

# MATH 532: Linear Algebra

## Chapter 5: Norms, Inner Products and Orthogonality

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Spring 2015



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



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# Vector Norms

## Definition

Let  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$  ( $\mathbb{C}^n$ ). Then

$$\mathbf{x}^T \mathbf{y} = \sum_{i=1}^n x_i y_i \in \mathbb{R}$$

$$\mathbf{x}^* \mathbf{y} = \sum_{i=1}^n \bar{x}_i y_i \in \mathbb{C}$$

is called the **standard inner product** for  $\mathbb{R}^n$  ( $\mathbb{C}^n$ ).



## Definition

Let  $\mathcal{V}$  be a vector space. A function  $\|\cdot\| : \mathcal{V} \rightarrow \mathbb{R}_{\geq 0}$  is called a **norm** provided for any  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  and  $\alpha \in \mathbb{R}$

- 1  $\|\mathbf{x}\| \geq 0$  and  $\|\mathbf{x}\| = 0$  if and only if  $\mathbf{x} = \mathbf{0}$ ,
- 2  $\|\alpha\mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ ,
- 3  $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ .

## Remark

The inequality in (3) is known as the **triangle inequality**.



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- *Any inner product  $\langle \cdot, \cdot \rangle$  induces a norm via (more later)*

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*Inner products let us define angles via*

$$\cos \theta = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|}.$$

*In particular,  $\mathbf{x}, \mathbf{y}$  are orthogonal if and only if  $\mathbf{x}^T \mathbf{y} = 0$ .*

## Example

Let  $\mathbf{x} \in \mathbb{R}^n$  and consider the **Euclidean norm**

$$\begin{aligned}\|\mathbf{x}\|_2 &= \sqrt{\mathbf{x}^T \mathbf{x}} \\ &= \left( \sum_{i=1}^n x_i^2 \right)^{1/2} .\end{aligned}$$

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1 Clearly,  $\|\mathbf{x}\|_2 \geq 0$ . Also,

$$\begin{aligned}\|\mathbf{x}\|_2 = 0 &\iff \|\mathbf{x}\|_2^2 = 0 \\ \iff \sum_{i=1}^n x_i^2 = 0 &\iff x_i = 0, \quad i = 1, \dots, n, \\ \iff \mathbf{x} = \mathbf{0}.\end{aligned}$$

## Example (cont.)

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3 To establish (3) we need

## Lemma

Let  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ . Then

$$|\mathbf{x}^T \mathbf{y}| \leq \|\mathbf{x}\|_2 \|\mathbf{y}\|_2. \quad (\text{Cauchy-Schwarz-Bunyakovsky})$$

Moreover, equality holds if and only if  $\mathbf{y} = \alpha \mathbf{x}$  with

$$\alpha = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}\|_2^2}.$$

# Motivation for Proof of Cauchy–Schwarz–Bunyakovsky

As already alluded to above, the **angle**  $\theta$  between two vectors  $\mathbf{a}$  and  $\mathbf{b}$  is **related to the inner product** by





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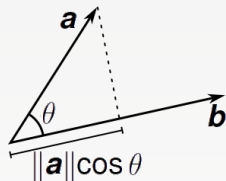
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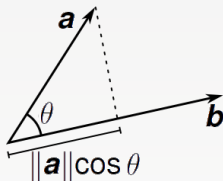
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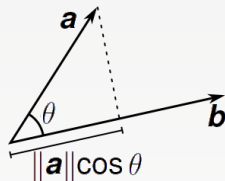
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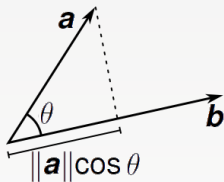
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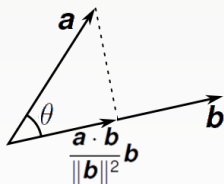
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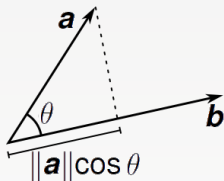
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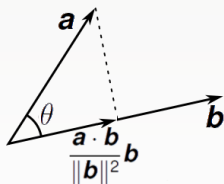
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Now, we let  $\mathbf{y} = \mathbf{a}$  and  $\mathbf{x} = \mathbf{b}$ , so that the projection of  $\mathbf{y}$  onto  $\mathbf{x}$  is given by

$$\alpha \mathbf{x}, \quad \text{where } \alpha = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}\|^2}.$$



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and the Cauchy–Schwarz–Bunyakovsky inequality follows by taking square roots.

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so that we have equality.  $\square$



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Now we just need to take square roots to have the triangle inequality.

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Let  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ . Then we have the *backward triangle inequality*

$$| \|\mathbf{x}\| - \|\mathbf{y}\| | \leq \|\mathbf{x} - \mathbf{y}\|.$$



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Together with the previous inequality we have

$$\|\|\mathbf{x}\| - \|\mathbf{y}\|\| \leq \|\mathbf{x} - \mathbf{y}\|.$$



# Other common norms



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- $\ell_1$ -norm (or taxi-cab norm, Manhattan norm):

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### Remark

In the homework you will use *Hölder's* and *Minkowski's inequalities* to show that the  $p$ -norm is a norm.

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This implies that

$$\frac{\tilde{x}_i}{\tilde{x}_1} < 1, \quad \text{for } i = k + 1, \dots, n.$$



Remark (cont.)

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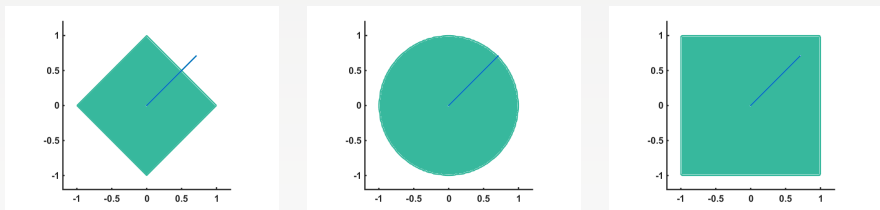
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$$\|\mathbf{x}\|_p \rightarrow |\tilde{x}_1| = \max_{1 \leq i \leq n} |x_i| = \|\mathbf{x}\|_\infty.$$



**Figure:** Unit “balls” in  $\mathbb{R}^2$  for the  $l_1$ ,  $l_2$  and  $l_\infty$  norms.

Note that  $B_1 \subseteq B_2 \subseteq B_\infty$  since, e.g.,

$$\left\| \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix} \right\|_1 = \sqrt{2}, \quad \left\| \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix} \right\|_2 = \sqrt{\frac{1}{2} + \frac{1}{2}} = 1, \quad \left\| \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix} \right\|_\infty = \frac{\sqrt{2}}{2},$$





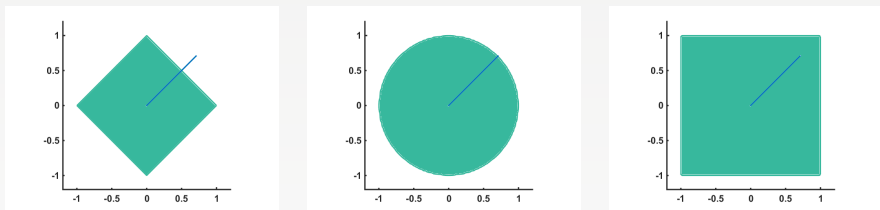


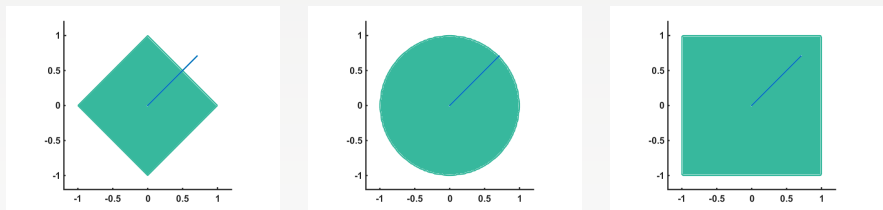
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In fact, we have in general (similar to HW)

$$\|\mathbf{x}\|_1 \geq \|\mathbf{x}\|_2 \geq \|\mathbf{x}\|_\infty, \quad \text{for any } \mathbf{x} \in \mathbb{R}^n.$$



# Norm equivalence

## Definition

Two norms  $\|\cdot\|$  and  $\|\cdot\|'$  on a vector space  $\mathcal{V}$  are called **equivalent** if there exist constants  $\alpha, \beta$  such that

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$\|\cdot\|_1$  and  $\|\cdot\|_2$  are equivalent since from above  $\|\mathbf{x}\|_1 \geq \|\mathbf{x}\|_2$  and also  $\|\mathbf{x}\|_1 \leq \sqrt{n}\|\mathbf{x}\|_2$  (see HW) so that



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### Remark

*In fact, all norms on finite-dimensional vector spaces are equivalent.*

# Outline

- 1 Vector Norms
- 2 Matrix Norms**
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



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i.e., the **Frobenius norm is just a 2-norm for the vector that contains all elements of the matrix.**



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We can **generalize this to matrices**, i.e., we have

$$\|AB\|_F \leq \|A\|_F \|B\|_F,$$

which motivates us to **require this submultiplicativity for any matrix norm**.



## Definition

A **matrix norm** is a function  $\| \cdot \|$  from the set of all real (or complex) matrices of finite size into  $\mathbb{R}_{\geq 0}$  that satisfies

- 1  $\|A\| \geq 0$  and  $\|A\| = 0$  if and only if  $A = O$  (a matrix of all zeros).
- 2  $\|\alpha A\| = |\alpha| \|A\|$  for all  $\alpha \in \mathbb{R}$ .
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## Remark

*This definition is usually **too general**. In addition to the Frobenius norm, **most useful matrix norms are induced by a vector norm**.*



# Induced matrix norms

## Theorem

Let  $\|\cdot\|_{(m)}$  and  $\|\cdot\|_{(n)}$  be vector norms on  $\mathbb{R}^m$  and  $\mathbb{R}^n$ , respectively, and let  $A$  be an  $m \times n$  matrix. Then

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Here the *vector norm could be any vector norm*. In particular, any  $p$ -norm. For example, we could have

$$\|A\|_2 = \max_{\|x\|_{2,(n)}=1} \|Ax\|_{2,(m)}.$$

To keep notation simple we often drop indices.

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since  $A_{*k} \neq O$ .



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$$\begin{aligned} \|\mathbf{A} + \mathbf{B}\| &= \max \|(\mathbf{A} + \mathbf{B})\mathbf{x}\| = \max \|\mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{x}\| \\ &\leq \max (\|\mathbf{A}\mathbf{x}\| + \|\mathbf{B}\mathbf{x}\|) \\ &= \max \|\mathbf{A}\mathbf{x}\| + \max \|\mathbf{B}\mathbf{x}\| = \|\mathbf{A}\| + \|\mathbf{B}\|. \end{aligned}$$



## Proof (cont.)

4 First note that

$$\max_{\|\mathbf{x}\|=1} \|\mathbf{A}\mathbf{x}\| = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|}$$

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$$\|\mathbf{Ax}\| \leq \|\mathbf{A}\| \|\mathbf{x}\|. \quad (1)$$

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## Remark

- One can show (see HW) that — if  $A$  is invertible —

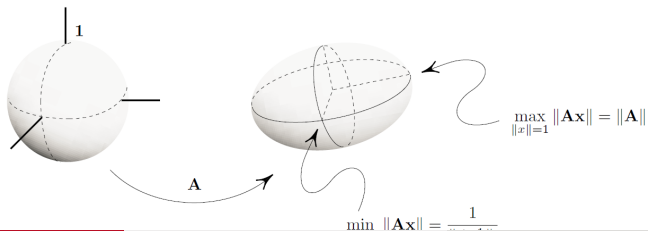
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## Remark

- One can show (see HW) that — if  $A$  is invertible —

$$\min_{\|x\|=1} \|Ax\| = \frac{1}{\|A^{-1}\|}.$$

- The induced matrix norm can be *interpreted geometrically*:
  - $\|A\|$ : the most a vector on the unit sphere can be stretched when transformed by  $A$ .
  - $\frac{1}{\|A^{-1}\|}$ : the most a vector on the unit sphere can be shrunk when transformed by  $A$ .



# Matrix 2-norm

## Theorem

Let  $A$  be an  $m \times n$  matrix. Then

$$\textcircled{1} \quad \|A\|_2 = \max_{\|x\|=1} \|Ax\|_2 = \sqrt{\lambda_{\max}}.$$

$$\textcircled{2} \quad \|A^{-1}\|_2 = \frac{1}{\min_{\|x\|=1} \|Ax\|_2} = \frac{1}{\sqrt{\lambda_{\min}}}.$$

where  $\lambda_{\max}$  and  $\lambda_{\min}$  are the *largest and smallest eigenvalues of  $A^T A$* , respectively.



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where  $\lambda_{\max}$  and  $\lambda_{\min}$  are the *largest and smallest eigenvalues of  $A^T A$* , respectively.

## Remark

We also have

$$\sqrt{\lambda_{\max}} = \sigma_1, \quad \text{the largest singular value of } A,$$

$$\sqrt{\lambda_{\min}} = \sigma_n, \quad \text{the smallest singular value of } A.$$

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We will show only (1), the largest singular value ((2) goes similarly).



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The idea is to **solve a constrained optimization problem** (as in calculus), i.e.,

$$\begin{aligned} \text{maximize} \quad & f(\mathbf{x}) = \|\mathbf{Ax}\|_2^2 = (\mathbf{Ax})^T \mathbf{Ax} \\ \text{subject to} \quad & g(\mathbf{x}) = \|\mathbf{x}\|_2^2 = \mathbf{x}^T \mathbf{x} = 1. \end{aligned}$$





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We do this by introducing a **Lagrange multiplier**  $\lambda$  and define

$$h(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda g(\mathbf{x}) = \mathbf{x}^T \mathbf{A}^T \mathbf{Ax} - \lambda \mathbf{x}^T \mathbf{x}.$$



Proof (cont.)

Necessary and sufficient (since quadratic) condition for maximum:

$$\frac{\partial h}{\partial x_i} = 0, i = 1, \dots, n, g(\mathbf{x}) = 1$$

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Together this yields

$$\mathbf{A}^T \mathbf{A} \mathbf{x} - \lambda \mathbf{x} = \mathbf{0} \quad \iff \quad (\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I}) \mathbf{x} = \mathbf{0},$$

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so that  $\lambda$  must be an eigenvalue of  $\mathbf{A}^T \mathbf{A}$  (since  $g(\mathbf{x}) = \mathbf{x}^T \mathbf{x} = 1$  ensures  $\mathbf{x} \neq \mathbf{0}$ ).



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so that

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$$\begin{aligned} \|A\|_2 &= \max_{\|\mathbf{x}\|_2=1} \|A\mathbf{x}\|_2 = \max_{\|\mathbf{x}\|_2^2=1} \|A\mathbf{x}\|_2 \\ &= \max \sqrt{\lambda} = \sqrt{\lambda_{\max}}. \end{aligned}$$



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### Remark

*The proof is a HW problem.*



# Matrix 1-norm and $\infty$ -norm

## Theorem

Let  $A$  be an  $m \times n$  matrix. Then we have

1 the *column sum norm*

$$\|A\|_1 = \max_{\|x\|_1=1} \|Ax\|_1 = \max_{j=1,\dots,n} \sum_{i=1}^m |a_{ij}|,$$

2 and the *row sum norm*

$$\|A\|_\infty = \max_{\|x\|_\infty=1} \|Ax\|_\infty = \max_{i=1,\dots,m} \sum_{j=1}^n |a_{ij}|.$$





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## Remark

We know these are norms, so what we need to do is *verify that the formulas hold*. We will show (1).

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First we look at  $\|A\mathbf{x}\|_1$ .

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Since we actually need to look at  $\|\mathbf{Ax}\|_1$  for  $\|\mathbf{x}\|_1 = 1$  we note that  $\|\mathbf{x}\|_1 = \sum_{j=1}^n |x_j|$  and therefore have

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$$\begin{aligned} \|\mathbf{Ax}\|_1 &= \sum_{i=1}^m |(\mathbf{Ax})_i| = \sum_{i=1}^m |\mathbf{A}_{i*} \mathbf{x}| = \sum_{i=1}^m \left| \sum_{j=1}^n a_{ij} x_j \right| \\ &\stackrel{\text{reg.}\Delta}{\leq} \sum_{i=1}^m \sum_{j=1}^n |a_{ij}| |x_j| \\ &= \sum_{j=1}^n \left[ |x_j| \sum_{i=1}^m |a_{ij}| \right] \leq \left[ \max_{j=1, \dots, n} \sum_{i=1}^m |a_{ij}| \right] \sum_{j=1}^n |x_j|. \end{aligned}$$

Since we actually need to look at  $\|\mathbf{Ax}\|_1$  for  $\|\mathbf{x}\|_1 = 1$  we note that  $\|\mathbf{x}\|_1 = \sum_{j=1}^n |x_j|$  and therefore have

$$\|\mathbf{Ax}\|_1 \leq \max_{j=1, \dots, n} \sum_{i=1}^m |a_{ij}|.$$

Proof (cont.)

We even have equality since for  $\mathbf{x} = \mathbf{e}_k$ , where  $k$  is the index such that  $A_{*k}$  has maximum column sum, we get



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Since  $\|\mathbf{e}_k\|_1 = 1$  we indeed have the desired formula.  $\square$





# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces**
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



## Definition

A general **inner product** in a real (complex) vector space  $\mathcal{V}$  is a **symmetric (Hermitian) bilinear form**  $\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R} (\mathbb{C})$ , i.e.,

- 1  $\langle \mathbf{x}, \mathbf{x} \rangle \in \mathbb{R}_{\geq 0}$  with  $\langle \mathbf{x}, \mathbf{x} \rangle = 0$  if and only if  $\mathbf{x} = \mathbf{0}$ .
- 2  $\langle \mathbf{x}, \alpha \mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle$  for all scalars  $\alpha$ .
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## Remark

*The following two properties (providing **bilinearity**) are implied (see HW)*

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

$$\langle \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle.$$

As before, **any** inner product induces a norm via

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In particular, we have a general **Cauchy–Schwarz–Bunyakovsky** inequality

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



## Example

①  $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y}$  (or  $\mathbf{x}^* \mathbf{y}$ ), the standard inner product for  $\mathbb{R}^n$  ( $\mathbb{C}^n$ ).

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with

$$\|f\| = \sqrt{\langle f, f \rangle} = \left( \int_a^b (f(t))^2 dt \right)^{1/2}.$$



# Parallelogram identity

In any inner product space the so-called **parallelogram identity** holds, i.e.,

$$\|\mathbf{x} + \mathbf{y}\|^2 + \|\mathbf{x} - \mathbf{y}\|^2 = 2 \left( \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 \right). \quad (2)$$





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The following theorem shows that we

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### Theorem

Let  $\mathcal{V}$  be a real vector space with norm  $\|\cdot\|$ . If the parallelogram identity (2) holds then

$$\langle \mathbf{x}, \mathbf{y} \rangle = \frac{1}{4} \left( \|\mathbf{x} + \mathbf{y}\|^2 - \|\mathbf{x} - \mathbf{y}\|^2 \right) \quad (3)$$

is an inner product on  $\mathcal{V}$ .



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Moreover,  $\langle \mathbf{x}, \mathbf{x} \rangle > 0$  if and only if  $\mathbf{x} \neq \mathbf{0}$  since  $\langle \mathbf{x}, \mathbf{x} \rangle = \|\mathbf{x}\|^2$ .



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2 **Symmetry:**

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

is clear since  $\|\mathbf{x} - \mathbf{y}\| = \|\mathbf{y} - \mathbf{x}\|$ .



Proof (cont.)

③ Additivity: The parallelogram identity implies

$$\|\mathbf{x} + \mathbf{y}\|^2 + \|\mathbf{x} + \mathbf{z}\|^2 = \frac{1}{2} \left( \|\mathbf{x} + \mathbf{y} + \mathbf{x} + \mathbf{z}\|^2 + \|\mathbf{y} - \mathbf{z}\|^2 \right). \quad (4)$$



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**Subtracting** (5) from (4) we get

$$\begin{aligned} \|\mathbf{x} + \mathbf{y}\|^2 - \|\mathbf{x} - \mathbf{y}\|^2 + \|\mathbf{x} + \mathbf{z}\|^2 - \|\mathbf{x} - \mathbf{z}\|^2 \\ = \frac{1}{2} \left( \|2\mathbf{x} + \mathbf{y} + \mathbf{z}\|^2 - \|2\mathbf{x} - \mathbf{y} - \mathbf{z}\|^2 \right). \end{aligned} \quad (6)$$

Proof (cont.)

The specific form of the polarized inner product implies

$$\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{z} \rangle = \frac{1}{4} \left( \|\mathbf{x} + \mathbf{y}\|^2 - \|\mathbf{x} - \mathbf{y}\|^2 + \|\mathbf{x} + \mathbf{z}\|^2 - \|\mathbf{x} - \mathbf{z}\|^2 \right)$$

(7)

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 &= \frac{1}{2} \left( \left\| \mathbf{x} + \frac{\mathbf{y} + \mathbf{z}}{2} \right\|^2 - \left\| \mathbf{x} - \frac{\mathbf{y} + \mathbf{z}}{2} \right\|^2 \right)
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Setting  $\mathbf{z} = \mathbf{0}$  in (7) yields

$$\langle \mathbf{x}, \mathbf{y} \rangle = 2 \left\langle \mathbf{x}, \frac{\mathbf{y}}{2} \right\rangle \tag{8}$$

since  $\langle \mathbf{x}, \mathbf{z} \rangle = 0$ .

Proof (cont.)

To summarize, we have

$$\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{z} \rangle = 2\langle \mathbf{x}, \frac{\mathbf{y} + \mathbf{z}}{2} \rangle. \quad (7)$$

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This, however, is the right-hand side of (7) so that we end up with

$$\langle \mathbf{x}, \mathbf{y} + \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{z} \rangle,$$

as desired.

## Proof (cont.)

## ② Scalar multiplication:

To show  $\langle \mathbf{x}, \alpha \mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle$  for integer  $\alpha$  we can just repeatedly apply the additivity property just proved.



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We let  $\alpha = \frac{\beta}{\gamma}$  with integer  $\beta, \gamma \neq 0$  so that

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Dividing by  $\gamma^2$  we get

$$\frac{\beta}{\gamma} \langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \frac{\beta}{\gamma} \mathbf{y} \rangle.$$



**Proof** (cont.)

Finally, for **real**  $\alpha$  we use the continuity of the norm function (see HW) which implies that our **inner product**  $\langle \cdot, \cdot \rangle$  also is **continuous**.



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Now we **take a sequence  $\{\alpha_n\}$  of rational numbers** such that  $\alpha_n \rightarrow \alpha$  for  $n \rightarrow \infty$  and have — by continuity

$$\langle \mathbf{x}, \alpha_n \mathbf{y} \rangle \rightarrow \langle \mathbf{x}, \alpha \mathbf{y} \rangle \quad \text{as } n \rightarrow \infty.$$





## Theorem

*The only vector  $p$ -norm induced by an inner product is the 2-norm.*



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## Remark

*Since many problems are more easily dealt with in inner product spaces (since we then have lengths **and** angles, see next section) the 2-norm has a clear advantage over other  $p$ -norms.*



## Proof

We know that the 2-norm does induce an inner product, i.e.,

$$\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^T \mathbf{x}}.$$



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We do this by showing that the parallelogram identity

$$\|\mathbf{x} + \mathbf{y}\|^2 + \|\mathbf{x} - \mathbf{y}\|^2 = 2 \left( \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 \right)$$

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We will do this for  $1 \leq p < \infty$ . You will work out the case  $p = \infty$  in a HW problem.



Proof (cont.)

All we need is a **counterexample**, so we take  $\mathbf{x} = \mathbf{e}_1$  and  $\mathbf{y} = \mathbf{e}_2$  so that

$$\|\mathbf{x} + \mathbf{y}\|_p^2 = \|\mathbf{e}_1 + \mathbf{e}_2\|_p^2$$



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and, similarly

$$\|\mathbf{x} - \mathbf{y}\|_p^2 = \|\mathbf{e}_1 - \mathbf{e}_2\|_p^2 = 2^{2/p}.$$

Together, the **left-hand side of the parallelogram identity** is  $2(2^{2/p}) = 2^{2/p+1}$ .



Proof (cont.)

For the right-hand side of the parallelogram identity we calculate

$$\|\mathbf{x}\|_{\rho}^2 = \|\mathbf{e}_1\|_{\rho}^2$$



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Finally, we have

$$2^{2/p+1} = 4$$





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so that the right-hand side comes out to 4.

Finally, we have

$$2^{2/p+1} = 4 \iff \frac{2}{p} + 1 = 2 \iff \frac{2}{p} = 1 \text{ or } p = 2.$$



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# Orthogonal Vectors

We will now work in a **general inner product space  $\mathcal{V}$**  with induced **norm**

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## Definition

Two vectors  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  are called **orthogonal** if

$$\langle \mathbf{x}, \mathbf{y} \rangle = 0.$$

We often use the notation  $\mathbf{x} \perp \mathbf{y}$ .



In the HW you will prove the Pythagorean theorem for the 2-norm and standard inner product  $\mathbf{x}^T \mathbf{y}$ , i.e.,

$$\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 = \|\mathbf{x} - \mathbf{y}\|^2 \iff \mathbf{x}^T \mathbf{y} = 0.$$



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$$\|\mathbf{x} - \mathbf{y}\|^2 = \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - 2\|\mathbf{x}\|\|\mathbf{y}\|\cos\theta,$$



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This motivates our general definition of angles:

### Definition

Let  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$ . The **angle** between  $\mathbf{x}$  and  $\mathbf{y}$  is defined via

$$\cos\theta = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\|\|\mathbf{y}\|}, \quad \theta \in [0, \pi].$$



# Orthonormal sets

## Definition

A set  $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\} \subseteq \mathcal{V}$  is called **orthonormal** if

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Every *orthonormal set* is *linearly independent*.

## Corollary

Every *orthonormal set of  $n$  vectors from an  $n$ -dimensional vector space  $\mathcal{V}$*  is an *orthonormal basis for  $\mathcal{V}$* .



**Proof** (of the theorem)

We want to **show linear independence**, i.e., that

$$\sum_{j=1}^n \alpha_j \mathbf{u}_j = \mathbf{0} \implies \alpha_j = 0, j = 1, \dots, n.$$

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To see this is true we **take the inner product with  $\mathbf{u}_i$** :

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Since  $i$  was arbitrary this holds for all  $i = 1, \dots, n$ , and we have linear independence.  $\square$

## Example

The standard orthonormal basis of  $\mathbb{R}^n$  is given by

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The **standard orthonormal basis** of  $\mathbb{R}^n$  is given by

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Using this basis we can express any  $\mathbf{x} \in \mathbb{R}^n$  as

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + \dots + x_n \mathbf{e}_n,$$

we get a **coordinate expansion** of  $\mathbf{x}$ .



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We therefore have proved

### Theorem

Let  $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$  be an orthonormal basis for an inner product space  $\mathcal{V}$ . Then any  $\mathbf{x} \in \mathcal{V}$  can be written as

$$\mathbf{x} = \sum_{j=1}^n \langle \mathbf{x}, \mathbf{u}_j \rangle \mathbf{u}_j.$$

This is a (finite) *Fourier expansion* with *Fourier coefficients*  $\langle \mathbf{x}, \mathbf{u}_j \rangle$ .



## Remark

The *classical* (infinite-dimensional) *Fourier series for continuous functions* on  $(-\pi, \pi)$  uses the *orthogonal* (but not yet orthonormal) *basis*

$$\{1, \sin t, \cos t, \sin 2t, \cos 2t, \dots, \}$$

and the *inner product*

$$\langle f, g \rangle = \int_{-\pi}^{\pi} f(t)g(t)dt.$$





## Example

Consider the basis

$$\mathcal{B} = \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right\}.$$

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It is **clear by inspection** that  $\mathcal{B}$  is an **orthogonal** subset of  $\mathbb{R}^3$ , i.e., using the **Euclidean inner product**, we have  $\mathbf{u}_i^T \mathbf{u}_j = 0$ ,  $i, j = 1, 2, 3$ ,  $i \neq j$ .

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This yields

$$\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$

## Example (cont.)

The Fourier expansion of  $\mathbf{x} = (1 \ 2 \ 3)^T$  is given by



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$$\begin{aligned}\mathbf{x} &= \sum_{i=1}^3 (\mathbf{x}^T \mathbf{v}_i) \mathbf{v}_i \\ &= \frac{4}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + 2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} - \frac{2}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\end{aligned}$$



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We want to convert an arbitrary basis  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  of  $\mathcal{V}$  to an orthonormal basis  $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$ .



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**Idea:** construct  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n$  successively so that  $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k\}$  is an ON basis for  $\text{span}\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$ ,  $k = 1, \dots, n$ .



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$k = 1$ :

$$\mathbf{u}_1 = \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}.$$



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In general, consider  $\{\mathbf{u}_1, \dots, \mathbf{u}_k\}$  as a given ON basis for  $\text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ .



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This vector, however is **not yet normalized**.



We now want  $\|\mathbf{u}_{k+1}\| = 1$ , i.e.,

$$\sqrt{\left\langle \frac{\mathbf{v}_{k+1}}{\langle \mathbf{u}_{k+1}, \mathbf{x}_{k+1} \rangle}, \frac{\mathbf{v}_{k+1}}{\langle \mathbf{u}_{k+1}, \mathbf{x}_{k+1} \rangle} \right\rangle} = \frac{1}{|\langle \mathbf{u}_{k+1}, \mathbf{x}_{k+1} \rangle|} \|\mathbf{v}_{k+1}\| = 1$$



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Therefore

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Since the factor  $\pm 1$  does not change the span, nor orthogonality, nor normalization we can pick the positive sign.



# Gram–Schmidt algorithm

Summarizing, we have

$$\begin{aligned}\mathbf{u}_1 &= \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}, \\ \mathbf{v}_k &= \mathbf{x}_k - \sum_{i=1}^{k-1} \langle \mathbf{u}_i, \mathbf{x}_k \rangle \mathbf{u}_i, \quad k = 2, \dots, n, \\ \mathbf{u}_k &= \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}.\end{aligned}$$



# Using matrix notation to describe Gram–Schmidt

We will assume  $\mathcal{V} \subseteq \mathbb{R}^m$  (but this also works in the complex case).  
Let

$$U_1 = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^m$$

and for  $k = 2, 3, \dots, n$  let

$$U_k = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_{k-1}) \in \mathbb{R}^{m \times k-1}.$$



Then

$$\mathbf{U}_k^T \mathbf{x}_k = \begin{pmatrix} \mathbf{u}_1^T \mathbf{x}_k \\ \mathbf{u}_2^T \mathbf{x}_k \\ \vdots \\ \mathbf{u}_{k-1}^T \mathbf{x}_k \end{pmatrix}$$



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and

$$\begin{aligned} \mathbf{U}_k \mathbf{U}_k^T \mathbf{x}_k &= (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_{k-1}) \begin{pmatrix} \mathbf{u}_1^T \mathbf{x}_k \\ \mathbf{u}_2^T \mathbf{x}_k \\ \vdots \\ \mathbf{u}_{k-1}^T \mathbf{x}_k \end{pmatrix} \\ &= \sum_{i=1}^{k-1} \mathbf{u}_i (\mathbf{u}_i^T \mathbf{x}_k) = \sum_{i=1}^{k-1} (\mathbf{u}_i^T \mathbf{x}_k) \mathbf{u}_i. \end{aligned}$$



Now, Gram–Schmidt says

$$\mathbf{v}_k = \mathbf{x}_k - \sum_{i=1}^{k-1} (\mathbf{u}_i^T \mathbf{x}_k) \mathbf{u}_i$$



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where the case  $k = 1$  is also covered by the special definition of  $\mathbf{U}_1$ .





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### Remark

$\mathbf{U}_k \mathbf{U}_k^T$  is a *projection matrix*, and  $\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^T$  is a *complementary projection*. We will cover these later.



# QR Factorization (via Gram–Schmidt)

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We want to convert the set of columns of  $A$ ,  $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\}$  to an ON basis  $\{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n\}$  of  $R(A)$ .



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From our discussion of Gram–Schmidt we know

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{\|\mathbf{a}_1\|},$$

$$\mathbf{v}_k = \mathbf{a}_k - \sum_{i=1}^{k-1} \langle \mathbf{q}_i, \mathbf{a}_k \rangle \mathbf{q}_i, \quad k = 2, \dots, n,$$

$$\mathbf{q}_k = \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}.$$



We now rewrite as follows:

$$\mathbf{a}_1 = \|\mathbf{a}_1\| \mathbf{q}_1$$

$$\mathbf{a}_k = \langle \mathbf{q}_1, \mathbf{a}_k \rangle \mathbf{q}_1 + \dots + \langle \mathbf{q}_{k-1}, \mathbf{a}_k \rangle \mathbf{q}_{k-1} + \|\mathbf{v}_k\| \mathbf{q}_k, \quad k = 2, \dots, n.$$



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Then

$$\begin{aligned} \mathbf{A} &= (\mathbf{a}_1 \quad \mathbf{a}_2 \quad \dots \quad \mathbf{a}_n) \\ &= \underbrace{(\mathbf{q}_1 \quad \mathbf{q}_2 \quad \dots \quad \mathbf{q}_n)}_{=Q} \underbrace{\begin{pmatrix} r_{11} & \langle \mathbf{q}_1, \mathbf{a}_2 \rangle & \dots & \langle \mathbf{q}_1, \mathbf{a}_n \rangle \\ & r_{22} & \dots & \langle \mathbf{q}_2, \mathbf{a}_n \rangle \\ & & \ddots & \vdots \\ \mathbf{0} & & & r_{nn} \end{pmatrix}}_{=R} \end{aligned}$$

and we have the **reduced QR factorization of A**.



## Remark

- The matrix  $Q$  is  $m \times n$  with *orthonormal columns*
- The matrix  $R$  is  $n \times n$  *upper triangular* with positive diagonal entries.
- The reduced QR factorization is *unique* (see HW).





## Example

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$$\Rightarrow \mathbf{q}_2 = \frac{\mathbf{v}_2}{\|\mathbf{v}_2\|} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

## Example (cont.)

$$\mathbf{v}_3 = \mathbf{a}_3 - (\mathbf{q}_1^T \mathbf{a}_3) \mathbf{q}_1 - (\mathbf{q}_2^T \mathbf{a}_3) \mathbf{q}_2$$

with

$$\mathbf{q}_1^T \mathbf{a}_3 = \frac{1}{\sqrt{2}} = r_{13}, \quad \mathbf{q}_2^T \mathbf{a}_3 = 0 = r_{23}$$

Thus

$$\mathbf{v}_3 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} - \frac{1}{\sqrt{2}\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - 0 = \frac{1}{2} \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}, \quad \|\mathbf{v}_3\| = \frac{\sqrt{6}}{2} = r_{33}$$

So

$$\mathbf{q}_3 = \frac{\mathbf{v}_3}{\|\mathbf{v}_3\|} = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}$$

## Example (cont.)

Together we have

$$Q = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \end{pmatrix}, \quad R = \begin{pmatrix} \sqrt{2} & \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \sqrt{3} & 0 \\ 0 & 0 & \sqrt{6} \end{pmatrix}$$



# Solving linear systems with the QR factorization

Recall the use of the LU factorization to solve  $A\mathbf{x} = \mathbf{b}$ .

Now,  $A = QR$  implies

$$A\mathbf{x} = \mathbf{b} \iff QR\mathbf{x} = \mathbf{b}.$$

In the special case of a nonsingular  $n \times n$  matrix  $A$  the matrix  $Q$  is also  $n \times n$  with ON columns so that

$$Q^{-1} = Q^T \quad (\text{since } Q^T Q = I)$$

and

$$QR\mathbf{x} = \mathbf{b} \iff R\mathbf{x} = Q^T \mathbf{b}.$$





Therefore we solve  $A\mathbf{x} = \mathbf{b}$  by the following steps:

- 1 Compute  $A = QR$ .
- 2 Compute  $\mathbf{y} = Q^T \mathbf{b}$ .
- 3 Solve the upper triangular system  $R\mathbf{x} = \mathbf{y}$ .

### Remark

*This procedure is comparable to the three-step LU solution procedure.*



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Consider  $\mathbf{Ax} = \mathbf{b}$  with  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\text{rank}(\mathbf{A}) = n$



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Consider  $A\mathbf{x} = \mathbf{b}$  with  $A \in \mathbb{R}^{m \times n}$  and  $\text{rank}(A) = n$  (so that a **unique least squares solution exists**).



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$$A^T A \mathbf{x} = A^T \mathbf{b}.$$

Using the QR factorization of  $A$  this becomes

$$(QR)^T QR \mathbf{x} = (QR)^T \mathbf{b}$$



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$$\begin{aligned} (\mathbf{QR})^T \mathbf{QRx} &= (\mathbf{QR})^T \mathbf{b} \\ \iff \mathbf{R}^T \underbrace{\mathbf{Q}^T \mathbf{Q}}_{=\mathbf{I}} \mathbf{Rx} &= \mathbf{R}^T \mathbf{Q}^T \mathbf{b} \end{aligned}$$



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Consider  $\mathbf{Ax} = \mathbf{b}$  with  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\text{rank}(\mathbf{A}) = n$  (so that a **unique least squares solution exists**).

We know that the least squares solution is given by the solution of the **normal equations**

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Now  $\mathbf{R}$  is **upper triangular with positive diagonal and therefore invertible**. Therefore solving the normal equations corresponds to solving (cf. the previous discussion)

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## Remark

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## Summary

The QR factorization provides a simple and efficient way to solve least squares problems.

The ill-conditioned matrix  $\mathbf{A}^T\mathbf{A}$  is *never computed*.

If it is required, then it can be computed from R as  $\mathbf{R}^T\mathbf{R}$  (in fact, this is the *Cholesky factorization*) of  $\mathbf{A}^T\mathbf{A}$ .



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**Idea:** rearrange the order of calculation, i.e., write the projection matrices

$$U_k U_k^T = \sum_{i=1}^{k-1} \mathbf{u}_i \mathbf{u}_i^T$$

as a **sum of rank-1 projections**.





# MGS Algorithm

$$k=1: \mathbf{u}_1 \leftarrow \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}, \quad \mathbf{u}_j \leftarrow \mathbf{x}_j, \quad j = 2, \dots, n$$

for  $k = 2 : n$

$$\mathbf{E}_k = \mathbf{I} - \mathbf{u}_{k-1} \mathbf{u}_{k-1}^T$$

for  $j = k, \dots, n$

$$\mathbf{u}_j \leftarrow \mathbf{E}_k \mathbf{u}_j$$

$$\mathbf{u}_k \leftarrow \frac{\mathbf{u}_k}{\|\mathbf{u}_k\|}$$



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- Most stable implementations of the QR factorization use *Householder reflections* or *Givens rotations* (more later).
- Householder reflections are also more efficient than MGS.



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices**
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



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A real (complex)  $n \times n$  matrix is called **orthogonal** (**unitary**) if its columns form an orthonormal basis for  $\mathbb{R}^n$  ( $\mathbb{C}^n$ ).



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Let  $U$  be an orthogonal  $n \times n$  matrix. Then

- 1  $U$  has orthonormal rows.
- 2  $U^{-1} = U^T$ .
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Analogous properties for unitary matrices are formulated and proved in [Mey00].



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1 Therefore the statement about orthonormal rows follows from

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so that  $\mathbf{u}_i^T \mathbf{u}_j = 0$  for  $i \neq j$  and the *columns of  $\mathbf{U}$  are orthogonal*.



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- **Permutation matrices are orthogonal**, e.g.,

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- An orthogonal matrix can be viewed as a unitary matrix, but **a unitary matrix may not be orthogonal**. For example for

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ -1 & i \end{pmatrix}$$

we have  $A^* A = AA^* = I$ , but  $A^T A \neq I \neq AA^T$ .

# Elementary Orthogonal Projectors

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A matrix  $Q$  of the form

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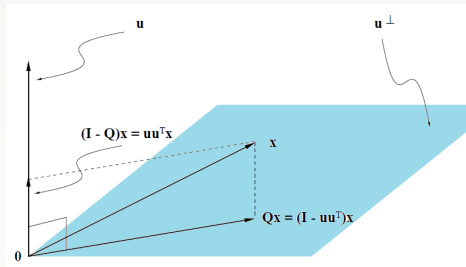


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$$\mathbf{x} = (\mathbf{I} - \mathbf{Q})\mathbf{x} + \mathbf{Q}\mathbf{x}$$

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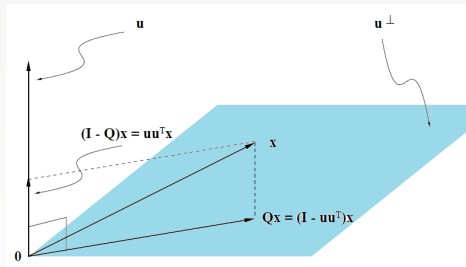
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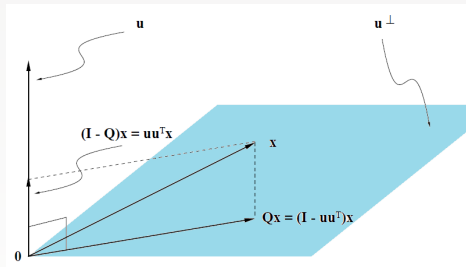
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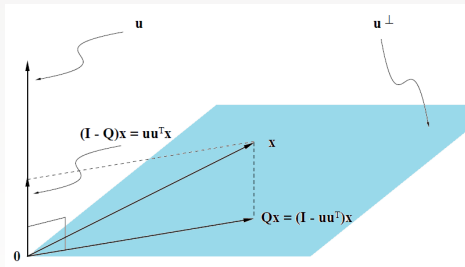
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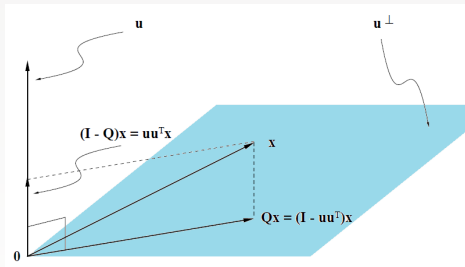
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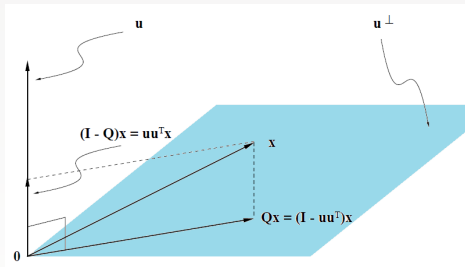
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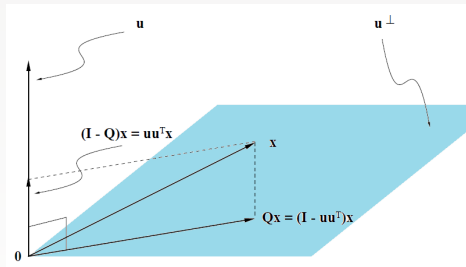
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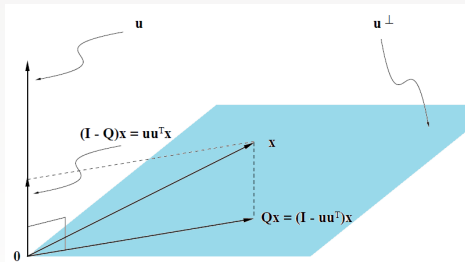
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Also note that  $\|(\mathbf{u}^T \mathbf{x})\mathbf{u}\| = |\mathbf{u}^T \mathbf{x}| \underbrace{\|\mathbf{u}\|_2}_{=1}$ , so that  $|\mathbf{u}^T \mathbf{x}|$  is the length of the orthogonal projection of  $\mathbf{x}$  onto  $\text{span}\{\mathbf{u}\}$ .



# Summary

- $(I - Q)\mathbf{x} \in \text{span}\{\mathbf{u}\}$ , so

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Above we assumed that  $\|\mathbf{u}\|_2 = 1$ .

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For an *arbitrary vector*  $\mathbf{v}$  we get a unit vector  $\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|_2} = \frac{\mathbf{v}}{\sqrt{\mathbf{v}^T \mathbf{v}}}$ .

Therefore, for general  $\mathbf{v}$

- $P_{\mathbf{v}} = \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T \mathbf{v}}$  is a *projection onto*  $\text{span}\{\mathbf{v}\}$ .



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# Elementary Reflections

## Definition

Let  $\mathbf{v} (\neq \mathbf{0}) \in \mathbb{R}^n$ . Then

$$R = I - 2 \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$$

is called the **elementary** (or **Householder**) **reflector** about  $\mathbf{v}^\perp$ .

## Remark

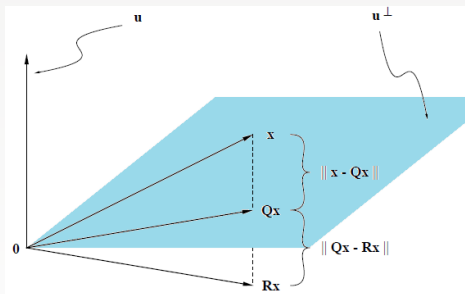
For  $\mathbf{u} \in \mathbb{R}^n$  with  $\|\mathbf{u}\|_2 = 1$  we have

$$R = I - 2\mathbf{u}\mathbf{u}^T.$$



## Geometric interpretation

Consider  $\|\mathbf{u}\|_2 = 1$ , and note that  $Q\mathbf{x} = (I - \mathbf{u}\mathbf{u}^T)\mathbf{x}$  is the orthogonal projection of  $\mathbf{x}$  onto  $\mathbf{u}^\perp$  as above.

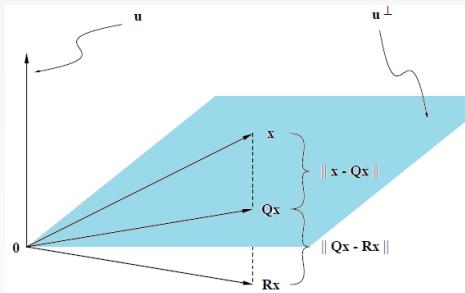


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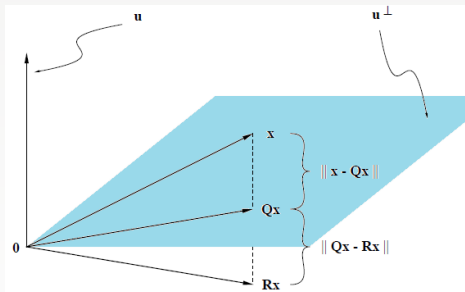


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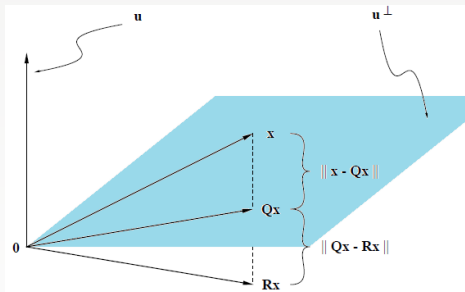


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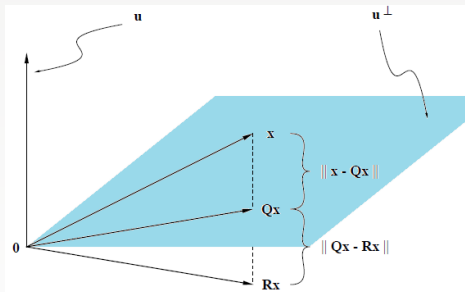


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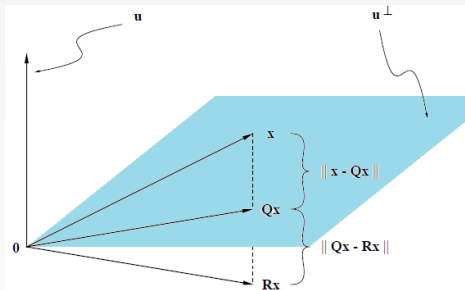
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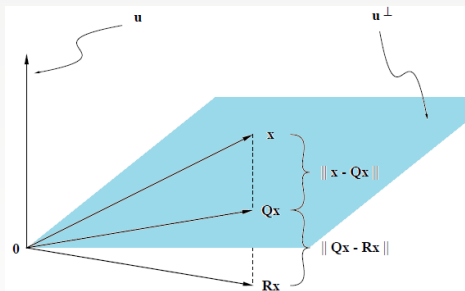
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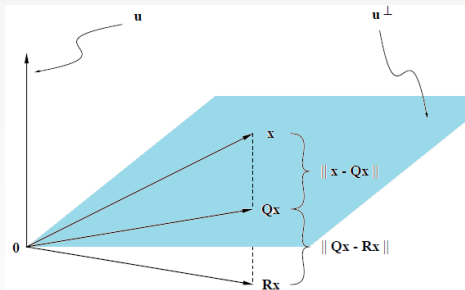
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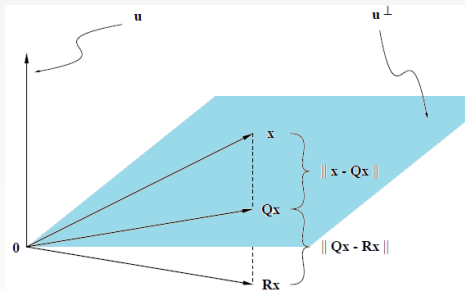
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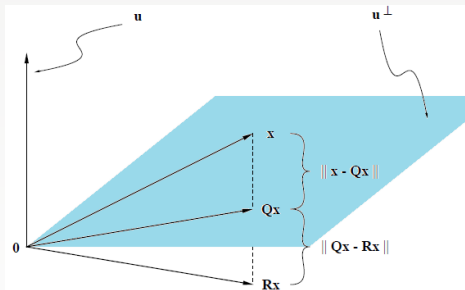
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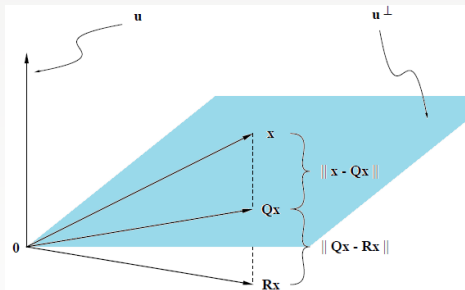
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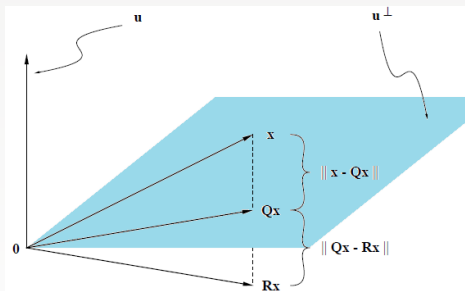
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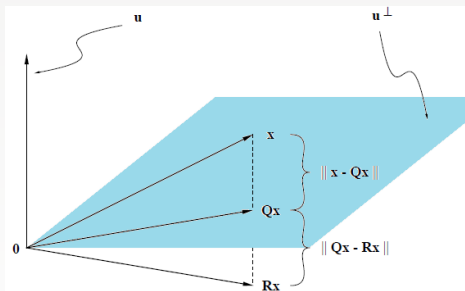
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Together,  $R\mathbf{x}$  is the reflection of  $\mathbf{x}$  about  $\mathbf{u}^\perp$ .





# Properties of elementary reflections

## Theorem

Let  $R$  be an elementary reflector. Then

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## Remark

However, *these properties do not characterize a reflection*, i.e., an orthogonal, symmetric and involutory matrix is not necessarily a reflection (see HW).



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## Reflection of $\mathbf{x}$ onto $\mathbf{e}_1$

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Our **Householder reflection** was defined as

$$R = I - 2 \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$$

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### Remark

*These special reflections are used in the Householder variant of the QR factorization. For optimal numerical stability of real matrices one lets  $\mp\mu = \text{sign}(x_1)$ .*

**Remark**

Since  $R^2 = I$  ( $R^{-1} = R$ ) we have — whenever  $\|\mathbf{x}\|_2 = 1$  —

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Thus, this allows us to construct an ON basis for  $\mathbb{R}^n$  that contains  $\mathbf{x}$  (see example in [Mey00]).



# Rotations

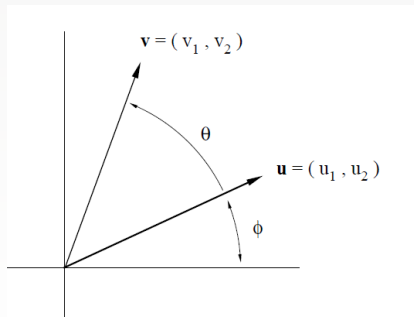
We give only a brief overview (more details can be found in [Mey00]).

We begin in  $\mathbb{R}^2$  and look for a **matrix representation of the rotation of a vector  $\mathbf{u}$  into another vector  $\mathbf{v}$** , counterclockwise by an angle  $\theta$ :

Here

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \|\mathbf{u}\| \cos \phi \\ \|\mathbf{u}\| \sin \phi \end{pmatrix} \quad (10)$$

$$\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \|\mathbf{v}\| \cos(\phi + \theta) \\ \|\mathbf{v}\| \sin(\phi + \theta) \end{pmatrix} \quad (11)$$



We use the trigonometric identities

$$\cos(A + B) = \cos A \cos B - \sin A \sin B$$

$$\sin(A + B) = \sin A \cos B + \sin B \cos A$$

with  $A = \phi$ ,  $B = \theta$  and  $\|\mathbf{v}\| = \|\mathbf{u}\|$  to get

$$\begin{aligned} \mathbf{v} &\stackrel{(11)}{=} \begin{pmatrix} \|\mathbf{v}\| \cos(\phi + \theta) \\ \|\mathbf{v}\| \sin(\phi + \theta) \end{pmatrix} \\ &= \begin{pmatrix} \|\mathbf{u}\| (\cos \phi \cos \theta - \sin \phi \sin \theta) \\ \|\mathbf{u}\| (\sin \phi \cos \theta + \sin \theta \cos \phi) \end{pmatrix} \end{aligned}$$



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where  $\mathbf{P}$  is the **rotation matrix**.



## Remark

- *Note that*

$$P^T P = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$





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- $P^T$  is also a rotation matrix (by an angle  $-\theta$ ).



Rotations about a coordinate axis in  $\mathbb{R}^3$  are very similar. Such rotations are referred to as **plane rotations**.



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For example, **rotation about the x-axis** (in the yz-plane) is accomplished with

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Rotation about the y and z-axes is done analogously.



We can use the same ideas for **plane rotations in higher dimensions**.









Usually we set

$$c = \frac{x_i}{\sqrt{x_i^2 + x_j^2}}, \quad s = \frac{x_j}{\sqrt{x_i^2 + x_j^2}}$$

since then for  $\mathbf{x} = (x_1 \ \cdots \ x_n)^T$

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This shows that  $P_{ij}$  zeros the  $j^{\text{th}}$  component of  $\mathbf{x}$ .



Note that  $\frac{x_i^2 + x_j^2}{\sqrt{x_i^2 + x_j^2}} = \sqrt{x_i^2 + x_j^2}$  so that repeatedly applying Givens rotations  $P_{ij}$  with the same  $i$ , but different values of  $j$  will zero out all but the  $i^{\text{th}}$  component of  $\mathbf{x}$ , and that component will become  $\sqrt{x_1^2 + \dots + x_n^2} = \|\mathbf{x}\|_2$ .



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Therefore, the sequence

$$P = P_{in} \cdots P_{i,i+1} P_{i,i-1} \cdots P_{i1}$$

of Givens rotations rotates the vector  $\mathbf{x} \in \mathbb{R}^n$  onto  $\mathbf{e}_i$ , i.e.,

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Moreover, the matrix  $P$  is orthogonal.



## Remark

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- *Givens rotations* can be used as an *alternative to Householder reflections* to construct a QR factorization.
- *Householder reflections* are in general more efficient, but *for sparse matrices Givens rotations are more efficient* because they can be applied more selectively.



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction**
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



# Orthogonal Reduction

Recall the form of **LU factorization** (Gaussian elimination):

$$T_{n-1} \cdots T_2 T_1 A = U,$$

where  $T_k$  are **lower triangular** and **U is upper triangular**, i.e., we have a **triangular reduction**.



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For the **QR factorization** we will use **orthogonal Householder reflectors**  $R_k$  to get

$$R_{n-1} \cdots R_2 R_1 A = T,$$

where  $T$  is **upper triangular**, i.e., we have an **orthogonal reduction**.



Recall Householder reflectors

$$R = I - 2 \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}, \quad \text{with } \mathbf{v} = \mathbf{x} \pm \mu\|\mathbf{x}\|\mathbf{e}_1,$$

so that

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Now we explain how to use these Householder reflectors to convert an  $m \times n$  matrix  $A$  to an upper triangular matrix of the same size, i.e., how to do a full QR factorization.



Apply Householder reflector to the first column of  $A$ :

$$\begin{aligned}
 R_1 A_{*1} &= \left( I - 2 \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} \right) A_{*1} && \text{with } \mathbf{v} = A_{*1} \pm \|A_{*1}\| \mathbf{e}_1 \\
 &= \mp \|A_{*1}\| \mathbf{e}_1 = \begin{pmatrix} t_{11} \\ 0 \\ \vdots \\ 0 \end{pmatrix}
 \end{aligned}$$



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$$= \mp \|A_{*1}\| \mathbf{e}_1 = \begin{pmatrix} t_{11} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Then,  $R_1$  applied to all of  $A$  yields

$$R_1 A = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1n} \\ 0 & * & \cdots & * \\ \vdots & \vdots & & \vdots \\ 0 & * & \cdots & * \end{pmatrix}$$





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Next, we apply the same idea to  $A_2$ , i.e., we let

$$R_2 = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \hat{R}_2 \end{pmatrix}$$

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We continue the process until we get an upper triangular matrix, i.e.,

$$\underbrace{R_n \cdots R_2 R_1}_=P A = \begin{pmatrix} t_{11} & & * \\ & \ddots & \vdots \\ 0 & & t_{nn} \\ & 0 & \end{pmatrix} \quad \text{whenever } m > n$$



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Since each  $R_k$  is orthogonal (unitary for complex A) we have

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$$A = QR \quad (Q = P^T, R = T)$$





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- This is similar to obtaining the QR factorization via MGS, but now  $Q$  is orthogonal (square) and  $R$  is rectangular.
- This gives us the *full QR factorization*, whereas MGS gave us the *reduced QR factorization* (with  $m \times n$   $Q$  and  $n \times n$   $R$ ).



## Example

We use Householder reflections to find the QR factorization (where  $R$  has positive diagonal elements) of

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Thus we take the  $\pm$  sign as “ $-$ ” so that  $t_{11} = \sqrt{2} > 0$ .

## Example ((cont.))

To find  $R_1 A$  we can either compute  $R_1$  using the formula above and then compute the matrix-matrix product, or — **more cheaply** — note that

$$R_1 \mathbf{x} = \left( I - 2 \frac{\mathbf{v}_1 \mathbf{v}_1^T}{\mathbf{v}_1^T \mathbf{v}_1} \right) \mathbf{x} = \mathbf{x} - 2 \mathbf{v}_1^T \mathbf{x} \frac{\mathbf{v}_1}{\mathbf{v}_1^T \mathbf{v}_1},$$

so that we can **compute**  $\mathbf{v}_1^T A_{*j}$ ,  $j = 2, 3$ , instead of the full  $R_1$ .

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so that we can **compute  $\mathbf{v}_1^T A_{*j}$ ,  $j = 2, 3$** , instead of the full  $R_1$ .

$$\mathbf{v}_1^T A_{*2} = (1 - \sqrt{2}) \cdot 2 + 0 \cdot 1 + 1 \cdot 0$$

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### Example ((cont.))

To find  $R_1 A$  we can either compute  $R_1$  using the formula above and then compute the matrix-matrix product, or — **more cheaply** — note that

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Also

$$2 \frac{\mathbf{v}_1}{\mathbf{v}_1^T \mathbf{v}_1} = \frac{1}{2 - \sqrt{2}} \begin{pmatrix} 1 - \sqrt{2} \\ 0 \\ 1 \end{pmatrix}$$

Example ((cont.))

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$$R_1 A = \begin{pmatrix} \sqrt{2} & \sqrt{2} & \frac{\sqrt{2}}{2} \\ 0 & 1 & 1 \\ 0 & \sqrt{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 1 \\ \sqrt{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$$

## Example ((cont.))

Next

$$\hat{R}_2 \mathbf{x} = \mathbf{x} - 2\mathbf{v}_2^T \mathbf{x} \frac{\mathbf{v}_2}{\mathbf{v}_2^T \mathbf{v}_2} \quad \text{with } \mathbf{v}_2 = (\mathbf{A}_2)_{*1} - \|(\mathbf{A}_2)_{*1}\| \mathbf{e}_1$$

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$$\hat{R}_2 (\mathbf{A}_2)_{*1} = \begin{pmatrix} \sqrt{3} \\ 0 \end{pmatrix}, \quad \hat{R}_2 (\mathbf{A}_2)_{*2} = \begin{pmatrix} 0 \\ \frac{\sqrt{6}}{2} \end{pmatrix}$$

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Using  $R_2 = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \hat{R}_2 \end{pmatrix}$  we get

$$\underbrace{R_2 R_1}_{=P} A = \begin{pmatrix} \sqrt{2} & \sqrt{2} & \frac{\sqrt{2}}{2} \\ 0 & \sqrt{3} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{2} \end{pmatrix} = T$$

## Remark

- *As mentioned earlier, the factor  $R$  of the QR factorization is given by the matrix  $T$ .*
- *The factor  $Q = P^T$  is not explicitly given in the example.*





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- *As mentioned earlier, the factor  $R$  of the QR factorization is given by the matrix  $T$ .*
- *The factor  $Q = P^T$  is not explicitly given in the example.*
- *One could also obtain the same answer using Givens rotations (compare [Mey00, Example 5.7.2]).*



## Theorem

Let  $A$  be an  $n \times n$  nonsingular real matrix. Then the factorization

$$A = QR$$

with  $n \times n$  orthogonal matrix  $Q$  and  $n \times n$  upper triangular matrix  $R$  with positive diagonal entries is *unique*.



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## Remark

*In this  $n \times n$  case the reduced and full QR factorizations coincide, i.e., the results obtained via Gram–Schmidt, Householder and Givens should be identical.*



## Proof

Assume we have two QR factorizations

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Since  $U$  is upper triangular

$$U_{*1} = \begin{pmatrix} u_{11} \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$



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Moreover, since  $U$  is orthogonal  $u_{11} = 1$ .

Proof (cont.)

Next,

$$U_{*1}^T U_{*2} = (1 \quad 0 \quad \dots \quad 0) \begin{pmatrix} u_{12} \\ u_{22} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$



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Comparing all the other pairs of columns of  $U$  shows that  $U = I$ , and therefore



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## Recommendations (so far) for solution of $Ax = b$

- 1 If  $A$  is square and nonsingular, then use LU factorization with partial pivoting. This is stable for most practical problems and requires  $\mathcal{O}(\frac{n^3}{3})$  operations.





## Recommendations (so far) for solution of $A\mathbf{x} = \mathbf{b}$

- 1 If  $A$  is square and nonsingular, then use LU factorization with partial pivoting. This is stable for most practical problems and requires  $\mathcal{O}(\frac{n^3}{3})$  operations.
- 2 To find a least square solution, use QR factorization:

$$A\mathbf{x} = \mathbf{b} \iff QR\mathbf{x} = \mathbf{b} \iff R\mathbf{x} = Q^T\mathbf{b}.$$

Usually the reduced QR factorization is all that's needed.



Even though (for square nonsingular  $A$ ) the Gram–Schmidt, Householder and Givens versions of the QR factorization are equivalent (due to the uniqueness theorem), we have — for general  $A$  — that

- classical GS is **not stable**,
- modified GS is **stable for least squares**, but unstable for QR (since it has problems maintaining orthogonality),
- Householder and Givens are **stable**, both for least squares and QR



## Computational cost (for $n \times n$ matrices)

- LU with partial pivoting:  $\mathcal{O}(\frac{n^3}{3})$
- Gram–Schmidt:  $\mathcal{O}(n^3)$
- Householder:  $\mathcal{O}(\frac{2n^3}{3})$
- Givens:  $\mathcal{O}(\frac{4n^3}{3})$

Householder reflections are often the preferred method since they provide both stability and also decent efficiency.



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces**
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections



# Complementary Subspaces

## Definition

Let  $\mathcal{V}$  be a vector space and  $\mathcal{X}, \mathcal{Y} \subseteq \mathcal{V}$  be **subspaces**.  $\mathcal{X}$  and  $\mathcal{Y}$  are called **complementary** provided

$$\mathcal{V} = \mathcal{X} + \mathcal{Y} \quad \text{and} \quad \mathcal{X} \cap \mathcal{Y} = \{\mathbf{0}\}.$$

In this case,  $\mathcal{V}$  is also called the **direct sum** of  $\mathcal{X}$  and  $\mathcal{Y}$ , and we write

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## Example

- Any **two lines** through the origin in  $\mathbb{R}^2$  are complementary.
- Any **plane** through the origin in  $\mathbb{R}^3$  is complementary to any line through the origin not contained in the plane.
- Two planes through the origin in  $\mathbb{R}^3$  are **not complementary** since they must intersect in a line.

## Theorem

Let  $\mathcal{V}$  be a vector space, and  $\mathcal{X}, \mathcal{Y} \subseteq \mathcal{V}$  be subspaces with bases  $\mathcal{B}_\mathcal{X}$  and  $\mathcal{B}_\mathcal{Y}$ . The following are equivalent:

- 1  $\mathcal{V} = \mathcal{X} \oplus \mathcal{Y}$ .
- 2 For every  $\mathbf{v} \in \mathcal{V}$  there exist **unique**  $\mathbf{x} \in \mathcal{X}$  and  $\mathbf{y} \in \mathcal{Y}$  such that  $\mathbf{v} = \mathbf{x} + \mathbf{y}$ .
- 3  $\mathcal{B}_\mathcal{X} \cap \mathcal{B}_\mathcal{Y} = \{\}$  and  $\mathcal{B}_\mathcal{X} \cup \mathcal{B}_\mathcal{Y}$  is a basis for  $\mathcal{V}$ .



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## Proof.

See [Mey00].





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See [Mey00]. □

## Definition

Suppose  $\mathcal{V} = \mathcal{X} \oplus \mathcal{Y}$ , i.e., any  $\mathbf{v} \in \mathcal{V}$  can be uniquely decomposed as  $\mathbf{v} = \mathbf{x} + \mathbf{y}$ . Then

- 1  $\mathbf{x}$  is called the **projection of  $\mathbf{v}$  onto  $\mathcal{X}$  along  $\mathcal{Y}$** .
- 2  $\mathbf{y}$  is called the **projection of  $\mathbf{v}$  onto  $\mathcal{Y}$  along  $\mathcal{X}$** .

# Properties of projectors

## Theorem

Let  $\mathcal{X}, \mathcal{Y}$  be complementary subspaces of  $\mathcal{V}$ . Let  $P$ , defined by  $P\mathbf{v} = \mathbf{x}$ , be the *projector onto  $\mathcal{X}$  along  $\mathcal{Y}$* . Then

- 1  $P$  is unique.
- 2  $P^2 = P$ , i.e.,  $P$  is idempotent.
- 3  $I - P$  is the *complementary projector* (onto  $\mathcal{Y}$  along  $\mathcal{X}$ ).
- 4  $R(P) = \{\mathbf{x} : P\mathbf{x} = \mathbf{x}\} = \mathcal{X}$  ("fixed points" for  $P$ ).
- 5  $N(I - P) = \mathcal{X} = R(P)$  and  $R(I - P) = N(P) = \mathcal{Y}$ .
- 6 If  $\mathcal{V} = \mathbb{R}^n$  (or  $\mathbb{C}^n$ ), then

$$\begin{aligned} P &= (X \ 0) (X \ Y)^{-1} \\ &= (X \ Y) \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} (X \ Y)^{-1}, \end{aligned}$$

where the columns of  $X$  and  $Y$  are bases for  $\mathcal{X}$  and  $\mathcal{Y}$ .

## Proof

① Assume  $P_1 \mathbf{v} = \mathbf{x} = P_2 \mathbf{v}$  for all  $\mathbf{v} \in \mathcal{V}$ . But then  $P_1 = P_2$ .



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Together we therefore have  $P^2 = P$ .



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$$\mathbf{v} = \mathbf{x} + \mathbf{y} = P\mathbf{v} + \mathbf{y}$$



## Proof

1 Assume  $P_1 \mathbf{v} = \mathbf{x} = P_2 \mathbf{v}$  for all  $\mathbf{v} \in \mathcal{V}$ . But then  $P_1 = P_2$ .

2 We know

$$P\mathbf{v} = \mathbf{x} \quad \text{for every } \mathbf{v} \in \mathcal{V}$$

so that

$$P^2 \mathbf{v} = P(P\mathbf{v}) = P\mathbf{x} = \mathbf{x}.$$

Together we therefore have  $P^2 = P$ .

3 Using the **unique decomposition of  $\mathbf{v}$**  we can write

$$\begin{aligned} \mathbf{v} &= \mathbf{x} + \mathbf{y} = P\mathbf{v} + \mathbf{y} \\ \iff (I - P)\mathbf{v} &= \mathbf{y}, \end{aligned}$$

the projection of  $\mathbf{v}$  onto  $\mathcal{V}$  along  $\mathcal{X}$ .



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The claim  $R(I - P) = \mathcal{Y} = N(P)$  is shown similarly.

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The second part follows by noting that

$$B \begin{pmatrix} I & O \\ O & O \end{pmatrix} = (X \ Y) \begin{pmatrix} I & O \\ O & O \end{pmatrix} = (X \ 0).$$



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### Remark

*This theorem is sometimes used to **define** projectors.*



# Angle between subspaces

In some applications, e.g., when determining the convergence rates of iterative algorithms, it is useful to know the **angle between subspaces**.



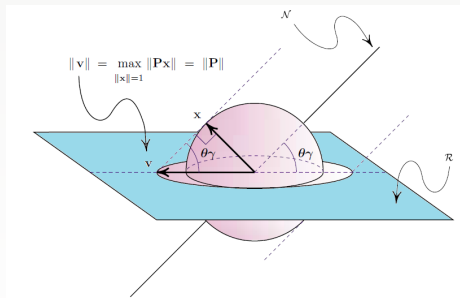
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If  $\mathcal{R}, \mathcal{N}$  are complementary then

$$\sin \theta = \frac{1}{\|P\|_2} = \frac{1}{\lambda_{\max}} = \frac{1}{\sigma_1},$$

where  $P$  is the projector onto  $\mathcal{R}$  along  $\mathcal{N}$ ,  $\lambda_{\max}$  is the largest eigenvalue of  $P^T P$  and  $\sigma_1$  is the largest singular value of  $P$ .



See [Mey00, Example 5.9.2] for more details.



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While the range–nullspace decomposition is theoretically important, its *practical usefulness is limited* because *computation is very unstable* due to lack of orthogonality.



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While the range–nullspace decomposition is theoretically important, its *practical usefulness is limited* because *computation is very unstable* due to lack of orthogonality.

This also means we *will not discuss nilpotent matrices* and — later on — the *Jordan normal form*.



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition**
- 10 Singular Value Decomposition
- 11 Orthogonal Projections

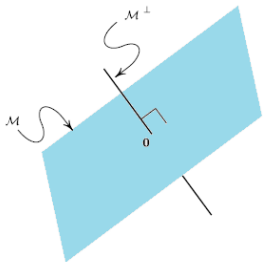
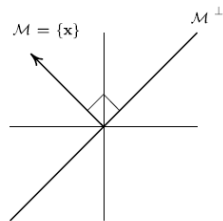




## Definition

Let  $\mathcal{V}$  be an inner product space and  $\mathcal{M} \subseteq \mathcal{V}$ . The **orthogonal complement**  $\mathcal{M}^\perp$  of  $\mathcal{M}$  is

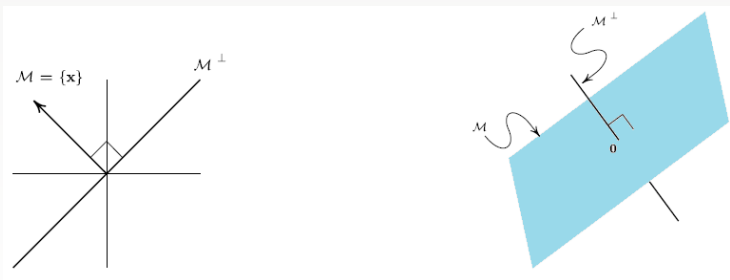
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## Remark

Even if  $\mathcal{M}$  is not a subspace of  $\mathcal{V}$  (i.e., only a subset),  $\mathcal{M}^\perp$  is (see HW).

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Let  $\mathcal{V}$  be an inner product space and  $\mathcal{M} \subseteq \mathcal{V}$ . If  $\mathcal{M}$  is a subspace of  $\mathcal{V}$ , then

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## Proof

According to the definition of complementary subspaces we need to show

- 1  $\mathcal{M} \cap \mathcal{M}^\perp = \{\mathbf{0}\},$
- 2  $\mathcal{M} + \mathcal{M}^\perp = \mathcal{V}.$



**Proof** (cont.)

- 1 Let's assume there exists an  $\mathbf{x} \in \mathcal{M} \cap \mathcal{M}^\perp$ , i.e.,  $\mathbf{x} \in \mathcal{M}$  and  $\mathbf{x} \in \mathcal{M}^\perp$ .



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This is true for any  $\mathbf{x} \in \mathcal{M} \cap \mathcal{M}^\perp$ , so  $\mathbf{x} = \mathbf{0}$  is the only such vector.





## Proof (cont.)

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However, **any vector in the extension must be orthogonal to  $\mathcal{M}$** , i.e., in  $\mathcal{M}^\perp$ , but this is not possible since the extended basis must be linearly independent.

Therefore, the extension set is empty.



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Let  $\mathcal{V}$  be an inner product space with  $\dim(\mathcal{V}) = n$  and  $\mathcal{M}$  be a subspace of  $\mathcal{V}$ . Then

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Also, since  $\mathcal{M}$  is a subspace of  $\mathcal{V}$  we have  $\mathcal{V} = \mathcal{M} + \mathcal{M}^\perp$  and the dimension formula implies (1).





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But

$$\langle \mathbf{n}, \mathbf{n} \rangle = 0 \quad \iff \quad \mathbf{n} = \mathbf{0},$$

and therefore  $\mathbf{x} = \mathbf{m}$  is in  $\mathcal{M}$ .

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Now, recall from Chapter 4 that for subspaces  $\mathcal{X} \subseteq \mathcal{Y}$

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Now, recall from Chapter 4 that for subspaces  $\mathcal{X} \subseteq \mathcal{Y}$

$$\dim \mathcal{X} = \dim \mathcal{Y} \implies \mathcal{X} = \mathcal{Y}.$$

We take  $\mathcal{X} = \mathcal{M}^{\perp\perp}$  and  $\mathcal{Y} = \mathcal{M}$  (and know from the work just performed that  $\mathcal{M}^{\perp\perp}$  is a subspace of  $\subseteq \mathcal{M}$ ).

From (1) we know

$$\begin{aligned}\dim \mathcal{M}^{\perp} &= n - \dim \mathcal{M} \\ \dim \mathcal{M}^{\perp\perp} &= n - \dim \mathcal{M}^{\perp} \\ &= n - (n - \dim \mathcal{M}) = \dim \mathcal{M}.\end{aligned}$$

But then  $\mathcal{M}^{\perp\perp} = \mathcal{M}$ .  $\square$



# Back to Fundamental Subspaces

## Theorem

Let  $A$  be a real  $m \times n$  matrix. Then

- 1  $R(A)^\perp = N(A^T)$ ,
- 2  $N(A)^\perp = R(A^T)$ .



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## Corollary

$$\mathbb{R}^m = \underbrace{R(A)}_{\subseteq \mathbb{R}^m} \oplus R(A)^\perp = R(A) \oplus N(A^T),$$

$$\mathbb{R}^n = \underbrace{N(A)}_{\subseteq \mathbb{R}^n} \oplus N(A)^\perp = N(A) \oplus R(A^T).$$



## Proof (of Theorem)

1 We show that  $\mathbf{x} \in R(\mathbf{A})^\perp$  implies  $\mathbf{x} \in N(\mathbf{A}^T)$  and vice versa.

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 &\stackrel{\mathbf{A} \rightarrow \mathbf{A}^T}{\iff} R(\mathbf{A}^T) = N(\mathbf{A})^\perp.
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# Starting to think about the SVD

The decompositions of  $\mathbb{R}^m$  and  $\mathbb{R}^n$  from the corollary help prepare for the SVD of an  $m \times n$  matrix  $A$ .



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Assume  $\text{rank}(A) = r$  and let

$$\mathcal{B}_{R(A)} = \{\mathbf{u}_1, \dots, \mathbf{u}_r\}$$

ON basis for  $R(A) \subseteq \mathbb{R}^m$ ,

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By the corollary

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and therefore the following are **orthogonal matrices**

$$U = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_m)$$

$$V = (\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n).$$



Consider

$$R = U^T A V = \left( \mathbf{u}_i^T A \mathbf{v}_j \right)_{i,j=1}^{m,n}.$$

Note that

$$A \mathbf{v}_j = \mathbf{0}, \quad j =$$



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so

$$R = \begin{pmatrix} \mathbf{u}_1^T A \mathbf{v}_1 & \cdots & \mathbf{u}_1^T A \mathbf{v}_r & \mathbf{0} \\ \vdots & & \vdots & \mathbf{0} \\ \mathbf{u}_r^T A \mathbf{v}_1 & \cdots & \mathbf{u}_r^T A \mathbf{v}_r & \mathbf{0} \\ \mathbf{0} & & \mathbf{0} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{r \times r} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$





Thus

$$R = U^T A V = \begin{pmatrix} C_{r \times r} & O \\ O & O \end{pmatrix}$$
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### Remark

The matrix  $C_{r \times r}$  is nonsingular since

$$\text{rank}(C) = \text{rank}(U^T A V) = \text{rank}(A) = r$$

because multiplication by the orthogonal (and therefore nonsingular) matrices  $U^T$  and  $V$  does not change the rank of  $A$ .



We have now shown that the ON bases for the fundamental subspaces of  $A$  yield the URV factorization.



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As we show next, the converse is also true, i.e., any URV factorization of  $A$  yields a ON bases for the fundamental subspaces of  $A$ .



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As we show next, the converse is also true, i.e., any URV factorization of  $A$  yields a ON bases for the fundamental subspaces of  $A$ .

However, the URV factorization is not unique. Different ON bases result in different factorizations.



Consider  $A = URV^T$  with  $U, V$  orthogonal  $m \times m$  and  $n \times n$  matrices, respectively, and  $R = \begin{pmatrix} C & O \\ O & O \end{pmatrix}$  with  $C$  nonsingular.



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We **partition**

$$U = \begin{pmatrix} \underbrace{U_1}_{m \times r} & \underbrace{U_2}_{m \times m-r} \end{pmatrix}, \quad V = \begin{pmatrix} \underbrace{V_1}_{n \times r} & \underbrace{V_2}_{n \times n-r} \end{pmatrix}$$



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Then  **$V$  (and therefore also  $V^T$ ) is nonsingular** and we see that

$$R(A) = R(URV^T)$$

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so that the **columns of  $U_1$  are an ON basis for  $R(A)$ .**



Moreover,

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This implies that the **columns of  $U_2$  are an ON basis for  $N(A^T)$** .

The **other two cases can be argued similarly** using  $N(AB) = N(B)$  provided  $\text{rank}(A) = n$ .



The main difference between a URV factorization and the SVD is that the SVD will contain a diagonal matrix  $\Sigma$  with  $r$  nonzero singular values, while  $R$  contains the full  $r \times r$  block  $C$ .



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Idea: use Householder reflections (or Givens rotations)



Consider an  $m \times n$  matrix  $A$ .

We apply an  $m \times m$  orthogonal (Householder reflection) matrix  $P$  so that

$$A \longrightarrow PA = \begin{pmatrix} B \\ O \end{pmatrix}, \quad \text{with } r \times m \text{ matrix } B, \text{ rank}(B) = r.$$



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$$BQ^T = (T^T \ O) \iff B = (T^T \ O)Q$$



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Then

$$BQ^T = (T^T \ O) \iff B = (T^T \ O)Q$$

and

$$\begin{pmatrix} B \\ O \end{pmatrix} = \begin{pmatrix} T^T & O \\ O & O \end{pmatrix} Q.$$



Together,

$$PA = \begin{pmatrix} T^T & O \\ O & O \end{pmatrix} Q$$
$$\iff A = P^T \begin{pmatrix} T^T & O \\ O & O \end{pmatrix} Q,$$

a URV factorization with lower triangular block  $T^T$ .



Together,

$$\begin{aligned} PA &= \begin{pmatrix} T^T & O \\ O & O \end{pmatrix} Q \\ \iff A &= P^T \begin{pmatrix} T^T & O \\ O & O \end{pmatrix} Q, \end{aligned}$$

a URV factorization with lower triangular block  $T^T$ .

### Remark

*See HW for an example of this process with numbers.*



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition**
- 11 Orthogonal Projections



# Singular Value Decomposition

We know

$$A = URV^T = U \begin{pmatrix} C & O \\ O & O \end{pmatrix} V^T,$$

where  $C$  is upper triangular and  $U, V$  are orthogonal.



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$$A = URV^T = U \begin{pmatrix} C & O \\ O & O \end{pmatrix} V^T,$$

where  $C$  is upper triangular and  $U, V$  are orthogonal.

Now we want to establish that  $C$  can even be made **diagonal**.



Note that

$$\|\mathbf{A}\|_2 = \|\mathbf{C}\|_2 =: \sigma_1$$

since multiplication by an orthogonal matrix does not change the 2-norm (see HW).





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Also,

$$\|\mathbf{C}\|_2 = \max_{\|\mathbf{z}\|_2=1} \|\mathbf{Cz}\|_2$$

so that

$$\|\mathbf{C}\|_2 = \|\mathbf{Cx}\|_2 \quad \text{for some } \mathbf{x}, \|\mathbf{x}\|_2 = 1.$$



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$$\|\mathbf{C}\|_2 = \max_{\|\mathbf{z}\|_2=1} \|\mathbf{C}\mathbf{z}\|_2$$

so that

$$\|\mathbf{C}\|_2 = \|\mathbf{C}\mathbf{x}\|_2 \quad \text{for some } \mathbf{x}, \|\mathbf{x}\|_2 = 1.$$

In fact (see Sect.5.2),  $\mathbf{x}$  is such that  $(\mathbf{C}^T\mathbf{C} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$ , i.e.,  $\mathbf{x}$  is an eigenvector of  $\mathbf{C}^T\mathbf{C}$  so that

$$\|\mathbf{C}\|_2 = \sigma_1 = \sqrt{\lambda} = \sqrt{\mathbf{x}^T\mathbf{C}^T\mathbf{C}\mathbf{x}}. \quad (13)$$



Since  $\mathbf{x}$  is a unit vector we can extend it to an orthogonal matrix

$$R_{\mathbf{x}} = (\mathbf{x} \ \mathbf{X}),$$

e.g., using Householder reflectors as discussed at the end of Sect.5.6.



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Similarly, let

$$\mathbf{y} = \frac{\mathbf{C}\mathbf{x}}{\|\mathbf{C}\mathbf{x}\|_2} = \frac{\mathbf{C}\mathbf{x}}{\sigma_1}. \quad (14)$$



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Then

$$R_{\mathbf{y}} = (\mathbf{y} \ \mathbf{Y})$$

is also orthogonal (and Hermitian/symmetric) since it's a Householder reflector.



Now

$$\underbrace{R_y^T}_{=R_y} C R_x = \begin{pmatrix} \mathbf{y}^T \\ \mathbf{Y}^T \end{pmatrix} C (\mathbf{x} \quad \mathbf{X}) = \begin{pmatrix} \mathbf{y}^T C \mathbf{x} & \mathbf{y}^T C \mathbf{X} \\ \mathbf{Y}^T C \mathbf{x} & \mathbf{Y}^T C \mathbf{X} \end{pmatrix}.$$



Now

$$\underbrace{R_y^T}_{=R_y} C R_x = \begin{pmatrix} \mathbf{y}^T \\ Y^T \end{pmatrix} C (\mathbf{x} \quad X) = \begin{pmatrix} \mathbf{y}^T C \mathbf{x} & \mathbf{y}^T C X \\ Y^T C \mathbf{x} & Y^T C X \end{pmatrix}.$$

From above

$$\begin{aligned} \sigma_1^2 &= \lambda \stackrel{(13)}{=} \mathbf{x}^T C^T C \mathbf{x} \stackrel{(14)}{=} \sigma_1 \mathbf{y}^T C \mathbf{x} \\ \implies \mathbf{y}^T C \mathbf{x} &= \sigma_1. \end{aligned}$$



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Also,

$$Y^T C \mathbf{x} \stackrel{(14)}{=} Y^T (\sigma_1 \mathbf{y}) = \mathbf{0}$$

since  $R_y$  is orthogonal, i.e.,  $\mathbf{y}$  is orthogonal to the columns of  $Y$ .





Let  $Y^T CX = C_2$  and  $\mathbf{y}^T CX = \mathbf{c}^T$  so that

$$R_{\mathbf{y}}CR_{\mathbf{x}} = \begin{pmatrix} \sigma_1 & \mathbf{c}^T \\ \mathbf{0} & C_2 \end{pmatrix}.$$



Let  $\mathbf{Y}^T \mathbf{C} \mathbf{X} = \mathbf{C}_2$  and  $\mathbf{y}^T \mathbf{C} \mathbf{X} = \mathbf{c}^T$  so that

$$\mathbf{R}_y \mathbf{C} \mathbf{R}_x = \begin{pmatrix} \sigma_1 & \mathbf{c}^T \\ \mathbf{0} & \mathbf{C}_2 \end{pmatrix}.$$

To show that  $\mathbf{c}^T = \mathbf{0}^T$  consider

$$\begin{aligned} \mathbf{c}^T &= \mathbf{y}^T \mathbf{C} \mathbf{X} \stackrel{(14)}{=} \left( \frac{\mathbf{C} \mathbf{x}}{\sigma_1} \right)^T \mathbf{C} \mathbf{X} \\ &= \frac{\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{X}}{\sigma_1}. \end{aligned} \tag{15}$$



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From (13)  $\mathbf{x}$  is an eigenvector of  $\mathbf{C}^T \mathbf{C}$ , i.e.,

$$\mathbf{C}^T \mathbf{C} \mathbf{x} = \lambda \mathbf{x} = \sigma_1^2 \mathbf{x} \iff \mathbf{x}^T \mathbf{C}^T \mathbf{C} = \sigma_1^2 \mathbf{x}^T.$$



Let  $Y^T C X = C_2$  and  $\mathbf{y}^T C X = \mathbf{c}^T$  so that

$$R_{\mathbf{y}} C R_{\mathbf{x}} = \begin{pmatrix} \sigma_1 & \mathbf{c}^T \\ \mathbf{0} & C_2 \end{pmatrix}.$$

To show that  $\mathbf{c}^T = \mathbf{0}^T$  consider

$$\begin{aligned} \mathbf{c}^T &= \mathbf{y}^T C X \stackrel{(14)}{=} \left( \frac{C \mathbf{x}}{\sigma_1} \right)^T C X \\ &= \frac{\mathbf{x}^T C^T C X}{\sigma_1}. \end{aligned} \tag{15}$$

From (13)  $\mathbf{x}$  is an eigenvector of  $C^T C$ , i.e.,

$$C^T C \mathbf{x} = \lambda \mathbf{x} = \sigma_1^2 \mathbf{x} \iff \mathbf{x}^T C^T C = \sigma_1^2 \mathbf{x}^T.$$

Plugging this into (15) yields

$$\mathbf{c}^T = \sigma_1 \mathbf{x}^T X = \mathbf{0}$$

since  $R_{\mathbf{x}} = (\mathbf{x} \ X)$  is orthogonal.



Moreover,  $\sigma_1 \geq \|C_2\|_2$  since

$$\sigma_1 = \|C\|_2 \stackrel{\text{HW}}{=} \|R_y C R_x\|_2 = \max\{\sigma_1, \|C_2\|_2\}.$$



Moreover,  $\sigma_1 \geq \|C_2\|_2$  since

$$\sigma_1 = \|C\|_2 \stackrel{\text{HW}}{=} \|R_y C R_x\|_2 = \max\{\sigma_1, \|C_2\|_2\}.$$

Next, we repeat this process for  $C_2$ , i.e.,

$$S_y C_2 S_x = \begin{pmatrix} \sigma_2 & \mathbf{0}^T \\ \mathbf{0} & C_3 \end{pmatrix} \quad \text{with} \quad \sigma_2 \geq \|C_3\|_2.$$



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Let

$$P_2 = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & S_y^T \end{pmatrix} R_y^T, \quad Q_2 = R_x \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & S_x \end{pmatrix}.$$

Then

$$P_2 C Q_2 = \begin{pmatrix} \sigma_1 & 0 & \mathbf{0}^T \\ 0 & \sigma_2 & \mathbf{0}^T \\ \mathbf{0} & \mathbf{0} & C_3 \end{pmatrix} \quad \text{with} \quad \sigma_1 \geq \sigma_2 \geq \|C_3\|_2.$$



We continue this until

$$P_{r-1}CQ_{r-1} = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \dots & \\ 0 & & & \sigma_r \end{pmatrix} = D, \quad \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r.$$





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Finally, let

$$\tilde{U}^T = \begin{pmatrix} P_{r-1} & 0 \\ 0 & I \end{pmatrix} U^T, \quad \text{and} \quad \tilde{V} = \begin{pmatrix} Q_{r-1} & 0 \\ 0 & I \end{pmatrix}.$$



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$$P_{r-1}CQ_{r-1} = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{pmatrix} = D, \quad \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r.$$

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Together,

$$\tilde{U}^T A \tilde{V} = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}$$

or — without the tildes — the **singular value decomposition** (SVD) of  $A$

$$A = U \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} V^T,$$

where  $A$  is  $m \times n$ ,  $U$  is  $m \times m$ ,  $D = r \times r$  and  $V = n \times n$ .



We use the following terminology:

**singular values:**  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$ ,

**left singular vectors:** columns of  $U$ ,

**right singular vectors:** columns of  $V$ .



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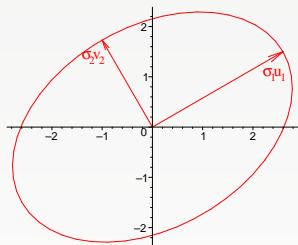
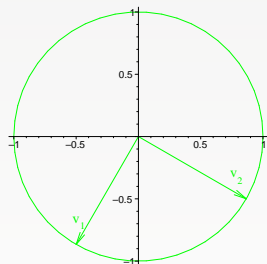
### Remark

*In Chapter 7 we will see that the columns of  $U$  and  $V$  are also special eigenvectors of  $A^T A$ .*



# Geometric interpretation of SVD

For the following we assume  $A \in \mathbb{R}^{n \times n}$ ,  $n = 2$ .



This picture is true since

$$A = UDV^T \iff AV = UD$$

and  $\sigma_1, \sigma_2$  are the lengths of the semi-axes of the ellipse because  $\|\mathbf{u}_1\| = \|\mathbf{u}_2\| = 1$ .

## Remark

See [Mey00] for more details.

For **general**  $n$ ,  $A$  transforms the 2-norm unit sphere to an ellipsoid whose semi-axes have lengths

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n.$$



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Therefore,

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Moreover,

$$\sigma_1 = \|\mathbf{A}\|_2, \quad \sigma_n = \frac{1}{\|\mathbf{A}^{-1}\|_2}$$

so that

$$\kappa_2(\mathbf{A}) = \|\mathbf{A}\|_2 \|\mathbf{A}^{-1}\|_2$$

is the **2-norm condition number of  $A$**  ( $\in \mathbb{R}^{n \times n}$ ).





## Remark

*The relations for  $\sigma_1$  and  $\sigma_n$  hold because*

$$\begin{aligned}\|A\|_2 &= \|UDV^T\|_2 \stackrel{HW}{=} \|D\|_2 = \sigma_1 \\ \|A^{-1}\|_2 &= \|VD^{-1}U^T\|_2 \stackrel{HW}{=} \|D^{-1}\|_2 = \frac{1}{\sigma_n}\end{aligned}$$



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## Remark

We *always have*  $\kappa_2(A) \geq 1$ , and  $\kappa_2(A) = 1$  if and only if  $A$  is a multiple of an orthogonal matrix (typo in [Mey00], see proof on next slide).



## Proof

“ $\Leftarrow$ ”: Assume  $A = \alpha Q$  with  $\alpha > 0$ ,  $Q$  orthogonal, i.e.,

$$\|A\|_2 = \alpha \|Q\|_2 = \alpha \max_{\|\mathbf{x}\|_2=1} \|Q\mathbf{x}\|_2 \stackrel{\text{invariance}}{=} \alpha \max_{\|\mathbf{x}\|_2=1} \|\mathbf{x}\|_2 = \alpha.$$



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Also

$$A^T A = \alpha^2 Q^T Q = \alpha^2 I \quad \implies \quad A^{-1} = \frac{1}{\alpha^2} A^T \quad \text{and} \quad \|A^T\|_2 = \|A\|_2$$

so that  $\|A^{-1}\|_2 = \frac{1}{\alpha}$  and

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2 = \alpha \frac{1}{\alpha} = 1.$$



## Proof (cont.)

“ $\implies$ ”: Assume  $\kappa_2(\mathbf{A}) = \frac{\sigma_1}{\sigma_n} = 1$  so that  $\sigma_1 = \sigma_n$  and therefore

$$\mathbf{D} = \sigma_1 \mathbf{I}.$$



Proof (cont.)

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$$\mathbf{D} = \sigma_1 \mathbf{I}.$$

Thus

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T = \sigma_1 \mathbf{U}\mathbf{V}^T$$

and

$$\begin{aligned}\mathbf{A}^T \mathbf{A} &= \sigma_1^2 (\mathbf{U}\mathbf{V}^T)^T \mathbf{U}\mathbf{V}^T \\ &= \sigma_1^2 \mathbf{V}\mathbf{U}^T \mathbf{U}\mathbf{V}^T = \sigma_1^2 \mathbf{I}.\end{aligned}$$



# Applications of the Condition Number

Let  $\tilde{\mathbf{x}}$  be the answer obtained by solving  $A\mathbf{x} = \mathbf{b}$  with  $A \in \mathbb{R}^{n \times n}$ .



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Let  $\tilde{\mathbf{x}}$  be the answer obtained by solving  $A\mathbf{x} = \mathbf{b}$  with  $A \in \mathbb{R}^{n \times n}$ .

Is a small residual

$$\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$$

a good indicator for the accuracy of  $\tilde{\mathbf{x}}$ ?





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Is a small residual

$$\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$$

a good indicator for the accuracy of  $\tilde{\mathbf{x}}$ ?

Since  $\mathbf{x}$  is the exact answer, and  $\tilde{\mathbf{x}}$  the computed answer we have the relative error

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|}.$$



Now

$$\begin{aligned}\|\mathbf{r}\| &= \|\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}\| = \|\mathbf{A}\mathbf{x} - \mathbf{A}\tilde{\mathbf{x}}\| \\ &= \|\mathbf{A}(\mathbf{x} - \tilde{\mathbf{x}})\| \leq \|\mathbf{A}\|\|\mathbf{x} - \tilde{\mathbf{x}}\|.\end{aligned}$$



Now

$$\begin{aligned}\|r\| &= \|b - A\tilde{x}\| = \|Ax - A\tilde{x}\| \\ &= \|A(x - \tilde{x})\| \leq \|A\| \|x - \tilde{x}\|.\end{aligned}$$

To get the relative error we multiply by  $\frac{\|A^{-1}b\|}{\|x\|} = 1$ .



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Then

$$\begin{aligned}\|r\| &\leq \|A\| \|A^{-1}b\| \frac{\|x - \tilde{x}\|}{\|x\|} \\ \frac{\|r\|}{\|b\|} &\leq \kappa(A) \frac{\|x - \tilde{x}\|}{\|x\|}.\end{aligned}\tag{16}$$



Moreover, using  $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = \mathbf{b} - \tilde{\mathbf{b}}$ ,

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| = \|A^{-1}(\mathbf{b} - \tilde{\mathbf{b}})\| \leq \|A^{-1}\| \|\mathbf{r}\|.$$



Moreover, using  $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = \mathbf{b} - \tilde{\mathbf{b}}$ ,

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Multiplying by  $\frac{\|A\mathbf{x}\|}{\|\mathbf{b}\|} = 1$  we have

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(A) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}. \quad (17)$$



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Multiplying by  $\frac{\|\mathbf{Ax}\|}{\|\mathbf{b}\|} = 1$  we have

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(\mathbf{A}) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}. \quad (17)$$

Combining (16) and (17) yields

$$\frac{1}{\kappa(\mathbf{A})} \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} \leq \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(\mathbf{A}) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}.$$



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Therefore, the **relative residual**  $\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}$  is a good indicator of relative error if **and only if A is well conditioned**, i.e.,  $\kappa(\mathbf{A})$  is small (close to 1).





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- 2 Low-rank approximation of A:  
The **Eckart–Young theorem** states that

$$\mathbf{A}_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

is the **best rank  $k$  approximation to A in the 2-norm** (also the Frobenius norm), i.e.,

$$\|\mathbf{A} - \mathbf{A}_k\|_2 = \min_{\text{rank}(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_2.$$

Moreover,

$$\|\mathbf{A} - \mathbf{A}_k\|_2 = \sigma_{k+1}.$$



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Run `SVD_movie.m`



- ③ Stable solution of least squares problems:  
Use Moore–Penrose pseudoinverse

### Definition

Let  $A \in \mathbb{R}^{m \times n}$  and

$$A = U \begin{pmatrix} D & O \\ O & O \end{pmatrix} V^T$$

be the SVD of  $A$ . Then

$$A^\dagger = V \begin{pmatrix} D^{-1} & O \\ O & O \end{pmatrix} U^T$$

is called the Moore–Penrose pseudoinverse of  $A$ .



- ③ **Stable solution of least squares problems:**  
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$$A^\dagger = V \begin{pmatrix} D^{-1} & O \\ O & O \end{pmatrix} U^T$$

is called the **Moore–Penrose pseudoinverse of  $A$** .

### Remark

Note that  $A^\dagger \in \mathbb{R}^{n \times m}$  and

$$A^\dagger = \sum_{i=1}^r \frac{\mathbf{v}_i \mathbf{u}_i^T}{\sigma_i}, \quad r = \text{rank}(A).$$

We now show that the least squares solution of

$$A\mathbf{x} = \mathbf{b}$$

is given by

$$\mathbf{x} = A^\dagger \mathbf{b}.$$



Start with normal equations and use

$$A = U \begin{pmatrix} D & O \\ O & O \end{pmatrix} V^T = \tilde{U} D \tilde{V}^T,$$

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$$\begin{aligned} A^T A \mathbf{x} = A^T \mathbf{b} &\iff \tilde{V} D \underbrace{\tilde{U}^T \tilde{U}}_{=I} D \tilde{V}^T \mathbf{x} = \tilde{V} D \tilde{U}^T \mathbf{b} \\ &\iff \tilde{V} D^2 \tilde{V}^T \mathbf{x} = \tilde{V} D \tilde{U}^T \mathbf{b} \end{aligned}$$



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Multiplication by  $D^{-1} \tilde{V}^T$  yields

$$D \tilde{V}^T \mathbf{x} = \tilde{U}^T \mathbf{b}.$$



Thus

$$D\tilde{V}^T \mathbf{x} = \tilde{U}^T \mathbf{b}$$

implies

$$\mathbf{x} = \tilde{V}D^{-1}\tilde{U}^T \mathbf{b}$$

$$\iff \mathbf{x} = V \begin{pmatrix} D^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} U^T \mathbf{b}$$

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## Remark

- If  $A$  is nonsingular then  $A^\dagger = A^{-1}$  (see HW).
- If  $\text{rank}(A) < n$  (i.e., the least squares solution is *not unique*), then  $\mathbf{x} = A^\dagger \mathbf{b}$  provides the *unique solution with minimum 2-norm* (see justification on following slide).



# Minimum norm solution of underdetermined systems

Note that the general solution of  $A\mathbf{x} = \mathbf{b}$  is given by

$$\mathbf{z} = A^\dagger \mathbf{b} + \mathbf{n}, \quad \mathbf{n} \in N(A).$$



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The Pythagorean theorem applies since (see HW)

$$A^\dagger \mathbf{b} \in R(A^\dagger) = R(A^T)$$

so that, using  $R(A^T) = N(A)^\perp$ ,

$$A^\dagger \mathbf{b} \perp \mathbf{n}.$$





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Instead we solve  $A\mathbf{x} = \mathbf{b}$ ,  $A \in \mathbb{R}^{m \times n}$ , by



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  - 1 Solve  $\mathbf{D}\mathbf{y} = \tilde{\mathbf{U}}^T\mathbf{b}$  for  $\mathbf{y}$
  - 2 Compute  $\mathbf{x} = \tilde{\mathbf{V}}\mathbf{y}$



## Other Applications

Also known as **principal component analysis (PCA)**, **(discrete) Karhunen-Loève (KL) transformation**, **Hotelling transform**, or **proper orthogonal decomposition (POD)**

- Data compression
- Noise filtering
- Regularization of inverse problems
  - Tomography
  - Image deblurring
  - Seismology
- Information retrieval and data mining (latent semantic analysis)
- Bioinformatics and computational biology
  - Immunology
  - Molecular dynamics
  - Microarray data analysis



# Outline

- 1 Vector Norms
- 2 Matrix Norms
- 3 Inner Product Spaces
- 4 Orthogonal Vectors
- 5 Gram–Schmidt Orthogonalization & QR Factorization
- 6 Unitary and Orthogonal Matrices
- 7 Orthogonal Reduction
- 8 Complementary Subspaces
- 9 Orthogonal Decomposition
- 10 Singular Value Decomposition
- 11 Orthogonal Projections**



# Orthogonal Projections

Earlier we discussed **orthogonal complementary subspaces** of an inner product space  $\mathcal{V}$ , i.e.,

$$\mathcal{V} = \mathcal{M} \oplus \mathcal{M}^\perp.$$

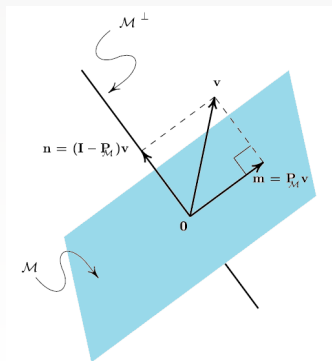
## Definition

Consider  $\mathcal{V} = \mathcal{M} \oplus \mathcal{M}^\perp$  so that for every  $\mathbf{v} \in \mathcal{V}$  there exist unique vectors  $\mathbf{m} \in \mathcal{M}$ ,  $\mathbf{n} \in \mathcal{M}^\perp$  such that

$$\mathbf{v} = \mathbf{m} + \mathbf{n}.$$

Then  $\mathbf{m}$  is called the **orthogonal projection of  $\mathbf{v}$  onto  $\mathcal{M}$** .

The matrix  $\mathbf{P}_\mathcal{M}$  such that  $\mathbf{P}_\mathcal{M}\mathbf{v} = \mathbf{m}$  is the **orthogonal projector onto  $\mathcal{M}$  along  $\mathcal{M}^\perp$** .





For **arbitrary complementary subspaces**  $\mathcal{X}, \mathcal{Y}$  we showed earlier that the projector onto  $\mathcal{X}$  along  $\mathcal{Y}$  is given by

$$\begin{aligned} P &= (X \ O) (X \ Y)^{-1} \\ &= (X \ Y) \begin{pmatrix} I & O \\ O & O \end{pmatrix} (X \ Y)^{-1}, \end{aligned}$$

where the columns of  $X$  and  $Y$  are bases for  $\mathcal{X}$  and  $\mathcal{Y}$ .



Now we let  $\mathcal{X} = \mathcal{M}$  and  $\mathcal{Y} = \mathcal{M}^\perp$  be **orthogonal complementary subspaces**, where M and N contain the basis vectors of  $\mathcal{M}$  and  $\mathcal{M}^\perp$  in their columns.



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Then

$$P = (M \ O) (M \ N)^{-1}. \quad (18)$$

To find  $(M \ N)^{-1}$  we note that

$$M^T N = N^T M = O$$

and if  $N$  is an orthogonal matrix (i.e., contains an ON basis), then

$$\begin{pmatrix} (M^T M)^{-1} M^T \\ N^T \end{pmatrix} (M \ N) = \begin{pmatrix} I & O \\ O & I \end{pmatrix}$$

(note that  $M^T M$  is invertible since  $M$  is full rank because its columns form a basis of  $\mathcal{M}$ ).



Thus

$$(\mathbf{M} \ \mathbf{N})^{-1} = \begin{pmatrix} (\mathbf{M}^T \mathbf{M})^{-1} \mathbf{M}^T \\ \mathbf{N}^T \end{pmatrix}. \quad (19)$$



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Inserting (19) into (18) yields

$$\begin{aligned} P_{\mathcal{M}} &= (M \ 0) \begin{pmatrix} (M^T M)^{-1} M^T \\ N^T \end{pmatrix} \\ &= M(M^T M)^{-1} M^T. \end{aligned}$$



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Inserting (19) into (18) yields

$$\begin{aligned} \mathbf{P}_{\mathcal{M}} &= (\mathbf{M} \ \mathbf{O}) \begin{pmatrix} (\mathbf{M}^T \mathbf{M})^{-1} \mathbf{M}^T \\ \mathbf{N}^T \end{pmatrix} \\ &= \mathbf{M}(\mathbf{M}^T \mathbf{M})^{-1} \mathbf{M}^T. \end{aligned}$$

### Remark

Note that  $\mathbf{P}_{\mathcal{M}}$  is unique so that this formula holds for an arbitrary basis of  $\mathcal{M}$  (collected in  $\mathbf{M}$ ).

In particular, if  $\mathbf{M}$  contains an ON basis for  $\mathcal{M}$ , then

$$\mathbf{P}_{\mathcal{M}} = \mathbf{M} \mathbf{M}^T.$$



Similarly,

$$P_{\mathcal{M}^\perp} = N(N^T N)^{-1} N^T \quad (\text{arbitrary basis for } \mathcal{N})$$

$$P_{\mathcal{M}^\perp} = N N^T \quad \text{ON basis}$$

As before,

$$P_{\mathcal{M}} = I - P_{\mathcal{M}^\perp}.$$





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As before,

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### Example

If  $\mathcal{M} = \text{span}\{\mathbf{u}\}$ ,  $\|\mathbf{u}\| = 1$  then

$$P_{\mathcal{M}} = P_{\mathbf{u}} = \mathbf{u}\mathbf{u}^T$$

and

$$P_{\mathbf{u}^\perp} = I - P_{\mathbf{u}} = I - \mathbf{u}\mathbf{u}^T$$

(cf. elementary orthogonal projectors earlier).

# Properties of orthogonal projectors

## Theorem

Let  $P \in \mathbb{R}^{n \times n}$  be a projector, i.e.,  $P^2 = P$ . Then the matrix  $P$  is an orthogonal projector if

- 1  $R(P) \perp N(P)$ ,
- 2  $P^T = P$ ,
- 3  $\|P\|_2 = 1$ .



## Proof

- 1 Follows directly from the definition.



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- 2 “ $\implies$ ”: Assume  $P$  is an orthogonal projector, i.e.,

$$P = M(M^T M)^{-1} M^T \quad \text{and} \quad P^T = M \underbrace{(M^T M)^{-T}}_{=(M^T M)^{-1}} M^T = P.$$



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“ $\impliedby$ ”: Assume  $P = P^T$ . Then

$$R(P) = R(P^T) \stackrel{\text{Orth.decomp.}}{=} N(P)^\perp$$

so that  $P$  is an orthogonal projector via (1).



## Proof (cont.)

- ③ For complementary subspaces  $\mathcal{X}, \mathcal{Y}$  we know the angle between  $\mathcal{X}$  and  $\mathcal{Y}$  is given by

$$\|\mathbf{P}\|_2 = \frac{1}{\sin \theta}, \quad \theta \in \left[0, \frac{\pi}{2}\right].$$



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Assume  $P$  is an orthogonal projector, then  $\theta = \frac{\pi}{2}$  so that  $\|P\|_2 = 1$ .

Conversely, if  $\|P\|_2 = 1$ , then  $\theta = \frac{\pi}{2}$  and  $\mathcal{X}, \mathcal{Y}$  are orthogonal complements, i.e.,  $P$  is an orthogonal projector.





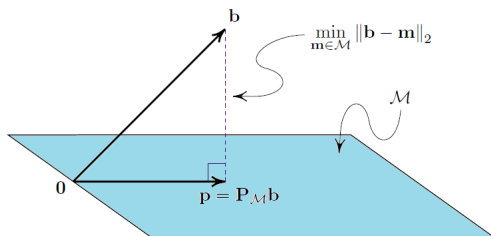
# Why is orthogonal projection so important?

## Theorem

Let  $\mathcal{V}$  be an inner product space with subspace  $\mathcal{M}$ , and let  $\mathbf{b} \in \mathcal{V}$ . Then

$$\text{dist}(\mathbf{b}, \mathcal{M}) = \min_{\mathbf{m} \in \mathcal{M}} \|\mathbf{b} - \mathbf{m}\|_2 = \|\mathbf{b} - P_{\mathcal{M}}\mathbf{b}\|_2,$$

i.e.,  $P_{\mathcal{M}}\mathbf{b}$  is the unique vector in  $\mathcal{M}$  closest to  $\mathbf{b}$ . The quantity  $\text{dist}(\mathbf{b}, \mathcal{M})$  is called the (orthogonal) **distance from  $\mathbf{b}$  to  $\mathcal{M}$** .



## Proof

Let  $\mathbf{p} = P_{\mathcal{M}}\mathbf{b}$ . Then  $\mathbf{p} \in \mathcal{M}$  and  $\mathbf{p} - \mathbf{m} \in \mathcal{M}$  for every  $\mathbf{m} \in \mathcal{M}$ .

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Moreover,

$$\mathbf{b} - \mathbf{p} = (\mathbf{I} - P_{\mathcal{M}})\mathbf{b} \in \mathcal{M}^{\perp},$$

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Therefore  $\min_{\mathbf{m} \in \mathcal{M}} \|\mathbf{b} - \mathbf{m}\|_2 = \|\mathbf{b} - \mathbf{p}\|_2$ .

Proof (cont.)

**Uniqueness:** Assume there exists a  $\mathbf{q} \in \mathcal{M}$  such that

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But then (20) implies that  $\|\mathbf{p} - \mathbf{q}\|_2^2 = 0$  and therefore  $\mathbf{p} = \mathbf{q}$ .  $\square$



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**Goal of least squares:** For  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , find

$$\min_{\mathbf{x} \in \mathbb{R}^n} \sqrt{\sum_{i=1}^m ((\mathbf{A}\mathbf{x})_i - b_i)^2} \iff \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2.$$



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Now  $A\mathbf{x} \in R(A)$ , so the **least squares error** is

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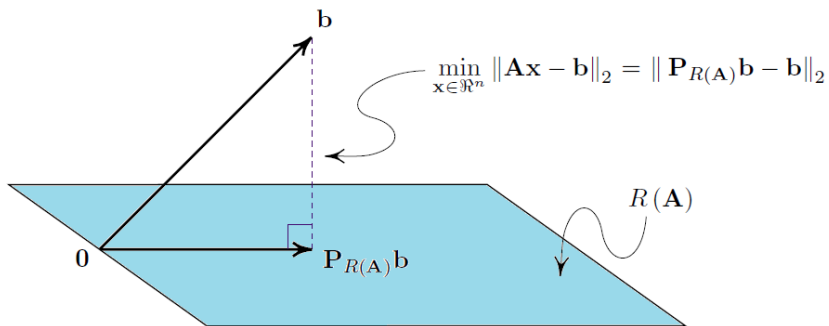
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Now  $A\mathbf{x} \in R(A)$ , so the **least squares error** is

$$\begin{aligned} \text{dist}(\mathbf{b}, R(A)) &= \min_{A\mathbf{x} \in R(A)} \|\mathbf{b} - A\mathbf{x}\|_2 \\ &= \|\mathbf{b} - P_{R(A)}\mathbf{b}\|_2 \end{aligned}$$

with  $P_{R(A)}$  the orthogonal projector onto  $R(A)$ .





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$$\begin{aligned} A\mathbf{x} &= P_{R(A)}\mathbf{b} \\ \iff P_{R(A)}A\mathbf{x} &= P_{R(A)}^2\mathbf{b} = P_{R(A)}\mathbf{b} \end{aligned}$$



Moreover, the **least squares solution** of  $A\mathbf{x} = \mathbf{b}$  is given by that  $\mathbf{x}$  for which

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### Remark

*No we are no longer limited to the real case.*

# References I

- [Mey00] Carl D. Meyer, *Matrix Analysis and Applied Linear Algebra*, SIAM, Philadelphia, PA, 2000.

