Lecture 02
Linear Algebra Basics

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

Some logistics

- Creating team.
- Plagiarism (we are very strict about this).
- Ruijia Wang, a new TA member.
- Please be nice to our TA team.
- Midterm exam will cover unsupervised learning and final exam will cover supervised. You already know the dates, please plan accordingly.
- Office hours will be started from next week.

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

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

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

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

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

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

Linear Algebra Basics

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

- 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 $A \in \mathbb{R}^{n \times n}$ 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.

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

$$G = G^T \rightsquigarrow (A+A^T)^T = A^T + (A^T)^T = A^T + A$$

$$H = -H^T \rightsquigarrow (A-A^T)^T = A^T - A$$

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Norms

- Norm of a vector $||x||$ is informally a measure of the "length" of a vector

- More formally, a norm is any function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ that satisfies
  - For all $x \in \mathbb{R}^n$, $f(x) \geq 0$ (non-negativity)
  - $f(x) = 0$ is and only if $x = 0$ (definiteness)
  - For $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, $f(tx) = |t| f(x)$ (homogeneity)
  - For all $x, y \in \mathbb{R}^n$, $f(x + y) \leq f(x) + f(y)$ (triangle inequality)

- Common norms used in machine learning are
  - ℓ_2 norm
    - $||x||_2 = \sqrt{\sum_{i=1}^{n} x_i^2} = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$

Norms

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

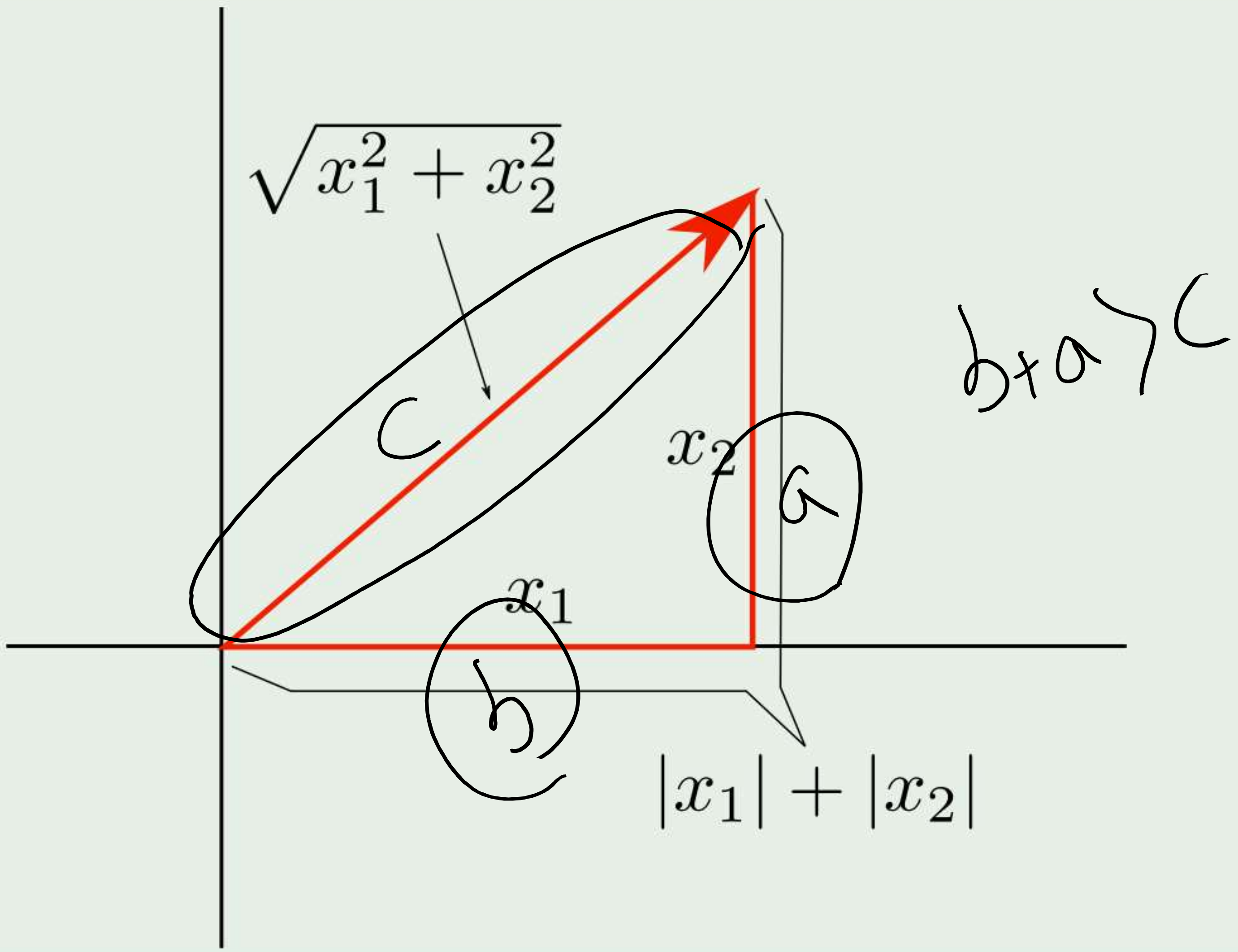
- ℓ_∞ norm
  - $\|x\|_\infty = max_i |x_i|$

- 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.
  - $\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} {A_{ij}}^2} = \sqrt{tr(A^\top A)}$

Vector Norm Examples

Example ℓ_1-norm and ℓ_2-norm



Special Matrices

- The identity matrix, denoted by $I \in \mathbb{R}^{n \times n}$ 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 = $diag(d_1, d_2, d_3, \ldots, d_n)$

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

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

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Multiplications

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

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

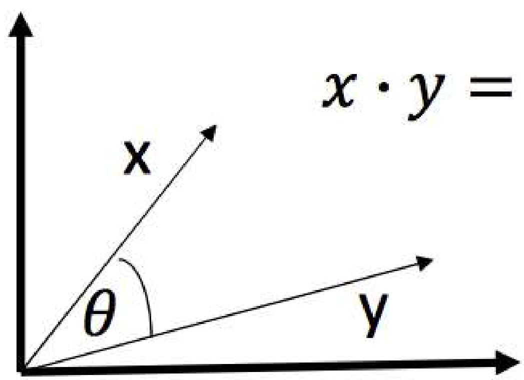
$$x^\top y = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \sum_{i=1}^{3} x_i y_i$$

- Given two vectors $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$, the term $xy^\top$ is called the **outer product** of the vectors, and is a matrix given by $(x_i y_j)^\top = x_i y_j$. For example,

Multiplications

$$xy^{\top} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} = \begin{bmatrix} x_1y_1 & x_1y_2 & x_1y_3 \\ x_2y_1 & x_2y_2 & x_2y_3 \\ x_3y_1 & x_3y_2 & x_3y_3 \end{bmatrix}$$

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

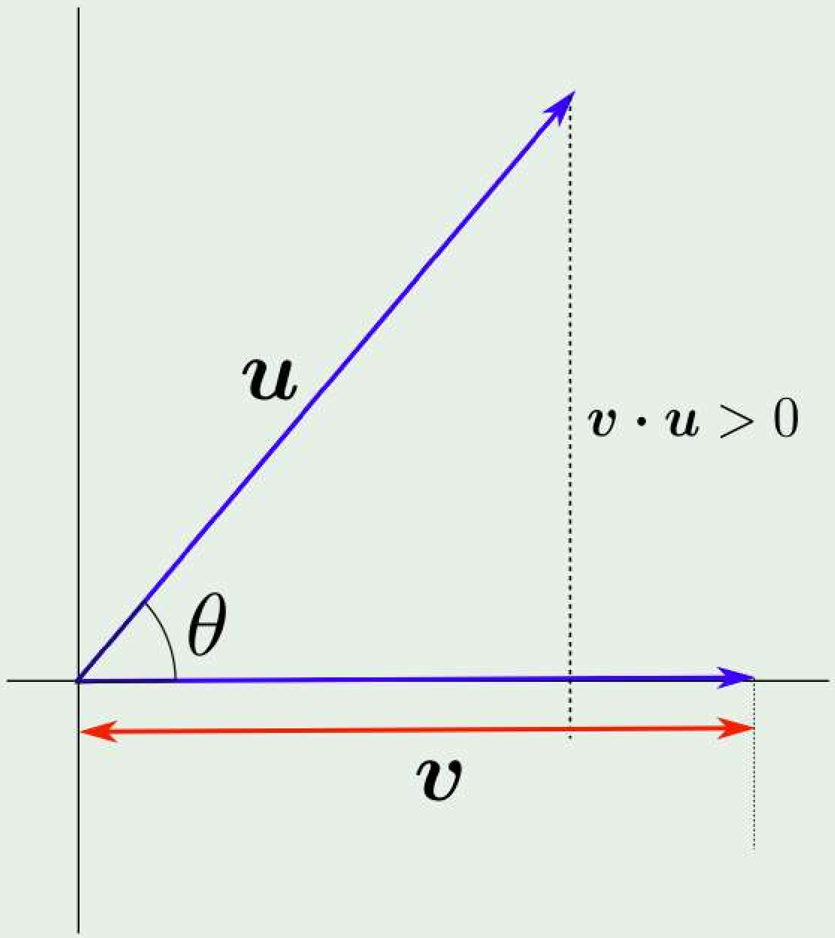


$$x \cdot y = |x||y| \cos\theta$$

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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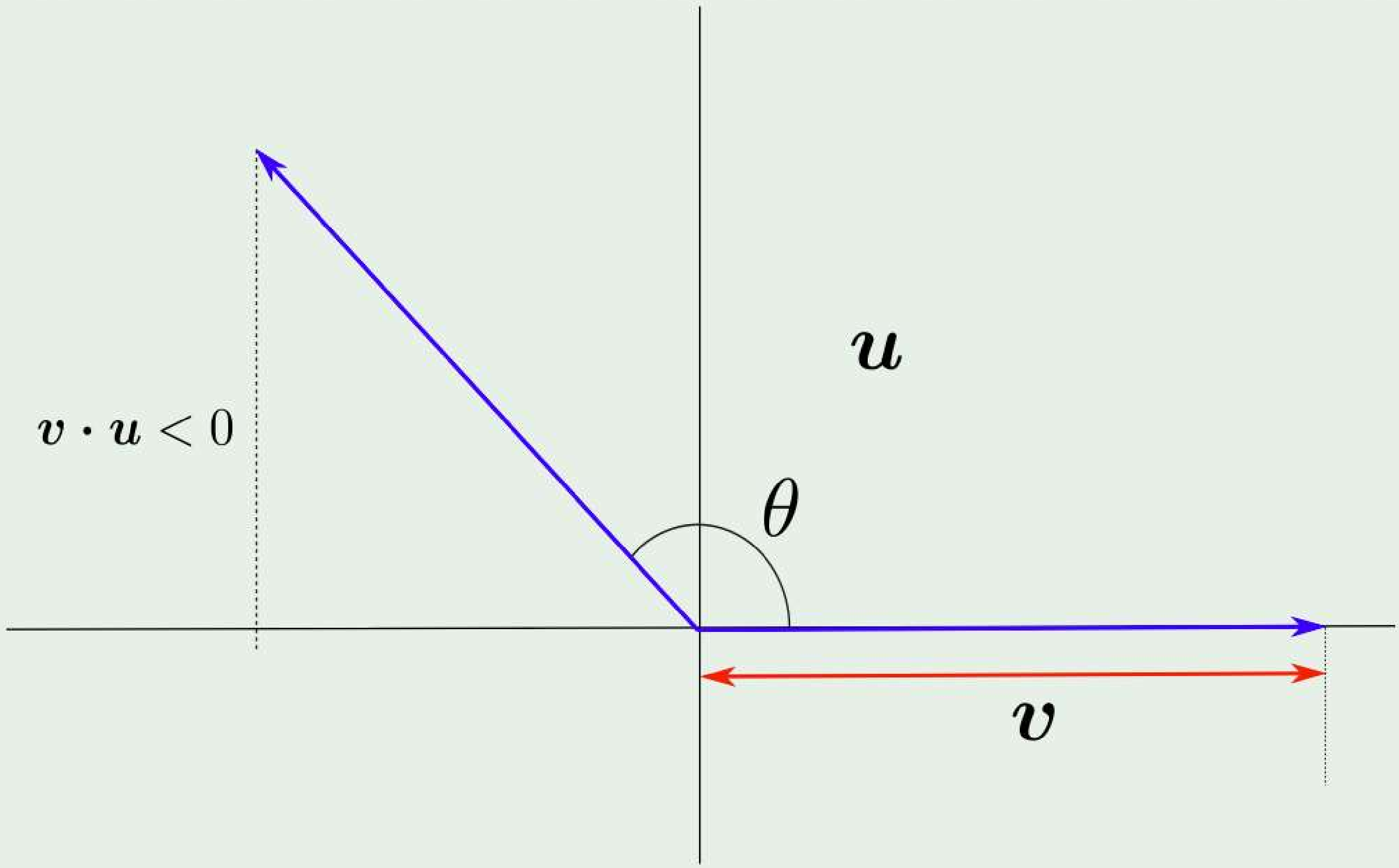

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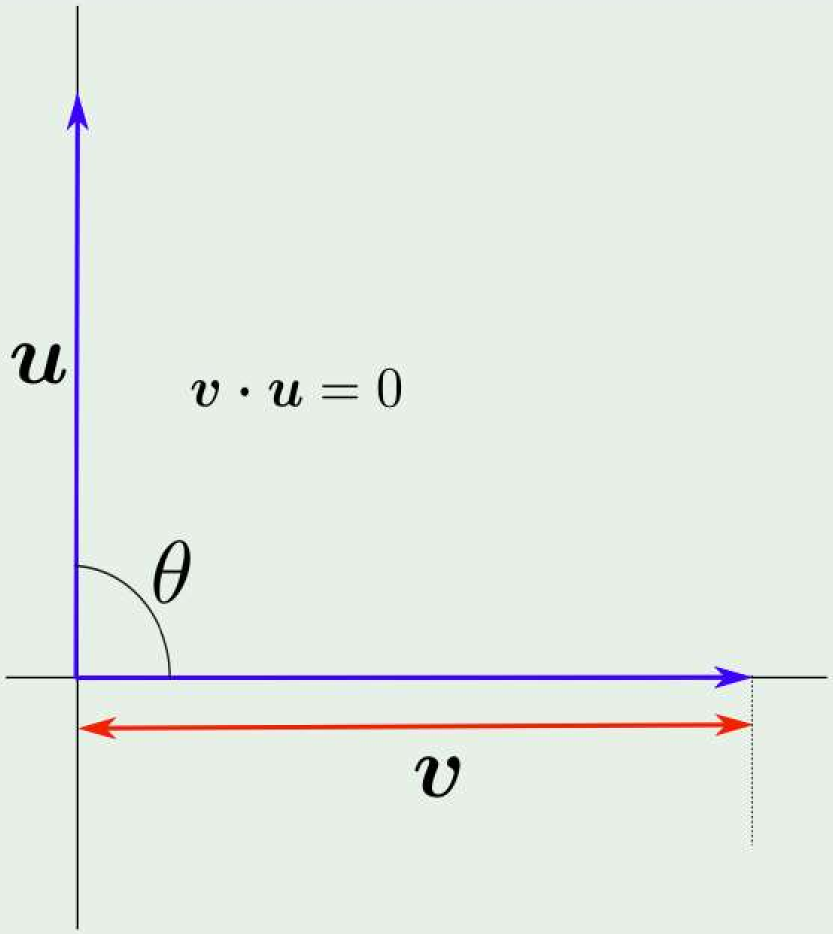

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Linear Independence and Matrix Rank

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

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i$$

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

- The **column rank** of a matrix $A \in \mathbb{R}^{m \times n}$ 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.

Range and Null Space

- The span of a set of vectors $\{x_1,\ x_2, \ldots, x_n\}$ is the set of all vectors that can be expressed as a linear combination of the set $\{v: v = \sum_{i=1}^{n} \alpha_i x_i \ , \alpha_i \ \in \ \mathbb{R}\}$

- If $\{x_1,\ x_2, \ldots, x_n\} \in \mathbb{R}^n$ is a set of linearly independent set of vectors, then span($\{x_1,\ x_2, \ldots, x_n\}$) = $\mathbb{R}^n$

- The range of a matrix $A \in \mathbb{R}^{m \times n}$, denoted as $\mathcal{R}(A)$, is the span of the columns of A

- The nullspace of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{N}(A)$, is the set of all vectors that equal 0 when multiplied by A
    - $\mathcal{N}(A) = \{x \ \in \ \mathbb{R}^n : Ax = 0\}$

Row and Column Space

- The row space and column space are the linear subspaces generated by row and column vectors of a matrix
- Linear subspace, is a vector space that is a subset of some other higher dimension vector space
- For a matrix $A \in \mathbb{R}^{m \times n}$
  - $Col\ space(A) = span(columns\ of\ A)$
  - $Rank(A) = \dim(row\ space(A)) = \dim(col\ space(A))$

Matrix Rank: Examples

What are the ranks for the following matrices?

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

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

Matrix Inverse

- The inverse of a square matrix $A \in \mathbb{R}^{n \times n}$ 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**

$$A_{n \times d}$$

$$\underbrace{A^T}_{d \times n}\underbrace{A}_{n \times d} = d \times d$$

$$(\cancel{A^T} A)^{-1} \cancel{A^T}$$

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Matrix Trace

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

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

- The trace has the following properties
  - For $A \in \mathbb{R}^{n \times n}$, $tr(A) = trA^{\top}$
  - For $A, B \in \mathbb{R}^{n \times n}$, $tr(A + B) = tr(A) + tr(B)$
  - For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, $tr(tA) = t \cdot tr(A)$
  - 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

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

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 $A \in \mathbb{R}^{n \times n}$ we say that $\lambda \in \mathbb{C}$ is an eigenvalue of A and $x \in \mathbb{C}^n$ is an eigenvector if

eigen value

eigen vector

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

- 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

Computing Eigenvalues and Eigenvectors

- We can rewrite the original equation in the following manner

$$Ax = \lambda x, \qquad x \neq 0$$

$$\Rightarrow (\lambda I - A)x = 0, \qquad x \neq 0$$

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

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

$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

Eigenvalue Example

$|\lambda I - A| = 0$

Eigenvalues

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

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

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

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

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

Eigenvector for λ_1 = -5

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

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

Eigenvector for λ_1 = 2

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

$Ax = \lambda x$

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

$$\begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_n \end{bmatrix}$$

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

- There are several properties of eigenvalues and eigenvectors
  - $Tr(A) = \sum_{i=1}^{n} \lambda_i$
  - $|A| = \prod_{i=1}^{n} \lambda_i$
  - 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!

Properties of Eigendecomposition

- For a symmetric matrix A, it can be shown that eigenvalues are real and the eigenvectors are orthonormal. Thus it can be represented as $U \Lambda U^\top$
- Considering quadratic form of A,
  - $x^\top A x = x^\top U \Lambda U^\top x = y^\top \Lambda y = \sum_{i=1}^{n} \lambda_i {y_i}^2$ (where $y = U^\top x$)

- Since ${y_i}^2$ is always positive the sign of the expression always depends on λ_i. If λ_i >0 then the matrix A is positive definite, if $\lambda_i \geq 0$ then the matrix A is positive semidefinite

- For a multivariate Gaussian, the variances of *x* and *y* do not fully describe the distribution. The eigenvectors of this covariance matrix capture the directions of highest variance and eigenvalues the variance

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$$
X = \begin{array}{ccc} \text{height} & \text{weight} & \text{gender} \\ \left[\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix}\right. & \begin{matrix} 5 \\ 6 \\ 7 \\ 8 \end{matrix} & \left.\begin{matrix} \text{female}=1 \\ \text{femal}=1 \\ \text{male}=0 \\ \text{male}=0 \end{matrix}\right] \end{array}_{n \times d}
$$

female = 1

male = 0

$$
\underbrace{X^T X}_{} = \begin{array}{c} \text{height} \\ \text{weight} \\ \text{gender} \end{array} \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{array}{ccc} \text{height} & \text{weight} & \text{gender} \\ \left[\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix}\right. & \begin{matrix} 5 \\ 6 \\ 7 \\ 8 \end{matrix} & \left.\begin{matrix} 1 \\ 1 \\ 9 \\ 0 \end{matrix}\right] \end{array}
$$

$$
\rightsquigarrow \begin{array}{c|ccc} & h & w & g \\ \hline \text{height} & & & \\ w & & & \\ g & & & \end{array}_{3 \times 3}
$$

$$\mathrm{Var}(x) = \frac{\sum_i (x_i - \mu)^2}{n}$$

average

$$X = [1 \quad 2 \quad 3 \quad 4]$$

$$\bar{X} = \begin{array}{ccc} h & w & g \\ \end{array}$$
$$\begin{bmatrix} 1-2.5 & & \\ 2-2.5 & & \\ 3-2.5 & & \\ 4-2.5 & & \end{bmatrix}$$

$\rightsquigarrow$ Covariance

Standardize

$$\frac{X - \mu}{\sigma}$$

$$\mathrm{Cov}(X) = \frac{\bar{X}^T \bar{X}}{n}$$

Singular Value Decomposition

$X_{n \times d}$

n: instances
d: dimensions
X is a centered matrix

$$X = U\Sigma V^T$$

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

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

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

$$C = \frac{X^T X}{m}$$

$$X = \begin{bmatrix} u_{1\times1} & \cdots & u_{1\times n} \\ \vdots & \ddots & \vdots \\ u_{n\times1} & \cdots & u_{n\times n} \end{bmatrix} \times \begin{bmatrix} \Sigma_{1\times1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \Sigma_{n\times d} \end{bmatrix} \times \begin{bmatrix} v_{1\times1} & \cdots & v_{1\times d} \\ \vdots & \ddots & \vdots \\ v_{d\times1} & \cdots & v_{d\times d} \end{bmatrix}$$

$CX = \Lambda X$

Covariance matrix:

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

C

X

$$X = U\Sigma V^T$$

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

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

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

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

$AV = \frac{\Sigma^2}{n} V$

According to Eigen-decomposition definition ➔ $AV = \Lambda V$

$AX = \Lambda X$

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

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

V is the right singular vectors (Principal directions)

$X = U\Sigma V$

Geometric Meaning of SVD

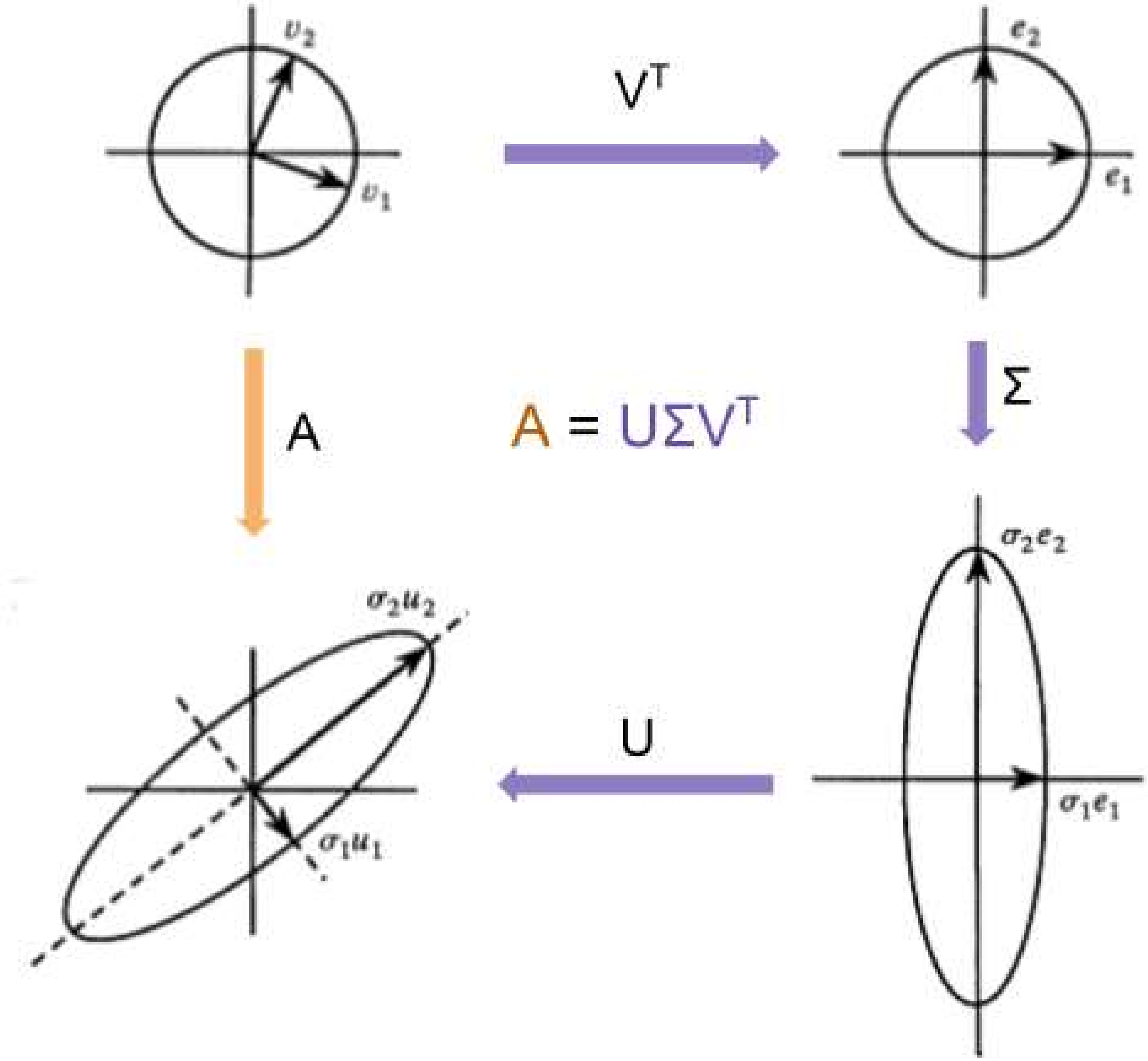

Image Credit: Kevin Binz

SVD Example

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

$$\mathbf{M} \qquad\qquad \mathbf{U} \qquad\qquad \mathbf{\Sigma} \qquad\qquad \mathbf{V}^{\mathrm{T}}$$

From [Strang]

Matrix Calculus

- For a vector x, b $\in \mathbb{R}^n$, let $f(x) = b^\top x$, then $\nabla_x b^\top x$ is equal to b
  - $\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} b_i x_i = b_k$
- Now for a quadratic function, $f(x) = x^\top A x$, with $A \in \mathbb{S}^n$, $\frac{\partial f(x)}{\partial x_k} = 2Ax$
  - $\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{i=1}^{n} A_{ij} x_i x_j$
  - $= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2A_{kk} x_k$
  - $= 2 \sum_{i=1}^{n} A_{ki} x_i$
- Let $f(X) = X^{-1}$, then $\partial(X^{-1}) = -X^{-1}(\partial X) X^{-1}$

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