Linear Algebra Basics

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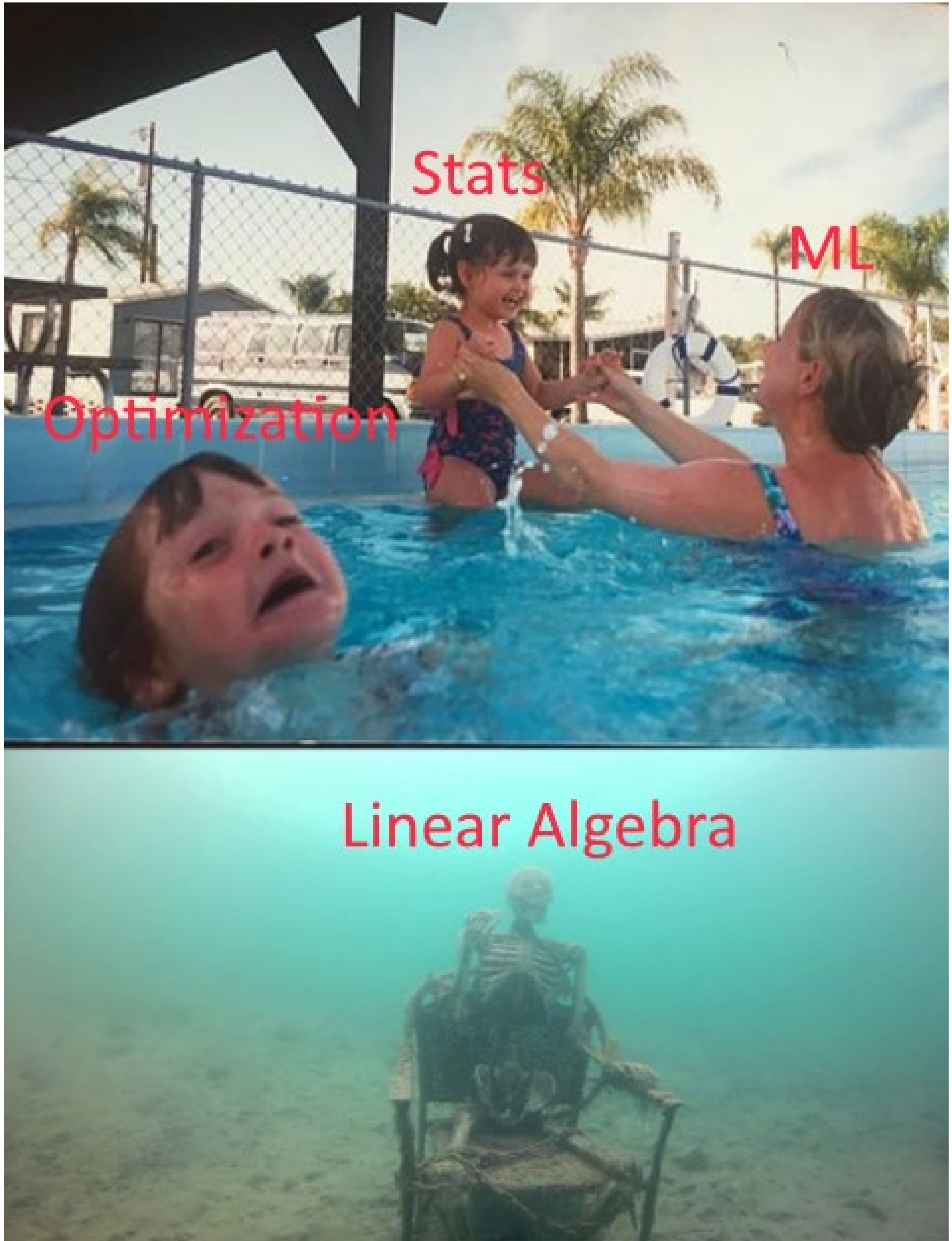
These slides are inspired based on slides from Le Song and Andres Mendez-Vazquez, Chao Zhang


Stats
ML
Optimization
Linear Algebra

Some logistics

- The syllabus quiz is out (was out at 8:00am). Unlike other quizzes, this quiz will have 25 questions and it also has 48-hour grace period. Also, unlike other quizzes, you have you have unlimited attempts before Friday night + 48-hour grace period
- OHs start this week
- Project Seminar will be on Friday at 11:00 am organized by Kevin. Will will go over Project's requirements and Julia will go over an example
- Quiz 0 is re-opened to those that signed up late during registration
- Creating your project's team.

Outline

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

Why Linear Algebra?

- Linear algebra provides a way of compactly representing and operating on sets of linear equations

  $4x_1 - 5x_2 = -13 \quad -2x_1 + 3x_2 = 9$

  can be written in the form of $Ax = b$

  $A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \quad b = \begin{bmatrix} -13 \\ 9 \end{bmatrix}$

- $A \in \mathbb{R}^{n \times d}$ denotes a matrix with n rows and d columns, where elements belong to real numbers.

- $x \in \mathbb{R}^d$ denotes a vector with d real entries. By convention an d dimensional vector is often thought as a matrix with 1 row and d column.

Linear Algebra Basics

- Transpose of a matrix results from flipping the rows and columns. Given A ∈ $\mathbb{R}^{n \times d}$, transpose is $A^\top \in \mathbb{R}^{d \times n}$

- For each element of the matrix, the transpose can be written as → $A^\top{}_{ij} = A_{ji}$

- The following properties of the transposes are easily verified
  - $(A^\top)^\top = A$
  - $(AB)^\top = B^\top A^\top$
  - $(A + B)^\top = A^\top + B^\top$

- A square matrix $A \in \mathbb{R}^{d \times d}$ is symmetric if $A = A^\top$ and it is anti-symmetric if $A = -A^\top$. Thus each matrix can be written as a sum of symmetric and anti-symmetric matrices.

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

$$G = G^T \Rightarrow \underbrace{(A + A^T)}_{G} = \underbrace{(A + A^T)^T}_{G^T} = A^T + (A^T)^T = \underbrace{A^T + A}_{}$$

$$H = -H^T \Rightarrow \underbrace{(A - A^T)}_{H} = -\underbrace{(A - A^T)^T}_{-H^T} = -(A^T - (A^T)^T) = \underbrace{A - A^T}_{}$$

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Norms

$\|x\| = \|x\|_2$

- Norm of a vector $\|x\|$ is informally a measure of the "length" of a vector
- More formally, a norm is any function $f \boxed{: \mathbb{R}^d \to \mathbb{R}}$ that satisfies
  - For all $x \in \mathbb{R}^d$, $f(x) \geq 0$ (non-negativity)
  - $f(x) = 0$ is and only if $x = 0$ (definiteness)
  - For $x \in \mathbb{R}^d$, $t \in \mathbb{R}$, $f(tx) = |t| f(x)$ (homogeneity)
  - For all $x, y \in \mathbb{R}^d$, $f(x + y) \leq f(x) + f(y)$ (triangle inequality)
- Common norms used in machine learning are
  - ℓ_2 norm
    - $\|x\|_2 = \sqrt{\sum_{i=1}^{d} x_i^2}$

$X = [1, 2, 3]$

$\|X\|_2 = \sqrt{1^2 + 2^2 + 3^2}$

Norms

$X = [1, 2, 3]$

- ℓ_1 norm
  - $\|x\|_1 = \sum_{i=1}^{d} |x_i|$

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

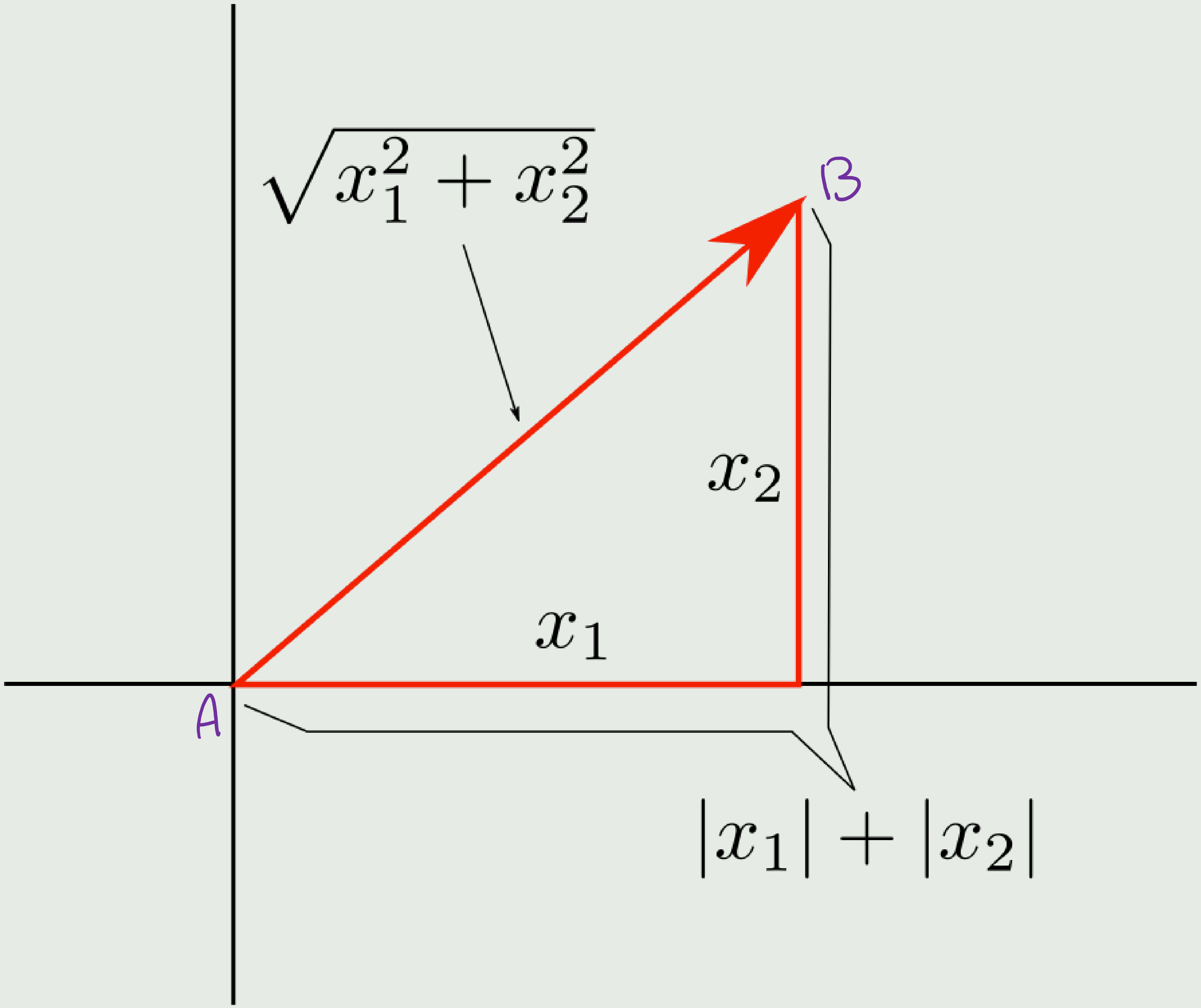
- ℓ_∞ norm
  - $\|x\|_\infty = max_i |x_i|$

$\|x\|_\infty = \text{argmax} \left| [1, 2, 3] \right| = |3|$

- All norms presented so far are examples of the family of ℓ_p norms, which are parameterized by a real number $p \geq 1$
  - $\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{\frac{1}{p}}$
- Norms can be defined for matrices, such as the Frobenius norm.
  - $\|A\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{d} A_{ij}^{2}} = \sqrt{tr(A^\top A)}$

Vector Norm Examples

Example ℓ_1-norm and ℓ_2-norm



Special Matrices

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

- 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 matrix where all non-diagonal matrices are 0. This is typically denoted as D = $diag(d_1, d_2, d_3, \ldots, d_d)$

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

Orthonormal = Unitary

$\begin{array}{ccc} x_1 & x_2 & \\ \end{array}$
$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

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

$U U^{-1} = I$

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

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Multiplications

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

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

$$xy^T = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \sum_{i=1}^{3} x_i y_i$$

- Given two vectors x $\in \mathbb{R}^d$, y $\in \mathbb{R}^n$, the term $x^T y$ is called the **outer product** of the vectors : $x \otimes y$

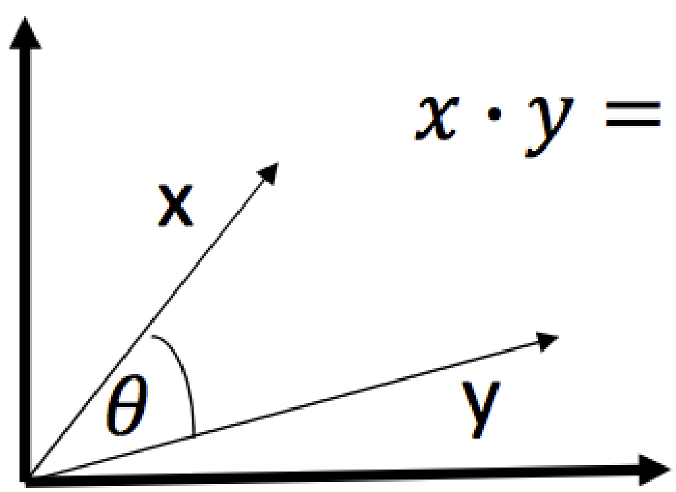
Is Dot Product a linear operation?

YES

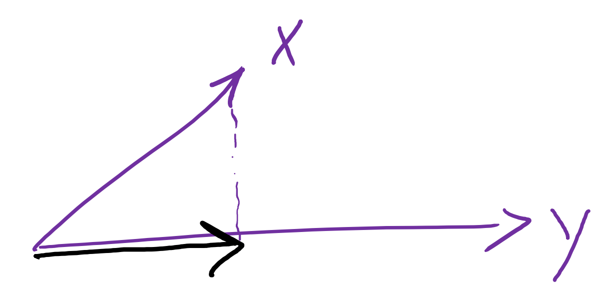
Multiplications

$$x \otimes y = x\,{}^{\mathrm{T}}y = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} = \begin{bmatrix} x_1y_1 & x_1y_2 & x_1y_3 \\ x_2y_1 & x_2y_2 & x_2y_3 \\ x_3y_1 & x_3y_2 & x_3y_3 \end{bmatrix}$$

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



$$x \cdot y = |x||y| \cos\theta$$

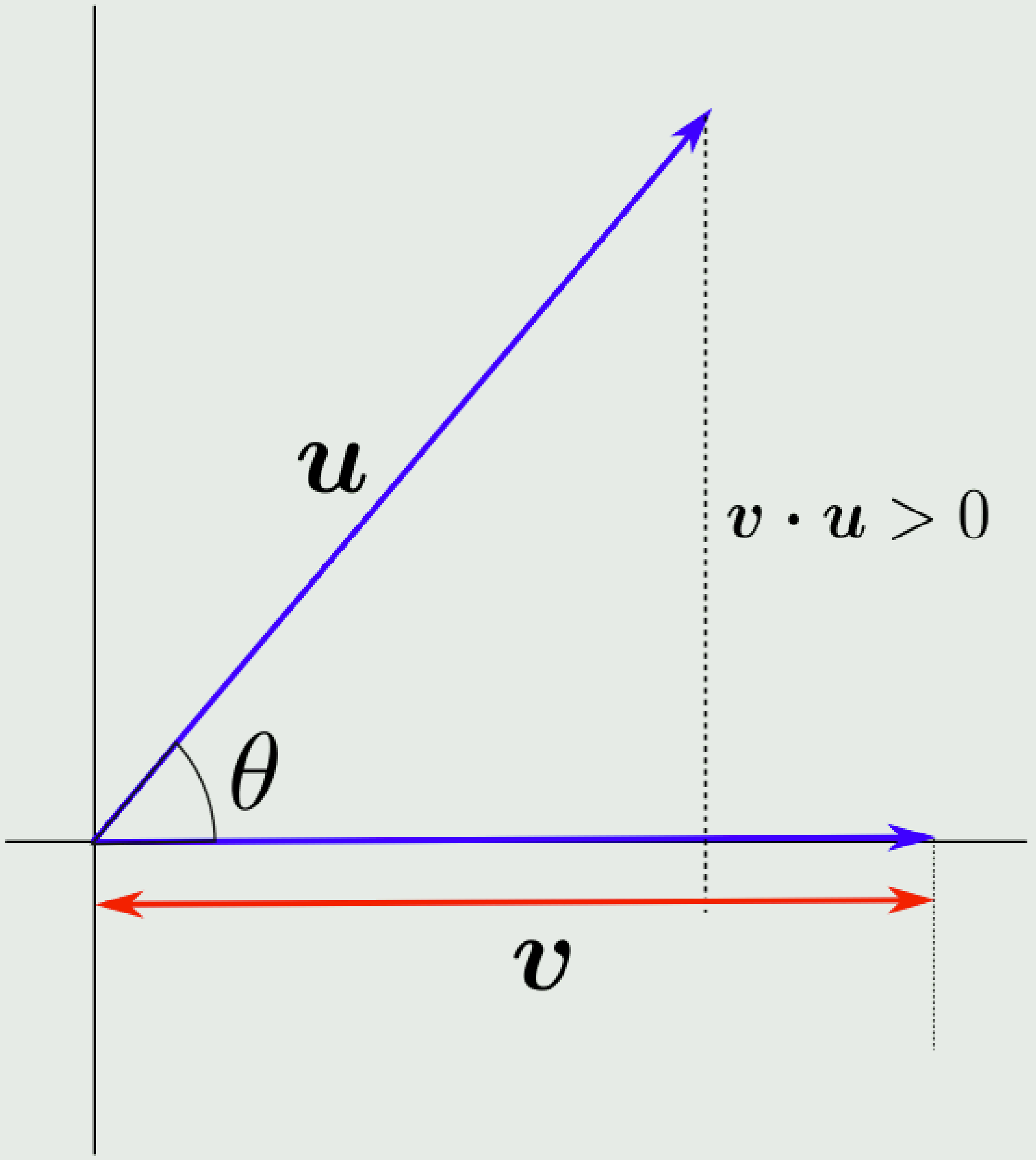


$\cancel{x.y}$ $\quad x.\frac{y}{\|y\|}$

which leads to use of dot product for testing orthogonality, getting the Euclidean norm of a vector, and scalar projections.

Inner Product Properties

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



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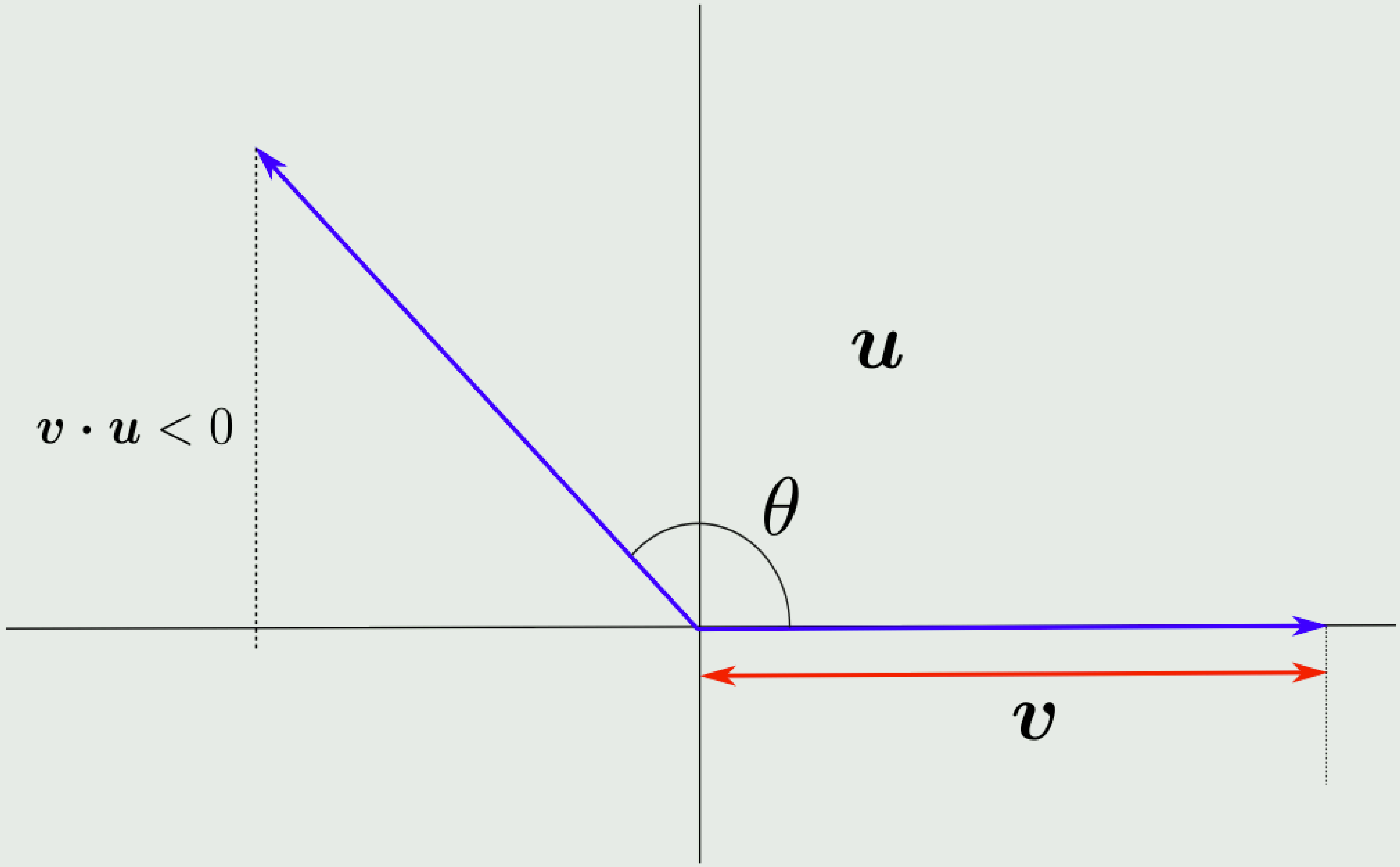

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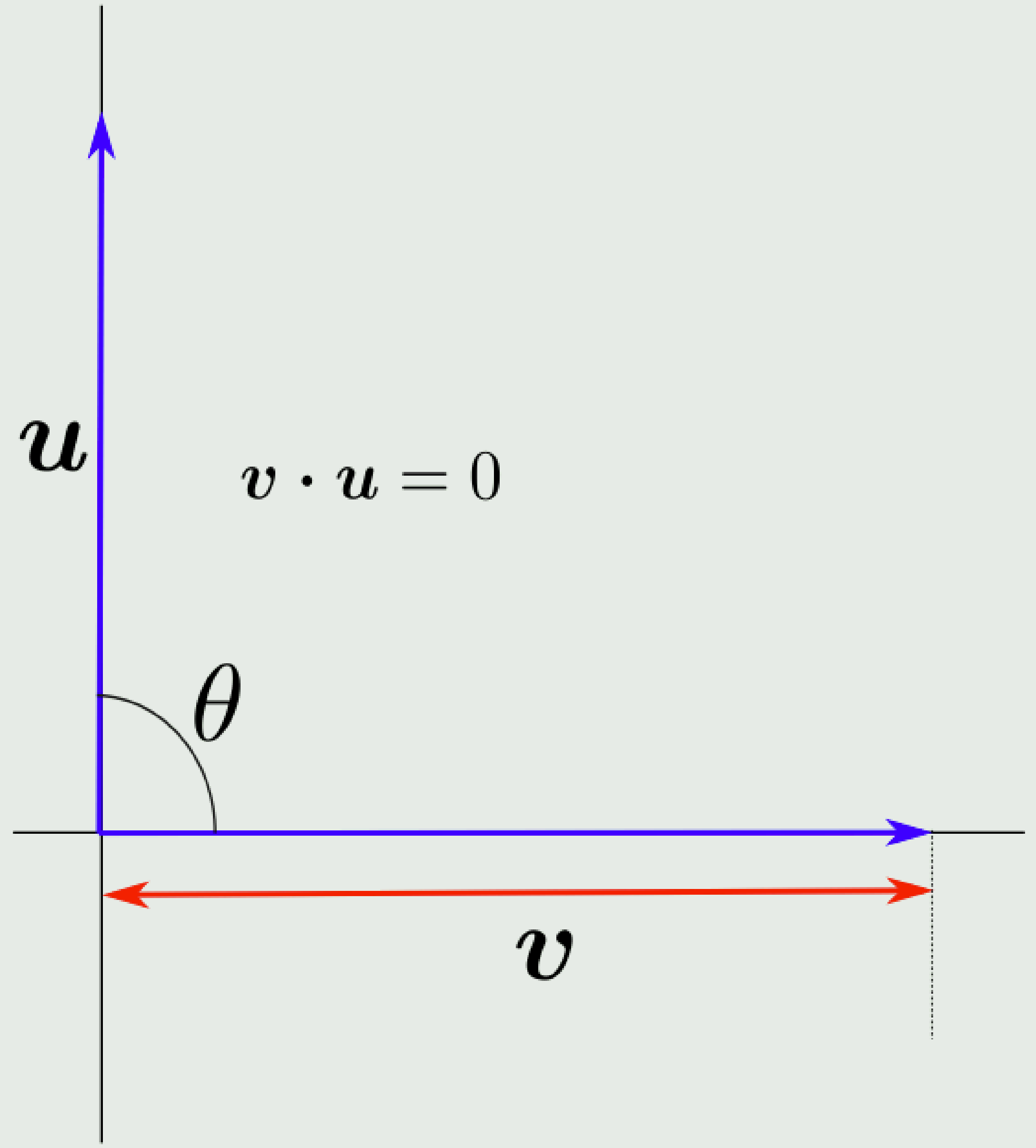

If two variables are uncorrelated, they are orthogonal and if two variables are orthogonal, they are uncorrelated.

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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

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

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

$A_{50 \times 100}$ $\quad$ $B_{100 \times 20}$

- 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 is a full rank if the rank is min{n,d}. This is the maximum rank.

Matrix Rank: Examples

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

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

$\times 2$ $\times 3$

Rank = 1 NOT a full rank

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

Rank = 3 or Full-rank

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**

$A_{n \times d}$ $\quad A^{T} \rightsquigarrow d \times n$ $\rightarrow$ my goal is to find pseudo inverse of $\boxed{A^{-1}}$

$(A^{T}A)_{d \times d} \rightsquigarrow (A^{T}A)^{-1} \rightsquigarrow \frac{1}{\cancel{A^{T}}A}\cancel{A^{T}} \approx \frac{1}{A}$

$\boxed{\mathrm{PInv}(A) = (A^{T}A)^{-1}A^{T}}$

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Matrix Trace

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

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 $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

$$|A| = ad - bc$$

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 $\left|A^{-1}\right| = \frac{1}{|A|}$.

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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

$$A = [\quad]_{5\times5} \qquad Ax = \lambda x, \qquad x \neq 0 \qquad AX = X\Lambda$$

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

- Geometrically, we are transforming the matrix A from its original orthonormal basis/co-ordinates to a new set of orthonormal basis x with magnitude as λ

$$x_1 = [\;]_{5\times1} \; \cdots \; x_5 = [\;]_{5\times1} \qquad \delta_1 \quad \delta_5$$

$$\Longrightarrow \quad X = \begin{bmatrix} x_1 & x_2 & \cdots & x_5 \end{bmatrix} \qquad \Lambda = \begin{bmatrix} \delta_1 & 0 & 0 & \cdots & 0 \\ & \delta_2 & & & 0 \\ & & & \ddots & \\ 0 & & & & \delta_5 \end{bmatrix}$$

Computing Eigenvalues and Eigenvectors

- We can rewrite the original equation in the following manner

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

- 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

Eigenvalues

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} \quad \lambda_1 = -5 \quad \lambda_2 = 2$$

Determine eigenvectors: $\mathbf{Ax} = \lambda \mathbf{x}$

$$\begin{aligned} x_1 + 2x_2 &= \lambda x_1 \\ 3x_1 - 4x_2 &= \lambda x_2 \end{aligned} \quad \Rightarrow \quad \begin{aligned} (1-\lambda)x_1 + 2x_2 &= 0 \\ 3x_1 - (4+\lambda)x_2 &= 0 \end{aligned}$$

Eigenvector for λ_1 = -5

$$\begin{aligned} 6x_1 + 2x_2 &= 0 \\ 3x_1 + x_2 &= 0 \end{aligned} \quad \Rightarrow \quad \mathbf{x}_1 = \begin{bmatrix} -0.3162 \\ 0.9487 \end{bmatrix} \text{ or } \mathbf{x}_1 = \begin{bmatrix} 1 \\ -3 \end{bmatrix}$$

Eigenvector for λ_1 = 2

$$\begin{aligned} -x_1 + 2x_2 &= 0 \\ 3x_1 - 6x_2 &= 0 \end{aligned} \quad \Rightarrow \quad \mathbf{x}_2 = \begin{bmatrix} 0.8944 \\ 0.4472 \end{bmatrix} \text{ or } \mathbf{x}_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$|A - \delta I| = 0 \Rightarrow \left| \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} - \delta \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| = \left| \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} - \begin{bmatrix} \delta & 0 \\ 0 & \delta \end{bmatrix} \right| =$$

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

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

$$\delta_1 = -5 \quad \text{and} \quad \delta_2 = 2$$

$$A x_1 = \delta x_1 \Rightarrow \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} \overset{x_1}{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}} = -5 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$x_1 + 2x_2 = -5x_1$$

$$3x_1 - 4x_2 = -5x_2$$

$$x_1 = \begin{bmatrix} 1 \\ -3 \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 2 \\ -3 & 1 \end{bmatrix} \quad \Lambda = \begin{bmatrix} -5 & 0 \\ 0 & 2 \end{bmatrix}$$

Slide credit: Shubham Kumbhar

Matrix Eigen Decomposition

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

- If the eigenvectors of A are invertible, then $A = X\Lambda X^{-1}$

- There are several properties of eigenvalues and eigenvectors
  - $Tr(A) = \sum_{i=1}^{d} \lambda_i$
  - $|A| = \prod_{i=1}^{d} \lambda_i$
  - Rank of A is the number of non-zero eigenvalues of A
  - 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!

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \qquad A^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$$

Can a matrix have the same eigenvalues?

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

Are the eigenvectors of a matrix orthogonal against each other?

It is yes if my matrix was symmetrical

NO

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Singular Value Decomposition

np.svd

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

n: instances
d: dimensions
X is a centered matrix

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

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

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

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

$$X = \underbrace{\begin{bmatrix} u_{1\times1} & \cdots & \cdots & \cdots & u_{1\times n} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ u_{1\times1} & \cdots & \cdots & \cdots & u_{n\times n} \end{bmatrix}}_{U} \times \underbrace{\begin{bmatrix} \sum_{1\times1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sum_{d\times d} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\Sigma} \times \underbrace{\begin{bmatrix} v_{1\times1} & \cdots & \cdots & \cdots & v_{1\times d} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ v_{d\times1} & \cdots & \cdots & \cdots & v_{d\times d} \end{bmatrix}}_{V^T}$$

$d < n$

Eigen decomposition of $C_{d\times d}$

Covariance matrix:

$$C_{d\times d} = \frac{\bar{X}^T\bar{X}}{n}$$

$(ABC)^T = C^T B^T A^T$

np.svd

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

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

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

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

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

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

$$\Lambda = \frac{\Sigma^2}{n}$$

$\frac{\Sigma^2}{n} = \Lambda$ V = eigenvectors for C

$$CV = V\Lambda$$

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 of a covariance matrix by having the singular value of matrix X **directly**

Geometric Meaning of SVD

Ax

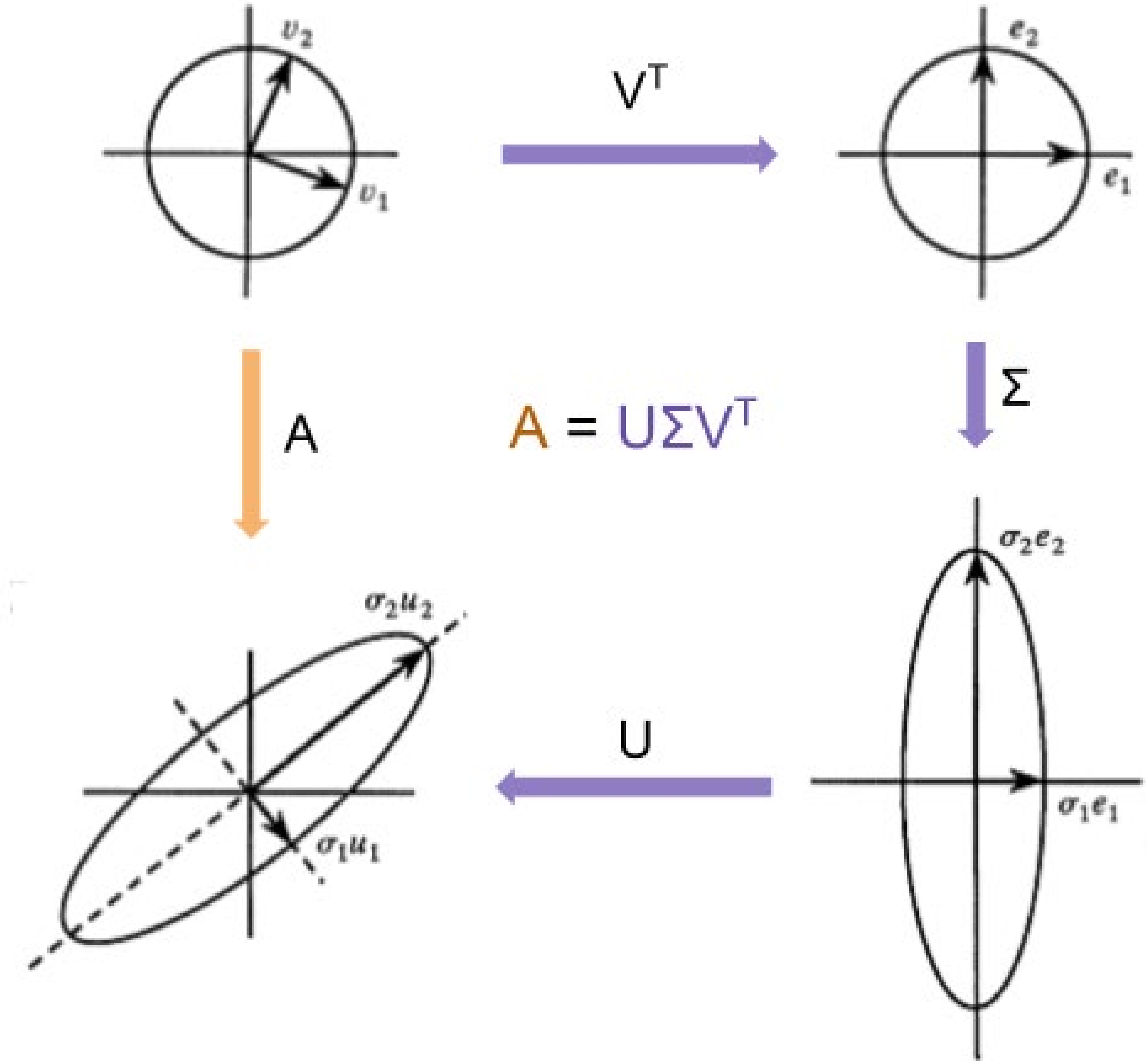

Image Credit: Kevin Binz

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