being a specific column of A).

Can we get the same space C(A) using less than three columns of A<sup>1</sup>? In this particular example, the third column of A is a linear combination of the first two columns of A. C(A) is therefore a 2-dimensional subspace of R<sup>4</sup>.

• In general, if A is an  $m \times n$  matrix, C(A) is a subspace of  $\Re^m$ .

<sup>&</sup>lt;sup>1</sup>In subsequent sections, we will refer to these columns as *pivot* columns.

## Null Space

- The null space N(A), is the space of all solutions to the equation  $A\mathbf{x} = 0$ .
- N(A) of an  $m \times n$  matrix A is a subspace of  $\Re^n$ .
- Eg: One obvious solution to the system below is 0 (which will always be  $\in N(A)$ ). Any other solution?

$$A\mathbf{x} = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 3 \\ 3 & 1 & 4 \\ 4 & 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
(7)

# Finding elements of N(A)

• Since columns of A are linearly dependent, a second solution  $\mathbf{x}^* \in N(A)$  is as follows (and so are  $c\mathbf{x}^*$  for any  $c \in \Re$ )

 $\mathbf{x}^* = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \xrightarrow{\mathbf{a}} \begin{bmatrix} \mathbf{a} & \mathbf{b}^{\mathbf{e}} & \mathbf{s} & \mathbf{n}^{\mathbf{e}} \\ \mathbf{j}^{\mathbf{o}\mathbf{u}\mathbf{n}\mathbf{d}} & \mathbf{g}^{\mathbf{u}\mathbf{n}} & \mathbf{s} \\ \mathbf{g}^{\mathbf{u}\mathbf{n}} & \mathbf{s} \end{bmatrix}$ The null space N(A) is the line passing through the zero N(A) is always a vector space
 N(A) is always a vector space
 N(A) is always of specifying a subspace

- Specify a bunch of vectors whose linear combinations will yield the subspace.
  - $\gtrsim$  Specify  $A\mathbf{x} = \mathbf{0}$  and any vector  $\mathbf{x}$  that satisfies the system is an element of the subspace.
  - Set of all solutions to the equation  $A\mathbf{x} = \mathbf{b}$  do NOT form a space?

## Independence, Basis, and Rank

- Independence: Vectors x<sub>1</sub>, x<sub>2</sub>,..., x<sub>n</sub> are independent if no linear combination gives the zero vector, except the zero combination. That is, ∀c<sub>1</sub>, c<sub>2</sub>,..., c<sub>n</sub> ∈ ℜ, such that not all of the c<sub>i</sub>'s are simultaneously 0, ∑<sub>i</sub><sup>n</sup> c<sub>i</sub>x<sub>i</sub> ≠ 0.
- Eg: x and 2x are dependent
- The columns v<sub>1</sub>, v<sub>2</sub>,..., v<sub>n</sub> of a matrix A are independent if the null-space of A is the zero vector. The columns of A are dependent only if Ac = 0 for some c ≠ 0.
- Space spanned by vectors: Vectors v<sub>1</sub>, v<sub>2</sub>,..., v<sub>n</sub> span a space means that the space consists of all linear combinations of the vectors. Thus, the space spanned by the columns v<sub>1</sub>, v<sub>2</sub>,..., v<sub>n</sub> is C(A).
- The rank of A (m × n) is the number of its maximally independent columns ≤ n and those columns form the basis of C(A). In the reduced echelon form, all columns will be pivot columns with no free variables.

Here is a matrix that is not invertible:

$$\mathsf{A} = \left[ \begin{array}{cc} 1 & 3 \\ 2 & 6 \end{array} \right] \tag{9}$$

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- If A<sup>-1</sup> exists, the solution will be x = A<sup>-1</sup>b and elimination must also produce an upper triangular matrix with non-zero pivots.
- Thus, the condition works both ways: if elimination produces non-zero pivots then the inverse exists and otherwise, the matrix is not invertible or singular (verify for (5))
- ⇔ Matrix will be singular iff its rows or columns are linearly dependent (rank < n)
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- ⇔ Matrix will be singular iff its "determinant" is 0 and is related to the elimination producing non-zero pivots.

- If  $A^{-1}$  exists, the only solution to  $A\mathbf{x} = \mathbf{b}$  is  $\mathbf{x} = A^{-1}\mathbf{b}$ .
- $\Leftrightarrow A$  is singular iff there are solutions other than  $\mathbf{x} = \mathbf{0}$  to  $A\mathbf{x} = \mathbf{0}$ .
- $\Leftrightarrow$  A is singular iff it has a non-singular null-space  $\mathcal{N}(A)$

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• Eg: For A in (5),  $\mathbf{x} = [3, -1]$  is a solution to  $A\mathbf{x} = \mathbf{0}$ .

## Computing Solution to Linear System (only example)

$$A = \begin{bmatrix} 1 & 2 & 2 & 2 \\ 2 & 4 & 6 & 8 \\ 3 & 6 & 8 & 10 \end{bmatrix}$$
(10)

elimination<sup>2</sup> changes C(A) while leaving N(A) intact:

$$A_{1} = \begin{bmatrix} 1 & 2 & 2 & 2 \\ 0 & 0 & 2 & 4 \\ 0 & 0 & 2 & 4 \end{bmatrix}$$
(11)
$$U = \begin{bmatrix} 1 & 2 & 2 & 2 \\ 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$
(12)

#### Row reduced Echelon Form

 $U\mathbf{x} = \mathbf{0}$ , which has the same solution as  $A\mathbf{x} = \mathbf{0}$ 

$$x_1 + 2x_2 + 2x_3 + 2x_4 = 0$$

 $2x_3 + 4x_4 = 0$ 

- Solution can be described by first separating out the two columns containing the pivots, referred to as *pivot columns* and the remaining columns, referred to as *free columns*.
- Variables corresponding to the free columns are called *free variables*, since they can be assigned any value.
- Variables corresponding to the pivot columns are called *pivot* variables
- Following assignment of values to free variables:  $x_2 = 1$ ,  $x_4 = 0 \Rightarrow$  by back substitution, we get the following values:  $x_1 = -2$  and  $x_3 = 0$ .

#### **General Procedure**



#### General Procedure

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## Computing the Inverse: From Gauss to Gauss Jordan

• A slight variant, which is invertible:

$$\mathsf{A} = \left[ \begin{array}{rrr} 1 & 3 \\ 2 & 7 \end{array} \right]$$

• How can we determine it's inverse  $A^{-1}$ ?

$$A^{-1} = \left[ \begin{array}{cc} a & c \\ b & d \end{array} \right] \tag{13}$$

The system of equations  $AA^{-1} = I$  can be written as:

$$\left[\begin{array}{rrr}1&3\\2&7\end{array}\right]\left[\begin{array}{rrr}a&c\\b&d\end{array}\right]=\left[\begin{array}{rrr}1&0\\0&1\end{array}\right]$$

• We can solve the two systems to assemble  $A^{-1}$ 

# Gauss Jordan Elimination contd.

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 The Guass-Jordan elimination method addresses the problem of solving several linear systems Ax<sub>i</sub> = b<sub>i</sub> (1 ≤ i ≤ N) at once, such that each linear system has the same coefficient matrix A but a different right hand side b<sub>i</sub>.

$$U = E_{32}(E_{31}(E_{21}A)) = (E_{32}E_{31}E_{21})A$$

• Now further apply elimination steps until *U* was transformed into the identity matrix:

$$I = E_{13}(E_{12}(E_{23}(E_{32}(E_{31}(E_{21}A))))) = (E_{13}E_{12}E_{23}E_{32}E_{31}E_{21})A = XA$$
(14)
By definition  $X = (E_{13}E_{12}E_{23}E_{32}E_{31}E_{21})$  must be  $A^{-1}$ .

## Illustration of Inversion

- Trick to carry out same elimination steps on two matrices *A* and *B*: Create an augmented matrix [*A B*] and carry out the elimination on this augmented matrix.
- Gauss-Jordan: perform elimination steps on the augmented matrix  $[A \ I]$  (representing the equation AX = I) to give the augmented matrix  $[I \ A^{-1}]$  (representing the equation  $IX = A^{-1}$ ).

$$\begin{bmatrix} 1 & 3 \\ 2 & 7 \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \xrightarrow{Row_2 - 2 \times Row_1} \begin{bmatrix} 1 & 3 \\ 0 & 1 \end{bmatrix} \xrightarrow{Aow_1 - 3 \times Row_2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \xrightarrow{Row_1 - 3 \times Row_2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \xrightarrow{Row_1 - 2 \times Row_2} \begin{bmatrix} 1 & 0 \\ -2 & 1 \end{bmatrix}$$
  
Verify that  $A^{-1}$  is

$$A^{-1} = \begin{bmatrix} 7 & -3 \\ -2 & 1 \end{bmatrix}$$
(15)

#### Dealing with Rectangular Matrices

- What if A is not a square matrix but rather a rectangular matrix of size m × n, such that m ≠ n. Does there exist a notion of A<sup>-1</sup>? The answer depends on the rank of A.
  - If A is full row rank and n > m, then AA<sup>T</sup> is a full rank m × m matrix ⇔ (AA<sup>T</sup>)<sup>-1</sup> exists with A<sup>T</sup>(AA<sup>T</sup>)<sup>-1</sup> = I and is therefore called the **right inverse of** A. When the right inverse of A is multiplied on its left, we get the projection matrix A<sup>T</sup>(AA<sup>T</sup>)<sup>-1</sup>A, which projects matrices onto the row space of A.
  - If A is full column rank and m > n, then  $A^T A$  is a full rank  $n \times n$  matrix  $\Leftrightarrow (A^T A)^{-1}$  exists with  $(A^T A)^{-1} A^T = I$  and is therefore called the **left inverse of** A. When the left inverse of A is multiplied on its right, we get the projection matrix  $A(A^T A)^{-1} A^T$ , which projects matrices onto the column space of A.
- Singular Value Decomposition: When A is neither full row rank nor full column rank

- If A is a full column rank matrix (that is, its columns are independent), A<sup>T</sup>A is invertible.
- We will show that the null space of A<sup>T</sup>A is {0}, which implies that the square matrix A<sup>T</sup>A is full column (as well as row) rank is invertible. That is, if A<sup>T</sup>Ax = 0, then x = 0. Note that if A<sup>T</sup>Ax = 0, then x<sup>T</sup>A<sup>T</sup>Ax = ||Ax|| = 0 which implies that Ax = 0. Since the columns of A are linearly independent, its null space is 0 and therefore, x = 0.