

# 线性代数

## 一、基本知识

1. 本书中所有的向量都是列向量的形式：

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

2. 矩阵的 **F** 范数：设  $\mathbf{A} = (a_{i,j})_{m \times n}$

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i,j} a_{i,j}^2}$$

它是向量的  $L_2$  范数的推广。

3. 矩阵的迹  $tr(\mathbf{A}) = \sum_i a_{i,i}$ 。其性质有：

- $\|\mathbf{A}\|_F = \sqrt{tr(\mathbf{A}\mathbf{A}^T)}$
- $tr(\mathbf{A}) = tr(\mathbf{A}^T)$
- 假设  $\mathbf{A} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{B} \in \mathbb{R}^{n \times m}$ , 则有：

$$tr(\mathbf{AB}) = tr(\mathbf{BA})$$

- $tr(\mathbf{ABC}) = tr(\mathbf{CAB}) = tr(\mathbf{BCA})$

## 二、向量操作

1. 一组向量  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_n$  是线性相关的：指存在一组不全为零的实数  $a_1, a_2, \dots, a_n$ ，使得：

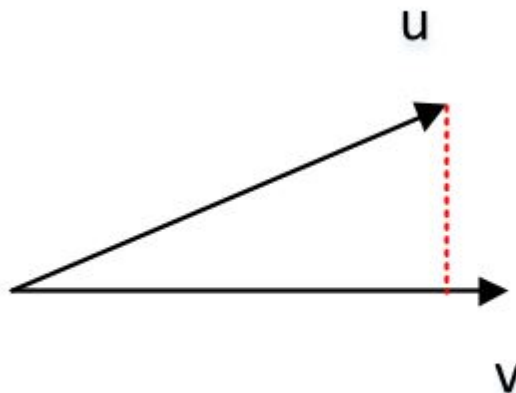
$$\sum_{i=1}^n a_i \vec{v}_i = \vec{0}$$

一组向量  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_n$  是线性无关的，当且仅当  $a_i = 0, i = 1, 2, \dots, n$  时，才有

$$\sum_{i=1}^n a_i \vec{v}_i = \vec{0}$$

2. 一个向量空间所包含的最大线性无关向量的数目，称作该向量空间的维数。
3. 三维向量的点积：

$$\vec{u} \cdot \vec{v} = u_x v_x + u_y v_y + u_z v_z = |\vec{u}| |\vec{v}| \cos(\angle(\vec{u}, \vec{v}))$$



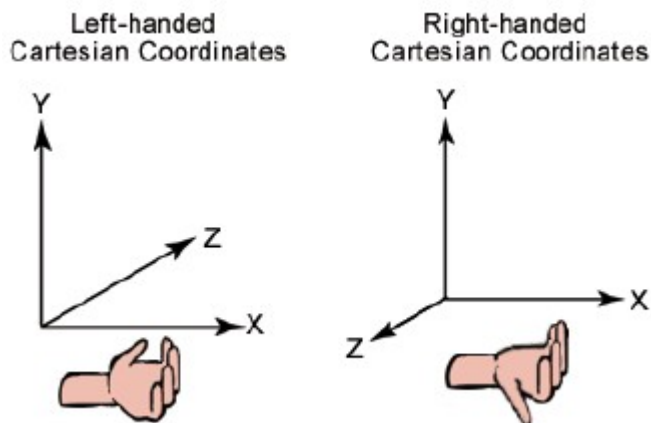
#### 4. 三维向量的叉积:

$$\vec{w} = \vec{u} \times \vec{v} = \begin{bmatrix} \vec{i} & \vec{j} & \vec{k} \\ u_x & u_y & u_z \\ v_x & v_y & v_z \end{bmatrix}$$

其中  $\vec{i}, \vec{j}, \vec{k}$  分别为  $x, y, z$  轴的单位向量。

$$\vec{u} = u_x \vec{i} + u_y \vec{j} + u_z \vec{k}, \quad \vec{v} = v_x \vec{i} + v_y \vec{j} + v_z \vec{k}$$

- $\vec{u}$  和  $\vec{v}$  的叉积垂直于  $\vec{u}, \vec{v}$  构成的平面, 其方向符合右手规则。
- 叉积的模等于  $\vec{u}, \vec{v}$  构成的平行四边形的面积
- $\vec{u} \times \vec{v} = -\vec{v} \times \vec{u}$
- $\vec{u} \times (\vec{v} \times \vec{w}) = (\vec{u} \cdot \vec{w})\vec{v} - (\vec{u} \cdot \vec{v})\vec{w}$



#### 5. 三维向量的混合积:

$$\begin{aligned} [\vec{u} \vec{v} \vec{w}] &= (\vec{u} \times \vec{v}) \cdot \vec{w} = \vec{u} \cdot (\vec{v} \times \vec{w}) \\ &= \begin{vmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix} = \begin{vmatrix} u_x & v_x & w_x \\ u_y & v_y & w_y \\ u_z & v_z & w_z \end{vmatrix} \end{aligned}$$

- 其物理意义为: 以  $\vec{u}, \vec{v}, \vec{w}$  为三个棱边所围成的平行六面体的体积。当  $\vec{u}, \vec{v}, \vec{w}$  构成右手系时, 该平行六面体的体积为正号。

#### 6. 两个向量的并矢: 给定两个向量 $\vec{x} = (x_1, x_2, \dots, x_n)^T, \vec{y} = (y_1, y_2, \dots, y_m)^T$ , 则向量的并矢记作:

$$\vec{x}\vec{y} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_m \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_m \\ \vdots & \vdots & \ddots & \vdots \\ x_n y_1 & x_n y_2 & \cdots & x_n y_m \end{bmatrix}$$

也记作  $\vec{x} \otimes \vec{y}$  或者  $\vec{x}\vec{y}^T$

### 三、矩阵运算

1. 给定两个矩阵  $\mathbf{A} = (a_{i,j}) \in \mathbb{R}^{m \times n}$ ,  $\mathbf{B} = (b_{i,j}) \in \mathbb{R}^{m \times n}$ , 定义:

◦ 阿达马积 Hadamard product (又称作逐元素积):

$$\mathbf{A} \circ \mathbf{B} = \begin{bmatrix} a_{1,1}b_{1,1} & a_{1,2}b_{1,2} & \cdots & a_{1,n}b_{1,n} \\ a_{2,1}b_{2,1} & a_{2,2}b_{2,2} & \cdots & a_{2,n}b_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1}b_{m,1} & a_{m,2}b_{m,2} & \cdots & a_{m,n}b_{m,n} \end{bmatrix}$$

◦ 克罗内积 Kronecker product:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{1,1}\mathbf{B} & a_{1,2}\mathbf{B} & \cdots & a_{1,n}\mathbf{B} \\ a_{2,1}\mathbf{B} & a_{2,2}\mathbf{B} & \cdots & a_{2,n}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1}\mathbf{B} & a_{m,2}\mathbf{B} & \cdots & a_{m,n}\mathbf{B} \end{bmatrix}$$

2. 设  $\vec{x}, \vec{a}, \vec{b}, \vec{c}$  为  $n$  阶向量,  $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{X}$  为  $n$  阶方阵, 则:

$$\frac{\partial(\vec{a}^T \vec{x})}{\partial \vec{x}} = \frac{\partial(\vec{x}^T \vec{a})}{\partial \vec{x}} = \vec{a}$$

$$\frac{\partial(\vec{a}^T \mathbf{X} \vec{b})}{\partial \mathbf{X}} = \vec{a} \vec{b}^T = \vec{a} \otimes \vec{b} \in \mathbb{R}^{n \times n}$$

$$\frac{\partial(\vec{a}^T \mathbf{X}^T \vec{b})}{\partial \mathbf{X}} = \vec{b} \vec{a}^T = \vec{b} \otimes \vec{a} \in \mathbb{R}^{n \times n}$$

$$\frac{\partial(\vec{a}^T \mathbf{X} \vec{a})}{\partial \mathbf{X}} = \frac{\partial(\vec{a}^T \mathbf{X}^T \vec{a})}{\partial \mathbf{X}} = \vec{a} \otimes \vec{a}$$

$$\frac{\partial(\vec{a}^T \mathbf{X}^T \mathbf{X} \vec{b})}{\partial \mathbf{X}} = \mathbf{X}(\vec{a} \otimes \vec{b} + \vec{b} \otimes \vec{a})$$

$$\frac{\partial[(\mathbf{A}\vec{x} + \vec{a})^T \mathbf{C}(\mathbf{B}\vec{x} + \vec{b})]}{\partial \vec{x}} = \mathbf{A}^T \mathbf{C}(\mathbf{B}\vec{x} + \vec{b}) + \mathbf{B}^T \mathbf{C}(\mathbf{A}\vec{x} + \vec{a})$$

$$\frac{\partial(\vec{x}^T \mathbf{A} \vec{x})}{\partial \vec{x}} = (\mathbf{A} + \mathbf{A}^T) \vec{x}$$

$$\frac{\partial[(\mathbf{X} \vec{b} + \vec{c})^T \mathbf{A} (\mathbf{X} \vec{b} + \vec{c})]}{\partial \mathbf{X}} = (\mathbf{A} + \mathbf{A}^T)(\mathbf{X} \vec{b} + \vec{c}) \vec{b}^T$$

$$\frac{\partial(\vec{b}^T \mathbf{X}^T \mathbf{A} \mathbf{X} \vec{c})}{\partial \mathbf{X}} = \mathbf{A}^T \mathbf{X} \vec{b} \vec{c}^T + \mathbf{A} \mathbf{X} \vec{c} \vec{b}^T$$

3. 如果  $f$  是一元函数, 则:

- 其逐元向量函数为:

$$f(\vec{x}) = (f(x_1), f(x_2), \dots, f(x_n))^T$$

- 其逐矩阵函数为:

$$f(\mathbf{X}) = [f(x_{i,j})]$$

- 其逐元导数分别为:

$$f'(\vec{x}) = (f'(x_1), f'(x_2), \dots, f'(x_n))^T$$

$$f'(\mathbf{X}) = [f'(x_{i,j})]$$

4. 各种类型的偏导数:

- 标量对标量的偏导数

$$\frac{\partial u}{\partial v}$$

- 标量对向量 ( $n$  维向量) 的偏导数

$$\frac{\partial u}{\partial \vec{v}} = \left( \frac{\partial u}{\partial v_1}, \frac{\partial u}{\partial v_2}, \dots, \frac{\partial u}{\partial v_n} \right)^T$$

- 标量对矩阵 ( $m \times n$  阶矩阵) 的偏导数

$$\frac{\partial u}{\partial \mathbf{V}} = \begin{bmatrix} \frac{\partial u}{\partial V_{1,1}} & \frac{\partial u}{\partial V_{1,2}} & \dots & \frac{\partial u}{\partial V_{1,n}} \\ \frac{\partial u}{\partial V_{2,1}} & \frac{\partial u}{\partial V_{2,2}} & \dots & \frac{\partial u}{\partial V_{2,n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u}{\partial V_{m,1}} & \frac{\partial u}{\partial V_{m,2}} & \dots & \frac{\partial u}{\partial V_{m,n}} \end{bmatrix}$$

- 向量 ( $m$  维向量) 对标量的偏导数

$$\frac{\partial \vec{u}}{\partial v} = \left( \frac{\partial u_1}{\partial v}, \frac{\partial u_2}{\partial v}, \dots, \frac{\partial u_m}{\partial v} \right)^T$$

- 向量 ( $m$  维向量) 对向量 ( $n$  维向量) 的偏导数 (雅可比矩阵, 行优先)

$$\frac{\partial \vec{u}}{\partial \vec{v}} = \begin{bmatrix} \frac{\partial u_1}{\partial v_1} & \frac{\partial u_1}{\partial v_2} & \cdots & \frac{\partial u_1}{\partial v_n} \\ \frac{\partial u_2}{\partial v_1} & \frac{\partial u_2}{\partial v_2} & \cdots & \frac{\partial u_2}{\partial v_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_m}{\partial v_1} & \frac{\partial u_m}{\partial v_2} & \cdots & \frac{\partial u_m}{\partial v_n} \end{bmatrix}$$

如果为列优先, 则为上面矩阵的转置

- 矩阵 ( $m \times n$  阶矩阵) 对标量的偏导数

$$\frac{\partial \mathbf{U}}{\partial v} = \begin{bmatrix} \frac{\partial U_{1,1}}{\partial v} & \frac{\partial U_{1,2}}{\partial v} & \cdots & \frac{\partial U_{1,n}}{\partial v} \\ \frac{\partial U_{2,1}}{\partial v} & \frac{\partial U_{2,2}}{\partial v} & \cdots & \frac{\partial U_{2,n}}{\partial v} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial U_{m,1}}{\partial v} & \frac{\partial U_{m,2}}{\partial v} & \cdots & \frac{\partial U_{m,n}}{\partial v} \end{bmatrix}$$

- 更复杂的情况依次类推。对于  $\frac{\partial \mathbf{u}}{\partial v}$ 。根据 `numpy` 的术语:

- 假设  $\mathbf{u}$  的 `ndim` (维度) 为  $d_u$

对于标量, `ndim` 为 0; 对于向量, `ndim` 为 1; 对于矩阵, `ndim` 为 2

- 假设  $\mathbf{v}$  的 `ndim` 为  $d_v$

- 则  $\frac{\partial \mathbf{u}}{\partial v}$  的 `ndim` 为  $d_u + d_v$

5. 对于矩阵的迹, 有下列偏导数成立:

$$\frac{\partial [\text{tr}(f(\mathbf{X}))]}{\partial \mathbf{X}} = (f'(\mathbf{X}))^T$$

$$\frac{\partial [\text{tr}(\mathbf{A}\mathbf{X}\mathbf{B})]}{\partial \mathbf{X}} = \mathbf{A}^T \mathbf{B}^T$$

$$\frac{\partial [\text{tr}(\mathbf{A}\mathbf{X}^T \mathbf{B})]}{\partial \mathbf{X}} = \mathbf{B}\mathbf{A}$$

$$\frac{\partial [\text{tr}(\mathbf{A} \otimes \mathbf{X})]}{\partial \mathbf{X}} = \text{tr}(\mathbf{A})\mathbf{I}$$

$$\frac{\partial [\text{tr}(\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X})]}{\partial \mathbf{X}} = \mathbf{A}^T \mathbf{X}^T \mathbf{B}^T + \mathbf{B}^T \mathbf{X} \mathbf{A}^T$$

$$\frac{\partial [\text{tr}(\mathbf{X}^T \mathbf{B}\mathbf{X}\mathbf{C})]}{\partial \mathbf{X}} = (\mathbf{B}^T + \mathbf{B})\mathbf{X}\mathbf{C}\mathbf{C}^T$$

$$\frac{\partial[\text{tr}(\mathbf{C}^T \mathbf{X}^T \mathbf{B} \mathbf{X} \mathbf{C})]}{\partial \mathbf{X}} = \mathbf{B} \mathbf{X} \mathbf{C} + \mathbf{B}^T \mathbf{X} \mathbf{C}^T$$

$$\frac{\partial[\text{tr}(\mathbf{A} \mathbf{X} \mathbf{B} \mathbf{X}^T \mathbf{C})]}{\partial \mathbf{X}} = \mathbf{A}^T \mathbf{C}^T \mathbf{X} \mathbf{B}^T + \mathbf{C} \mathbf{A} \mathbf{X} \mathbf{B}$$

$$\frac{\partial[\text{tr}((\mathbf{A} \mathbf{X} \mathbf{B} + \mathbf{C})(\mathbf{A} \mathbf{X} \mathbf{B} + \mathbf{C}))]}{\partial \mathbf{X}} = 2\mathbf{A}^T (\mathbf{A} \mathbf{X} \mathbf{B} + \mathbf{C}) \mathbf{B}^T$$

6. 假设  $\mathbf{U} = \mathbf{f}(\mathbf{X})$  是关于  $\mathbf{X}$  的矩阵值函数 ( $f: \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{m \times n}$ ) , 且  $g(\mathbf{U})$  是关于  $\mathbf{U}$  的实值函数 ( $g: \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ ) , 则下面链式法则成立:

$$\begin{aligned} \frac{\partial g(\mathbf{U})}{\partial \mathbf{X}} &= \left( \frac{\partial g(\mathbf{U})}{\partial x_{i,j}} \right) = \begin{bmatrix} \frac{\partial g(\mathbf{U})}{\partial x_{1,1}} & \frac{\partial g(\mathbf{U})}{\partial x_{1,2}} & \cdots & \frac{\partial g(\mathbf{U})}{\partial x_{1,n}} \\ \frac{\partial g(\mathbf{U})}{\partial x_{2,1}} & \frac{\partial g(\mathbf{U})}{\partial x_{2,2}} & \cdots & \frac{\partial g(\mathbf{U})}{\partial x_{2,n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g(\mathbf{U})}{\partial x_{m,1}} & \frac{\partial g(\mathbf{U})}{\partial x_{m,2}} & \cdots & \frac{\partial g(\mathbf{U})}{\partial x_{m,n}} \end{bmatrix} \\ &= \left( \sum_k \sum_l \frac{\partial g(\mathbf{U})}{\partial u_{k,l}} \frac{\partial u_{k,l}}{\partial x_{i,j}} \right) \\ &= \text{tr} \left[ \left( \frac{\partial g(\mathbf{U})}{\partial \mathbf{U}} \right)^T \frac{\partial \mathbf{U}}{\partial x_{i,j}} \right] \end{aligned}$$