

DDA3020 Machine Learning

Lecture 03 Linear Algebra

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September 09&11, 2025

Outline

- ① Vector, matrix, and their norms
- ② Matrix inverse, determinant, independence
- ③ Systems of linear equations

Reference

References for this lecture:

- [Book1] Stephen Boyd and Lieven Vandenberghe, “Introduction to Applied Linear Algebra”, Cambridge University Press, 2018 ([available online](#)).
- [Book2] Andreas C. Muller and Sarah Guido, “Introduction to Machine Learning with Python: A Guide for Data Scientists”, O’Reilly Media, Inc., 2017.

① Vector, matrix, and their norms

② Matrix inverse, determinant, independence

③ Systems of linear equations

Scalar

- A **scalar** is a simple numerical value, like 15 or -3.2 .
- **Variables** or **constants** that take **scalar** values are denoted by an **italic** letter, like x or a .
- We shall focus on **real** numbers.
- The **summation** over a collection $\{x_1, x_2, x_3, \dots, x_m\}$ is denoted like this:

$$\sum_{i=1}^m x_i = x_1 + x_2 + \dots + x_m$$

- The **product** over a collection $\{x_1, x_2, x_3, \dots, x_m\}$ is denoted like this:

$$\prod_{i=1}^m x_i = x_1 \cdot x_2 \cdot \dots \cdot x_m$$

Vector

- A **vector** is an **ordered list** of scalar values, called attributes. We denote a vector as a **bold character**, for example, **x** or **w**.
- Vectors can be visualized as **arrows** that point to some directions as well as **points** in a **multi-dimensional space**.
- In many books, vectors are written **column-wise**:

$$\mathbf{a} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -2 \\ 5 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Vector

Illustrations of three two-dimensional vectors, $\mathbf{a} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$, $\mathbf{b} = \begin{bmatrix} -2 \\ 5 \end{bmatrix}$, $\mathbf{c} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ are given in Figure 1 below.

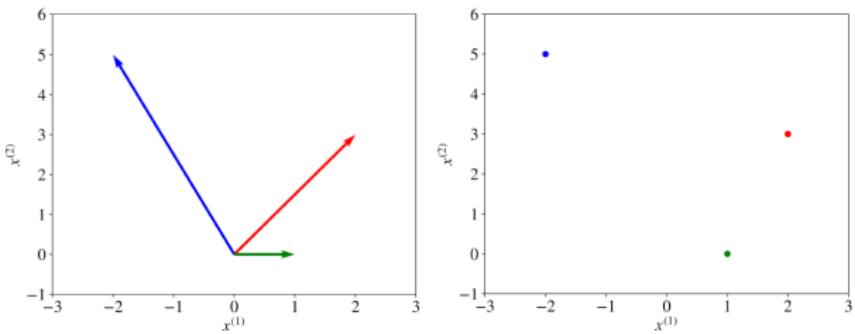


Figure: Three vectors visualized as directions and as points.

Vector

- We denote **an attribute of a vector** as an italic value with an index, like this: $w^{(j)}$ or $x^{(j)}$. The **index j** denotes a specific **dimension** of the vector, the position of an attribute in the list.
- For instance, in the vector **a** shown in **red** in Figure 1,

$$\mathbf{a} = \begin{bmatrix} a^{(1)} \\ a^{(2)} \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}, \text{ or more commonly, } \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

Note:

- The notation $x^{(j)}$ should not be confused with the power operator, such as the 2 in x^2 (squared) or 3 in x^3 (cubed).
- If we want to apply a power operator, say square, to an indexed attribute of a vector, we write like this: $(x^{(j)})^2$.

Matrix

- A **matrix** is a rectangular array of numbers arranged in rows and columns.
Below is an example of a matrix with two rows and three columns,

$$\mathbf{X} = \begin{bmatrix} 2 & 4 & -3 \\ 21 & -6 & -1 \end{bmatrix}$$

- Matrices are denoted with bold capital letters, such as \mathbf{X} or \mathbf{W} .

Note:

- A variable can have two or more indices, like this: $x_i^{(j)}$ or like this $x_{i,j}^{(k)}$.
- For example, in neural networks, we denote as $x_{l,u}^{(j)}$ the input feature j of unit u in layer l .

Vector and matrix operations

Operations on Vectors:

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \end{bmatrix}$$

$$\mathbf{x} - \mathbf{y} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x_1 - y_1 \\ x_2 - y_2 \end{bmatrix}$$

$$a\mathbf{x} = a \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} ax_1 \\ ax_2 \end{bmatrix}$$

$$\frac{1}{a}\mathbf{x} = \frac{1}{a} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{a}x_1 \\ \frac{1}{a}x_2 \end{bmatrix}$$

Vector and matrix operations

- Matrix or Vector Transpose:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \mathbf{x}^\top = [x_1 \quad x_2]$$

$$\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \end{bmatrix}, \quad \mathbf{X}^\top = \begin{bmatrix} x_{1,1} & x_{2,1} & x_{3,1} \\ x_{1,2} & x_{2,2} & x_{3,2} \\ x_{1,3} & x_{2,3} & x_{3,3} \end{bmatrix}$$

- Dot Product or Inner Product of Vectors:

$$\begin{aligned} \mathbf{x} \cdot \mathbf{y} &= \mathbf{x}^\top \mathbf{y} \\ &= [x_1 \quad x_2] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \\ &= x_1 y_1 + x_2 y_2 \end{aligned}$$

- Trace of (square) matrix:

$$\text{tr}(\mathbf{X}) = \sum_{i=1}^n x_{ii}$$

Vector and matrix operations

- Matrix-Vector Product

$$\begin{aligned}\mathbf{X}\mathbf{w} &= \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} \\ &= \begin{bmatrix} x_{1,1}w_1 + x_{1,2}w_2 + x_{1,3}w_3 \\ x_{2,1}w_1 + x_{2,2}w_2 + x_{2,3}w_3 \\ x_{3,1}w_1 + x_{3,2}w_2 + x_{3,3}w_3 \end{bmatrix}\end{aligned}$$

Vector and matrix operations

Matrix-Vector Product

$$\mathbf{x}^\top \mathbf{W} = [x_1 \quad x_2 \quad x_3] \begin{bmatrix} w_{1,1} & w_{1,2} & w_{1,3} \\ w_{2,1} & w_{2,2} & w_{2,3} \\ w_{3,1} & w_{3,2} & w_{3,3} \end{bmatrix}$$
$$= [(w_{1,1}x_1 + w_{2,1}x_2 + w_{3,1}x_3) \quad (w_{1,2}x_1 + w_{2,2}x_2 + w_{3,2}x_3) \quad (w_{1,3}x_1 + w_{2,3}x_2 + w_{3,3}x_3)]$$

Vector and matrix operations

Matrix-Matrix Product

$$\begin{aligned}\mathbf{XW} &= \begin{bmatrix} x_{1,1} & \dots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \dots & x_{m,d} \end{bmatrix} \begin{bmatrix} w_{1,1} & \dots & w_{1,h} \\ \vdots & \ddots & \vdots \\ w_{d,1} & \dots & w_{d,h} \end{bmatrix} \\ &= \begin{bmatrix} (x_{1,1}w_{1,1} + \dots + x_{1,d}w_{d,1}) & \dots & (x_{1,1}w_{1,h} + \dots + x_{1,d}w_{d,h}) \\ \vdots & \ddots & \vdots \\ (x_{m,1}w_{1,1} + \dots + x_{m,d}w_{d,1}) & \dots & (x_{m,1}w_{1,h} + \dots + x_{m,d}w_{d,h}) \end{bmatrix} \\ &= \begin{bmatrix} \sum_{i=1}^d x_{1,i}w_{i,1} & \dots & \sum_{i=1}^d x_{1,i}w_{i,h} \\ \vdots & \ddots & \vdots \\ \sum_{i=1}^d x_{m,i}w_{i,1} & \dots & \sum_{i=1}^d x_{m,i}w_{i,h} \end{bmatrix}\end{aligned}$$

Vector norms

- **Question:** How to compare two vectors with the same dimension? Which is larger? (**Answer:** use vector norms)
- In mathematics, a **norm**, usually denoted as $\|\cdot\|$, is a function from a real or complex vector space to the non-negative real numbers that behaves in certain ways like the distance from the origin: it commutes with scaling, obeys a form of the triangle inequality, and is zero only at the origin.
- Norm axioms:
 - Positivity: $\|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = \mathbf{0}$
 - Homogeneity: $\|\lambda\mathbf{x}\| = |\lambda|\|\mathbf{x}\|$
 - Triangle Inequality: $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$

Vector norms

- ℓ_2 -norm of vector (a.k.a. Euclidean norm or distance):

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^d x_i^2}$$

- ℓ_1 -norm of vector:

$$\|\mathbf{x}\|_1 = \sum_{i=1}^d |x_i|$$

- ℓ_p -norm of vector ($p \geq 1$):

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^d |x_i|^p \right)^{1/p}$$

- ℓ_0 -norm of vector:

$$\|\mathbf{x}\|_0 = \text{number of nonzero elements in } \mathbf{x}$$

Matrix norms

- In addition to the three axioms for vector norms, matrix norms may satisfy the sub-multiplicative property:

$$\|\mathbf{XY}\| \leq \|\mathbf{X}\| \|\mathbf{Y}\|$$

- Frobenius norm of matrix:

$$\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}$$

- Spectral norm of matrix:

$$\|\mathbf{X}\|_2 = \sigma_{\max}(\mathbf{X}) \quad (\text{largest singular value})$$

- Singular value decomposition: $\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^\top$, $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots)$

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Matrix inverse

Matrix Inverse

- Definition:

A $d \times d$ square matrix \mathbf{A} is called **invertible** (also **nonsingular**) if there exists a $d \times d$ square matrix \mathbf{B} such that $\mathbf{AB} = \mathbf{BA} = \mathbf{I}$ (**Identity matrix**) given by

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \quad \text{of } d \text{ by } d \text{ dimension}$$

Matrix inverse

Matrix Inverse Computation

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})} \text{adj}(\mathbf{A})$$

- $\det(\mathbf{A})$ is the determinant of \mathbf{A}
 - Example: $\det(\mathbf{A}) = |\mathbf{A}| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$
- $\text{adj}(\mathbf{A})$ is the adjugate or adjoint of \mathbf{A} which is the transpose of its cofactor matrix \mathbf{C} , i.e., $\text{adj}(\mathbf{A}) = \mathbf{C}^\top$
- The cofactor $\mathbf{C}_{i,j}$ of a matrix is the (i,j) -minor $\mathbf{M}_{i,j}$ times a sign factor $(-1)^{i+j}$, i.e., $\mathbf{C}_{i,j} = \mathbf{M}_{i,j} \times (-1)^{i+j}$
- $\mathbf{M}_{i,j}$ is computed through two-steps: removing the i -th row and j -th column from the original matrix to obtain a small matrix; computing the determinant of the small matrix
 - For example, $\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ then $\mathbf{C} = \begin{bmatrix} d & -c \\ -b & a \end{bmatrix}$, $\text{adj}(\mathbf{A}) = \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

Matrix inverse

- Matrix inverse (if invertible or non-singular) via SVD:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^\top, \quad \mathbf{A}^{-1} = \mathbf{V}\Sigma^{-1}\mathbf{U}^\top, \quad \Sigma^{-1} = \text{diag}(\sigma_1^{-1}, \sigma_2^{-1}, \dots)$$

- Determinant computation via SVD:

$$\det(\mathbf{A}) = \prod_i \sigma_i$$

Linear dependence and independence

Linear dependence and independence

- A collection of d -vectors $\mathbf{x}_1, \dots, \mathbf{x}_m$ (with $m \geq 1$) is called **linearly dependent** if

$$\beta_1 \mathbf{x}_1 + \dots + \beta_m \mathbf{x}_m = 0$$

holds for some β_1, \dots, β_m **that are not all zero.**

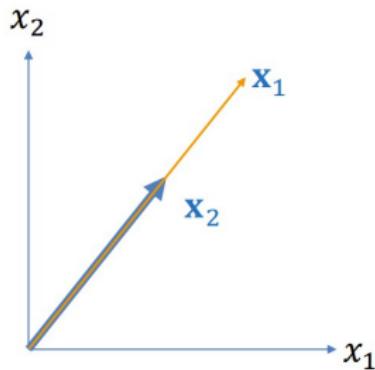
- A collection of d -vectors $\mathbf{x}_1, \dots, \mathbf{x}_m$ (with $m \geq 1$) is called **linearly independent**, which means that

$$\beta_1 \mathbf{x}_1 + \dots + \beta_m \mathbf{x}_m = 0$$

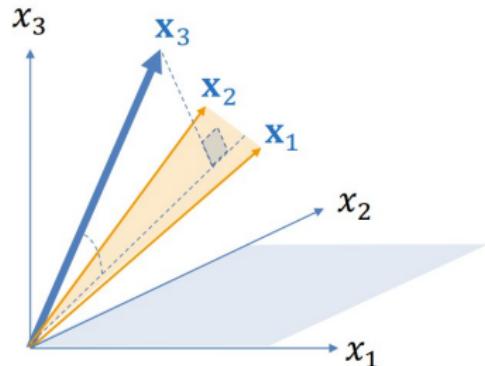
only holds for $\beta_1 = \dots = \beta_m = 0$.

Linear dependence and independence

Geometry of dependency and independency



$$\beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 = 0$$



$$\beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 \neq \beta_3 \mathbf{x}_3$$

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Systems of linear equations

- Consider a system of m linear **equations** in d variables w_1, \dots, w_d :

$$x_{1,1}w_1 + x_{1,2}w_2 + \dots + x_{1,d}w_d = y_1$$

$$x_{2,1}w_1 + x_{2,2}w_2 + \dots + x_{2,d}w_d = y_2$$

$$\vdots$$

$$x_{m,1}w_1 + x_{m,2}w_2 + \dots + x_{m,d}w_d = y_m$$

Systems of linear equations

These equations can be written compactly in matrix-vector notation:

$$\mathbf{X}\mathbf{w} = \mathbf{y},$$

where

$$\mathbf{X} = \begin{bmatrix} x_{1,1} & \dots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \dots & x_{m,d} \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

Note: \mathbf{X} is of $m \times d$ dimension.

Systems of linear equations

(i) **Square of even-determined system:** $m = d$ in $\mathbf{X}\mathbf{w} = \mathbf{y}$, $\mathbf{X} \in \mathbb{R}^{m \times d}$
(equal number of equations and unknowns, i.e., $\mathbf{X} \in \mathbb{R}^{d \times d}$)

If \mathbf{X} is invertible (or $\mathbf{X}^{-1}\mathbf{X} = \mathbf{I}$), then pre-multiply both sides by \mathbf{X}^{-1} , we have

$$\mathbf{X}^{-1}\mathbf{X}\mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$$

$$\Rightarrow \mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$$

If all rows or columns of \mathbf{X} are linearly independent, then \mathbf{X} is invertible.

Systems of linear equations

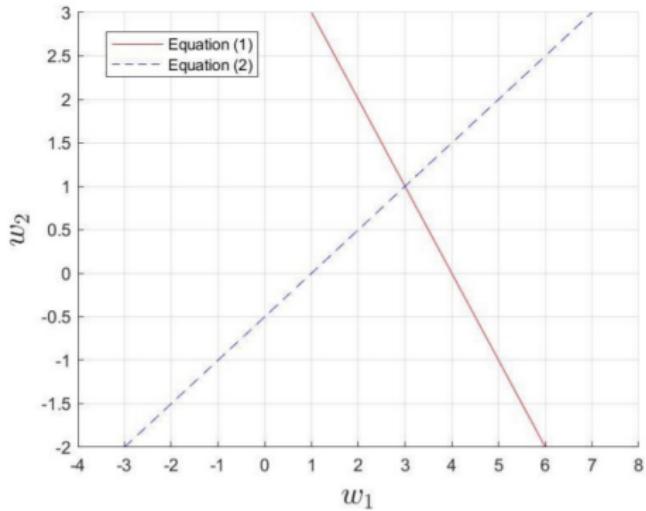
Example $w_1 + w_2 = 4 \quad (1)$
 $w_1 - 2w_2 = 1 \quad (2)$

Two unknowns and
two equations

$$\begin{bmatrix} 1 & 1 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

$$\mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$$

$$= \begin{bmatrix} 1 & 1 \\ 1 & -2 \end{bmatrix}^{-1} \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$$



Here, the rows or columns of \mathbf{X} are **linearly independent**, hence \mathbf{X} is **invertible**.

Systems of linear equations

(ii) Over-determined system: $m > d$ in $\mathbf{X}\mathbf{w} = \mathbf{y}$, $\mathbf{X} \in \mathbb{R}^{m \times d}$
(i.e., there are more equations than unknowns)

- This set of linear equations has **NO exact solution** (\mathbf{X} is non-square and hence not invertible). However, an **approximated solution** is yet available.
- If the **left-inverse** of \mathbf{X} exists such that $\mathbf{X}^\dagger \mathbf{X} = \mathbf{I}$, then **pre-multiply both sides by \mathbf{X}^\dagger** results in

$$\begin{aligned}\mathbf{X}^\dagger \mathbf{X}\mathbf{w} &= \mathbf{X}^\dagger \mathbf{y} \\ \Rightarrow \mathbf{w} &= \mathbf{X}^\dagger \mathbf{y}\end{aligned}$$

- **Definition:** a matrix \mathbf{B} that satisfies $\mathbf{B}\mathbf{A} = \mathbf{I}$ (**identity matrix**) is called a **left-inverse** of \mathbf{A} . (Note: \mathbf{A} is **m-by-d** and \mathbf{B} is **d-by-m**.)
- Note: The left-inverse can be computed as $\mathbf{X}^\dagger = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ given $\mathbf{X}^\top \mathbf{X}$ is invertible.

Systems of linear equations

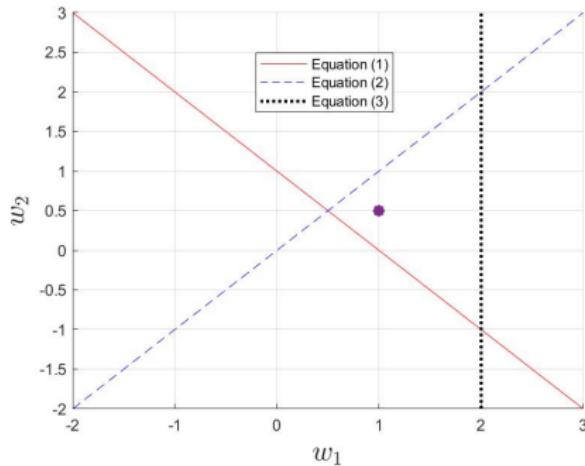
Example $w_1 + w_2 = 1 \quad (1)$
 $w_1 - w_2 = 0 \quad (2)$
 $w_1 = 2 \quad (3)$

Two unknowns and three equations

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$$

\mathbf{X} \mathbf{w} \mathbf{y}

This set of linear equations has NO exact solution.



$$\mathbf{w} = \mathbf{X}^\dagger \mathbf{y} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Here $\mathbf{X}^\top \mathbf{X}$ is invertible.

$$= \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}$$

(Approximation)

Systems of linear equations

(iii) **Under-determined system:** $m < d$ in $\mathbf{X}\mathbf{w} = \mathbf{y}$, $\mathbf{X} \in \mathbb{R}^{m \times d}$

(i.e., there are more unknowns than equations \Rightarrow infinite number of solutions)

- If the right-inverse of \mathbf{X} exists such that $\mathbf{X}\mathbf{X}^\dagger = \mathbf{I}$, then the d -vector $\mathbf{w} = \mathbf{X}^\dagger\mathbf{y}$ (one of the infinite cases) satisfies the equation $\mathbf{X}\mathbf{w} = \mathbf{y}$, i.e.,

$$\mathbf{X}\mathbf{X}^\dagger\mathbf{y} = \mathbf{y}$$

$$\Rightarrow \mathbf{y} = \mathbf{y}$$

- **Definition:** a matrix \mathbf{B} that satisfies $\mathbf{A}\mathbf{B} = \mathbf{I}$ (identity matrix) is called a right-inverse of \mathbf{A} . (Note: \mathbf{A} is m-by-d and \mathbf{B} is d-by-m).
- Note: The right-inverse can be computed as $\mathbf{X}^\dagger = \mathbf{X}^\top(\mathbf{X}\mathbf{X}^\top)^{-1}$ given $\mathbf{X}\mathbf{X}^\top$ is invertible.

Systems of linear equations

Derivation:

- Under-determined system: $m < d$ in $\mathbf{X}\mathbf{w} = \mathbf{y}$, $\mathbf{X} \in \mathbb{R}^{m \times d}$
(i.e., there are more unknowns than equations \Rightarrow infinite number of solutions \Rightarrow but a unique solution is yet possible by constraining the search using $\mathbf{w} = \mathbf{X}^\top \mathbf{a}$!)
- If $\mathbf{X}\mathbf{X}^\top$ is invertible, let $\mathbf{w} = \mathbf{X}^\top \mathbf{a}$, then

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

$$\Rightarrow \mathbf{a} = (\mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{y}$$

$$\mathbf{w} = \mathbf{X}^\top \mathbf{a} = \underbrace{\mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top)^{-1}}_{\mathbf{X}^\dagger} \mathbf{y}$$

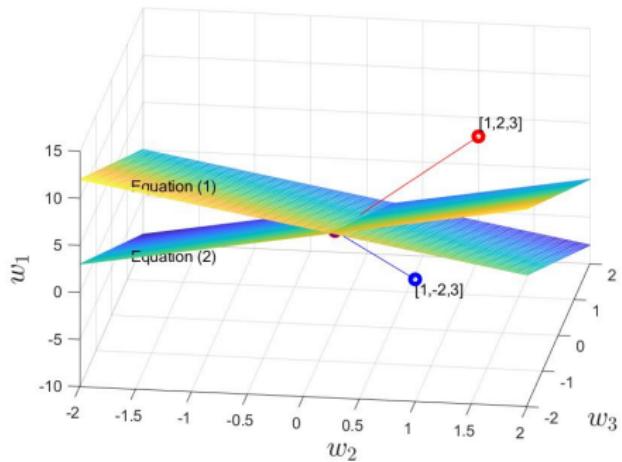
Systems of linear equations

Example $w_1 + 2w_2 + 3w_3 = 2 \quad (1)$
 $w_1 - 2w_2 + 3w_3 = 1 \quad (2)$

Three unknowns and two equations

$$\begin{bmatrix} 1 & 2 & 3 \\ 1 & -2 & 3 \\ X \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ y \end{bmatrix}$$

This set of linear equations has infinitely many solutions along the intersection line.



$$w = X^\top (X X^\top)^{-1} y \quad \text{Here } X X^\top \text{ is invertible.}$$

$$= \begin{bmatrix} 1 & 1 \\ 2 & -2 \\ 3 & 3 \end{bmatrix} \begin{bmatrix} 14 & 6 \\ 6 & 14 \end{bmatrix}^{-1} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.15 \\ 0.25 \\ 0.45 \end{bmatrix} \quad (\text{Constrained solution})$$

Systems of linear equations

Example $w_1 + 2w_2 + 3w_3 = 2 \quad (1)$
 $3w_1 + 6w_2 + 9w_3 = 1 \quad (2)$

Three unknowns and
two equations

$$\begin{bmatrix} 1 & 2 & 3 \\ 3 & 6 & 9 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

\mathbf{X} \mathbf{w} \mathbf{y}

Here both \mathbf{XX}^\top and $\mathbf{X}^\top\mathbf{X}$ are
NOT invertible!

There is **NO solution** for the
system.

