

# 模和内积

Norms and Inner Products

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# Vector Norms

- A significant portion of linear algebra is in fact geometric in nature.
- Much of the subject grew out of the need to generalize the basic geometry of  $\mathbb{R}^2$  and  $\mathbb{R}^3$  to nonvisual higher-dimensional spaces.
- The usual approach is to coordinatize geometric concepts in  $\mathbb{R}^2$  and  $\mathbb{R}^3$ , and then extend statements to ordered n-tuples in  $\mathbb{R}^n$  and  $\mathcal{C}^n$ .

## Euclidean Vector Norm

For a vector  $\mathbf{x}_{n \times 1}$ , the *euclidean norm* of  $\mathbf{x}$  is defined to be

- $\|\mathbf{x}\| = \left( \sum_{i=1}^n x_i^2 \right)^{1/2} = \sqrt{\mathbf{x}^T \mathbf{x}}$  whenever  $\mathbf{x} \in \mathbb{R}^{n \times 1}$ ,
- $\|\mathbf{x}\| = \left( \sum_{i=1}^n |x_i|^2 \right)^{1/2} = \sqrt{\mathbf{x}^* \mathbf{x}}$  whenever  $\mathbf{x} \in \mathcal{C}^{n \times 1}$ .

For example, if  $\mathbf{u} = \begin{pmatrix} 0 \\ -1 \\ 2 \\ -2 \\ 4 \end{pmatrix}$  and  $\mathbf{v} = \begin{pmatrix} i \\ 2 \\ 1-i \\ 0 \\ 1+i \end{pmatrix}$ , then

$$\|\mathbf{u}\| = \sqrt{\sum u_i^2} = \sqrt{\mathbf{u}^T \mathbf{u}} = \sqrt{0 + 1 + 4 + 4 + 16} = 5,$$

$$\|\mathbf{v}\| = \sqrt{\sum |v_i|^2} = \sqrt{\mathbf{v}^* \mathbf{v}} = \sqrt{1 + 4 + 2 + 0 + 2} = 3.$$

There are several points to note.

- The complex version of  $\|\mathbf{x}\|$  includes the real version as a special case because  $\|z\|^2 = z^2$  whenever  $z$  is a real number.
- The definition of euclidean norm guarantees that for all scalars  $\alpha$ ,

$$\|\mathbf{x}\| \geq 0, \quad \|\mathbf{x}\| = 0 \iff \mathbf{x} = 0, \quad \text{and} \quad \|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|.$$

- Given a vector  $\mathbf{x} \neq 0$ , we **normalize**  $\mathbf{x}$  by setting  $\mathbf{u} = \mathbf{x}/\|\mathbf{x}\|$ .
- The distance between vectors in  $\Re^3$  can be visualized with the aid of the parallelogram law. The distance between  $u$  and  $v$  is naturally defined to be  $\|\mathbf{u} - \mathbf{v}\|$ .

## Standard Inner Product

The scalar terms defined by

$$\mathbf{x}^T \mathbf{y} = \sum_{i=1}^n x_i y_i \in \Re \quad \text{and} \quad \mathbf{x}^* \mathbf{y} = \sum_{i=1}^n \bar{x}_i y_i \in \mathcal{C}$$

are called the ***standard inner products*** for  $\Re^n$  and  $\mathcal{C}^n$ , respectively.

- The Cauchy-Bunyakovskii-Schwarz(CBS) inequality is one of the most important inequalities, which relates inner product to norm.

## Cauchy–Bunyakovskii–Schwarz (CBS) Inequality

$$|\mathbf{x}^* \mathbf{y}| \leq \|\mathbf{x}\| \|\mathbf{y}\| \quad \text{for all } \mathbf{x}, \mathbf{y} \in \mathcal{C}^{n \times 1}.$$

Equality holds if and only if  $\mathbf{y} = \alpha \mathbf{x}$  for  $\alpha = \mathbf{x}^* \mathbf{y} / \mathbf{x}^* \mathbf{x}$ .

*Proof.* Set  $\alpha = \mathbf{x}^* \mathbf{y} / \mathbf{x}^* \mathbf{x} = \mathbf{x}^* \mathbf{y} / \|\mathbf{x}\|^2$  (assume  $\mathbf{x} \neq \mathbf{0}$  because there is nothing to prove if  $\mathbf{x} = \mathbf{0}$ ) and observe that  $\mathbf{x}^*(\alpha \mathbf{x} - \mathbf{y}) = 0$ , so

$$\begin{aligned} 0 &\leq \|\alpha \mathbf{x} - \mathbf{y}\|^2 = (\alpha \mathbf{x} - \mathbf{y})^* (\alpha \mathbf{x} - \mathbf{y}) = \bar{\alpha} \mathbf{x}^* (\alpha \mathbf{x} - \mathbf{y}) - \mathbf{y}^* (\alpha \mathbf{x} - \mathbf{y}) \\ &= -\mathbf{y}^* (\alpha \mathbf{x} - \mathbf{y}) = \mathbf{y}^* \mathbf{y} - \alpha \mathbf{y}^* \mathbf{x} = \frac{\|\mathbf{y}\|^2 \|\mathbf{x}\|^2 - (\mathbf{x}^* \mathbf{y})(\mathbf{y}^* \mathbf{x})}{\|\mathbf{x}\|^2}. \end{aligned}$$

Since  $\mathbf{y}^* \mathbf{x} = \overline{\mathbf{x}^* \mathbf{y}}$ , it follows that  $(\mathbf{x}^* \mathbf{y})(\mathbf{y}^* \mathbf{x}) = |\mathbf{x}^* \mathbf{y}|^2$ , so

$$0 \leq \frac{\|\mathbf{y}\|^2 \|\mathbf{x}\|^2 - |\mathbf{x}^* \mathbf{y}|^2}{\|\mathbf{x}\|^2}.$$

Now,  $0 < \|\mathbf{x}\|^2$  implies  $0 \leq \|\mathbf{y}\|^2 \|\mathbf{x}\|^2 - |\mathbf{x}^* \mathbf{y}|^2$ , and thus the CBS inequality is obtained. ■

# Triangle Inequality

$$\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\| \quad \text{for every } \mathbf{x}, \mathbf{y} \in \mathcal{C}^n.$$

*Proof.* Consider  $\mathbf{x}$  and  $\mathbf{y}$  to be column vectors, and write

$$\begin{aligned}\|\mathbf{x} + \mathbf{y}\|^2 &= (\mathbf{x} + \mathbf{y})^*(\mathbf{x} + \mathbf{y}) = \mathbf{x}^*\mathbf{x} + \mathbf{x}^*\mathbf{y} + \mathbf{y}^*\mathbf{x} + \mathbf{y}^*\mathbf{y} \\ &= \|\mathbf{x}\|^2 + \mathbf{x}^*\mathbf{y} + \mathbf{y}^*\mathbf{x} + \|\mathbf{y}\|^2.\end{aligned}$$

Recall that if  $z = a + ib$ , then  $z + \bar{z} = 2a = 2 \operatorname{Re}(z)$  and  $|z|^2 = a^2 + b^2 \geq a^2$ , so that  $|z| \geq \operatorname{Re}(z)$ . Using the fact that  $\mathbf{y}^*\mathbf{x} = \overline{\mathbf{x}^*\mathbf{y}}$  together with the CBS inequality yields

$$\mathbf{x}^*\mathbf{y} + \mathbf{y}^*\mathbf{x} = 2 \operatorname{Re}(\mathbf{x}^*\mathbf{y}) \leq 2 |\mathbf{x}^*\mathbf{y}| \leq 2 \|\mathbf{x}\| \|\mathbf{y}\|.$$

Consequently, we may infer that

$$\|\mathbf{x} + \mathbf{y}\|^2 \leq \|\mathbf{x}\|^2 + 2 \|\mathbf{x}\| \|\mathbf{y}\| + \|\mathbf{y}\|^2 = (\|\mathbf{x}\| + \|\mathbf{y}\|)^2. \blacksquare$$

- It's not difficult to see that the triangle inequality can be extended to any number of vectors in the sense that  $\|\sum_i \mathbf{x}_i\| \leq \sum_i \|\mathbf{x}_i\|$ .
- Furthermore, for real or complex numbers,  $|\sum_i \alpha_i| \leq \sum_i |\alpha_i|$ .

**Backward Triangle Inequality.** The triangle inequality produces an upper bound for a sum, but it also yields the following lower bound for a difference:

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

This is a consequence of the triangle inequality because

$$\|\mathbf{x}\| = \|\mathbf{x} - \mathbf{y} + \mathbf{y}\| \leq \|\mathbf{x} - \mathbf{y}\| + \|\mathbf{y}\| \implies \|\mathbf{x}\| - \|\mathbf{y}\| \leq \|\mathbf{x} - \mathbf{y}\|$$

and

$$\|\mathbf{y}\| = \|\mathbf{x} - \mathbf{y} - \mathbf{x}\| \leq \|\mathbf{x} - \mathbf{y}\| + \|\mathbf{x}\| \implies -(\|\mathbf{x}\| - \|\mathbf{y}\|) \leq \|\mathbf{x} - \mathbf{y}\|.$$

## p-Norms

For  $p \geq 1$ , the  **$p$ -norm** of  $\mathbf{x} \in \mathcal{C}^n$  is defined as  $\|\mathbf{x}\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$ .

It can be proven that the following properties of the euclidean norm are in fact valid for all p-norms:

$$\|\mathbf{x}\|_p \geq 0 \quad \text{and} \quad \|\mathbf{x}\|_p = 0 \iff \mathbf{x} = \mathbf{0},$$

$$\|\alpha\mathbf{x}\|_p = |\alpha| \|\mathbf{x}\|_p \quad \text{for all scalars } \alpha,$$

$$\|\mathbf{x} + \mathbf{y}\|_p \leq \|\mathbf{x}\|_p + \|\mathbf{y}\|_p$$

- The generalized version of the CBS inequality for p-norm is Hölder's inequality.
- If  $p > 1$  and  $q > 1$  are real numbers such that  $1/p + 1/q = 1$ , then  $|\mathbf{x}^*\mathbf{y}| \leq \|\mathbf{x}\|_p \|\mathbf{y}\|_q$ .

In practice, only three of the p-norms are used, and they are

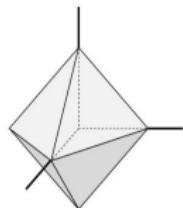
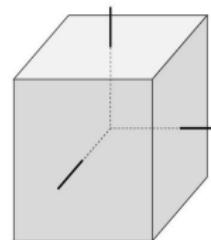
$$\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i| \quad (\text{the grid norm}), \quad \|\mathbf{x}\|_2 = \left( \sum_{i=1}^n |x_i|^2 \right)^{1/2} \quad (\text{the euclidean norm}),$$

and

$$\|\mathbf{x}\|_\infty = \lim_{p \rightarrow \infty} \|\mathbf{x}\|_p = \lim_{p \rightarrow \infty} \left( \sum_{i=1}^n |x_i|^p \right)^{1/p} = \max_i |x_i| \quad (\text{the max norm}).$$

- To get a feel for the 1-, 2- and  $\infty$ -norms, it helps to know the shapes and relative sizes of the unit p-sphere  $S_P = \{\mathbf{x} \mid \|\mathbf{x}\|_p = 1\}$  for  $p = 1, 2, \infty$ .
- the unit 1-, 2- and  $\infty$ -spheres in  $\Re^3$  are an octahedron, a ball and a cube, respectively.

- It's visually evident that  $S_1$  fits inside  $S_2$ , which in turn fits inside  $S_\infty$ .

 $S_1$  $S_2$  $S_\infty$ 

- This means that  $\|\mathbf{x}\|_1 \geq \|\mathbf{x}\|_2 \geq \|\mathbf{x}\|_\infty$  for all  $\mathbf{x} \in \Re^3$ .
- In general, this is true in  $\Re^n$ .
- Because the p-norms are defined in terms of coordinates, their use is limited to coordinate spaces.
- It's desirable to have a general notion of norm that works for all vector spaces.
- In other words, we need a coordinate-free definition of norm that includes the standard p-norms as a special case.

## General Vector Norms

A **norm** for a real or complex vector space  $\mathcal{V}$  is a function  $\|\star\|$  mapping  $\mathcal{V}$  into  $\mathbb{R}$  that satisfies the following conditions.

$$\begin{aligned}\|\mathbf{x}\| &\geq 0 \quad \text{and} \quad \|\mathbf{x}\| = 0 \iff \mathbf{x} = \mathbf{0}, \\ \|\alpha \mathbf{x}\| &= |\alpha| \|\mathbf{x}\| \quad \text{for all scalars } \alpha, \\ \|\mathbf{x} + \mathbf{y}\| &\leq \|\mathbf{x}\| + \|\mathbf{y}\|.\end{aligned}$$

- Vector norms are basic tools for defining and analyzing limiting behavior in vector spaces  $\mathcal{V}$ .
- A sequence  $\{\mathbf{x}_k\} \subset \mathcal{V}$  is said to converge to  $\mathbf{x}$  if  $\|\mathbf{x}_k - \mathbf{x}\| \rightarrow 0$ .
- This depends on the choice of the norm, so, we might have  $\mathbf{x}_k \rightarrow \mathbf{x}$  with one norm but not with another.
- Fortunately, this is impossible in finite-dimensional spaces because all norms are equivalent in the following sense.
- For each pair of norms,  $\|\cdot\|_a$ ,  $\|\cdot\|_b$  on an  $n$ -dimensional space  $\mathcal{V}$ , they are equivalent if there exist constants  $\alpha$  and  $\beta$  such that for all nonzero vectors,

$$\alpha \|\mathbf{x}\|_b \leq \|\mathbf{x}\|_a \leq \beta \|\mathbf{x}\|_b.$$

# Matrix Norms

- Because  $\mathcal{C}^{m \times n}$  is a vector space of dimension  $mn$ , magnitudes of  $\mathbf{A} \in \mathcal{C}^{m \times n}$  can be measured by employing any vector norm on  $\mathcal{C}^{mn}$ .
- This is one of the simplest notions of a matrix norm, called the *Frobenius norm (or Schur norm)*.

## Frobenius Matrix Norm

The *Frobenius norm* of  $\mathbf{A} \in \mathcal{C}^{m \times n}$  is defined by the equations

$$\|\mathbf{A}\|_F^2 = \sum_{i,j} |a_{ij}|^2 = \sum_i \|\mathbf{A}_{i*}\|_2^2 = \sum_j \|\mathbf{A}_{*j}\|_2^2 = \text{trace}(\mathbf{A}^* \mathbf{A}).$$

- The Frobenius matrix norm is not well suited for all applications.
- Similar to the situation for vector norms, alternatives need to be explored.
- It makes sense to first formulate a general definition a matrix norm.

- Matrix multiplication distinguishes matrix spaces from more general vector spaces, but the three vector-norm properties say nothing about products.
- So, an extra property that relates  $\|\mathbf{AB}\|$  to  $\|\mathbf{A}\|$  and  $\|\mathbf{B}\|$  is needed.
- Frobenius norm suggests the nature of this extra property.
- The CBS inequality insures that

$$\|\mathbf{Ax}\|_2^2 = \sum_i |\mathbf{A}_{i*} \mathbf{x}|^2 \leq \sum_i \|\mathbf{A}_{i*}\|_2^2 \|\mathbf{x}\|_2^2 = \|\mathbf{A}\|_F^2 \|\mathbf{x}\|_2^2. \text{ That is,}$$

$$\|\mathbf{Ax}\|_2 \leq \|\mathbf{A}\|_F \|\mathbf{x}\|_2,$$

and we express this by saying that the Frobenius matrix norm  $\|\star\|_F$  and the Euclidean vector norm  $\|\star\|_2$  are *compatible*. The compatibility condition implies that for all conformable matrices  $\mathbf{A}$  and  $\mathbf{B}$ ,

$$\begin{aligned} \|\mathbf{AB}\|_F^2 &= \sum_j \|[\mathbf{AB}]_{*j}\|_2^2 = \sum_j \|\mathbf{AB}_{*j}\|_2^2 \leq \sum_j \|\mathbf{A}\|_F^2 \|\mathbf{B}_{*j}\|_2^2 \\ &= \|\mathbf{A}\|_F^2 \sum_j \|\mathbf{B}_{*j}\|_2^2 = \|\mathbf{A}\|_F^2 \|\mathbf{B}\|_F^2 \implies \|\mathbf{AB}\|_F \leq \|\mathbf{A}\|_F \|\mathbf{B}\|_F. \end{aligned}$$

## General Matrix Norms

A **matrix norm** is a function  $\|\star\|$  from the set of all complex matrices (of all finite orders) into  $\mathbb{R}$  that satisfies the following properties.

$$\|\mathbf{A}\| \geq 0 \quad \text{and} \quad \|\mathbf{A}\| = 0 \iff \mathbf{A} = \mathbf{0}.$$

$$\|\alpha \mathbf{A}\| = |\alpha| \|\mathbf{A}\| \quad \text{for all scalars } \alpha.$$

$$\|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\| \quad \text{for matrices of the same size.}$$

$$\|\mathbf{AB}\| \leq \|\mathbf{A}\| \|\mathbf{B}\| \quad \text{for all conformable matrices.}$$

- The Frobenius norm satisfies the above definition, but where do other matrix norms come from?
- In fact, every legitimate vector norm generates a matrix norm.

## Induced Matrix Norms

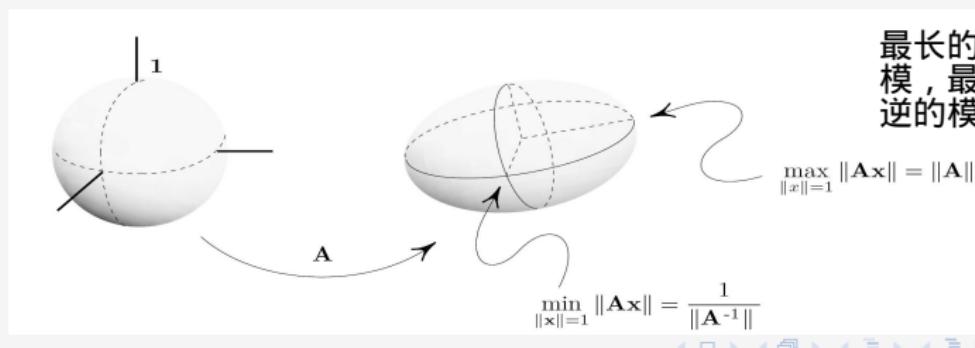
A vector norm that is defined on  $\mathcal{C}^p$  for  $p = m, n$  *induces* a matrix norm on  $\mathcal{C}^{m \times n}$  by setting

$$\|\mathbf{A}\| = \max_{\|\mathbf{x}\|=1} \|\mathbf{Ax}\| \quad \text{for } \mathbf{A} \in \mathcal{C}^{m \times n}, \quad \mathbf{x} \in \mathcal{C}^{n \times 1}.$$

- It's apparent that an induced matrix norm is compatible with its underlying vector norm in the sense that

$$\|\mathbf{Ax}\| \leq \|\mathbf{A}\| \|\mathbf{x}\|.$$

- When  $\mathbf{A}$  is nonsingular,  $\min_{\|\mathbf{x}\|=1} \|\mathbf{Ax}\| = \frac{1}{\|\mathbf{A}^{-1}\|}$ .
- In words, an induced norm  $\|\mathbf{A}\|$  represents the maximum extent to which a vector on the unit sphere can be stretched by  $\mathbf{A}$ .
- $1/\|\mathbf{A}^{-1}\|$  measures the extent to which a nonsingular matrix  $\mathbf{A}$  can shrink vectors on the unit sphere.



## Matrix 2-Norm

- The matrix norm induced by the Euclidean vector norm is

$$\|\mathbf{A}\|_2 = \max_{\|\mathbf{x}\|_2=1} \|\mathbf{Ax}\|_2 = \sqrt{\lambda_{\max}},$$

where  $\lambda_{\max}$  is the largest number  $\lambda$  such that  $\mathbf{A}^* \mathbf{A} - \lambda \mathbf{I}$  is singular.

- When  $\mathbf{A}$  is nonsingular,

$$\|\mathbf{A}^{-1}\|_2 = \frac{1}{\min_{\|\mathbf{x}\|_2=1} \|\mathbf{Ax}\|_2} = \frac{1}{\sqrt{\lambda_{\min}}},$$

where  $\lambda_{\min}$  is the smallest number  $\lambda$  such that  $\mathbf{A}^* \mathbf{A} - \lambda \mathbf{I}$  is singular.

**Problem:** Determine the induced norm  $\|\mathbf{A}\|_2$  as well as  $\|\mathbf{A}^{-1}\|_2$  for the nonsingular matrix

$$\mathbf{A} = \frac{1}{\sqrt{3}} \begin{pmatrix} 3 & -1 \\ 0 & \sqrt{8} \end{pmatrix}.$$

**Solution:** Find the values of  $\lambda$  that make  $\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I}$  singular by applying Gaussian elimination to produce

$$\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I} = \begin{pmatrix} 3-\lambda & -1 \\ -1 & 3-\lambda \end{pmatrix} \rightarrow \begin{pmatrix} -1 & 3-\lambda \\ 3-\lambda & -1 \end{pmatrix} \rightarrow \begin{pmatrix} -1 & 3-\lambda \\ 0 & -1 + (3-\lambda)^2 \end{pmatrix}.$$

This shows that  $\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I}$  is singular when  $-1 + (3-\lambda)^2 = 0$  or, equivalently, when  $\lambda = 2$  or  $\lambda = 4$ , so  $\lambda_{\min} = 2$  and  $\lambda_{\max} = 4$ . Consequently,

$$\|\mathbf{A}\|_2 = \sqrt{\lambda_{\max}} = 2 \quad \text{and} \quad \|\mathbf{A}^{-1}\|_2 = \frac{1}{\sqrt{\lambda_{\min}}} = \frac{1}{\sqrt{2}}.$$

- Note:  $\lambda_{\max}$  and  $\lambda_{\min}$  are the largest and smallest eigenvalues of  $\mathbf{A}^* \mathbf{A}$ .

## Properties of the 2-Norm

In addition to the properties shared by all induced norms, the 2-norm enjoys the following special properties.

- $\|\mathbf{A}\|_2 = \max_{\|\mathbf{x}\|_2=1} \max_{\|\mathbf{y}\|_2=1} |\mathbf{y}^* \mathbf{A} \mathbf{x}|.$
- $\|\mathbf{A}\|_2 = \|\mathbf{A}^*\|_2.$
- $\|\mathbf{A}^* \mathbf{A}\|_2 = \|\mathbf{A}\|_2^2.$
- $\left\| \begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{B} \end{pmatrix} \right\|_2 = \max \{ \|\mathbf{A}\|_2, \|\mathbf{B}\|_2 \}.$
- $\|\mathbf{U}^* \mathbf{A} \mathbf{V}\|_2 = \|\mathbf{A}\|_2$  when  $\mathbf{U} \mathbf{U}^* = \mathbf{I}$  and  $\mathbf{V}^* \mathbf{V} = \mathbf{I}$ .

- Let's investigate the nature of the matrix norms that are induced by the vector 1-norm and the vector  $\infty$ -norm.

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

The matrix norms induced by the vector 1-norm and  $\infty$ -norm are as follows.

- $\|\mathbf{A}\|_1 = \max_{\|\mathbf{x}\|_1=1} \|\mathbf{Ax}\|_1 = \max_j \sum_i |a_{ij}|$   
= the largest absolute column sum.
- $\|\mathbf{A}\|_\infty = \max_{\|\mathbf{x}\|_\infty=1} \|\mathbf{Ax}\|_\infty = \max_i \sum_j |a_{ij}|$   
= the largest absolute row sum.

For all  $\mathbf{x}$  with  $\|\mathbf{x}\|_1 = 1$ , the scalar triangle inequality yields

$$\begin{aligned}\|\mathbf{Ax}\|_1 &= \sum_i |\mathbf{A}_{i*} \mathbf{x}| = \sum_i \left| \sum_j a_{ij} x_j \right| \leq \sum_i \sum_j |a_{ij}| |x_j| = \sum_j \left( |x_j| \sum_i |a_{ij}| \right) \\ &\leq \left( \sum_j |x_j| \right) \left( \max_j \sum_i |a_{ij}| \right) = \max_j \sum_i |a_{ij}|.\end{aligned}$$

Equality can be attained because if  $\mathbf{A}_{*k}$  is the column with largest absolute sum, set  $\mathbf{x} = \mathbf{e}_k$ , and note that  $\|\mathbf{e}_k\|_1 = 1$  and  $\|\mathbf{Ae}_k\|_1 = \|\mathbf{A}_{*k}\|_1 = \max_j \sum_i |a_{ij}|$ .

- For all  $n \times n$  matrices, it can be shown that  $\|\mathbf{A}\|_i \leq \alpha \|\mathbf{A}\|_j$ , where  $\alpha$  is the  $(i,j)$ -entry in the following matrix

|          | 1          | 2          | $\infty$   | $F$        |
|----------|------------|------------|------------|------------|
| 1        | *          | $\sqrt{n}$ | $n$        | $\sqrt{n}$ |
| 2        | $\sqrt{n}$ | *          | $\sqrt{n}$ | 1          |
| $\infty$ | $n$        | $\sqrt{n}$ | *          | $\sqrt{n}$ |
| $F$      | $\sqrt{n}$ | $\sqrt{n}$ | $\sqrt{n}$ | *          |

矩阵范数的等价性

- $\|\mathbf{A}\|_2$  is difficult to compute in comparison with  $\|\mathbf{A}\|_1$ ,  $\|\mathbf{A}\|_\infty$  and  $\|\mathbf{A}\|_F$ .

**Problem:** Determine the induced matrix norms  $\|\mathbf{A}\|_1$  and  $\|\mathbf{A}\|_\infty$  for

$$\mathbf{A} = \frac{1}{\sqrt{3}} \begin{pmatrix} 3 & -1 \\ 0 & \sqrt{8} \end{pmatrix},$$

and compare the results with  $\|\mathbf{A}\|_2$  and  $\|\mathbf{A}\|_F$ .

- $\|\mathbf{A}\|_1 = \frac{1}{\sqrt{3}} + \frac{\sqrt{8}}{\sqrt{3}} \approx 2.21$ ,  $\|\mathbf{A}\|_\infty = \frac{4}{\sqrt{3}} \approx 2.31$ ,  $\|\mathbf{A}\|_F = \sqrt{6} \approx 2.45$ .
- Now, compute  $\|\mathbf{A}\|_2$ .

Find the values of  $\lambda$  that make  $\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I}$  singular by applying Gaussian elimination to produce

$$\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I} = \begin{pmatrix} 3-\lambda & -1 \\ -1 & 3-\lambda \end{pmatrix} \xrightarrow{\quad} \begin{pmatrix} -1 & 3-\lambda \\ 3-\lambda & -1 \end{pmatrix} \xrightarrow{\quad} \begin{pmatrix} -1 & 3-\lambda \\ 0 & -1 + (3-\lambda)^2 \end{pmatrix}.$$

This shows that  $\mathbf{A}^T \mathbf{A} - \lambda \mathbf{I}$  is singular when  $-1 + (3-\lambda)^2 = 0$  or, equivalently, when  $\lambda = 2$  or  $\lambda = 4$ , so  $\lambda_{\min} = 2$  and  $\lambda_{\max} = 4$ .

$$\|\mathbf{A}\|_2 = \sqrt{\lambda_{\max}} = 2 \quad \text{and} \quad \|\mathbf{A}^{-1}\|_2 = \frac{1}{\sqrt{\lambda_{\min}}} = \frac{1}{\sqrt{2}}.$$

# Inner-Product Spaces

## General Inner Product

An **inner product** on a real (or complex) vector space  $\mathcal{V}$  is a function that maps each ordered pair of vectors  $\mathbf{x}, \mathbf{y}$  to a real (or complex) scalar  $\langle \mathbf{x} | \mathbf{y} \rangle$  such that the following four properties hold.

- $\langle \mathbf{x} | \mathbf{x} \rangle$  is real with  $\langle \mathbf{x} | \mathbf{x} \rangle \geq 0$ , and  $\langle \mathbf{x} | \mathbf{x} \rangle = 0$  if and only if  $\mathbf{x} = \mathbf{0}$ ,
- $\langle \mathbf{x} | \alpha \mathbf{y} \rangle = \alpha \langle \mathbf{x} | \mathbf{y} \rangle$  for all scalars  $\alpha$ ,
- $\langle \mathbf{x} | \mathbf{y} + \mathbf{z} \rangle = \langle \mathbf{x} | \mathbf{y} \rangle + \langle \mathbf{x} | \mathbf{z} \rangle$ ,
- $\langle \mathbf{x} | \mathbf{y} \rangle = \overline{\langle \mathbf{y} | \mathbf{x} \rangle}$  (for real spaces, this becomes  $\langle \mathbf{x} | \mathbf{y} \rangle = \langle \mathbf{y} | \mathbf{x} \rangle$ ).

Notice that for each fixed value of  $\mathbf{x}$ , the second and third properties say that  $\langle \mathbf{x} | \mathbf{y} \rangle$  is a linear function of  $\mathbf{y}$ .

Any real or complex vector space that is equipped with an inner product is called an **inner-product space**.

## Some examples:

- ▶ The standard inner products  $\langle \mathbf{x} | \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y}$  for  $\Re^{n \times 1}$  and  $\langle \mathbf{x} | \mathbf{y} \rangle = \mathbf{x}^* \mathbf{y}$  for  $\mathcal{C}^{n \times 1}$ , satisfy the above four defining conditions.
- ▶ If  $\mathbf{A}_{n \times n}$  is a nonsingular matrix, then  $\langle \mathbf{x} | \mathbf{y} \rangle = \mathbf{x}^* \mathbf{A}^* \mathbf{A} \mathbf{y}$  is an inner product for  $\mathcal{C}^{n \times 1}$ . This inner product is sometimes called an **A-inner product** or an **elliptical inner product**.

- ▶ Consider the vector space of  $m \times n$  matrices. The functions defined by

$$\langle \mathbf{A} | \mathbf{B} \rangle = \text{trace}(\mathbf{A}^T \mathbf{B}) \quad \text{and} \quad \langle \mathbf{A} | \mathbf{B} \rangle = \text{trace}(\mathbf{A}^* \mathbf{B})$$

are inner products for  $\mathfrak{R}^{m \times n}$  and  $\mathcal{C}^{m \times n}$ , respectively. These are referred to as the **standard inner products for matrices**.

- ▶ If  $\mathcal{V}$  is the vector space of real-valued continuous functions defined on the interval  $(a, b)$ , then

$$\langle f | g \rangle = \int_a^b f(t)g(t)dt$$

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

- Every general inner product in an inner-product space  $\mathcal{V}$  defines a norm on  $\mathcal{V}$  by setting

$$\| * \| = \sqrt{\langle * | * \rangle}.$$

## General CBS Inequality

If  $\mathcal{V}$  is an inner-product space, and if we set  $\| \star \| = \sqrt{\langle \star | \star \rangle}$ , then

$$| \langle \mathbf{x} | \mathbf{y} \rangle | \leq \| \mathbf{x} \| \| \mathbf{y} \| \quad \text{for all } x, y \in \mathcal{V}.$$

Equality holds if and only if  $\mathbf{y} = \alpha \mathbf{x}$  for  $\alpha = \langle \mathbf{x} | \mathbf{y} \rangle / \| \mathbf{x} \|^2$ .

*Proof.* Set  $\alpha = \langle \mathbf{x} | \mathbf{y} \rangle / \|\mathbf{x}\|^2$  (assume  $\mathbf{x} \neq \mathbf{0}$ , for otherwise there is nothing to prove), and observe that  $\langle \mathbf{x} | \alpha \mathbf{x} - \mathbf{y} \rangle = 0$ , so

$$\begin{aligned} 0 &\leq \|\alpha \mathbf{x} - \mathbf{y}\|^2 = \langle \alpha \mathbf{x} - \mathbf{y} | \alpha \mathbf{x} - \mathbf{y} \rangle \\ &= \bar{\alpha} \langle \mathbf{x} | \alpha \mathbf{x} - \mathbf{y} \rangle - \langle \mathbf{y} | \alpha \mathbf{x} - \mathbf{y} \rangle \\ &= -\langle \mathbf{y} | \alpha \mathbf{x} - \mathbf{y} \rangle = \langle \mathbf{y} | \mathbf{y} \rangle - \alpha \langle \mathbf{y} | \mathbf{x} \rangle = \frac{\|\mathbf{y}\|^2 \|\mathbf{x}\|^2 - \langle \mathbf{x} | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{x} \rangle}{\|\mathbf{x}\|^2}. \end{aligned}$$

Since  $\langle \mathbf{y} | \mathbf{x} \rangle = \overline{\langle \mathbf{x} | \mathbf{y} \rangle}$ , it follows that  $\langle \mathbf{x} | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{x} \rangle = |\langle \mathbf{x} | \mathbf{y} \rangle|^2$ , so

$$0 \leq \frac{\|\mathbf{y}\|^2 \|\mathbf{x}\|^2 - |\langle \mathbf{x} | \mathbf{y} \rangle|^2}{\|\mathbf{x}\|^2} \implies |\langle \mathbf{x} | \mathbf{y} \rangle| \leq \|\mathbf{x}\| \|\mathbf{y}\|. \blacksquare$$

## Norms in Inner-Product Spaces

If  $\mathcal{V}$  is an inner-product space with an inner product  $\langle \mathbf{x} | \mathbf{y} \rangle$ , then

$$\|\star\| = \sqrt{\langle \star | \star \rangle} \text{ defines a norm on } \mathcal{V}.$$

## ■ The norms generated by the above inner products.

- Given a nonsingular matrix  $\mathbf{A} \in \mathcal{C}^{n \times n}$ , the  **$\mathbf{A}$ -norm** (or *elliptical norm*) generated by the  $\mathbf{A}$ -inner product on  $\mathcal{C}^{n \times 1}$  is

$$\|\mathbf{x}\|_{\mathbf{A}} = \sqrt{\langle \mathbf{x} | \mathbf{x} \rangle} = \sqrt{\mathbf{x}^* \mathbf{A}^* \mathbf{A} \mathbf{x}} = \|\mathbf{A}\mathbf{x}\|_2.$$

- The standard inner product for matrices generates the Frobenius matrix norm because

$$\|\mathbf{A}\| = \sqrt{\langle \mathbf{A} | \mathbf{A} \rangle} = \sqrt{\text{trace}(\mathbf{A}^* \mathbf{A})} = \|\mathbf{A}\|_F.$$

- For the space of real-valued continuous functions defined on  $(a, b)$ , the norm of a function  $f$  generated by the inner product  $\langle f | g \rangle = \int_a^b f(t)g(t)dt$  is

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

- To illustrate the utility of the ideas presented above, consider how to prove

$$\text{trace}(\mathbf{A}^T \mathbf{B})^2 \leq \text{trace}(\mathbf{A}^T \mathbf{A}) \text{trace}(\mathbf{B}^T \mathbf{B})$$

- Since each inner product generates a norm, it's natural to ask if the reverse is also true.
- That is, for each vector norm, does there exist a corresponding inner product?
- If not, under what conditions will a given norm be generated by an inner product?
- Maurice R. Fréchet and John Von Neumann provide the answer.

## Parallelogram Identity

For a given norm  $\|\star\|$  on a vector space  $\mathcal{V}$ , there exists an inner product on  $\mathcal{V}$  such that  $\langle \star | \star \rangle = \|\star\|^2$  if and only if the *parallelogram identity*

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

holds for all  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$ .

- The parallelogram identity expresses the fact that the sum of the squares of the diagonals in a parallelogram is twice the sum of the squares of the sides.

- **Problem:** Except for the euclidean norm, is any other vector p-norm generated by an inner product?
- No, because the parallelogram identity doesn't hold when  $p \neq 2$ . When  $p \neq 2$ , consider  $\mathbf{x} = \mathbf{e}_1$  and  $\mathbf{y} = \mathbf{e}_2$ . It's apparent that

$$\|\mathbf{e}_1 + \mathbf{e}_2\|_p^2 = 2^{2/p} = \|\mathbf{e}_1 - \mathbf{e}_2\|_p^2,$$

so

$$\|\mathbf{e}_1 + \mathbf{e}_2\|_p^2 + \|\mathbf{e}_1 - \mathbf{e}_2\|_p^2 = 2^{(p+2)/p} \quad \text{and} \quad 2(\|\mathbf{e}_1\|_p^2 + \|\mathbf{e}_2\|_p^2) = 4.$$

Clearly,  $2^{(p+2)/p} = 4$  only when  $p = 2$ .

- For applications that are best analyzed in the context of an inner product space (e.g., least squares problems), we are limited to the euclidean norm or else to one of its variation such as the elliptical norm.

# Orthogonal Vectors

- Two vectors in  $\Re^3$  are orthogonal (perpendicular) if the angle between them is a right angle ( $90^\circ$ ).
- $\mathbf{u}$  and  $\mathbf{v}$  are orthogonal if and only if  $\|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 = \|\mathbf{u} - \mathbf{v}\|^2$ .
- we can rewrite

$$\begin{aligned} 0 &= \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - \|\mathbf{u} - \mathbf{v}\|^2 = \mathbf{u}^T \mathbf{u} + \mathbf{v}^T \mathbf{v} - (\mathbf{u} - \mathbf{v})^T (\mathbf{u} - \mathbf{v}) \\ &= \mathbf{u}^T \mathbf{u} + \mathbf{v}^T \mathbf{v} - (\mathbf{u}^T \mathbf{u} - \mathbf{u}^T \mathbf{v} - \mathbf{v}^T \mathbf{u} + \mathbf{v}^T \mathbf{v}) = 2\mathbf{u}^T \mathbf{v} \end{aligned}$$

- Therefore,  $\mathbf{u}$  and  $\mathbf{v}$  are orthogonal vectors in  $\Re^3$  if and only if  $\mathbf{u}^T \mathbf{v} = 0$ .
- The natural extension of this provides us with a definition in more general spaces.

## Orthogonality

In an inner-product space  $\mathcal{V}$ , two vectors  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  are said to be ***orthogonal*** (to each other) whenever  $\langle \mathbf{x} | \mathbf{y} \rangle = 0$ , and this is denoted by writing  $\mathbf{x} \perp \mathbf{y}$ .

- For  $\Re^n$  with the standard inner product,  $\mathbf{x} \perp \mathbf{y} \iff \mathbf{x}^T \mathbf{y} = 0$ .
- For  $\mathcal{C}^n$  with the standard inner product,  $\mathbf{x} \perp \mathbf{y} \iff \mathbf{x}^* \mathbf{y} = 0$ .



- Now that "right angles" in higher dimensions make sense, how can more general angles be defined?

## Angles

In a real inner-product space  $\mathcal{V}$ , the radian measure of the *angle* between nonzero vectors  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  is defined to be the number  $\theta \in [0, \pi]$  such that

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

## Orthonormal Sets

$\mathcal{B} = \{ \mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n \}$  is called an *orthonormal set* whenever  $\| \mathbf{u}_i \| = 1$  for each  $i$ , and  $\mathbf{u}_i \perp \mathbf{u}_j$  for all  $i \neq j$ . In other words,

$$\langle \mathbf{u}_i | \mathbf{u}_j \rangle = \begin{cases} 1 & \text{when } i = j, \\ 0 & \text{when } i \neq j. \end{cases}$$

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

- The set  $\mathcal{B} = \{\mathbf{u}_1 = (1, -1, 0)^T, \mathbf{u}_2 = (1, 1, 1)^T, \mathbf{u}_3 = (-1, -1, 2)^T\}$  is a set of mutually orthogonal vectors, but it is not an orthonormal set.
- The most common orthonormal basis is  $\mathcal{S} = \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ , the standard basis for  $\mathbb{R}^n$  and  $\mathcal{S}^n$ .
- An important function of the standard basis  $\mathcal{S}$  for  $\mathbb{R}^n$  is to provide coordinate representations.
- Another orthonormal basis  $\mathcal{B}$  must amount to some rotation of  $\mathcal{S}$ , which is expected to provide essentially the same advantages as the standard basis.

## Fourier Expansions

If  $\mathcal{B} = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$  is an orthonormal basis for an inner-product space  $\mathcal{V}$ , then each  $\mathbf{x} \in \mathcal{V}$  can be expressed as

$$\mathbf{x} = \langle \mathbf{u}_1 | \mathbf{x} \rangle \mathbf{u}_1 + \langle \mathbf{u}_2 | \mathbf{x} \rangle \mathbf{u}_2 + \cdots + \langle \mathbf{u}_n | \mathbf{x} \rangle \mathbf{u}_n.$$

x在各个基  
上的投影

This is called the ***Fourier expansion*** of  $\mathbf{x}$ . The scalars  $\xi_i = \langle \mathbf{u}_i | \mathbf{x} \rangle$  are the coordinates of  $\mathbf{x}$  with respect to  $\mathcal{B}$ , and they are called the ***Fourier coefficients***. Geometrically, the Fourier expansion resolves  $\mathbf{x}$  into  $n$  mutually orthogonal vectors  $\langle \mathbf{u}_i | \mathbf{x} \rangle \mathbf{u}_i$ , each of which represents the orthogonal projection of  $\mathbf{x}$  onto the space (line) spanned by  $\mathbf{u}_i$ .

## ■ Fourier Series

- ▶ Let  $\mathcal{V}$  be the inner-product space of real-valued functions that are integrable on the interval  $(-\pi, \pi)$  and where the inner product and norm are given by

$$\langle f|g \rangle = \int_{-\pi}^{\pi} f(t)g(t) \quad \text{and} \quad \|f\| = \left( \int_{-\pi}^{\pi} f^2(t)dt \right)^{1/2}.$$

- ▶ The set of

$$\mathcal{B} = \left\{ \frac{1}{\sqrt{2\pi}}, \frac{\cos t}{\sqrt{\pi}}, \frac{\cos 2t}{\sqrt{\pi}}, \dots, \frac{\sin t}{\sqrt{\pi}}, \frac{\sin 2t}{\sqrt{\pi}}, \dots \right\}$$

produces the orthonormal set.

- ▶ Given an arbitrary  $f \in \mathcal{V}$ , we construct its Fourier expansion

$$F(t) = \alpha_0 \frac{1}{\sqrt{2\pi}} + \sum_{k=1}^{\infty} \alpha_k \frac{\cos kt}{\sqrt{\pi}} + \sum_{k=1}^{\infty} \beta_k \frac{\sin kt}{\sqrt{\pi}},$$

- The Fourier coefficients are given by

$$\alpha_0 = \left\langle \frac{1}{\sqrt{2\pi}} \Big| f \right\rangle, \quad \alpha_k = \left\langle \frac{\cos kt}{\sqrt{\pi}} \Big| f \right\rangle, \quad \beta_k = \left\langle \frac{\sin kt}{\sqrt{\pi}} \Big| f \right\rangle.$$

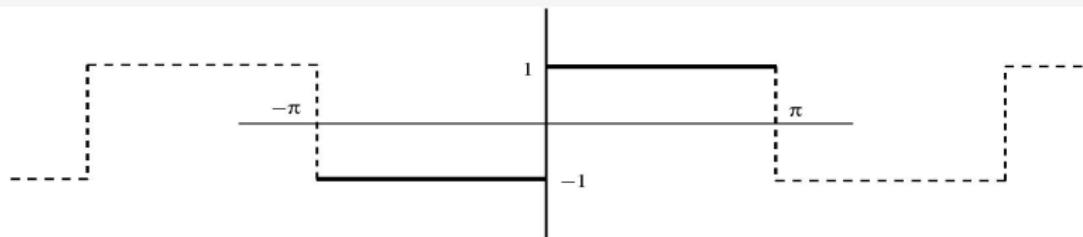
- Substituting these coefficients produces the infinite series

$$F(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nt + b_n \sin nt),$$

where  $a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos nt dt$  and  $b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sin nt dt$ .

- It is called the Fourier series expansion for  $f(t)$ .
- $F(t)$  need not agree with the original function  $f(t)$ .
- If  $f(t)$  is aperiodic function with period  $2\pi$  that is sectionally continuous on the interval  $(-\pi, \pi)$ , then the Fourier series  $F(t)$  converges to  $f(t)$  at each  $t \in (-\pi, \pi)$ , where  $f$  is continuous.
- For example,  $f(t) = \begin{cases} -1 & \text{when } -\pi < t < 0, \\ 1 & \text{when } 0 < t < \pi \end{cases}$ ,  $a_n = 0$ ,

$$b_n = \frac{2}{n\pi} (1 - \cos n\pi)$$



To find the Fourier series expansion for  $f$ , compute the coefficients as

$$\begin{aligned} a_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos nt dt = \frac{1}{\pi} \int_{-\pi}^0 -\cos nt dt + \frac{1}{\pi} \int_0^{\pi} \cos nt dt \\ &= 0, \end{aligned}$$

$$\begin{aligned} b_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sin nt dt = \frac{1}{\pi} \int_{-\pi}^0 -\sin nt dt + \frac{1}{\pi} \int_0^{\pi} \sin nt dt \\ &= \frac{2}{n\pi} (1 - \cos n\pi) = \begin{cases} 0 & \text{when } n \text{ is even,} \\ 4/n\pi & \text{when } n \text{ is odd,} \end{cases} \end{aligned}$$

so that

$$F(t) = \frac{4}{\pi} \sin t + \frac{4}{3\pi} \sin 3t + \frac{4}{5\pi} \sin 5t + \dots = \sum_{n=1}^{\infty} \frac{4}{(2n-1)\pi} \sin((2n-1)t).$$

# Gram-Schmidt Procedure

- Orthonormal bases possess significant advantages over bases that are not orthonormal.
- Does every finite dimensional space possess an orthonormal basis, and, if so, how can one be produced?
- The GramSchmidt orthogonalization procedure developed below answers these questions.

Let  $\mathcal{B} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  be an arbitrary basis (not necessarily orthonormal) for an  $n$ -dimensional inner-product space  $\mathcal{S}$ , and remember that  $\|\star\| = \langle \star | \star \rangle^{1/2}$ .

**Objective:** Use  $\mathcal{B}$  to construct an orthonormal basis  $\mathcal{O} = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$  for  $\mathcal{S}$ .

**Strategy:** Construct  $\mathcal{O}$  sequentially so that  $\mathcal{O}_k = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k\}$  is an orthonormal basis for  $\mathcal{S}_k = \text{span}\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$  for  $k = 1, \dots, n$ .

For  $k = 1$ , simply take  $\mathbf{u}_1 = \mathbf{x}_1 / \|\mathbf{x}_1\|$ . It's clear that  $\mathcal{O}_1 = \{\mathbf{u}_1\}$  is an orthonormal set whose span agrees with that of  $\mathcal{S}_1 = \{\mathbf{x}_1\}$ . Now reason inductively. Suppose that  $\mathcal{O}_k = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k\}$  is an orthonormal basis for  $\mathcal{S}_k = \text{span}\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$ , and consider the problem of finding one additional vector  $\mathbf{u}_{k+1}$  such that  $\mathcal{O}_{k+1} = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k, \mathbf{u}_{k+1}\}$  is an orthonormal basis for  $\mathcal{S}_{k+1} = \text{span}\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k, \mathbf{x}_{k+1}\}$ . For this to hold, the Fourier expansion of  $\mathbf{x}_{k+1}$  with respect to  $\mathcal{O}_{k+1}$  must be

$$\mathbf{x}_{k+1} = \sum_{i=1}^{k+1} \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i,$$

which in turn implies that

$$\mathbf{u}_{k+1} = \frac{\mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i}{\langle \mathbf{u}_{k+1} | \mathbf{x}_{k+1} \rangle}.$$

Since  $\|\mathbf{u}_{k+1}\| = 1$ , it follows that

$$|\langle \mathbf{u}_{k+1} | \mathbf{x}_{k+1} \rangle| = \left\| \mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i \right\|,$$

so  $\langle \mathbf{u}_{k+1} | \mathbf{x}_{k+1} \rangle = e^{i\theta} \left\| \mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i \right\|$  for some  $0 \leq \theta < 2\pi$ , and

$$\mathbf{u}_{k+1} = \frac{\mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i}{e^{i\theta} \left\| \mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i \right\|}.$$

Since the value of  $\theta$  in the scalar  $e^{i\theta}$  neither affects  $\text{span}\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_{k+1}\}$  nor the facts that  $\|\mathbf{u}_{k+1}\| = 1$  and  $\langle \mathbf{u}_{k+1} | \mathbf{u}_i \rangle = 0$  for all  $i \leq k$ , we can arbitrarily define  $\mathbf{u}_{k+1}$  to be the vector corresponding to the  $\theta = 0$  or, equivalently,  $e^{i\theta} = 1$ . For the sake of convenience, let

$$\nu_{k+1} = \left\| \mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i \right\|$$

so that we can write

$$\mathbf{u}_1 = \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|} \quad \text{and} \quad \mathbf{u}_{k+1} = \frac{\mathbf{x}_{k+1} - \sum_{i=1}^k \langle \mathbf{u}_i | \mathbf{x}_{k+1} \rangle \mathbf{u}_i}{\nu_{k+1}} \text{ for } k > 0.$$

This sequence of vectors is called the **Gram–Schmidt sequence**. A straightforward induction argument proves that  $\mathcal{O}_k = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k\}$  is indeed an orthonormal basis for  $\text{span}\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$  for each  $k = 1, 2, \dots$

## Gram-Schmidt Orthogonalization Procedure

If  $\mathcal{B} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  is a basis for a general inner-product space  $\mathcal{S}$ , then the **Gram-Schmidt sequence** defined by

$$\mathbf{u}_1 = \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|} \quad \text{and} \quad \mathbf{u}_k = \frac{\mathbf{x}_k - \sum_{i=1}^{k-1} \langle \mathbf{u}_i | \mathbf{x}_k \rangle \mathbf{u}_i}{\left\| \mathbf{x}_k - \sum_{i=1}^{k-1} \langle \mathbf{u}_i | \mathbf{x}_k \rangle \mathbf{u}_i \right\|} \quad \text{for } k = 2, \dots, n$$

is an orthonormal basis for  $\mathcal{S}$ . When  $\mathcal{S}$  is an  $n$ -dimensional subspace of  $\mathcal{C}^{m \times 1}$ , the Gram-Schmidt sequence can be expressed as

$$\mathbf{u}_k = \frac{(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k}{\|(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k\|} \quad \text{for } k = 1, 2, \dots, n$$

in which  $\mathbf{U}_1 = \mathbf{0}_{m \times 1}$  and  $\mathbf{U}_k = (\mathbf{u}_1 | \mathbf{u}_2 | \cdots | \mathbf{u}_{k-1})_{m \times k-1}$  for  $k > 1$ .

Suppose that  $\mathcal{B} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  is a basis for an  $n$ -dimensional subspace  $\mathcal{S}$  of  $\mathcal{C}^{m \times 1}$  so that the Gram-Schmidt sequence becomes

$$\mathbf{u}_1 = \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|} \quad \text{and} \quad \mathbf{u}_k = \frac{\mathbf{x}_k - \sum_{i=1}^{k-1} (\mathbf{u}_i^* \mathbf{x}_k) \mathbf{u}_i}{\left\| \mathbf{x}_k - \sum_{i=1}^{k-1} (\mathbf{u}_i^* \mathbf{x}_k) \mathbf{u}_i \right\|} \quad \text{for } k = 2, 3, \dots, n.$$

To express this in matrix notation, set

$$\mathbf{U}_1 = \mathbf{0}_{m \times 1} \quad \text{and} \quad \mathbf{U}_k = (\mathbf{u}_1 | \mathbf{u}_2 | \cdots | \mathbf{u}_{k-1})_{m \times k-1} \quad \text{for } k > 1,$$

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

Since

$$\mathbf{x}_k - \sum_{i=1}^{k-1} (\mathbf{u}_i^* \mathbf{x}_k) \mathbf{u}_i = \mathbf{x}_k - \mathbf{U}_k \mathbf{U}_k^* \mathbf{x}_k = (\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k,$$

$$\mathbf{u}_k = \frac{(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k}{\|(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k\|} \quad \text{for } k = 1, 2, \dots, n.$$

**Classical Gram–Schmidt Algorithm.** The following formal algorithm is the straightforward or “classical” implementation of the Gram–Schmidt procedure. Interpret  $\mathbf{a} \leftarrow \mathbf{b}$  to mean that “ $\mathbf{a}$  is defined to be (or overwritten by)  $\mathbf{b}$ .”

For  $k = 1$ :

$$\mathbf{u}_1 \leftarrow \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}$$

For  $k > 1$ :

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

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

**Problem:** Use the classical formulation of the Gram–Schmidt procedure given above to find an orthonormal basis for the space spanned by the following three linearly independent vectors.

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{x}_2 = \begin{pmatrix} 1 \\ 2 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{x}_3 = \begin{pmatrix} 3 \\ 1 \\ 1 \\ -1 \end{pmatrix}.$$

**Solution:**

$$k = 1: \quad \mathbf{u}_1 \leftarrow \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

$$k = 2: \quad \mathbf{u}_2 \leftarrow \mathbf{x}_2 - (\mathbf{u}_1^T \mathbf{x}_2) \mathbf{u}_1 = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{u}_2 \leftarrow \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$k = 3: \quad \mathbf{u}_3 \leftarrow \mathbf{x}_3 - (\mathbf{u}_1^T \mathbf{x}_3) \mathbf{u}_1 - (\mathbf{u}_2^T \mathbf{x}_3) \mathbf{u}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{u}_3 \leftarrow \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

Thus

$$\mathbf{u}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{u}_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

is the desired orthonormal basis.

- The GramSchmidt process frequently appears in the disguised form of a matrix factorization.
- Let  $\mathbf{A}_{m \times n} = (\mathbf{a}_1 | \mathbf{a}_2 | \cdots | \mathbf{a}_n)$  be a matrix with linearly independent columns.
- When Gram-Schmidt is applied to the columns of  $\mathbf{A}$ , the result is an orthonormal basis  $\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n\}$  for  $R(\mathbf{A})$ , where

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{\nu_1} \quad \text{and} \quad \mathbf{q}_k = \frac{\mathbf{a}_k - \sum_{i=1}^{k-1} \langle \mathbf{q}_i | \mathbf{a}_k \rangle \mathbf{q}_i}{\nu_k} \quad \text{for } k = 2, 3, \dots, n,$$

where  $\nu_1 = \|\mathbf{a}_1\|$  and  $\nu_k = \|\mathbf{a}_k - \sum_{i=1}^{k-1} \langle \mathbf{q}_i | \mathbf{a}_k \rangle \mathbf{q}_i\|$  for  $k > 1$ .

- The above relationships can be rewritten as

$$\mathbf{a}_1 = \nu_1 \mathbf{q}_1 \quad \text{and} \quad \mathbf{a}_k = \langle \mathbf{q}_1 | \mathbf{a}_k \rangle \mathbf{q}_1 + \cdots + \langle \mathbf{q}_{k-1} | \mathbf{a}_k \rangle \mathbf{q}_{k-1} + \nu_k \mathbf{q}_k \quad \text{for } k > 1,$$

which in turn can be expressed in matrix form by writing

$$(\mathbf{a}_1 | \mathbf{a}_2 | \cdots | \mathbf{a}_n) = (\mathbf{q}_1 | \mathbf{q}_2 | \cdots | \mathbf{q}_n) \begin{pmatrix} \nu_1 & \langle \mathbf{q}_1 | \mathbf{a}_2 \rangle & \langle \mathbf{q}_1 | \mathbf{a}_3 \rangle & \cdots & \langle \mathbf{q}_1 | \mathbf{a}_n \rangle \\ 0 & \nu_2 & \langle \mathbf{q}_2 | \mathbf{a}_3 \rangle & \cdots & \langle \mathbf{q}_2 | \mathbf{a}_n \rangle \\ 0 & 0 & \nu_3 & \cdots & \langle \mathbf{q}_3 | \mathbf{a}_n \rangle \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \nu_n \end{pmatrix}.$$

- This says that it's possible to factor a matrix with independent columns as  $\mathbf{A}_{m \times n} = \mathbf{Q}_{m \times n} \mathbf{R}_{n \times n}$ 
  - The columns of  $\mathbf{Q}$  are an orthonormal basis for  $R(\mathbf{A})$
  - $\mathbf{R}$  is an upper-triangular matrix with positive diagonal elements.

## QR Factorization

Every matrix  $\mathbf{A}_{m \times n}$  with linearly independent columns can be uniquely factored as  $\mathbf{A} = \mathbf{Q}\mathbf{R}$  in which the columns of  $\mathbf{Q}_{m \times n}$  are an orthonormal basis for  $R(\mathbf{A})$  and  $\mathbf{R}_{n \times n}$  is an upper-triangular matrix with positive diagonal entries.

- The QR factorization is the complete “road map” of the Gram–Schmidt process because the columns of  $\mathbf{Q} = (\mathbf{q}_1 | \mathbf{q}_2 | \cdots | \mathbf{q}_n)$  are the result of applying the Gram–Schmidt procedure to the columns of  $\mathbf{A} = (\mathbf{a}_1 | \mathbf{a}_2 | \cdots | \mathbf{a}_n)$  and  $\mathbf{R}$  is given by

$$\mathbf{R} = \begin{pmatrix} \nu_1 & \mathbf{q}_1^* \mathbf{a}_2 & \mathbf{q}_1^* \mathbf{a}_3 & \cdots & \mathbf{q}_1^* \mathbf{a}_n \\ 0 & \nu_2 & \mathbf{q}_2^* \mathbf{a}_3 & \cdots & \mathbf{q}_2^* \mathbf{a}_n \\ 0 & 0 & \nu_3 & \cdots & \mathbf{q}_3^* \mathbf{a}_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \nu_n \end{pmatrix},$$

where  $\nu_1 = \|\mathbf{a}_1\|$  and  $\nu_k = \|\mathbf{a}_k - \sum_{i=1}^{k-1} \langle \mathbf{q}_i | \mathbf{a}_k \rangle \mathbf{q}_i\|$  for  $k > 1$ .



■ **Problem:** Determine the QR factors of

$$\mathbf{A} = \begin{pmatrix} 0 & -20 & -14 \\ 3 & 27 & -4 \\ 4 & 11 & -2 \end{pmatrix}.$$

$$k = 1: \quad r_{11} \leftarrow \|\mathbf{a}_1\| = 5 \quad \text{and} \quad \mathbf{q}_1 \leftarrow \frac{\mathbf{a}_1}{r_{11}} = \begin{pmatrix} 0 \\ 3/5 \\ 4/5 \end{pmatrix}$$

$$k = 2: \quad r_{12} \leftarrow \mathbf{q}_1^T \mathbf{a}_2 = 25$$

$$\mathbf{q}_2 \leftarrow \mathbf{a}_2 - r_{12} \mathbf{q}_1 = \begin{pmatrix} -20 \\ 12 \\ -9 \end{pmatrix}$$

$$r_{22} \leftarrow \|\mathbf{q}_2\| = 25 \quad \text{and} \quad \mathbf{q}_2 \leftarrow \frac{\mathbf{q}_2}{r_{22}} = \frac{1}{25} \begin{pmatrix} -20 \\ 12 \\ -9 \end{pmatrix}$$

$$k = 3: \quad r_{13} \leftarrow \mathbf{q}_1^T \mathbf{a}_3 = -4 \quad \text{and} \quad r_{23} \leftarrow \mathbf{q}_2^T \mathbf{a}_3 = 10$$

$$\mathbf{q}_3 \leftarrow \mathbf{a}_3 - r_{13} \mathbf{q}_1 - r_{23} \mathbf{q}_2 = \frac{2}{5} \begin{pmatrix} -15 \\ -16 \\ 12 \end{pmatrix}$$

$$r_{33} \leftarrow \|\mathbf{q}_3\| = 10 \quad \text{and} \quad \mathbf{q}_3 \leftarrow \frac{\mathbf{q}_3}{r_{33}} = \frac{1}{25} \begin{pmatrix} -15 \\ -16 \\ 12 \end{pmatrix}$$

Therefore,

$$\mathbf{Q} = \frac{1}{25} \begin{pmatrix} 0 & -20 & -15 \\ 15 & 12 & -16 \\ 20 & -9 & 12 \end{pmatrix} \quad \text{and} \quad \mathbf{R} = \begin{pmatrix} 5 & 25 & -4 \\ 0 & 25 & 10 \\ 0 & 0 & 10 \end{pmatrix}.$$

- We now have two important matrix factorizations, namely, the LU factorization, discussed and the QR factorization. They are not the same, but some striking analogies exist.
  - ▶ Each factorization represents a reduction to upper-triangular form LU by Gaussian elimination, and QR by Gram-Schmidt.
  - ▶ When they exist, both factorizations  $\mathbf{A} = \mathbf{LU}$  and  $\mathbf{A} = \mathbf{QR}$  are uniquely determined by  $\mathbf{A}$ .
  - ▶ Once the LU factors (assuming they exist) of a nonsingular matrix  $\mathbf{A}$  are known, the solution of  $\mathbf{Ax} = \mathbf{b}$  is easily computed solve  $\mathbf{Ly} = \mathbf{b}$  by forward substitution, and then solve  $\mathbf{Ux} = \mathbf{y}$  by back substitution.
  - ▶ The QR factors can be used in a similar manner. If  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is nonsingular, then  $\mathbf{Q}^T = \mathbf{Q}^{-1}$ , so  $\mathbf{Ax} = \mathbf{b} \iff \mathbf{QRx} = \mathbf{b} \Leftrightarrow \mathbf{Rx} = \mathbf{Q}^T \mathbf{b}$ , which is also a triangular system that is solved by back substitution.
  - ▶ Things are different for singular and rectangular cases because  $\mathbf{Ax} = \mathbf{b}$  might be inconsistent.
    - the LU factors of  $\mathbf{A}$  don't exist when  $\mathbf{A}$  is rectangular.
    - Even if  $\mathbf{A}$  is square and has an LU factorization, the LU factors of  $\mathbf{A}$  are not much help in solving the system of normal equations  $\mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}$  that produces least squares solutions.
    - But the QR factors of  $\mathbf{A}_{m \times n}$  always exist as long as  $\mathbf{A}$  has linearly independent columns.

## Linear Systems and the QR Factorization

If  $\text{rank}(\mathbf{A}_{m \times n}) = n$ , and if  $\mathbf{A} = \mathbf{Q}\mathbf{R}$  is the QR factorization, then the solution of the nonsingular triangular system

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

is either the solution or the least squares solution of  $\mathbf{Ax} = \mathbf{b}$  depending on whether or not  $\mathbf{Ax} = \mathbf{b}$  is consistent.

- The GramSchmidt procedure is a powerful theoretical tool, but it's not a good numerical algorithm when implemented in the straightforward or "classical" sense.
- When floating-point arithmetic is used, the classical GramSchmidt algorithm applied to a set of vectors that is not already close to being an orthogonal set can produce a set of vectors that is far from being an orthogonal set.

**Problem:** Using 3-digit floating-point arithmetic, apply the classical Gram–Schmidt algorithm to the set

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 10^{-3} \\ 10^{-3} \end{pmatrix}, \quad \mathbf{x}_2 = \begin{pmatrix} 1 \\ 10^{-3} \\ 0 \end{pmatrix}, \quad \mathbf{x}_3 = \begin{pmatrix} 1 \\ 0 \\ 10^{-3} \end{pmatrix}.$$



**Solution:**

$k = 1$ :  $fl \|\mathbf{x}_1\| = 1$ , so  $\mathbf{u}_1 \leftarrow \mathbf{x}_1$ .

$k = 2$ :  $fl (\mathbf{u}_1^T \mathbf{x}_2) = 1$ , so

$$\mathbf{u}_2 \leftarrow \mathbf{x}_2 - (\mathbf{u}_1^T \mathbf{x}_2) \mathbf{u}_1 = \begin{pmatrix} 0 \\ 0 \\ -10^{-3} \end{pmatrix} \quad \text{and} \quad \mathbf{u}_2 \leftarrow fl \left( \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \right) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}.$$

$k = 3$ :  $fl (\mathbf{u}_1^T \mathbf{x}_3) = 1$  and  $fl (\mathbf{u}_2^T \mathbf{x}_3) = -10^{-3}$ , so

$$\mathbf{u}_3 \leftarrow \mathbf{x}_3 - (\mathbf{u}_1^T \mathbf{x}_3) \mathbf{u}_1 - (\mathbf{u}_2^T \mathbf{x}_3) \mathbf{u}_2 = \begin{pmatrix} 0 \\ -10^{-3} \\ -10^{-3} \end{pmatrix} \quad \text{and} \quad \mathbf{u}_3 \leftarrow fl \left( \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \right) = \begin{pmatrix} 0 \\ -.709 \\ -.709 \end{pmatrix}.$$

Therefore, classical Gram–Schmidt with 3-digit arithmetic returns

$$\mathbf{u}_1 = \begin{pmatrix} 1 \\ 10^{-3} \\ 10^{-3} \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{u}_3 = \begin{pmatrix} 0 \\ -.709 \\ -.709 \end{pmatrix},$$

which is unsatisfactory because  $\mathbf{u}_2$  and  $\mathbf{u}_3$  are far from being orthogonal.

It's possible to improve the numerical stability of the orthogonalization process by rearranging the order of the calculations. Recall from that

$$\mathbf{u}_k = \frac{(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k}{\|(\mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*) \mathbf{x}_k\|}, \quad \text{where } \mathbf{U}_1 = \mathbf{0} \text{ and } \mathbf{U}_k = (\mathbf{u}_1 \mid \mathbf{u}_2 \mid \cdots \mid \mathbf{u}_{k-1}).$$

If  $\mathbf{E}_1 = \mathbf{I}$  and  $\mathbf{E}_i = \mathbf{I} - \mathbf{u}_{i-1} \mathbf{u}_{i-1}^*$  for  $i > 1$ , then the orthogonality of the  $\mathbf{u}_i$ 's insures that

$$\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 = \mathbf{I} - \mathbf{u}_1 \mathbf{u}_1^* - \mathbf{u}_2 \mathbf{u}_2^* - \cdots - \mathbf{u}_{k-1} \mathbf{u}_{k-1}^* = \mathbf{I} - \mathbf{U}_k \mathbf{U}_k^*,$$

so the Gram-Schmidt sequence can also be expressed as

$$\mathbf{u}_k = \frac{\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{x}_k}{\|\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{x}_k\|} \quad \text{for } k = 1, 2, \dots, n.$$

This means that the Gram-Schmidt sequence can be generated as follows:

$$\begin{aligned} \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\} &\xrightarrow{\text{Normalize 1-st}} \{\mathbf{u}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\} \\ &\xrightarrow{\text{Apply } \mathbf{E}_2} \{\mathbf{u}_1, \mathbf{E}_2 \mathbf{x}_2, \mathbf{E}_2 \mathbf{x}_3, \dots, \mathbf{E}_2 \mathbf{x}_n\} \\ &\xrightarrow{\text{Normalize 2-nd}} \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{E}_2 \mathbf{x}_3, \dots, \mathbf{E}_2 \mathbf{x}_n\} \\ &\xrightarrow{\text{Apply } \mathbf{E}_3} \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{E}_3 \mathbf{E}_2 \mathbf{x}_3, \dots, \mathbf{E}_3 \mathbf{E}_2 \mathbf{x}_n\} \\ &\xrightarrow{\text{Normalize 3-rd}} \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{E}_3 \mathbf{E}_2 \mathbf{x}_4, \dots, \mathbf{E}_3 \mathbf{E}_2 \mathbf{x}_n\}, \\ &\quad \text{etc.} \end{aligned}$$

## Modified Gram–Schmidt Algorithm

For a linearly independent set  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\} \subset \mathcal{C}^{m \times 1}$ , the Gram–Schmidt sequence can be alternately described as

$$\mathbf{u}_k = \frac{\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{x}_k}{\|\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{x}_k\|} \text{ with } \mathbf{E}_1 = \mathbf{I}, \quad \mathbf{E}_i = \mathbf{I} - \mathbf{u}_{i-1} \mathbf{u}_{i-1}^* \text{ for } i > 1,$$

and this sequence is generated by the following algorithm.

For  $k = 1$ :  $\mathbf{u}_1 \leftarrow \mathbf{x}_1 / \|\mathbf{x}_1\|$  and  $\mathbf{u}_j \leftarrow \mathbf{x}_j$  for  $j = 2, 3, \dots, n$

For  $k > 1$ :  $\mathbf{u}_j \leftarrow \mathbf{E}_k \mathbf{u}_j = \mathbf{u}_j - (\mathbf{u}_{k-1}^* \mathbf{u}_j) \mathbf{u}_{k-1}$  for  $j = k, k+1, \dots, n$   
 $\mathbf{u}_k \leftarrow \mathbf{u}_k / \|\mathbf{u}_k\|$

- While there is no theoretical difference, this “modified” algorithm is numerically more stable than the classical algorithm when floating-point arithmetic is used.
- The  $k^{th}$  step of the classical algorithm alters only the  $k^{th}$  vector, but the  $k^{th}$  step of the modified algorithm “updates” all vectors from the  $k^{th}$  through the last, and conditioning the unorthogonalized tail in this way makes a difference.

**Solution:**  $\mathbf{x}_1 = \begin{pmatrix} 1 \\ 10^{-3} \\ 10^{-3} \end{pmatrix}$ ,  $\mathbf{x}_2 = \begin{pmatrix} 1 \\ 10^{-3} \\ 0 \end{pmatrix}$ ,  $\mathbf{x}_3 = \begin{pmatrix} 1 \\ 0 \\ 10^{-3} \end{pmatrix}$ .

$k = 1$ :  $fl \|\mathbf{x}_1\| = 1$ , so  $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\} \leftarrow \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ .

$k = 2$ :  $fl(\mathbf{u}_1^T \mathbf{u}_2) = 1$  and  $fl(\mathbf{u}_1^T \mathbf{u}_3) = 1$ , so

$$\mathbf{u}_2 \leftarrow \mathbf{u}_2 - (\mathbf{u}_1^T \mathbf{u}_2) \mathbf{u}_1 = \begin{pmatrix} 0 \\ 0 \\ -10^{-3} \end{pmatrix}, \quad \mathbf{u}_3 \leftarrow \mathbf{u}_3 - (\mathbf{u}_1^T \mathbf{u}_3) \mathbf{u}_1 = \begin{pmatrix} 0 \\ -10^{-3} \\ 0 \end{pmatrix},$$

and

$$\mathbf{u}_2 \leftarrow \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}.$$

$k = 3$ :  $\mathbf{u}_2^T \mathbf{u}_3 = 0$ , so

$$\mathbf{u}_3 \leftarrow \mathbf{u}_3 - (\mathbf{u}_2^T \mathbf{u}_3) \mathbf{u}_2 = \begin{pmatrix} 0 \\ -10^{-3} \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{u}_3 \leftarrow \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} = \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}.$$

Thus the modified Gram-Schmidt algorithm produces

$$\mathbf{u}_1 = \begin{pmatrix} 1 \\ 10^{-3} \\ 10^{-3} \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{u}_3 = \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix},$$

# Unitary and Orthogonal Matrices

- The purpose of this section is to examine square matrices whose columns (or rows) are orthonormal.
- The standard inner product and the euclidean 2-norm are the only ones used in this section, so distinguishing subscripts are omitted.

## Unitary and Orthogonal Matrices

- A *unitary matrix* is defined to be a *complex* matrix  $\mathbf{U}_{n \times n}$  whose columns (or rows) constitute an orthonormal basis for  $\mathcal{C}^n$ .
- An *orthogonal matrix* is defined to be a *real* matrix  $\mathbf{P}_{n \times n}$  whose columns (or rows) constitute an orthonormal basis for  $\mathbb{R}^n$ .

- Unitary and orthogonal matrices have some nice features, one of which is the fact that they are easy to invert.
- Notice  $\mathbf{U}^* \mathbf{U} = \mathbf{I} \iff \mathbf{U}^{-1} = \mathbf{U}^*, \iff \mathbf{U} \mathbf{U}^* = \mathbf{I}$ .
- The columns of  $\mathbf{U}$  are orthonormal if and only if the rows of  $\mathbf{U}$  are orthonormal.

- Another nice feature is that multiplication by a unitary matrix doesn't change the length of a vector.
- Only the direction can be altered because

$$\|\mathbf{U}\mathbf{x}\|^2 = \mathbf{x}^*\mathbf{U}^*\mathbf{U}\mathbf{x} = \mathbf{x}^*\mathbf{x} = \|\mathbf{x}\|^2 \quad \forall \mathbf{x} \in \mathcal{C}^n.$$

- Conversely, if the above equation holds, then  $\mathbf{U}$  must be unitary.
  - To see this, set  $\mathbf{x} = \mathbf{e}_i$  to observe  $\mathbf{u}_i^*\mathbf{u}_i = 1$  for each  $i$ .
  - Then set  $\mathbf{x} = \mathbf{e}_j + \mathbf{e}_k$  for  $j \neq k$  to obtain  $0 = 2\operatorname{Re}(\mathbf{u}_j^*\mathbf{u}_k)$ .
  - By setting  $\mathbf{x} = \mathbf{e}_j + i\mathbf{e}_k$ , it follows that  $0 = 2\operatorname{Im}(\mathbf{u}_j^*\mathbf{u}_k)$ .
  - So  $\mathbf{u}_j^*\mathbf{u}_k = 0$  for each  $j \neq k$ .
- In the case of orthogonal matrices, everything is real so that  $(\star)^*$  can be replaced by  $(\star)^T$ .

## Characterizations

- The following statements are equivalent to saying that a complex matrix  $\mathbf{U}_{n \times n}$  is unitary.
  - ▷  $\mathbf{U}$  has orthonormal columns.
  - ▷  $\mathbf{U}$  has orthonormal rows.
  - ▷  $\mathbf{U}^{-1} = \mathbf{U}^*$ .
  - ▷  $\|\mathbf{U}\mathbf{x}\|_2 = \|\mathbf{x}\|_2$  for every  $\mathbf{x} \in \mathbb{C}^{n \times 1}$ .
- The following statements are equivalent to saying that a real matrix  $\mathbf{P}_{n \times n}$  is orthogonal.
  - ▷  $\mathbf{P}$  has orthonormal columns.
  - ▷  $\mathbf{P}$  has orthonormal rows.
  - ▷  $\mathbf{P}^{-1} = \mathbf{P}^T$ .
  - ▷  $\|\mathbf{P}\mathbf{x}\|_2 = \|\mathbf{x}\|_2$  for every  $\mathbf{x} \in \mathbb{R}^{n \times 1}$ .

## Some Examples

- The identity matrix  $\mathbf{I}$  is an orthogonal matrix.
- All permutation matrices are orthogonal.
- An orthogonal matrix can be considered to be unitary, but a unitary matrix is generally not orthogonal.

- In general, a linear operator  $\mathbf{T}$  on a vector space  $\mathcal{V}$  with the property that  $\|\mathbf{T}\mathbf{x}\| = \|\mathbf{x}\|$  for all  $\mathbf{x} \in \mathcal{V}$  is called an **isometry** on  $\mathcal{V}$ .
- The term isometry can be used to treat the real and complex cases simultaneously.
- The isometries on  $\mathbb{R}^n$  are precisely the orthogonal matrices, and the isometries on  $\mathcal{C}^n$  are the unitary matrices.
- The geometrical concepts of projection, reflection, and rotation are among the most fundamental of all linear transformations in  $\mathbb{R}^2$  and  $\mathbb{R}^3$ .
- The reflector and rotator are isometries, but the projector is not.

## Elementary Orthogonal Projectors

For a vector  $\mathbf{u} \in \mathcal{C}^{n \times 1}$  such that  $\|\mathbf{u}\| = 1$ , a matrix of the form

$$\mathbf{Q} = \mathbf{I} - \mathbf{u}\mathbf{u}^*$$

$$\mathbf{Q}^2 = \mathbf{Q}$$

is called an *elementary orthogonal projector*.

## Geometry of Elementary Projectors

For vectors  $\mathbf{u}, \mathbf{x} \in \mathcal{C}^{n \times 1}$  such that  $\|\mathbf{u}\| = 1$ ,

- $(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{x}$  is the orthogonal projection of  $\mathbf{x}$  onto the orthogonal complement  $\mathbf{u}^\perp$ , the space of all vectors orthogonal to  $\mathbf{u}$ ;
- $\mathbf{u}\mathbf{u}^*\mathbf{x}$  is the orthogonal projection of  $\mathbf{x}$  onto the one-dimensional space  $\text{span}\{\mathbf{u}\}$ ;      的扩张
- $|\mathbf{u}^*\mathbf{x}|$  represents the length of the orthogonal projection of  $\mathbf{x}$  onto the one-dimensional space  $\text{span}\{\mathbf{u}\}$ .

- Note that elementary projectors are never isometries
- They are not unitary matrices in the complex case and not orthogonal matrices in the real case.
- Furthermore, isometries are nonsingular but elementary projectors are singular.
- For every nonzero vector  $\mathbf{u} \in \mathcal{C}^{n \times 1}$ , the orthogonal projectors onto  $\text{span}\{\mathbf{u}\}$  and  $\mathbf{u}^\perp$  are

$$\mathbf{P}_{\mathbf{u}} = \frac{\mathbf{u}\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}} \quad \text{and} \quad \mathbf{P}_{\mathbf{u}^\perp} = \mathbf{I} - \frac{\mathbf{u}\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}$$

## Elementary Reflectors

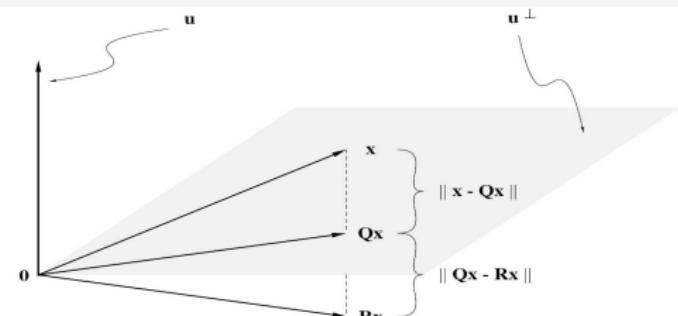
For  $\mathbf{u}_{n \times 1} \neq \mathbf{0}$ , the *elementary reflector* about  $\mathbf{u}^\perp$  is defined to be

$$\mathbf{R} = \mathbf{I} - 2 \frac{\mathbf{u}\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}$$

or, equivalently,

$$\mathbf{R} = \mathbf{I} - 2\mathbf{u}\mathbf{u}^* \quad \text{when} \quad \|\mathbf{u}\| = 1.$$

- Elementary reflectors are also called **Householder transformations**, and they are analogous to the simple reflector. 豪斯赫尔德
- It is easy to observe that  $\mathbf{Q}(\mathbf{R}\mathbf{x}) = \mathbf{Q}\mathbf{x}$ .
- Together with  $\|\mathbf{x} - \mathbf{Q}\mathbf{x}\| = |\mathbf{u}^T \mathbf{x}| = \|\mathbf{Q}\mathbf{x} - \mathbf{R}\mathbf{x}\|$ .
- This implies that  $\mathbf{R}\mathbf{x}$  is the reflection of  $\mathbf{x}$  about the plane  $\mathbf{u}^\perp$ .



## Properties of Elementary Reflectors

- All elementary reflectors  $\mathbf{R}$  are unitary, hermitian, and involutory ( $\mathbf{R}^2 = \mathbf{I}$ ). That is,

$$\mathbf{R} = \mathbf{R}^* = \mathbf{R}^{-1}.$$

- If  $\mathbf{x}_{n \times 1}$  is a vector whose first entry is  $x_1 \neq 0$ , and if

$$\mathbf{u} = \mathbf{x} \pm \mu \|\mathbf{x}\| \mathbf{e}_1, \quad \text{where } \mu = \begin{cases} 1 & \text{if } x_1 \text{ is real,} \\ x_1/|x_1| & \text{if } x_1 \text{ is not real,} \end{cases}$$

is used to build the elementary reflector  $\mathbf{R}$

$$\mathbf{R}\mathbf{x} = \mp\mu \|\mathbf{x}\| \mathbf{e}_1.$$

In other words, this  $\mathbf{R}$  “reflects”  $\mathbf{x}$  onto the first coordinate axis.

**Computational Note:** To avoid cancellation when using floating-point arithmetic for real matrices, set  $\mathbf{u} = \mathbf{x} + \text{sign}(x_1) \|\mathbf{x}\| \mathbf{e}_1$ .

- **Problem:** Given  $\mathbf{x} \in \mathbb{C}^{n \times 1}$  such  $\|\mathbf{x}\| = 1$ , construct an orthonormal basis for  $\mathbb{C}^n$  that contains  $\mathbf{x}$ .
- **Solution:** An efficient solution is to build a unitary matrix that contains  $\mathbf{x}$  as its first column.
  - Set  $\mathbf{u} = \mathbf{x} \pm \mu \mathbf{e}_1$  in  $\mathbf{R}$  which guarantees  $\mathbf{Rx} = \mp \mu \mathbf{e}_1$ .
  - Multiplication on the left by  $\mathbf{R}$  produces  $\mathbf{x} = \mp \mu \mathbf{Re}_1 = [\mp \mu \mathbf{R}]_{*1}$ .
  - Since  $|\mp \mu| = 1$ ,  $\mathbf{U} = \mp \mu \mathbf{R}$  is a unitary matrix with  $\mathbf{U}_{*1} = \mathbf{x}$ , so the columns of  $\mathbf{U}$  provide the desired orthonormal basis.
- For example, to construct an orthonormal basis for  $\mathbb{R}^4$  that includes  $\mathbf{x} = 1/3(-1 \ 2 \ 0 \ -2)^T$ .
- Set  $\mathbf{u} = \mathbf{x} - \mathbf{e}_1 = \frac{1}{3}(-4 \ 2 \ 0 \ -2)^T$ .
- Compute

$$\mathbf{R} = \mathbf{I} - 2 \frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}} = \frac{1}{3} \begin{pmatrix} -1 & 2 & 0 & -2 \\ 2 & 2 & 0 & 1 \\ 0 & 0 & 3 & 0 \\ -2 & 1 & 0 & 2 \end{pmatrix}.$$

The columns of  $\mathbf{R}$  do the job.

- Now consider rotation, and begin with a basic problem in  $\mathbb{R}^2$ .
- If a nonzero vector  $\mathbf{u} = (u_1, u_2)$  is rotated counterclockwise through an angle  $\theta$  to  $\mathbf{v} = (v_1, v_2)$ .
- $\mathbf{v} = \mathbf{P}\mathbf{u}$ , where  $\mathbf{P}$  is the rotator (rotation operator)

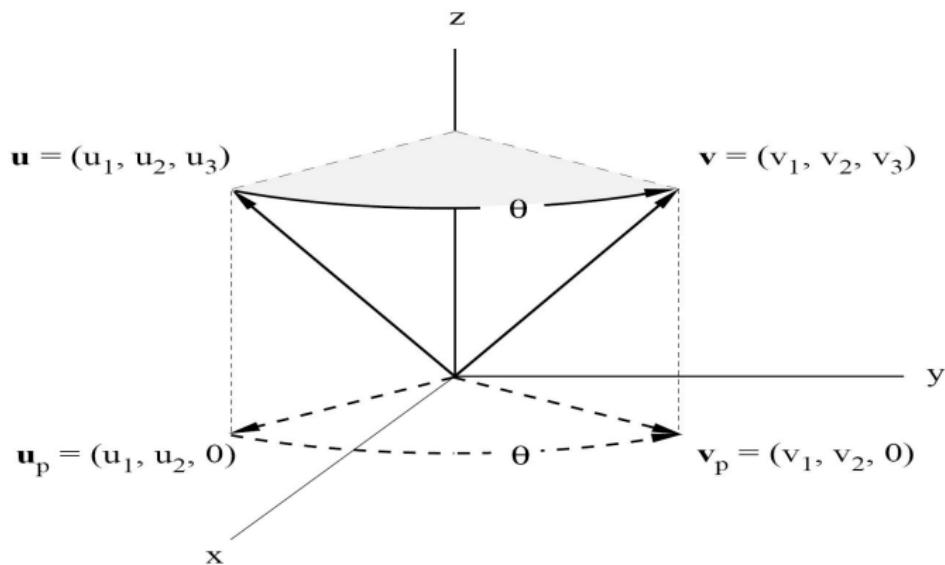
$$\mathbf{P} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

- Notice that  $\mathbf{P}$  is an orthogonal matrix because  $\mathbf{P}^T \mathbf{P} = \mathbf{I}$ .
- This means that if  $\mathbf{v} = \mathbf{P}\mathbf{u}$ , then  $\mathbf{u} = \mathbf{P}^T \mathbf{v}$ , and hence  $\mathbf{P}^T$  is also a rotator, but in the opposite direction of the associated with  $\mathbf{P}$ .
- That is ,  $\mathbf{P}^T$  is the rotator associated with the angle  $-\theta$ .
- Rotating vectors in  $\mathbb{R}^3$  around and one of the coordinate axes is similar.
- For example, cosider rotation around the  $z$ -axis.
- Suppose that  $\mathbf{v} = (v_1, v_2, v_3)$  is obtained by rotating  $\mathbf{u} = (u_1, u_2, u_3)$  counterclockwise through an angle  $\theta$  around the  $z$ -axis.

- It is evident that the third coordinates are unaffected, i.e.  $v_3 = u_3$ .
- To see how the  $xy$ -coordinates of  $\mathbf{u}$  and  $\mathbf{v}$  are related, consider the orthogonal projections

$$\mathbf{u}_p = (u_1, u_2, 0) \quad \text{and} \quad \mathbf{v}_p = (v_1, v_2, 0)$$

of  $\mathbf{u}$  and  $\mathbf{v}$  onto the  $xy$ -plane.



- It's apparent that the problem has been reduced to rotation in the  $xy$ -plane.
- Combining with the fact the  $v_3 = u_3$  produces the equation

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix},$$

so

$$\mathbf{P}_z = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

is the matrix that rotates vectors in  $\mathbb{R}^3$  counterclockwise around the  $z$ -axis through an angle  $\theta$ . It is easy to verify that  $\mathbf{P}_z$  is an orthogonal matrix and that  $\mathbf{P}_z^{-1} = \mathbf{P}_z^T$  rotates vectors *clockwise* around the  $z$ -axis.

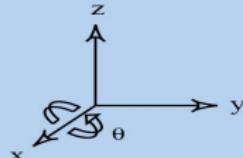
- By using similar techniques, it is possible to derive orthogonal matrices that rotate vectors around the  $x$ -axis or around  $y$ -axis.

## Rotations in $\mathbb{R}^3$

A vector  $\mathbf{u} \in \mathbb{R}^3$  can be rotated counterclockwise through an angle  $\theta$  around a coordinate axis by means of a multiplication  $\mathbf{P}_\star \mathbf{u}$  in which  $\mathbf{P}_\star$  is an appropriate orthogonal matrix as described below.

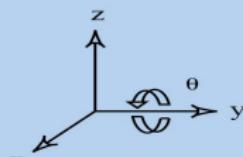
### Rotation around the x-Axis

$$\mathbf{P}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}$$



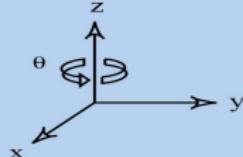
### Rotation around the y-Axis

$$\mathbf{P}_y = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}$$



### Rotation around the z-Axis

$$\mathbf{P}_z = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



**Note:** The minus sign appears above the diagonal in  $\mathbf{P}_x$  and  $\mathbf{P}_z$ , but below the diagonal in  $\mathbf{P}_y$ . This is not a mistake—it's due to the orientation of the positive  $x$ -axis with respect to the  $yz$ -plane.

- Rotations in higher dimensions are straightforward generalizations of rotations in  $\mathbb{R}^3$ .

## Plane Rotations

Orthogonal matrices of the form

$$\mathbf{P}_{ij} = \begin{pmatrix} & \text{col } i & \text{col } j \\ & \downarrow & \downarrow \\ 1 & \ddots & & & \\ & c & 1 & s & \\ & & & & \\ & -s & & c & 1 \\ & & & & \ddots \\ & & & & & 1 \end{pmatrix} \quad \begin{array}{l} \longleftarrow \text{row } i \\ \longleftarrow \text{row } j \end{array}$$

in which  $c^2 + s^2 = 1$  are called ***plane rotation matrices*** because they perform a rotation in the  $(i, j)$ -plane of  $\mathbb{R}^n$ . The entries  $c$  and  $s$  are meant to suggest cosine and sine, respectively, but designating a rotation angle  $\theta$  as is done in  $\mathbb{R}^2$  and  $\mathbb{R}^3$  is not useful in higher dimensions.

- Plane rotations matrices  $P_{ij}$  are also called **Givens rotations**.
- Applying  $P_{ij}$  to  $0 \neq x \in \Re^n$  rotates the  $(i,j)$ -coordinates of  $x$  in the sense that

$$P_{ij}x = \begin{pmatrix} x_1 \\ \vdots \\ cx_i + sx_j \\ \vdots \\ -sx_i + cx_j \\ \vdots \\ x_n \end{pmatrix}$$

- If  $x_i$  and  $x_j$  are not both zero, and if we set

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

then

$$\mathbf{P}_{ij}\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ \sqrt{x_i^2 + x_j^2} \\ \vdots \\ 0 \\ \vdots \\ x_n \end{pmatrix}$$

- This means that we can selectively annihilate any component  $x_j$  in this case by a rotation in the  $(i, j)$ -plane without affecting any entry except  $x_i$  and  $x_j$ .
- Consequently, plane rotations can be applied to annihilate all components below any particular “pivot.”

- For example, to annihilate all entries below the first position in  $\mathbf{x}$ , apply a sequence of plane rotations as follows:

$$\mathbf{P}_{12}\mathbf{x} = \begin{pmatrix} \sqrt{x_1^2 + x_2^2} \\ 0 \\ x_3 \\ x_4 \\ \vdots \\ x_n \end{pmatrix}, \quad \mathbf{P}_{13}\mathbf{P}_{12}\mathbf{x} = \begin{pmatrix} \sqrt{x_1^2 + x_2^2 + x_3^2} \\ 0 \\ 0 \\ x_4 \\ \vdots \\ x_n \end{pmatrix}, \quad \dots, \quad \mathbf{P}_{1n} \cdots \mathbf{P}_{13}\mathbf{P}_{12}\mathbf{x} = \begin{pmatrix} \|\mathbf{x}\| \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

- The product of plane rotations is generally not another plane rotation, but is always an orthogonal matrix, and hence an isometry.
- If we are willing to interpret rotation in  $\mathbb{R}^n$  as a sequence of plane rotations, then we can say that it is always possible to rotate each nonzero vector onto the first coordinate axis.

### Rotations in $\mathbb{R}^n$

Every nonzero vector  $\mathbf{x} \in \mathbb{R}^n$  can be rotated to the  $i^{th}$  coordinate axis by a sequence of  $n - 1$  plane rotations. In other words, there is an orthogonal matrix  $\mathbf{P}$  such that

$$\mathbf{Px} = \|\mathbf{x}\| \mathbf{e}_i,$$

where  $\mathbf{P}$  has the form

$$\mathbf{P} = \mathbf{P}_{in} \cdots \mathbf{P}_{i,i+1} \mathbf{P}_{i,i-1} \cdots \mathbf{P}_{i1}.$$

- **Problem:** If  $x \in \mathbb{R}^n$  is a vector such that  $\|x\| = 1$ , explain how to use plane rotations to construct an orthonormal basis for  $\mathbb{R}^n$  that contains  $x$ .
- **Solution:** The goal is to construct an orthogonal matrix  $Q$  such that  $Q_{*1} = x$ . But this time we need to use plane rotations rather than an elementary reflector.
  - Build an orthogonal matrix from a sequence of plane rotations  $P = P_{1n} \cdots P_{13}P_{12}$  such that  $Px = e_1$ .
  - Thus  $x = P^T e_1 = P_{*1}^T$ , and the columns of  $Q = P^T$  serve the purpose.
- For example, extend  $x = 1/3(-1 \ 2 \ 0 \ -2)^T$  to an orthonormal basis in  $\mathbb{R}^4$ .

$$P_{12} = \begin{pmatrix} \frac{-1}{\sqrt{5}} & \frac{2}{\sqrt{5}} & 0 & 0 \\ \frac{\sqrt{5}}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 & 0 \\ \frac{-2}{\sqrt{5}} & \frac{\sqrt{5}}{\sqrt{5}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad P_{14} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & 0 & \frac{-2}{3} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{2}{3} & 0 & 0 & \frac{\sqrt{5}}{3} \end{pmatrix}.$$

- $Q = (P_{14}P_{12})^T = P_{12}^T P_{14}^T$ .

# Exercises

- Find the 1-, 2- and  $\infty$ -norms of  $\mathbf{x} = (2, 1, -4, -2)^T$  and  $\mathbf{x} = (1+i, 1-i, 1, 4i)$ .
- Explain why  $\|\mathbf{x} - \mathbf{y}\| = \|\mathbf{y} - \mathbf{x}\|$  is true for all norms.
- Evaluate the Frobenius matrix norm, 1-norm, 2-norm and  $\infty$ -norm for each matrix below.

$$\mathbf{A} = \begin{pmatrix} 1 & -2 \\ -1 & 2 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 4 & -2 & 4 \\ -2 & 1 & -2 \\ 4 & -2 & 4 \end{pmatrix}.$$

- Explain why  $\|\mathbf{A}\|_F = \|\mathbf{A}^*\|_F$  for Frobenius matrix norm.
- For  $\mathbf{x} = (x_1, x_2, x_3)^T$ ,  $\mathbf{y} = (y_1, y_2, y_3)^T$  determine which of the following are inner products for  $\mathbb{R}^{3 \times 1}$ .
  - $\langle \mathbf{x} | \mathbf{y} \rangle = x_1y_1 + x_3y_3$ ,
  - $\langle \mathbf{x} | \mathbf{y} \rangle = x_1y_1 - x_2y_2 + x_3y_3$ ,
  - $\langle \mathbf{x} | \mathbf{y} \rangle = 2x_1y_1 + x_2y_2 + 4x_3y_3$ .

6. Explain why there does not exist an inner product on  $\mathcal{C}^n (n \geq 2)$  such that  $\| * \|_\infty = \sqrt{\langle * | * \rangle}$ .
7. For a general inner-product space  $\mathcal{V}$ , explain why each of the following statements must be true.
- If  $\langle \mathbf{x} | \mathbf{y} \rangle = 0$  for all  $\mathbf{x} \in \mathcal{V}$ , then  $\mathbf{y} = 0$ .
  - $\langle \alpha \mathbf{x} | \mathbf{y} \rangle = \bar{\alpha} \langle \mathbf{x} | \mathbf{y} \rangle$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  and for all scalars  $\alpha$ .
  - $\langle \mathbf{x} + \mathbf{y} | \mathbf{z} \rangle = \langle \mathbf{x} | \mathbf{z} \rangle + \langle \mathbf{y} | \mathbf{z} \rangle$ .
8. Find two vectors of unit norm that are orthogonal to  $\mathbf{u} = (3, -2)^T$ .
9. Using the standard inner product, determine the Fourier expansion of  $\mathbf{x} = (1, 0, -2)^T$  with respect to

$$\mathcal{B} = \left\{ \frac{1}{\sqrt{2}}(1, -1, 0)^T, \frac{1}{\sqrt{3}}(1, 1, 1)^T, \frac{1}{\sqrt{6}}(-1, -1, 2)^T \right\}$$

10. Let  $\mathcal{S} = \text{span}\{\mathbf{x}_1 = (1, 1, 1, -1)^T, \mathbf{x}_2 = (2, -1, -1, 1)^T, \mathbf{x}_3 = (-1, 2, 2, 1)^T\}$ .
- (a) Use the classical GramSchmidt algorithm (with exact arithmetic) to determine an orthonormal basis for  $\mathcal{S}$ .
  - (b) Repeat part (a) using the modified GramSchmidt algorithm, and compare the results.
11. Explain what happens when the GramSchmidt process is applied to an orthonormal set of vectors.
12. Let  $\mathbf{A} = \begin{pmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 1 & 1 & -3 \\ 0 & 1 & 1 \end{pmatrix}$  and  $\mathbf{b} = (1 \ 1 \ 1 \ 1)$
- (a) Determine the rectangular QR factorization of  $\mathbf{A}$ .
  - (b) Use the QR factor from part (a) to determine the least squares solution to  $\mathbf{Ax} = \mathbf{b}$ .
13. Under what conditions on the real numbers  $\alpha$  and  $\beta$  will  $\mathbf{P} = \begin{pmatrix} \alpha + \beta & \beta - \alpha \\ \alpha - \beta & \beta + \alpha \end{pmatrix}$  be an orthogonal matrix?

14. How many  $3 \times 3$  matrices are both diagonal and orthogonal?
15. Let  $\mathbf{U}$  and  $\mathbf{V}$  be two  $n \times n$  unitary (orthogonal) matrices, explain why the product  $\mathbf{UV}$  must be unitary(orthogonal).
16. Let  $\mathbf{u} = (-2 \ 1 \ 3 \ -1)^T$  and  $\mathbf{v} = (1 \ 4 \ 0 \ -1)^T$ .
- (a) Determine the orthogonal projection of  $\mathbf{u}$  onto  $\text{span}\{\mathbf{v}\}$  .
  - (b) Determine the orthogonal projection of  $\mathbf{v}$  onto  $\text{span}\{\mathbf{u}\}$  .
  - (c) Determine the orthogonal projection of  $\mathbf{u}$  onto  $\mathbf{v}^\perp$ .
  - (d) Determine the orthogonal projection of  $\mathbf{v}$  onto  $\mathbf{u}^\perp$ .