Machine Learning CS 4641

Linear Algebra Basics

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Outline

- Linear Algebra Basics
- Norms
- Multiplications
- Matrix Inversion
- Trace and Determinant
- Eigen Values and Eigen Vectors
- Singular Value Decomposition
- Matrix Calculus

Why linear algebra?

$X = \begin{bmatrix} \\ \\ \end{bmatrix}_{n \times d}$

dimensions

features

no. of datapoints

model training

⇓

Optimization

- Most data can be represented or stored in matrix-vector form
- Provides compact representation for sets of linear equations

$$\boxed{\begin{matrix} 4x_1 - 5x_2 = -13 \\ -2x_1 + 3x_2 = 9 \end{matrix}} \rightarrow \underbrace{\begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} -13 \\ 9 \end{bmatrix}}_{c_1, c_2} \rightarrow \mathbf{Ax} = \mathbf{b}$$

$c_1, c_2 \in \mathbb{R}$

2 2

- $\mathbf{A} \in \boxed{\mathbb{R}^{N \times D}}$ denotes a matrix with *N* rows and *D* columns, where elements belong to real numbers
- $\mathbf{x} \in \boxed{\mathbb{R}^{D}}$ denotes a vector with *D* real entries.

Linear algebra basics

- Transpose of a matrix results from flipping the rows and the columns. Given $\boxed{\mathbf{A} \in \mathbb{R}^{N \times D}}$, the transpose is $\boxed{\mathbf{A}^{\mathrm{T}} \in \mathbb{R}^{D \times N}}$

$$\mathbf{A} = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \rightarrow \underline{\mathbf{A}^{\mathrm{T}}} = \begin{bmatrix} 4 & -2 \\ -5 & 3 \end{bmatrix}$$

- For each element of the matrix, the transpose can be written as $\mathrm{A}_{ij}^{T} = \mathrm{A}_{ji}$
- The following properties of the transposes are easily verified
  - $\left(\mathbf{A}^{\mathrm{T}}\right)^{\mathrm{T}} = \mathbf{A}$
  - $(\mathbf{AB})^{\mathrm{T}} = \mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}$
  - $(\mathbf{A} + \mathbf{B})^{\mathrm{T}} = \mathbf{A}^{\mathrm{T}} + \mathbf{B}^{\mathrm{T}}$

Linear algebra basics

- A square matrix $\boxed{\mathbf{A} \in \mathbb{R}^{D \times D}}$ is symmetric if $\boxed{\mathbf{A} = \mathbf{A}^{\mathrm{T}}}$ and it is skew-symmetric if $\boxed{\mathbf{A} = -\mathbf{A}^{\mathrm{T}}}$. Thus each matrix can be written as a sum of symmetric and anti-symmetric matrices:

$$\mathbf{A} = \underbrace{\frac{1}{2}(\mathbf{A} - \mathbf{A}^T)}_{H} + \underbrace{\frac{1}{2}(\mathbf{A} + \mathbf{A}^T)}_{G}$$

$\boxed{A = A^T}$ ← A is symmetric

$\boxed{A = -A^T}$ ← A is skew-symmetric

$\boxed{H = -H^T}$ ← H is skew symmetric

$\boxed{G = G^T}$ ← G is symmetric

$H = A - A^T$

$H^T = (A - A^T)^T = A^T - A^{T^T} = A^T - A$

$= -(A - A^T)$

$= -H$

$G = A + A^T$

$G^T = (A + A^T)^T = A^T + A^{T^T} = A^T + A$

$= G$

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Norms

$\mathbb{R}^D \to \mathbb{R}$ $\quad \|\cdot\|$

Vector

$\|x\|$

- Norm of a vector $\|\mathbf{x}\|$ is informally a measure of the length of a vector
- More formally, a norm is any function $f: \mathbb{R}^D \to \mathbb{R}$ that satisfies:
    - For all $\mathbf{x} \in \mathbb{R}^D, f(\mathbf{x}) \geq 0$ (non-negativity)
    - $f(\mathbf{x}) = 0$ is and only if $x = 0$ (definiteness)
    - For $\mathbf{x} \in \mathbb{R}^D, t \in \mathbb{R}, f(t\mathbf{x}) = |t| f(\mathbf{x})$ (homogeneity)
    - For all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D, f(\mathbf{x}+\mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$ (triangle inequality)

Norms

ℓ_p norms $\quad p = 1, 2, 3 \ldots$

$p=1 \rightarrow \ell_1$ norm $\rightarrow$ Manhattan distance

ℓ_2 norm $\rightarrow$ Euclidean distance

$x = [1, 3, -2]$

- Common norms used in machine learning are:
  - ℓ_2-norm: $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{D} x_i^2}$
  - ℓ_1-norm: $\|\mathbf{x}\|_1 = \sum_{i=1}^{D} |x_i|$
  - ℓ_∞-norm: $\|\mathbf{x}\|_\infty = \max_i |x_i|$

$\|x\|_2 = \sqrt{1^2 + 3^2 + (-2)^2} = \sqrt{14}$

$\|x\|_1 = |1| + |3| + |-2|$

$= 6$

$\|x\|_\infty = \max(|1|, |3|, |-2|)$

$= 3$

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Norms

$\|x\| \sim \|x\|_2$

generally, we use $(\ell_2 \text{ norm})^2$

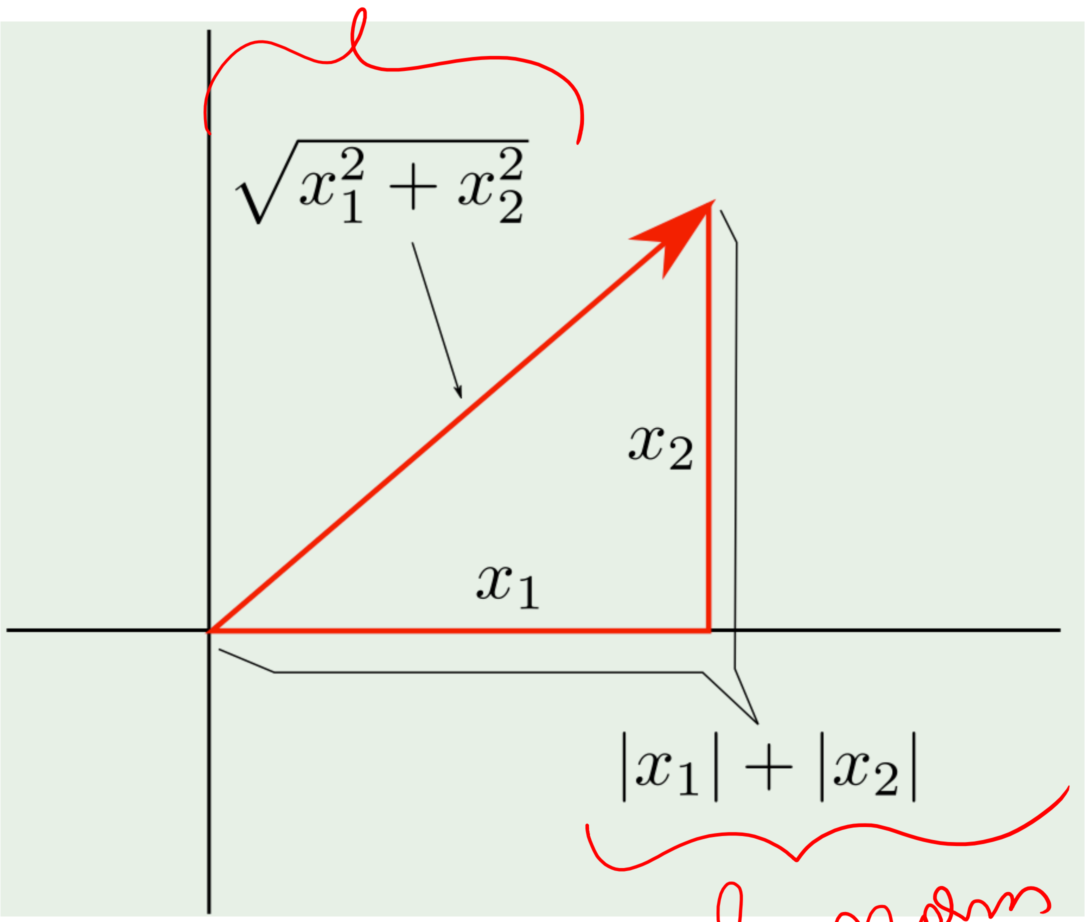
- All norms presented so far are examples of the family of ℓ_p norms, which are parametrized by a real number $p \geq 1$
  - $\boxed{\ell_p\text{-norm: } \|\mathbf{x}\|_p = \left(\sum_{i=1}^{D} |x_i|^p\right)^{\frac{1}{p}}}$
- Norms can be defined for matrices, such as the Frobenius norm
  - $\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{D} \mathrm{A}_{\mathrm{ij}}^2} = \sqrt{\mathrm{tr}(\mathbf{A}^{\mathbf{T}}\mathbf{A})}$

$\|A\|_F$

Vector norm examples

- ℓ_1-norm and ℓ_2-norm

ℓ_2 norm

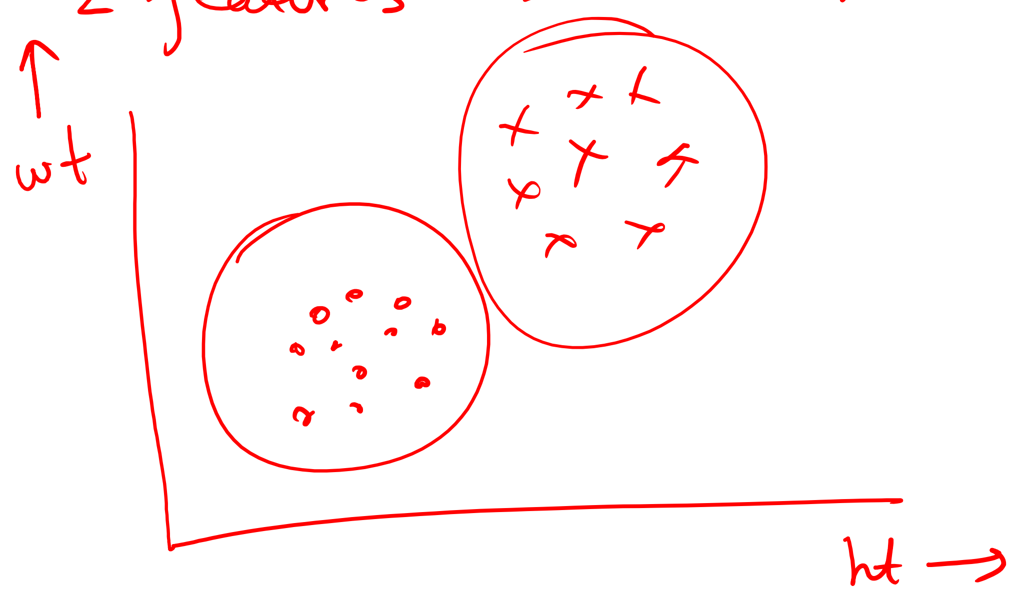


ℓ_1 norm

In context: how are norms useful in ML?

Unsupervised learning

X with 2 features → ht. & wt. .

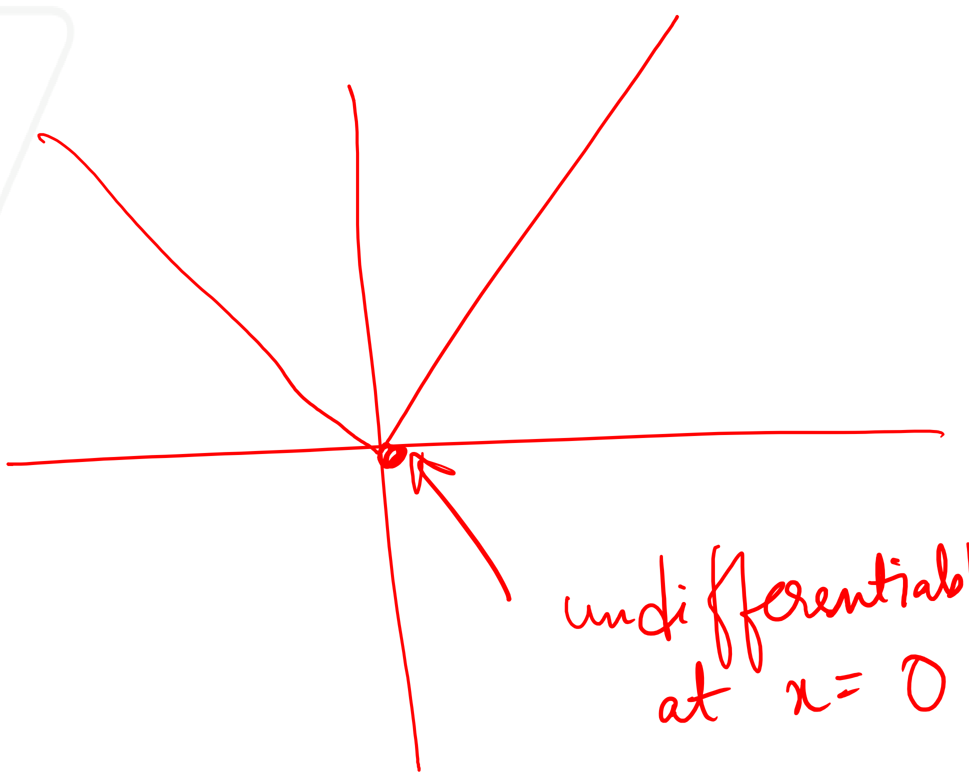


In context: choosing an appropriate norm

Manhattan vs. Euclidean

ℓ_1

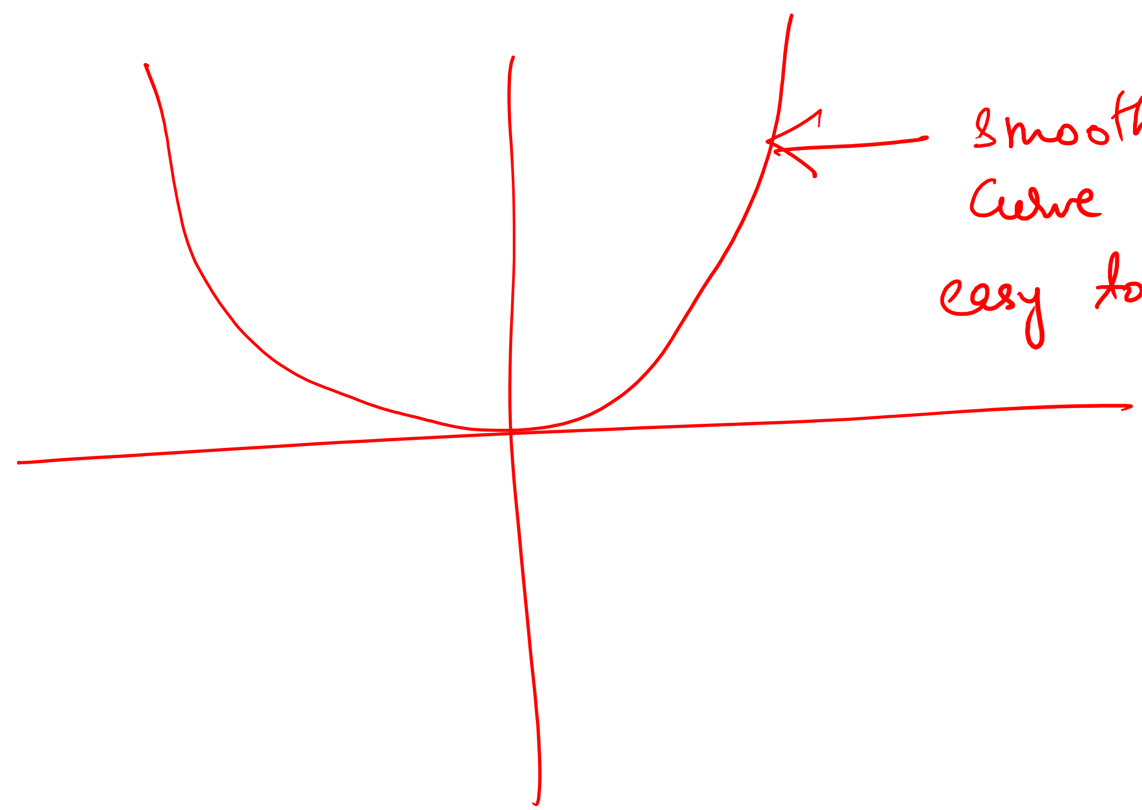
$y = |x|$



undifferentiable at $x = 0$

ℓ_2

$y = x^2$



smooth curve & very easy to differentiate

Special Matrices

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Do not Like List

1. For loops
2. Inverse

- The identity matrix, denoted by $I \in \mathbb{R}^{d \times d}$ is a square matrix with ones on the diagonal and zeros everywhere else

- A diagonal matrix is a matrix where all non-diagonal 'ELEMENTS' are 0. This is typically denoted as $D = diag\,(d_1, d_2, \ldots, d_d)$

$$\begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} = \begin{bmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$$

Why is diagonal matrix helpful?

- $\boxed{A^T A}$= elementwise squaring or all diagonal elements
- A^{-1} =1/A (elementwise)

$$A^{-1} = \begin{bmatrix} 1/a & 0 & 0 \\ 0 & 1/b & 0 \\ 0 & 0 & 1/c \end{bmatrix}$$

Special Matrices

$x \cdot y = 0$

$$U = \begin{array}{c} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\ \begin{array}{ccc} c_1 & c_2 & c_3 \end{array} \end{array}$$

- Two vectors x, y ∈ $\mathbb{R}^d$ are orthogonal if $x.y$ = 0. A square matrix U ∈ $\mathbb{R}^{d \times d}$ is **Orthonormal** if all its columns are orthogonal to each other and are normalized

$c_1 \cdot c_2 = 0$

$c_1 \cdot c_3 = 0$

$c_2 \cdot c_3 = 0$

$\|c_1\|_2 = 1$

$\|c_2\|_2 = \|c_3\|_2 = 1$

unitary ≈ orthonormal

- It follows from orthogonality and normality that
  - $\boxed{U^T U = I = U U^T}$
  - $\|Ux\|_2 = \|x\|_2$

Is the inverse of a unitary matrix equal to its transpose?

$U^T U = I = U U^T$ $\quad U^T = U^{-1}$ $\quad U U^{-1} = I$

Orthonormal Matrices do not STRETCH OR SHRINK a vector. It only ROTATES it.

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Multiplications

Matrix multiplication is a bunch of dot products

$$A = \begin{bmatrix} a_1 & b_1 & c_1 \\ d_1 & e_1 & f_1 \\ g_1 & h_1 & i_1 \end{bmatrix} \quad B = \begin{bmatrix} a_2 & b_2 & c_2 \\ d_2 & e_2 & f_2 \\ g_2 & h_2 & i_2 \end{bmatrix}$$

$A*B$

$A*B_{(1,1)} = a_1a_2 + b_1d_2 + c_1g_2$

- The product of two matrices $\mathbf{A} \in \mathbb{R}^{N\times D}$ and $\mathbf{B} \in \mathbb{R}^{D\times P}$ is given by $\mathbf{C} \in \mathbb{R}^{N\times P}$, where $C_{ij} = \sum_{k=1}^{D} A_{ik}B_{kj}$

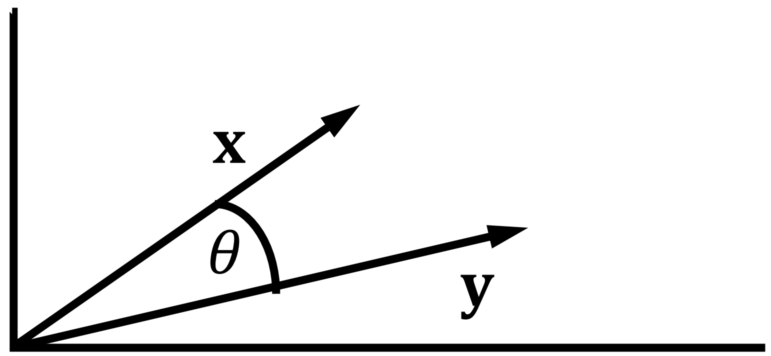
- Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$, the term $\mathbf{x} \cdot \mathbf{y}$ (or $\mathbf{x}^{\mathrm{T}}\mathbf{y}$) is called the inner product or dot product of the vectors, and is a real number given by $\sum_{k=1}^{D} x_i y_i$. For example,

$$\underset{1\times 3}{\mathbf{x}^{\mathrm{T}}}\,\underset{3\times 1}{\mathbf{y}} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \sum_{i=1}^{3} x_i y_i$$

Multiplications

project x onto y $= x \cdot \frac{y}{\|y\|_2}$

- The dot product also has a geometrical interpretation, for vectors in $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ with an angle θ between them:

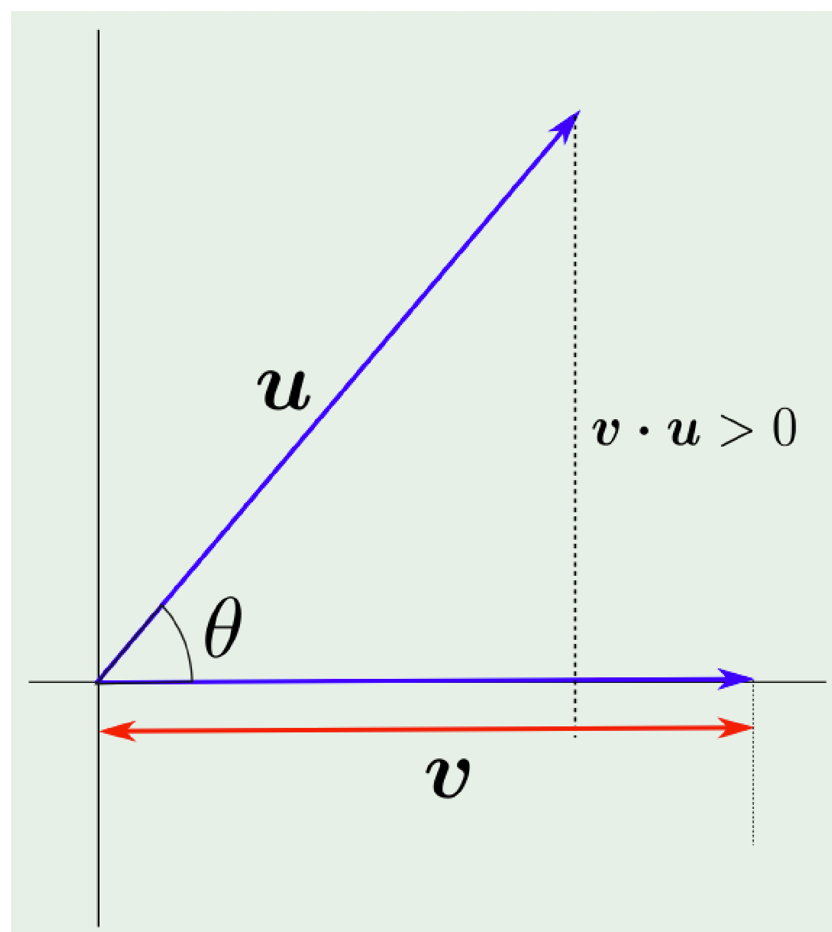


$$\mathbf{x} \cdot \mathbf{y} = \|\mathbf{x}\|_2 \|\mathbf{y}\|_2 \cos\theta$$

$\|x\|_2 \cos\theta$

Inner product properties

- The inner product is a measure of correlation between two vectors scaled by the norms of the vectors
- Here correlation term is used in the loose sense of directional alignment – not statistical sense



$>0 \quad >0$

$$u \cdot v = \|u\|_2 \cdot \|v\|_2 \cdot \cos\theta$$

>0

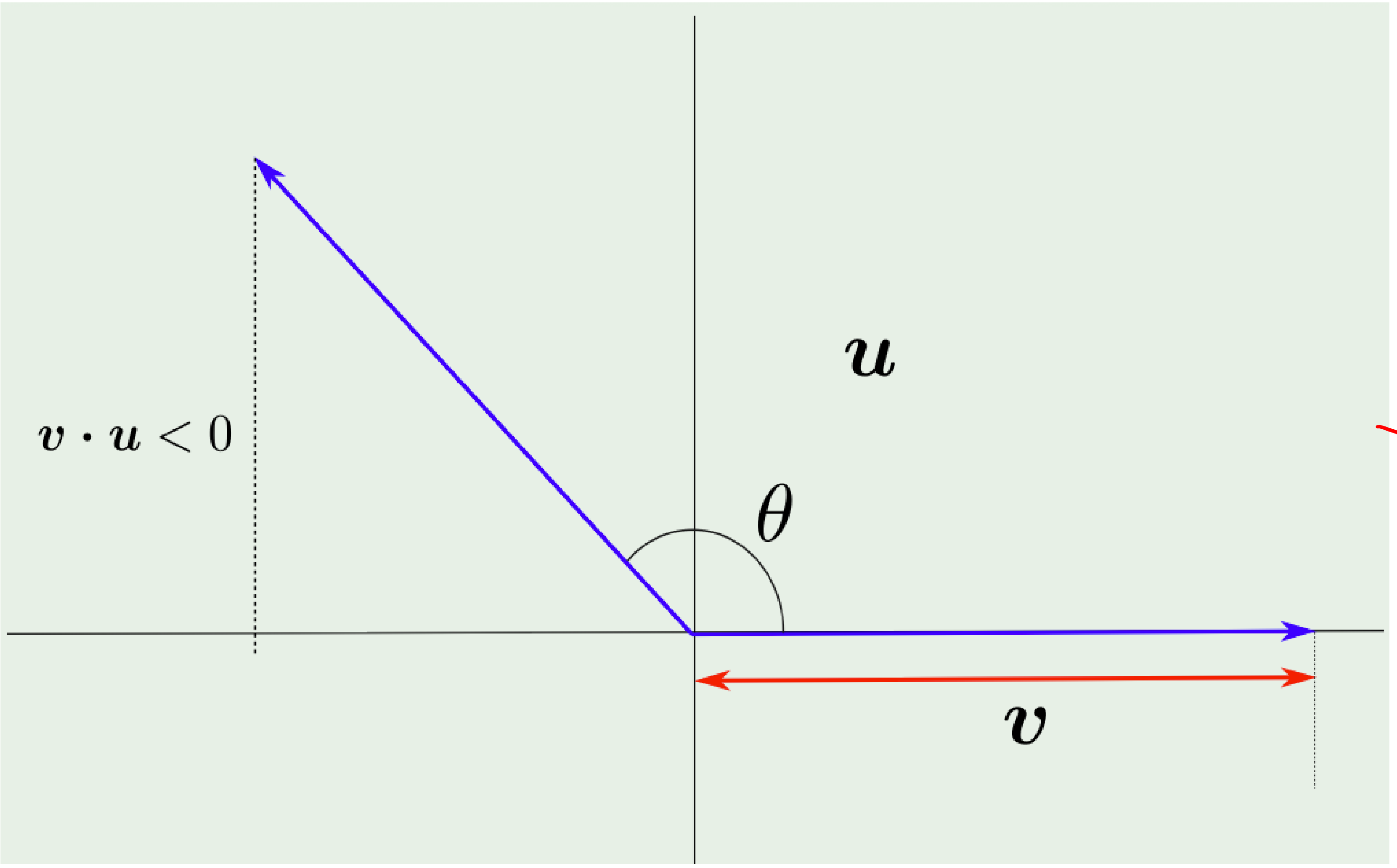
$\theta < 90$

$\cos\theta > 0$

$u \cdot v > 0$

Inner product properties

- The inner product is a measure of correlation between two vectors, scaled by the norms of the vectors



$\theta > 90^\circ$

$\cos\theta < 0$

>0

$u \cdot v = \|u\|_2 \cdot \|v\|_2 \cdot \cos\theta$

>0

$-ve$

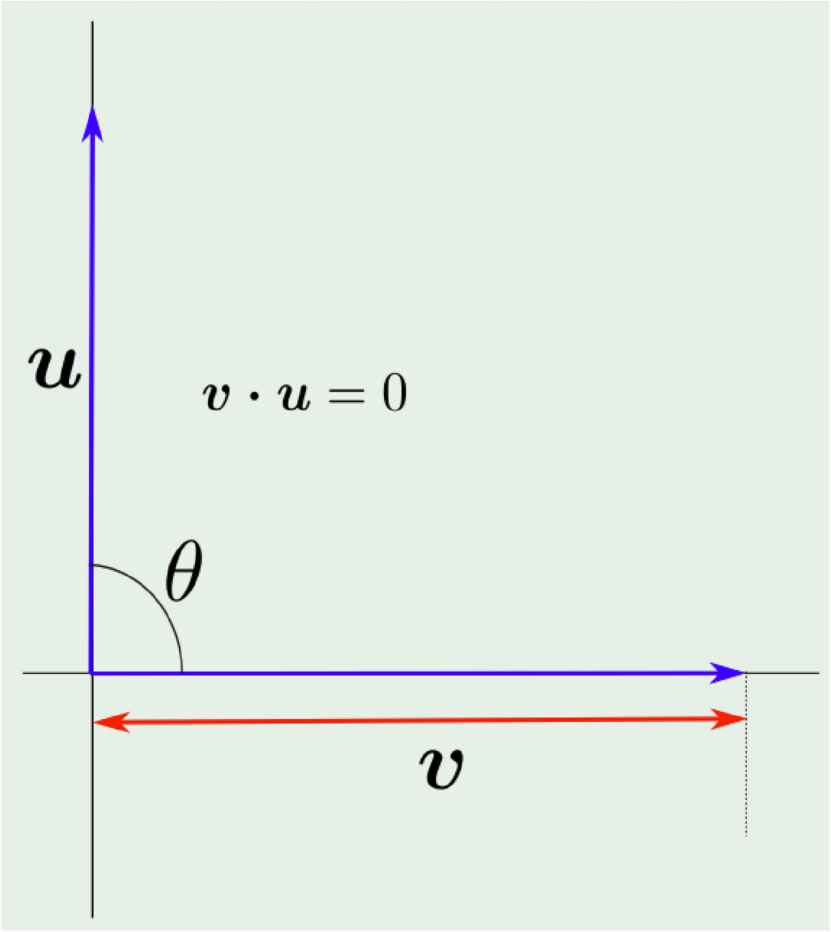
Hence,
$u \cdot v < 0$

Inner product properties

Dot product is a linear operation.

- The inner product is a measure of correlation between two vectors scaled by the norms of the vectors

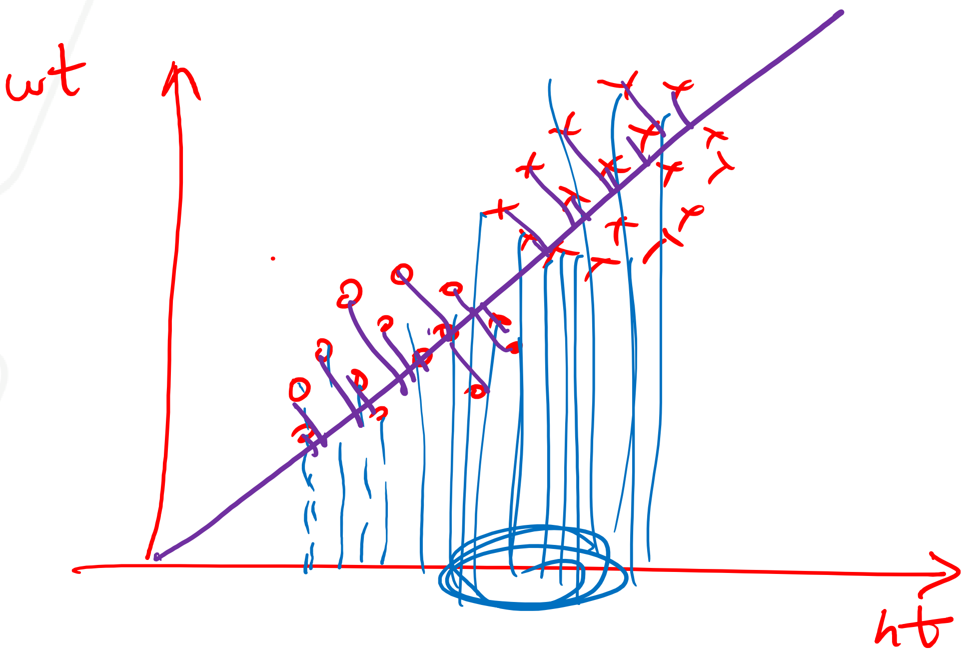
Linearly independent vectors

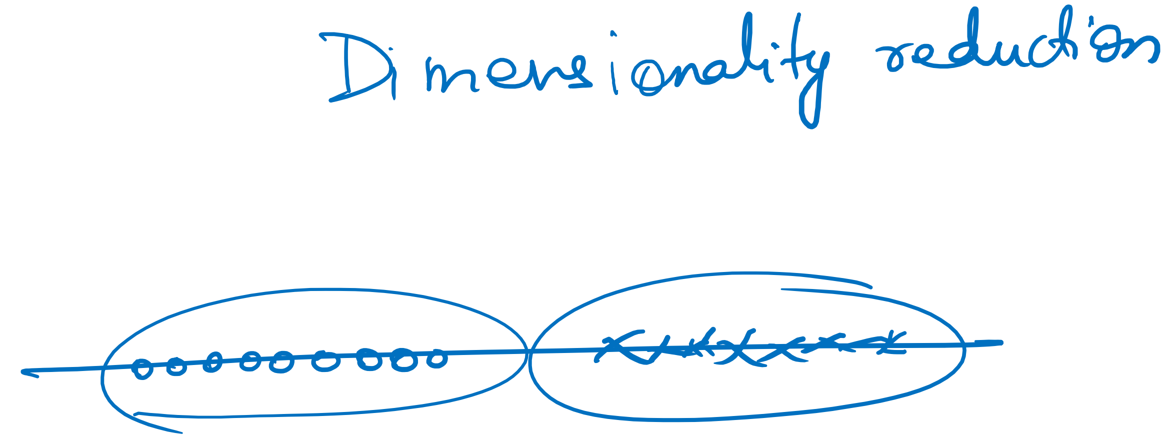


$u \cdot v = 0$

$\cos 90 = 0$

In context: how is the inner product useful in ML?
Projecting data onto a new direction





This will be helpful in dimensionality reduction, classification and feature engineering

Multiplications

- Given two vectors $\mathbf{x} \in \mathbb{R}^N$ and $\mathbf{y} \in \mathbb{R}^D$ the term $\mathbf{x}\mathbf{y}^\mathrm{T} \in \mathbb{R}^{N\times D}$ is called the outer product of the vectors and is a matrix given by $\left(x_i y_j\right)^\mathrm{T} = x_i y_j$.
- For example, $\mathbf{x} \in \mathbb{R}^3$ and $\mathbf{y} \in \mathbb{R}^2$

$$\mathbf{x}\mathbf{y}^\mathrm{T} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} [y1 \quad y2] = \begin{bmatrix} x_1y_1 & x_1y_2 \\ x_2y_1 & x_2y_2 \\ x_3y_1 & x_3y_2 \end{bmatrix}$$

3x1 1x2

3x2

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$A^{-1}Aw = A^{-1}b$

$w = A^{-1}b$ —— X^TX

Linear Independence and Matrix Rank

- A set of vectors $\{x_1, \ x_2, \ldots, x_d\} \subset \mathbb{R}^d$ are said to be ***(linearly) independent*** if no vector can be represented as a linear combination of the remaining vectors. That is if

$$x_d = \sum_{i=1}^{d-1} \alpha_i x_i$$

$$A = \begin{array}{c} \begin{array}{ccc} c_1 & c_2 & c_3 \end{array} \\ \begin{bmatrix} \quad & \quad & \quad \\ & & \\ & & \end{bmatrix} \end{array}$$

for some scalar values $\alpha_1, \alpha_2, \ldots \in \mathbb{R}$ then we say that the vectors are linearly ***dependent***; otherwise the vectors are linearly independent

$$A = \begin{array}{c} \begin{array}{ccc} c_1 & c_2 & c_3 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{array} \quad \text{rank}(A) = 3$$

A is a linearly independent matrix

full rank

$$B = \begin{array}{c} \begin{array}{ccc} c_1 & c_2 & c_3 \end{array} \\ \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 10 \end{bmatrix} \end{array}$$

$c_1 = \alpha_1 c_2 + \alpha_2 c_3$

$c_2 = 2c_1 + 0 \cdot c_3$

c_3 ✗

$\text{rank}(B) = 2$

In ML, we want as many linearly independent columns as possible

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tall matrix $C = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 5 & 8 \end{bmatrix}$ column rank = 2, row rank = 2

wide matrix $D = \begin{bmatrix} 1 & 2 & 3 & 5 \\ 2 & 4 & 6 & 7 \end{bmatrix}$ row rank = 2 = column rank

Linear Independence and Matrix Rank

- The **column rank** of a matrix $A \in \mathbb{R}^{n \times d}$ is the size of the largest subset of columns of A that constitute a linearly independent set. **Row rank** of a matrix is defined similarly for rows of a matrix.

It can be easily shown that the row and column ranks are equivalent, therefore we shall refer only to the **rank** of a matrix.

In general, for a full rank rectangular matrix, rank is the min of number of rows and number of columns.

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Matrix Rank: Examples

What are the ranks for the following matrices? How about an identity matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \end{bmatrix}$$

$\text{rank}(A) = 1$

Rank Deficiency means that the number of linearly independent vectors in our set is smaller than the smallest dimension

$$\mathbf{B} = \begin{bmatrix} 1 & 0 & 2 \\ 2 & 1 & 0 \\ 3 & 2 & 1 \end{bmatrix}$$

$\text{rank}(B) = 3$

$c_1 - 1 = c_2$

$c_1 + (-1)c_4 = c_2$

full rank matrix

Matrix Inverse

- The inverse of a square matrix $A \in \mathbb{R}^{d \times d}$ is denoted A^{-1} and is the unique matrix such that $A^{-1}A = I = AA^{-1}$

- For some square matrices A^{-1} may not exist, and we say that A is **singular or non-invertible.** In order for A to have an inverse, A must be **full rank.**

- For non-square matrices the inverse, denoted by A^{+} ,is given by $A^{+} = (A^{\top}A)^{-1}A^{\top}$ called the **pseudo inverse**

$\left(A^{T}_{d \times n} A_{n \times d}\right)^{-1} \cdot A^{T}$

In context: why is matrix rank important in ML?
Dataset preprocessing

If full rank $\longrightarrow$ V. Good

If not full rank $\longrightarrow$ Either combine dependent features or just get rid of it

$\underbrace{\hphantom{xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx}}$

No redundancy

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Matrix Trace

- The trace of a matrix $A \in \mathbb{R}^{d \times d}$, denoted as $\boldsymbol{tr(A)}$, is the sum of the diagonal elements in the matrix

$$tr(A) = \sum_{i=1}^{d} A_{ii}$$

- The trace has the following properties
  - For $A \in \mathbb{R}^{d \times d}$, $tr(A) = trA^{\top}$
  - For $A, B \in \mathbb{R}^{d \times d}$, $tr(A + B) = tr(A) + tr(B)$
  - For $A \in \mathbb{R}^{d \times d}$, $t \in \mathbb{R}$, $tr(tA) = t \cdot tr(A)$
  - For A, B, C such that ABC is a square matrix $tr(ABC) = tr(BCA) = tr(CAB)$

- The trace of a matrix helps us easily compute norms and eigenvalues of matrices as we will see later

Matrix Determinant

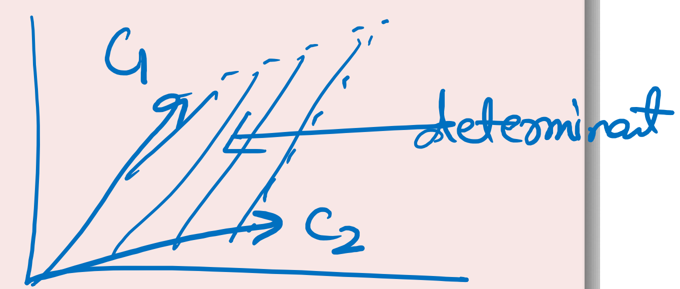
$$\begin{bmatrix} \cancel{a} & \cancel{b} & \cancel{c} \\ d & e & f \\ g & h & i \end{bmatrix}$$

$$a(ei - fh) - b(di - fg) + c(dh - eg)$$

Definition (Determinant)

The determinant of a square matrix A, denoted by $|A|$, is defined as

$$\det(A) = \sum_{j=1}^{d} (-1)^{i+j} a_{ij} M_{ij}$$



where M_{ij} is determinant of matrix A without the row i and column j.

For a 2×2 matrix $A = \begin{array}{c} \begin{array}{cc} c_1 & c_2 \end{array} \\ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \end{array}$

$$|A| = ad - bc$$

Linearly dependent columns → matrix is not full rank → determinant 0 → non-invertible matrix

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Properties of Matrix Determinant

Basic Properties

- $|A| = \left|A^T\right|$
- $|AB| = |A|\,|B|$
- $|A| = 0$ if and only if A is not invertible
- If A is invertible, then $\left|A^{-1}\right| = \frac{1}{|A|}$.

In context: how is the determinant useful in ML?
Matrix inversion

$A w = b$ $\quad w = A^{-1} b \quad$ A is not invertible

linear regression

Testing out if det(A) = 0 before trying to invert a matrix saves on computation

In that case, we can try out numerical methods

Gradient Descent

Recap

- Special Matrices

diagonal → $X^T X$ → square the diagonal terms

diagonal → X^{-1} → reciprocal of diagonal entries

Orthonormal → $X^{-1} = X^T$

Orthonormal → $\|Xx\|_2 = \|x\|_2$ → only allow rotation

- Norms

$\mathbb{R}^d \rightarrow \mathbb{R}$

"length"

$l_p \rightarrow l_2$ norm

To compute distances between datapoints in clustering

- Matrix Multiplications → is a bunch of dot product

gives us information about directional alignment / projection

$x \cdot y > 0$

$x \cdot y < 0$

$x \cdot y = 0$ → LINEARLY INDEPENDENT

- Matrix Inversion

$Aw = b$

$w = A^{-1} b$

2 indications of non-invertible matrix

Rank deficient → X not invertible

determinant is 0 → X not invertible

- Trace and Determinant

→ Area of formed by vectors

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Eigenvalues and Eigenvectors

- Given a square matrix $A \in \mathbb{R}^{d \times d}$ we say that $\lambda \in \mathbb{C}$ is an eigenvalue of A and $x \in \mathbb{C}^d$ is an eigenvector if

eigenvector eigenvalue

$$\boxed{Ax = \lambda x,} \qquad x \neq 0$$

dxd

- Intuitively this means that upon multiplying the matrix A with a vector x, we get the same vector, but scaled by a parameter λ

stretch or shrink ONLY

- So, eigenvectors are the special vectors whose direction is preserved under transformation (no rotation)

Matrix Eigen Decomposition

- All the eigenvectors can be written together as $\boxed{AX = X\Lambda}$ where the columns of X are the eigenvectors of A, and Λ is a diagonal matrix whose elements are eigenvalues of A

$A_{d\times d}$

$$\underbrace{\begin{bmatrix} A \end{bmatrix}}_{d\times d} \underbrace{\begin{bmatrix} e_1 & e_2 & \cdots & e_d \end{bmatrix}}_{X \quad d\times d} = \underbrace{\begin{bmatrix} X \end{bmatrix}}_{d\times d} \underbrace{\begin{bmatrix} \lambda_1 & 0 & 0 & & \\ 0 & \lambda_2 & 0 & & \\ 0 & & \lambda_3 & 0 & \\ & & & \ddots & \\ & & & & \lambda_d \end{bmatrix}}_{\Lambda \quad d\times d}$$

$$\boxed{AX = X\Lambda}$$

$$AXX^{-1} = X\Lambda X^{-1}$$

$$\boxed{A = X\Lambda X^{-1}}$$

Matrix Eigen Decomposition

- If the eigenvectors of A are invertible, then $\boxed{A = X\Lambda X^{-1}}$
- There are several properties of eigenvalues and eigenvectors
  - $Tr(A) = \sum_{i=1}^{d} \lambda_i$
  - $|A| = \prod_{i=1}^{d} \lambda_i$
  - If A is non-singular then $1/\lambda_i$ are the eigenvalues of A^{-1}
  - The eigenvalues of a diagonal matrix are the diagonal elements of the matrix itself!

3rd important property diagonal matrix

Matrix Eigen Decomposition

- For a symmetric matrix $\mathbf{A}$ it can be shown that eigenvalues are real and the eigenvectors are orthonormal. Thus it can be represented as $X\boldsymbol{\Lambda}\boldsymbol{X}^{\mathrm{T}}$

$A \leftarrow$ square

also symmetric

$X \leftarrow$ bunch of eigenvectors

ORTHONORMAL

$X^{-1} = X^{T}$

$$\boxed{A = X \Lambda X^{T}}$$

square

symmetric

orthonormal

diagonal

Eigenvalues and Eigenvectors

Geometrically, we are transforming the matrix A (if symmetric) from its original orthonormal basis/coordinates to a new set of orthonormal basis x with magnitude as **λ**

- If A is symmetric, eigenvectors are orthogonal. So, eigenvectors form an orthonormal basis
- Eigenvectors define the directions along which the transformation acts independently
- In the eigenvector basis, there is no rotation or shear, only scaling by the eigenvalues
- Each eigenvalue λi controls the amount of stretching or compression along eigenvector xi

Computing Eigenvalues and Eigenvectors

- We can rewrite the original equation in the following manner

$|A-\lambda I| \neq 0$

$(A-\lambda I)^{-1}$

$|A-\lambda I| = 0$

$$Ax = \lambda x, \qquad x \neq 0$$
$$\Rightarrow \boxed{(A-\lambda I)\,x = 0,} \qquad x \neq 0$$

$(A-\lambda I)^{-1}(A-\lambda I)\,x = 0$

$I \cdot x = 0 \Rightarrow x = 0$

- This is only possible if $(A-\lambda I)$ is singular, that is $|(A-\lambda I)| = 0$.

- Thus, eigenvalues and eigenvectors can be computed.
  - Compute the determinant of $A - \lambda I$.
    - This results in a polynomial of degree d.
  - Find the roots of the polynomial by equating it to zero.
    - The d roots are the d eigenvalues of A. They make $A - \lambda I$ singular.
  - For each eigenvalue λ, solve $(A-\lambda I)\,x$ to find an eigenvector x

Eigenvalue Example

$|A - \lambda I| = 0$

$\left| \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| = 0$

$= \left| \begin{bmatrix} 1-\lambda & 2 \\ 3 & -4-\lambda \end{bmatrix} \right| = 0$

$= (1-\lambda)(-4-\lambda) - 6 = 0$

$= -4 - \lambda + 4\lambda + \lambda^2 - 6 = 0$

Matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix}_{2\times 2}$

1. Compute the determinant of $\mathbf{A} - \lambda\mathbf{I}$

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

$$|\mathbf{A} - \lambda\mathbf{I}| = (1-\lambda)(-4-\lambda) - 6$$

2. Find the roots of the polynomial equating it to zero

$$|\mathbf{A} - \lambda\mathbf{I}| = 0 \rightarrow (1-\lambda)(-4-\lambda) - 6 = 0 \rightarrow \begin{cases} \lambda_1 = -5 \\ \lambda_2 = 2 \end{cases}$$

Eigenvalue Example

eigenvectors $\rightarrow$ we only care about direction

$Ax = \lambda x$

$A cx = c Ax = c \lambda x$

$= \lambda (cx)$

$A(cx) = \lambda (cx)$

λ is an eigenvalue for x & cx

3. For each eigenvalue λ solve $(\mathbf{A} - \lambda \mathbf{I})\mathbf{x} = \mathbf{0}$ to find eigenvector $\mathbf{x}$

$$\begin{bmatrix} 1-\lambda & 2 \\ 3 & -4-\lambda \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \begin{cases} (1-\lambda)x_1 + 2x_2 = 0 \\ 3x_1 - (4+\lambda)x_2 = 0 \end{cases}$$

Eigenvector for $\lambda_1 = -5$

$$\boxed{\begin{cases} 6x_1 + 2x_2 = 0 \\ 3x_1 + x_2 = 0 \end{cases}} \rightarrow \mathbf{x}_1 = \boxed{\begin{bmatrix} 1 \\ -3 \end{bmatrix}} \text{ or } \boxed{\begin{bmatrix} 0.3162 \\ -0.9487 \end{bmatrix}}$$

Eigenvector for $\lambda_2 = 2$

$$\begin{cases} -x_1 + 2x_2 = 0 \\ 3x_1 - 6x_2 = 0 \end{cases} \rightarrow \boxed{\mathbf{x}_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \text{ or } \begin{bmatrix} 0.8944 \\ 0.4472 \end{bmatrix}}$$

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Can a matrix have the same eigenvalues?

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$(1, 1, 1)$

If two vectors are linearly independent, does it mean they are orthogonal to each other?

if orthogonal

$\downarrow$

linearly independent

$$\begin{bmatrix} 1 & 5 \\ 2 & 7 \\ 3 & 9 \end{bmatrix}$$

Vice Versa is correct

In context: how is eigenvalues and eigenvectors helpful in ML?

- Eigenvectors are “special directions” where a matrix doesn’t rotate or shear — it only stretches or shrinks.
- The stretch amount is the eigenvalue.

- Many ML tools boil down to understanding **data transformations** (via matrices). Eigenvectors/eigenvalues tell us the **essential structure** of those transformations:

- Eigenvectors reveal the fundamental directions along which the transformation acts independently.
- Eigenvalues quantify the strength of that action (how much stretching or shrinking occurs).
- This decomposition simplifies complex transformations into basic “rotate–stretch–rotate back” operations, making it easier to analyze patterns, reduce dimensionality, or understand stability and sensitivity in models.

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Outline

- Linear Algebra Basics
- Norms
- Multiplications
- Matrix Inversion
- Trace and Determinant
- Eigen Values and Eigen Vectors
- Singular Value Decomposition

Eigenvalue decomposition

$$A = X \Lambda X^T$$

Square & symmetric

Singular Value Decomposition

$$\bar{X} = \begin{bmatrix} a_1 - \mu_1 \\ a_2 - \mu_1 \\ a_3 - \mu_1 \\ \vdots \\ a_n - \mu_1 \end{bmatrix}_{n \times d} \qquad \mu_1 = \frac{a_1 + \cdots + a_n}{n}$$

c_1

center

$$\bar{X}_{n\times d}$$

n: datapoints
d: dimensions
X is a centered matrix

orthonormal

$$\bar{X} = \boxed{U\Sigma V^T}$$

$$U_{n\times n} \rightarrow unitary\ matrix \rightarrow U \times U^T = I$$

$$\Sigma_{n\times d} \rightarrow diagonal\ matrix$$

$$X = [\ ]_{100{,}000 \times 100}$$

$$np.svd(X_{n\times d}) = \underset{n\times n}{U}\ \underset{n\times d}{\Sigma}\ \underset{d\times d}{V}$$

$$V_{d\times d} \rightarrow unitary\ matrix \rightarrow V \times V^T = I$$

$$X = \begin{bmatrix} u_{1\times 1} & \cdots & \cdots & \cdots & u_{1\times n} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ u_{1\times 1} & \cdots & \cdots & \cdots & u_{n\times n} \end{bmatrix} \times \begin{bmatrix} \sum_{1\times 1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sum_{d\times d} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} v_{1\times 1} & \cdots & \cdots & \cdots & v_{1\times d} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ v_{d\times 1} & \cdots & \cdots & \cdots & v_{d\times d} \end{bmatrix}$$

$n \times d$ $\qquad U \qquad \boxed{n\times n} \qquad \Sigma \qquad n\times d \qquad V^T \qquad d\times d$

$$d < n$$

Covariance matrix:

$(ab)^T = b^T a^T$

$\frac{\bar{X}^T \bar{X}}{n}$

DO NOT LIKE LIST
① FOR LOOP
② INVERSE
③ MATRIX MULP.

$C = \frac{\bar{X}^T \bar{X}}{N}$

$$\boxed{C_{d\times d} = \frac{\underset{10000\times 100}{\bar{X}^T}\ \underset{100\times 10000}{\bar{X}}}{n}} = C_{100k \times 100k}$$

$n \leftarrow$ no. of datapoints

$\bar{X} = U \Sigma V^T$

$C = \frac{(U\Sigma V^T)^T (U \Sigma V^T)}{N} = \frac{V \Sigma^T \boxed{U^T U} \Sigma V^T}{N} = \frac{V \Sigma^T \Sigma V^T}{N} = \frac{V \Sigma^2 V^T}{N}$

$$\bar{X} = U\Sigma V^T$$

$$C = \frac{\bar{X}^T \bar{X}}{n}$$

$$C = \frac{V\Sigma^T U^T U \Sigma V^T}{n} = \frac{V\Sigma^2 V^T}{n}$$

diagonal

$AX = X\Lambda$

square

Orthonormal

diagonal

$$\boxed{C V = V \frac{\Sigma^2}{N}}$$

square

$C = \frac{V \Sigma^2 V^T}{N}$

$CV = \frac{V \Sigma^2 V^T V}{N} = \frac{V \Sigma^2}{n}$

$$C = \frac{V\Sigma^2V^T}{n} = V\frac{\Sigma^2}{n}V^T$$

$$\begin{bmatrix} \Sigma_1 & & & \\ & \Sigma_2 & & \\ & & \ddots & \\ & & & \Sigma_d \\ 0 & 0 & 0 & 0 \end{bmatrix}_{n \times d}$$

$$CV = V\frac{\Sigma^2}{n}V^TV = V\frac{\Sigma^2}{n}$$

$$CV = V\Lambda$$

Remember: $$AX = X\Lambda$$

$\lambda_i = \frac{\Sigma_i^2}{n}$ ➔ The eigenvalues of covariance matrix

λ_i: Eigenvalue of C or covariance matrix

Σ_i: Singular value of X matrix

So, we can **directly** calculate eigenvalue and eigenvectors of a covariance matrix by having the singular value decomposition of matrix X

So, we can **directly** calculate eigenvalue and eigenvectors of a covariance matrix by having the singular value decomposition of matrix X

Why is this helpful?

Because SVD **always exists** for **any** matrix (rectangular, non-symmetric) and is **more numerically stable**. That's why in ML (e.g., PCA) we usually prefer **SVD of X** over eigen-decomposition of $\boldsymbol{X^T X}$.

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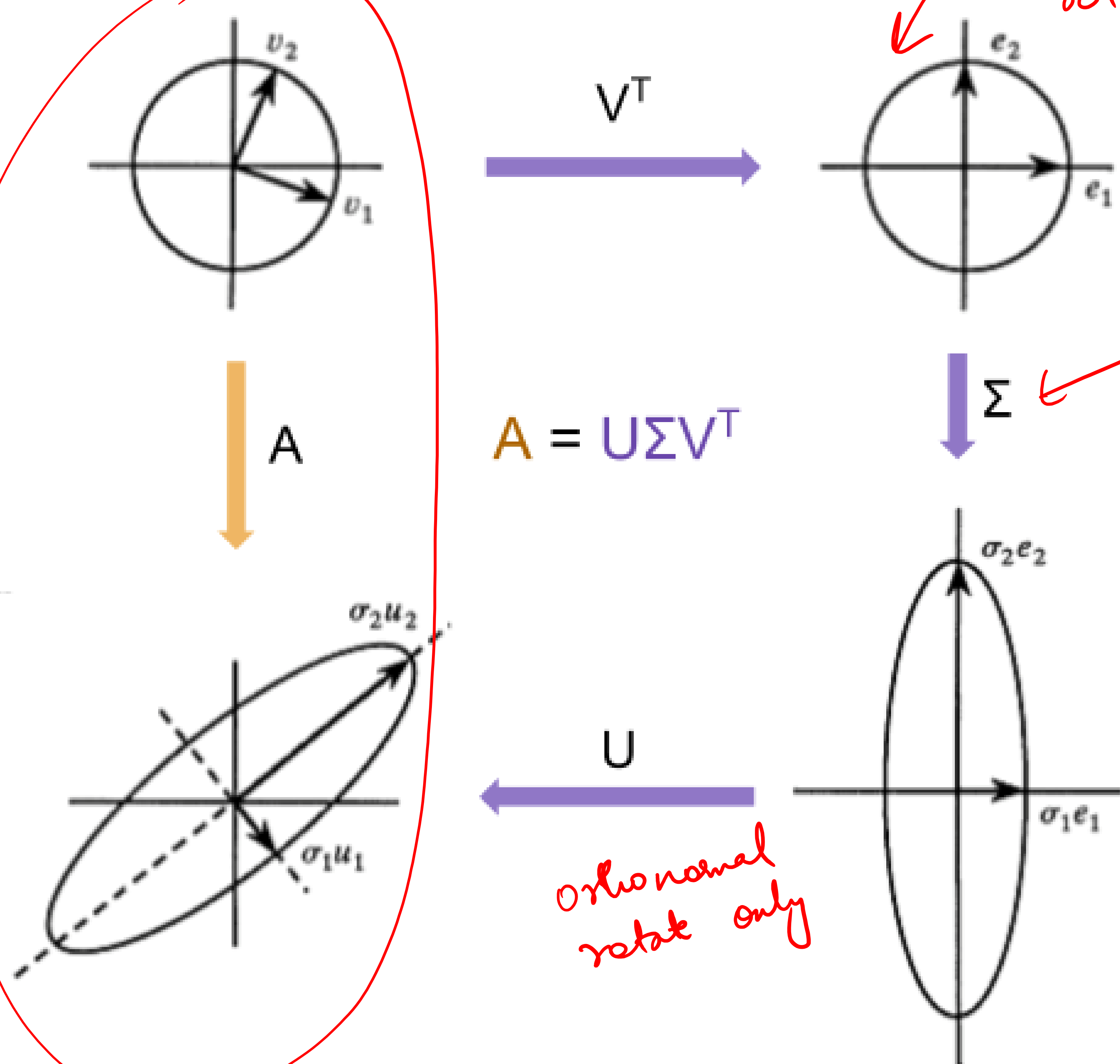
Geometric Meaning of SVD

$Xx = U\Sigma V^T x$

SVD tells us that *any* linear transformation can be decomposed into:
a rotation → a scaling → another rotation.

rotating only



diagonal stretching only

orthonormal rotate only

Image Credit: Kevin Binz

In context: why is SVD and covariance matrix useful in ML?

SVD (X=$U\Sigma V^T$)

•Finds the **most informative directions** in the data (columns of V); σ_i tell how strong each is.
•Gives the **best low-rank approximation** → dimensionality reduction, compression, **denoising** (Low values of σ_i means often represents noise)

Covariance (C= $\frac{X^T X}{n}$ with centered X)

•Summarizes **spread** (variances) and **relationships** (correlations) between features.
•Drives **PCA**: eigenvectors = principal components; eigenvalues = **explained variance**.
•Basis for **whitening/standardization**, which helps many models.

→ Covariance tells us what varies; **SVD** shows how to **use** it—rotate to those directions and keep the big values.

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Quick Knowledge Check

What property defines an orthonormal matrix Q?

A. $Q^T Q = I$ |B. $Q = Q^T$ |C. Entries are 0 or 1 | D. Determinant always positive

$Q^T = Q^{-1}$

When is a square matrix not invertible?

A. Columns linearly dependent | B. Matrix symmetric | C. Determinant nonzero | D. Columns orthogonal

What happens when a matrix acts on its eigenvector?

A. Direction unchanged | B. Vector rotates | C. Stretch or Shrink only| D. Direction becomes random

Why is SVD useful in machine learning?

A. Finds key directions | B. Removes all noise | C. Makes matrix invertible | D. Avoids multiplication

$C = X^T X$