Mathematics for Machine Learning

— Linear Algebra: Norms, Inner Products & Orthogonality

Joseph Chuang-Chieh Lin

Department of Computer Science & Information Engineering,
Tamkang University

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Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning.
  https://arxiv.org/abs/1912.13213

Outline

Outline

Norm

Norm

A norm on a vector space V is a function

$$\begin{aligned} \|\cdot\| : V &\mapsto \mathbb{R} \\ \mathbf{x} &\mapsto \|\mathbf{x}\| \end{aligned}$$

such that for $\lambda \in \mathbb{R}$ and $\mathbf{x}, \mathbf{y} \in V$ the following hold:

- $\|\lambda \mathbf{x}\| = |\lambda| \|\mathbf{x}\|$.
- $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$.
- $\|\mathbf{x}\| \geq 0$ and $\|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = \mathbf{0}$.

ℓ_1 norm & ℓ_2 norm

ℓ_1 norm (Manhattan Norm)

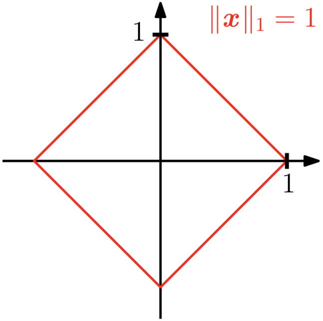
For $\mathbf{x} \in \mathbb{R}^n$,

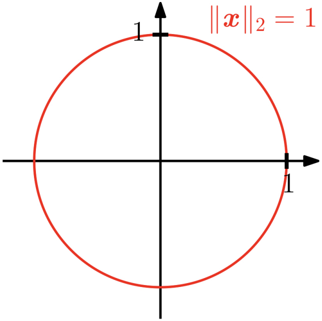
$$\|\mathbf{x}\|_1 := \sum_{i=1}^{n} |x_i|.$$

ℓ_2 norm

For $\mathbf{x} \in \mathbb{R}^n$,

$$\|\mathbf{x}\|_2 := \sqrt{\sum_{i=1}^{n} x_i^2} = \sqrt{\mathbf{x}^\top \mathbf{x}}.$$


$\|\boldsymbol{x}\|_1 = 1$
1
1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1

Outline

Dot Product

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For $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,

$$\mathbf{x}^\top \mathbf{y} = \sum_{i=1}^{n} x_i y_i.$$

General Inner Products

Bilinear Mapping f

Given a vector space V. For all $\mathbf{x}, \mathbf{y}, \mathbf{z} \in V$, $\lambda, \psi \in \mathbb{R}$, such that

$$f(\lambda\mathbf{x} + \psi\mathbf{y}, \mathbf{z}) = \lambda f(\mathbf{x}, \mathbf{z}) + \psi f(\mathbf{y}, \mathbf{z})$$
$$f(\mathbf{x}, \lambda\mathbf{y} + \psi\mathbf{z}) = \lambda f(\mathbf{x}, \mathbf{y}) + \psi f(\mathbf{x}, \mathbf{z})$$

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$$f(\lambda\mathbf{x} + \psi\mathbf{y}, \mathbf{z}) = \lambda f(\mathbf{x}, \mathbf{z}) + \psi f(\mathbf{y}, \mathbf{z}) \quad \text{(linear in the 1st argument)}$$
$$f(\mathbf{x}, \lambda\mathbf{y} + \psi\mathbf{z}) = \lambda f(\mathbf{x}, \mathbf{y}) + \psi f(\mathbf{x}, \mathbf{z}) \quad \text{(linear in the 2nd argument)}$$

Symmetric & Positive Definite (1/6)

Symmetric

Let V be a vector space and $f : V \times V \mapsto \mathbb{R}$ be a bilinear mapping. Then f is symmetric if $f(\mathbf{x}, \mathbf{y}) = f(\mathbf{y}, \mathbf{x})$.

Positive Definite

Let V be a vector space and $f : V \times V \mapsto \mathbb{R}$ be a bilinear mapping. Then f is positive definite if $\forall \mathbf{x} \in V \setminus \{\mathbf{0}\}$, we have

$$f(\mathbf{x}, \mathbf{x}) > 0 \quad \text{and} \quad f(\mathbf{0}, \mathbf{0}) = 0.$$

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Inner Product

A positive definite & symmetric bilinear mapping $f : V \times V \mapsto \mathbb{R}$ is called an inner product on V and we write $f(\mathbf{x}, \mathbf{y})$ as $\langle \mathbf{x}, \mathbf{y} \rangle$.

Symmetric & Positive Definite (2/6)

- Important in machine learning.
  - Matrix decompositions.
  - Key in defining kernels in the SVM (support vector machine).

An Exercise

Exercise

Consider $V = \mathbb{R}^2$. Define that

$$\langle \mathbf{x}, \mathbf{y} \rangle := x_1 y_1 - (x_1 y_2 + x_2 y_1) + 2 x_2 y_2.$$

Show that $\langle \cdot, \cdot \rangle$ is an inner product.

Symmetric & Positive Definite (3/6)

Consider an n-dimensional vector space V with an inner product $\langle\cdot\rangle : V \times V \mapsto \mathbb{R}$ and an ordered basis $B = (\mathbf{b}_1, \ldots, \mathbf{b}_n)$ of V.

- Assume that for $\mathbf{x}, \mathbf{y} \in V$,
  - $\mathbf{x} = \sum_{i=1}^{n} \psi_i \mathbf{b}_i$
  - $\mathbf{y} = \sum_{j=1}^{n} \lambda_j \mathbf{b}_j$

  for suitable $\psi_i, \lambda_j \in \mathbb{R}$.
- By the bilinearity of the inner product, we have

$$\langle \mathbf{x}, \mathbf{y} \rangle = \left\langle \sum_{i=1}^{n} \psi_i \mathbf{b}_i, \sum_{j=1}^{n} \lambda_j \mathbf{b}_j \right\rangle$$

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  where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are the coordinates of $\mathbf{b}$ w.r.t. the basis B.

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⋆ Note that the symmetry of the inner product implies that $\boldsymbol{A}$ is symmetric.

Example

Consider $V = \mathbb{R}^2$ with an inner product $\langle\cdot\rangle : V \times V \mapsto \mathbb{R}$ and an ordered basis $B = (\mathbf{q}_1, \mathbf{q}_2)$ of V, where $\mathbf{q}_1 = [1, 1]^\top, \mathbf{q}_2 = [1, -2]^\top$.
Compute $\langle \mathbf{x}, \mathbf{y} \rangle$, where

$$\begin{aligned} \mathbf{x} &= 2\mathbf{q}_1 + 3\mathbf{q}_2 \\ \mathbf{y} &= -\mathbf{q}_1 + 2\mathbf{q}_2 \end{aligned}$$

- $\langle \mathbf{x}, \mathbf{y} \rangle =$

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- W.r.t. the standard basis,

$$\begin{aligned} \mathbf{x} &= 5\mathbf{e}_1 - 4\mathbf{e}_2 \\ \mathbf{y} &= \mathbf{e}_1 - 5\mathbf{e}_2 \end{aligned}$$

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- W.r.t. the standard basis,

$$\begin{aligned} \mathbf{x} &= 5\mathbf{e}_1 - 4\mathbf{e}_2 \implies \hat{\mathbf{x}} = [5, -4]^\top \\ \mathbf{y} &= \mathbf{e}_1 - 5\mathbf{e}_2 \implies \hat{\mathbf{y}} = [1, -5]^\top \end{aligned}$$

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$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

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$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \implies \hat{\mathbf{x}}^\top \boldsymbol{A}\hat{\mathbf{y}} = [5, -4]\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ -5 \end{bmatrix} = 25.$$

Symmetric & Positive Definite (4/6)

The positive definiteness of the inner product implies that

$$\forall \mathbf{x} \in V \setminus \{\mathbf{0}\} : \quad \mathbf{x}^\top \boldsymbol{A}\mathbf{x} > 0.$$

Symmetric, Positive Definite Matrix

A symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ that satisfies the property:

$$\forall \mathbf{x} \in V \setminus \{\mathbf{0}\} : \quad \mathbf{x}^\top \boldsymbol{A}\mathbf{x} > 0.$$

is called symmetric, positive definite (or just positive definite).

If only $\geq$ holds, then $\boldsymbol{A}$ is called symmetric, positive semidefinite.

Example

Consider the matrices $\boldsymbol{A}_1 = \begin{bmatrix} 9 & 6 \\ 6 & 5 \end{bmatrix}$, $\boldsymbol{A}_2 = \begin{bmatrix} 9 & 6 \\ 6 & 3 \end{bmatrix}$

- $\boldsymbol{A}_1$ is positive definite (why?)

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- $\boldsymbol{A}_1$ is positive definite (why?)
- $\boldsymbol{A}_2$ is NOT positive definite (why?)

Symmetric & Positive Definite (5/6)

If $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric, positive definite, then

$$\langle \mathbf{x}, \mathbf{y} \rangle = \hat{\mathbf{x}}^\top \boldsymbol{A} \hat{\mathbf{y}}.$$

Symmetric & Positive Definite (5/6)

If $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric, positive definite, then

$$\langle \mathbf{x}, \mathbf{y} \rangle = \hat{\mathbf{x}}^\top \boldsymbol{A} \hat{\mathbf{y}}.$$

This defines an inner product w.r.t. an ordered basis B, where $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ are the coordinates of $\mathbf{x}, \mathbf{y}$ w.r.t. B.

Remark

Semidefinite Matrix

If $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric and for all $\mathbf{x}$ we have $\mathbf{x}^\top \boldsymbol{A}\mathbf{x} \geq 0$, we call $\boldsymbol{A}$ a semidefinite matrix.

Remark: If $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is not necessarily symmetric & positive definite:

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- Try $\hat{\boldsymbol{A}} := \boldsymbol{A}\boldsymbol{A}^\top$.
- $\hat{\boldsymbol{A}}$ must be semidefinite (why?).

Symmetric & Positive Definite (6/6)

The following properties hold if $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric and positive definite.

- $\text{null}(\boldsymbol{A}) = \{\mathbf{0}\}$.

Symmetric & Positive Definite (6/6)

The following properties hold if $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric and positive definite.

- $\text{null}(\boldsymbol{A}) = \{\mathbf{0}\}$.
  - Since $\mathbf{x}^\top \boldsymbol{A}\mathbf{x} > 0$ for all $\mathbf{x} > 0 \Rightarrow \boldsymbol{A}\mathbf{x} \neq \mathbf{0}$ if $\mathbf{x} \neq \mathbf{0}$.
- For the diagonal elements a_{ii} of $\boldsymbol{A}$, $a_{ii} = \mathbf{e}_i^\top \boldsymbol{A}\mathbf{e}_i > 0$.
  - $\mathbf{e}_i$: the ith vector of the standard basis of $\mathbb{R}^n$.

Outline

Remark

- Note that any inner product induces a norm:

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}.$$

Cauchy-Schwarz Inequality

For an inner product vector space $(V, \langle \cdot \rangle)$, the induced norm $\| \cdot \|$ satisfies the Cauchy-Schwarz inequality

$$|\langle \mathbf{x}, \mathbf{y} \rangle| \leq \|\mathbf{x}\| \|\mathbf{y}\|.$$

Lengths of Vectors

Example

Compute the length of a vector $\mathbf{x} = [1, 1]^\top \in \mathbb{R}^2$ using

- Dot product
- $\langle \mathbf{x}, \mathbf{y} \rangle := \mathbf{x}^\top \begin{bmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix} \mathbf{y} = x_1 y_1 - \frac{1}{2}(x_1 y_2 + x_2 y_1) + x_2 y_2.$

Distance & Metric

Distance

Consider an inner product space $(V, \langle\cdot\rangle)$. Then, the distance between $\mathbf{x}$ and $\mathbf{y}$ for $\mathbf{x}, \mathbf{y} \in V$ is

$$d(\mathbf{x}, \mathbf{y}) := \|\mathbf{x} - \mathbf{y}\| = \sqrt{\langle \mathbf{x} - \mathbf{y}, \mathbf{x} - \mathbf{y} \rangle}.$$

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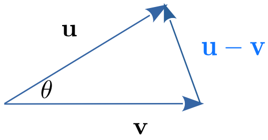
- The mapping $d : V \times V \mapsto \mathbb{R}$ for which $(\mathbf{x}, \mathbf{y})$ maps to $d(\mathbf{x}, \mathbf{y})$ is called a metric, which satisfies:
  - *positive definite*: $d(\mathbf{x}, \mathbf{y}) \geq 0$ for all $\mathbf{x}, \mathbf{y} \in V$ and $d(\mathbf{x}, \mathbf{y}) = 0$ iff $\mathbf{x} = \mathbf{y}$.
  - *symmetric*: $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}, \mathbf{y} \in V$.
  - *triangular inequality*: $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$.

Outline

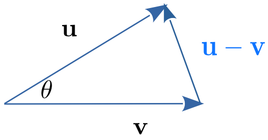
Recall from Senior High School Math



Law of Cosines

$$\|\mathbf{u}-\mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - 2\|\mathbf{u}\|\,\|\mathbf{v}\|\cos\theta$$

Recall from Senior High School Math



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Note:

$$\langle \mathbf{u}-\mathbf{v},\, \mathbf{u}-\mathbf{v}\rangle = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - 2\langle \mathbf{u},\mathbf{v}\rangle.$$

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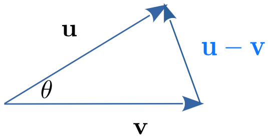
Recall from Senior High School Math



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Thus,

$$\langle \mathbf{u}, \mathbf{v}\rangle = \|\mathbf{u}\| \cdot \|\mathbf{v}\| \cos\theta.$$

Angles

Assume that $\mathbf{x} \neq \mathbf{0}, \mathbf{y} \neq \mathbf{0}$. Then by the Cauchy-Schwarz inequality,

$$-1 \leq \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|} \leq 1.$$

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Thus, there exists a unique $\theta \in [0, \pi]$, such that

$$\cos(\theta) = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|}.$$

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$$-1 \leq \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|} \leq 1.$$

Thus, there exists a unique $\theta \in [0, \pi]$, such that

$$\cos(\theta) = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|}.$$

We call θ the angle between $\mathbf{x}$ and $\mathbf{y}$.

Orthogonality

Orthogonality

- Two vectors $\mathbf{x}$ and $\mathbf{y}$ are orthogonal if and only if $\langle \mathbf{x}, \mathbf{y} \rangle = 0$.
  - We write $\mathbf{x} \perp \mathbf{y}$.
- If $\mathbf{x}$ and $\mathbf{y}$ are orthogonal and $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$, then $\mathbf{x}$ and $\mathbf{y}$ are both orthonormal.

Orthogonal Matrix

Orthogonal Matrix

A square matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is an orthogonal matrix iff its columns are orthonormal so that

$$\boldsymbol{A}\boldsymbol{A}^\top = \boldsymbol{I} = \boldsymbol{A}^\top \boldsymbol{A},$$

which implies

$$\boldsymbol{A}^{-1} = \boldsymbol{A}^\top.$$

Remark

Transformations by orthogonal matrices do NOT change the length of a vector.

$$\|\boldsymbol{A}\mathbf{x}\|^2 = (\boldsymbol{A}\mathbf{x})^\top (\boldsymbol{A}\mathbf{x}) =$$

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Let θ be the angle between $\boldsymbol{A}\mathbf{x}$ and $\boldsymbol{A}\mathbf{y}$, what is $\cos\theta$?

Outline

Orthonormal Basis

Orthonormal Basis

Consider an n-dimensional vector space V and a basis $\{\mathbf{b}_1, \ldots, \mathbf{b}_n\}$ of V. If for all $i, j = 1, \ldots, n$

$$\langle \mathbf{b}_i, \mathbf{b}_j \rangle = 0 \quad \text{for } i \neq j \tag{1}$$

$$\langle \mathbf{b}_i, \mathbf{b}_i \rangle = 1, \tag{2}$$

then the basis is called an orthonormal basis.

- Only (1) is satisfied $\Rightarrow$ orthogonal basis.

Example

- The standard basis for $\mathbb{R}^n$.
- $\mathbf{b}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \mathbf{b}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$

Outline

Inner Product of Functions

Inner Product of Functions

Given two functions $u, v : \mathbb{R} \mapsto \mathbb{R}$, the inner product of u and v can be defined as

$$\langle u, v \rangle := \int_a^b u(x)v(x)\mathrm{d}x$$

for lower and upper limits $a, b < \infty$.

Example

Example (Exercise)

- Choose $u(x) = \sin(x)$ and $v(x) = \cos(x)$.
- Define $f(x) = u(x)v(x)$.

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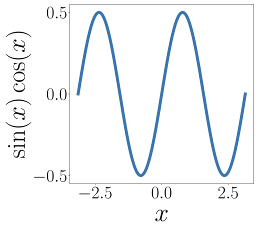

  - We can observe that $f(-x) = -f(x)$
- $\int_{-\pi}^{\pi} u(x)v(x)\mathrm{d}x = 0.$

⋆ **Note:** $\displaystyle\int \sin(x)\cos(x)\mathrm{d}x =$

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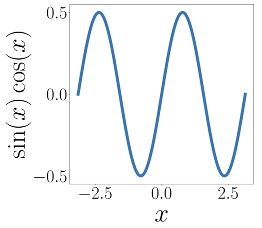

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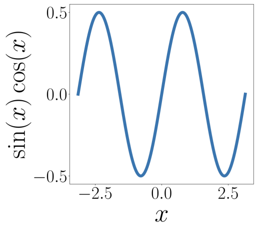

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⋆ **Note:** $\displaystyle\int \sin(x)\cos(x)\mathrm{d}x = \int u\,\mathrm{d}u = \frac{1}{2}u^2$, where $u = \sin(x)$.

Discussions