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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?

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

$$\begin{matrix} 4x_1 - 5x_2 = -13 \\ -2x_1 + 3x_2 = 9 \end{matrix} \rightarrow \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -13 \\ 9 \end{bmatrix} \rightarrow \mathbf{Ax} = \mathbf{b}$$

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

Linear algebra basics

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

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

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

$$\mathbf{A} = \frac{1}{2}\left(\mathbf{A} - \mathbf{A}^{T}\right) + \frac{1}{2}\left(\mathbf{A} + \mathbf{A}^{T}\right)$$

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Norms

- Norm of a vector $||\mathbf{x}||$ is informally a measure of the length of a vector
- More formally, a norm is any function $f: \mathbb{R}^D \rightarrow \mathbb{R}$ 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

- 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: $\|\mathbf{x}\|_\infty = \max_i |x_i|$

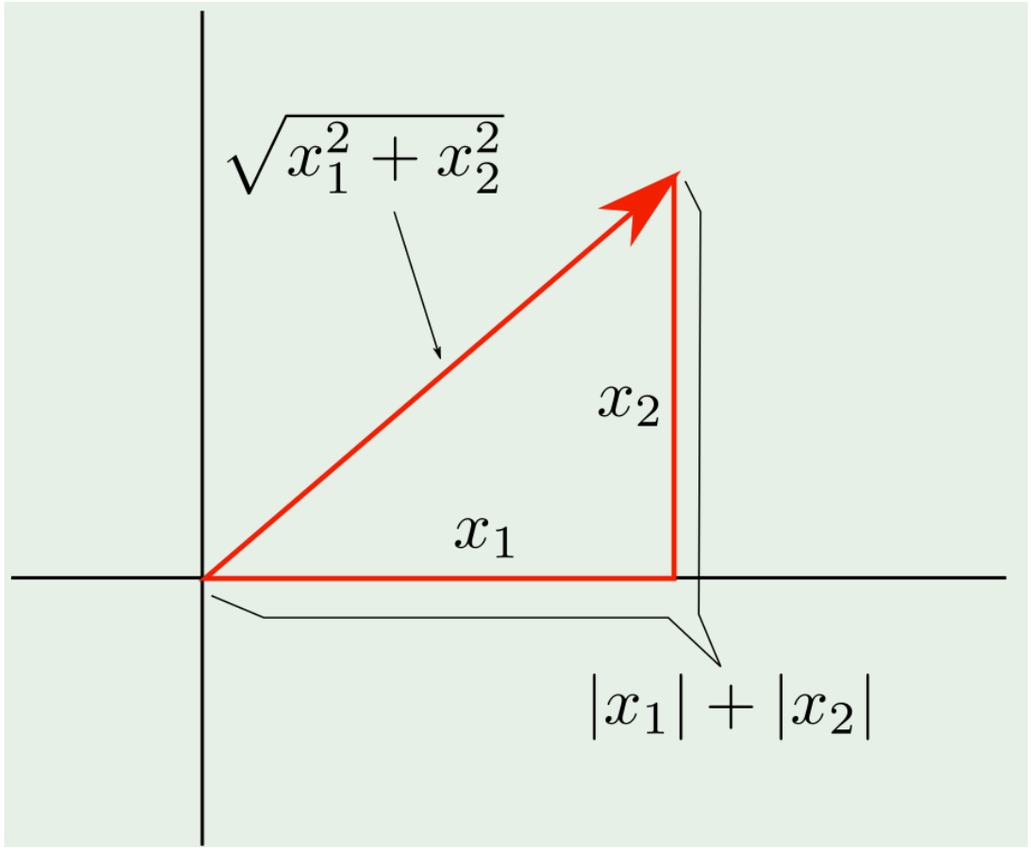
Norms

- All norms presented so far are examples of the family of ℓ_p norms, which are parametrized by a real number $p \geq 1$
  - ℓ_p-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
  - $\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^{N}\sum_{j=1}^{D} \mathrm{A}_{\mathrm{ij}}^2} = \sqrt{\mathrm{tr}(\mathbf{A}^\mathbf{T}\mathbf{A})}$

Vector norm examples

- ℓ_1-norm and ℓ_2-norm



In context: how are norms useful in ML?
Unsupervised learning

In context: choosing an appropriate norm

Manhattan vs. Euclidean

Special Matrices

- 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 $D = diag\,(d_1, d_2, \ldots, d_d)$

Why is diagonal matrix helpful?

- A^TA= elementwise squaring or all diagonal elements
- A^{-1} =1/A (elementwise)

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Special Matrices

- 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

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

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

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Multiplications

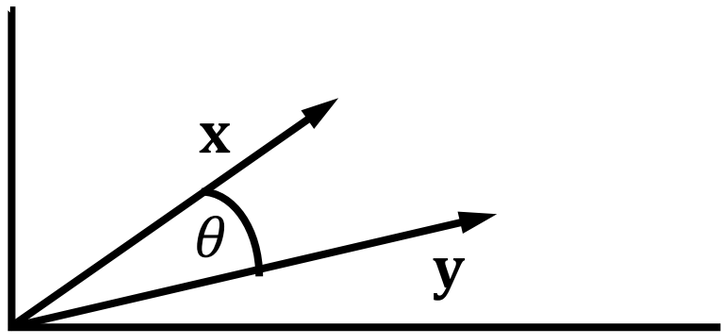
- The product of two matrices $\mathbf{A} \in \mathbb{R}^{N \times D}$ and $\mathbf{B} \in \mathbb{R}^{D \times P}$ is given by $\mathbf{C} \in \mathbb{R}^{N \times P}$, where $C_{ij} = \sum_{k=1}^{D} A_{ik} B_{kj}$

- Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{D}$, the term $\mathbf{x} \cdot \mathbf{y}$ $(\text{or } \mathbf{x}^{\mathrm{T}}\mathbf{y})$ 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,

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

Multiplications

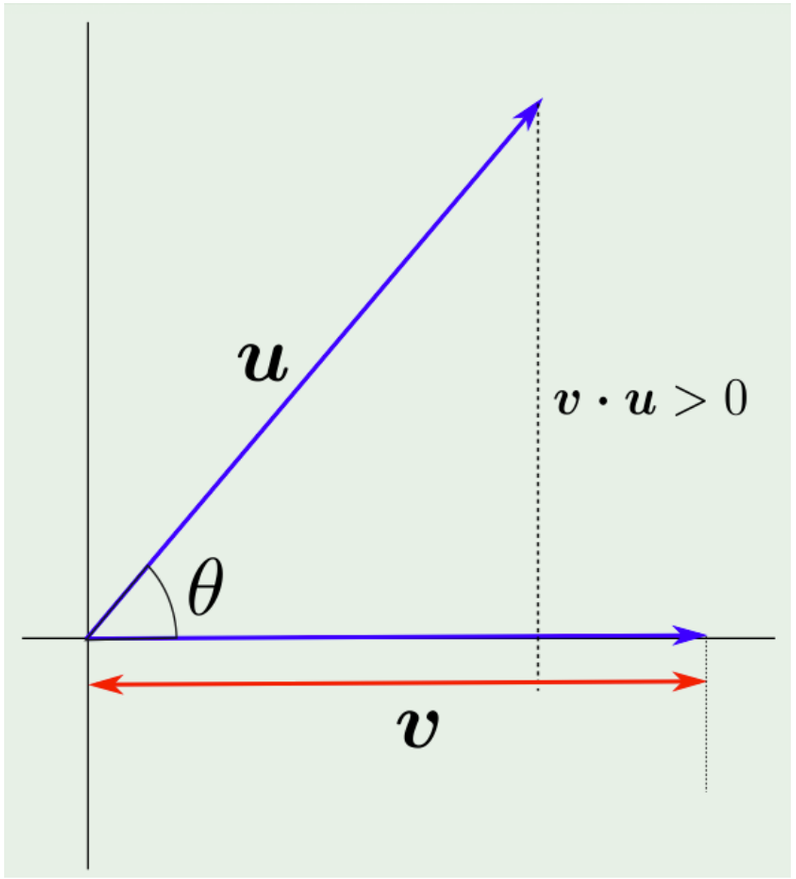
- The dot product also has a geometrical interpretation, for vectors in $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ with an angle θ between them:



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

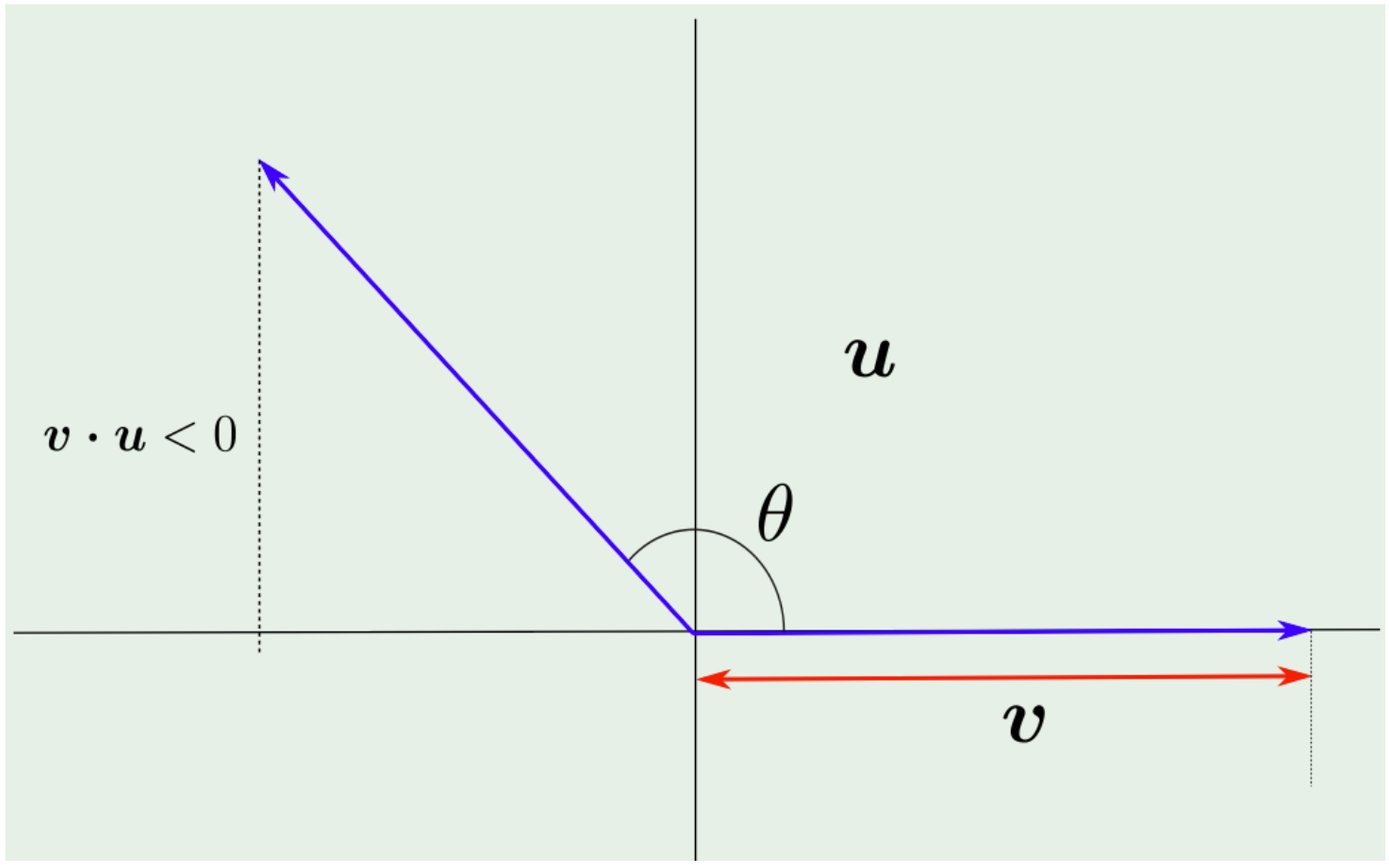
Inner product properties

- 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



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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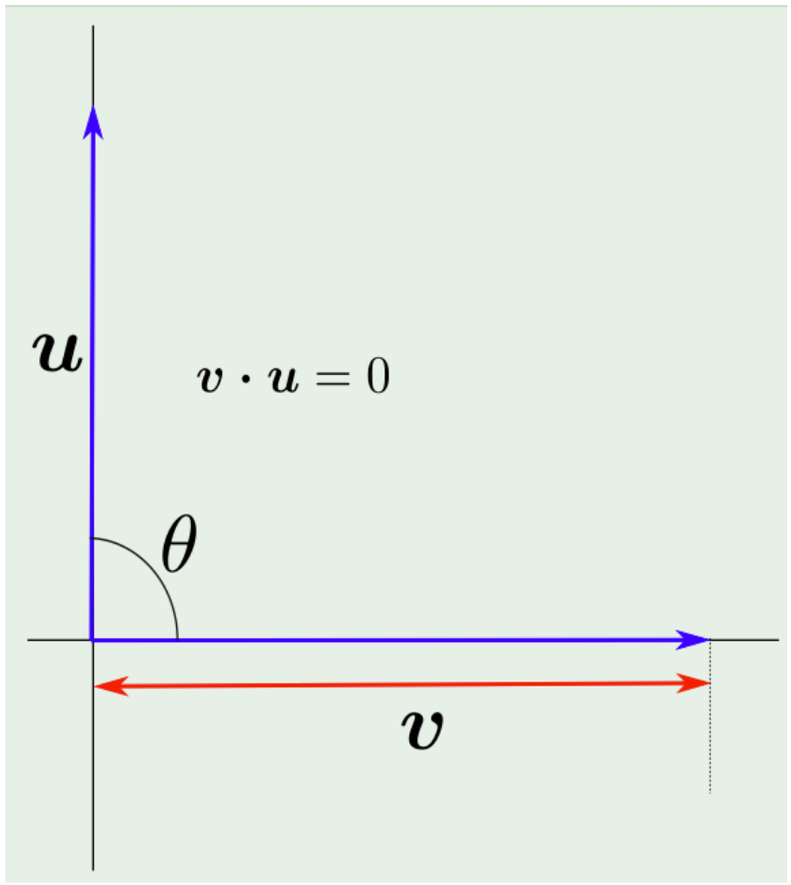

In context: how is the inner product useful in ML?
Projecting data onto a new direction

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 $\mathbf{y} \in \mathbb{R}^2$

$$\mathbf{x}\mathbf{y}^{\mathrm{T}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} [y1 \quad y2] = \begin{bmatrix} x_1 y_1 & x_1 y_2 \\ x_2 y_1 & x_2 y_2 \\ x_3 y_1 & x_3 y_2 \end{bmatrix}$$

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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

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

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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

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

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

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

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**

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

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

$$|A| = ad - bc$$

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

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

Recap

- Special Matrices
- Norms
- Matrix Multiplications
- Matrix Inversion
- Trace and Determinant

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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

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

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

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

Matrix Eigen Decomposition

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

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

- 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!

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 $X\boldsymbol{\Lambda}\boldsymbol{X}^{\mathrm{T}}$

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

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Computing Eigenvalues and Eigenvectors

- We can rewrite the original equation in the following manner

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

- 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

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

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

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 $\lambda_1=-5$

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

Eigenvector for $\lambda_2=2$

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

Can a matrix have the same eigenvalues?

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

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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Singular Value Decomposition

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

n: datapoints
d: dimensions
X is a centered matrix

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

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

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

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

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

U Σ V^T

$d < n$

Covariance matrix:

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

$$\left.\begin{aligned} \bar{X} &= U\Sigma V^T \\ C &= \frac{\bar{X}^T \bar{X}}{n} \end{aligned}\right\} \quad C = \frac{V\Sigma^T U^T U\Sigma V^T}{n} = \frac{V\Sigma^2 V^T}{n}$$

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

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

$$CV = V\Lambda$$

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

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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

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

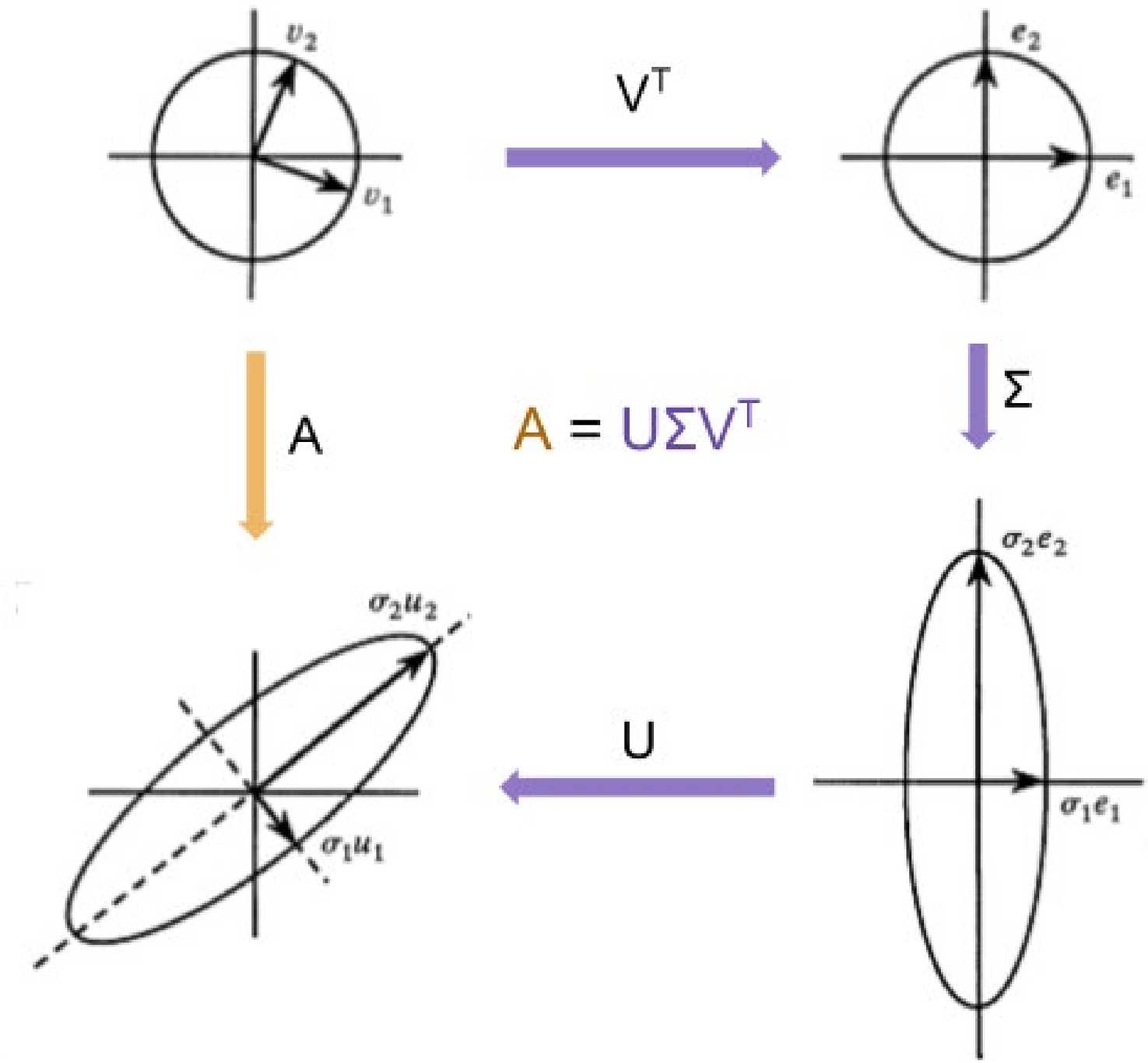

Image Credit: Kevin Binz

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 $\sigma_i$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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