矩阵求导

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2020 年 12 月 1 日

标量、向量、矩阵间的求导共有 9 种可能：

∂标量/∂标量	∂标量/∂向量	∂标量/∂矩阵
∂向量/∂标量	∂向量/∂向量	∂向量/∂矩阵
∂矩阵/∂标量	∂矩阵/∂向量	∂矩阵/∂矩阵

表 1: 9 种求导情形

∂标量/∂标量就是我们熟悉的单变量微积分，∂向量/∂矩阵、∂矩阵/∂向量、∂矩阵/∂矩阵会涉及高阶张量，处理更为麻烦，因此本文只考虑剩下的 5 种情形。

设 $\boldsymbol{u} \in \mathbb{R}^l$，$\mathbf{U} \in \mathbb{R}^{m \times n}$，则向量、矩阵对标量求导的定义为

$$\frac{\partial \boldsymbol{u}}{\partial x} \triangleq \begin{bmatrix} \frac{\partial u_1}{\partial x} \\ \frac{\partial u_2}{\partial x} \\ \vdots \\ \frac{\partial u_l}{\partial x} \end{bmatrix}, \quad \frac{\partial \mathbf{U}}{\partial x} \triangleq \begin{bmatrix} \frac{\partial u_{11}}{\partial x} & \frac{\partial u_{12}}{\partial x} & \cdots & \frac{\partial u_{1n}}{\partial x} \\ \frac{\partial u_{21}}{\partial x} & \frac{\partial u_{22}}{\partial x} & \cdots & \frac{\partial u_{2n}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}}{\partial x} & \frac{\partial u_{m2}}{\partial x} & \cdots & \frac{\partial u_{mn}}{\partial x} \end{bmatrix}$$

设 $\boldsymbol{x} \in \mathbb{R}^l$，$\mathbf{X} \in \mathbb{R}^{m \times n}$，则标量对向量、矩阵求导的定义为

$$\frac{\partial u}{\partial \boldsymbol{x}} \triangleq \begin{bmatrix} \frac{\partial u}{\partial x_1} & \frac{\partial u}{\partial x_2} & \cdots & \frac{\partial u}{\partial x_l} \end{bmatrix}, \quad \frac{\partial u}{\partial \mathbf{X}} \triangleq \begin{bmatrix} \frac{\partial u}{\partial x_{11}} & \frac{\partial u}{\partial x_{21}} & \cdots & \frac{\partial u}{\partial x_{m1}} \\ \frac{\partial u}{\partial x_{12}} & \frac{\partial u}{\partial x_{22}} & \cdots & \frac{\partial u}{\partial x_{m2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u}{\partial x_{1n}} & \frac{\partial u}{\partial x_{2n}} & \cdots & \frac{\partial u}{\partial x_{mn}} \end{bmatrix}$$

即向量、矩阵对标量求导的结果与分子尺寸相同，标量对向量、矩阵求导的结果与分母的转置尺寸相同。向量对向量求导的定义为 Jacobian 矩阵：

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}} \triangleq \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \cdots & \frac{\partial u_1}{\partial x_l} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \cdots & \frac{\partial u_2}{\partial x_l} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_l}{\partial x_1} & \frac{\partial u_l}{\partial x_2} & \cdots & \frac{\partial u_l}{\partial x_l} \end{bmatrix}$$

即行数与分子尺寸相同、列数与分母尺寸相同。

以上即为分子布局，其好处是链式法则跟单变量微积分中的顺序一样，坏处是计算标量值函数 $f(\boldsymbol{x})$ 关于向量变量 $\boldsymbol{x}$ 的梯度时要多做一个转置：$\nabla f = (\frac{\partial f}{\partial \boldsymbol{x}})^\top$，因为我们更习惯梯度是列向量。分母布局的结果均是分子布局的转置，好处就是算梯度时不用做转置，坏处就是链式法则的顺序要完全反过来。

1 基本结果

以下结果根据定义和单变量微积分的求导法则都是显然的。

单变量微积分中常量的导数为零

$$\frac{\partial a}{\partial x} = 0$$

类似的这里有

$$\frac{\partial \boldsymbol{a}}{\partial x} = \mathbf{0}, \quad \frac{\partial a}{\partial \boldsymbol{x}} = \mathbf{0}^\top, \quad \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} = \mathbf{0}, \quad \frac{\partial \mathbf{A}}{\partial x} = \mathbf{0}, \quad \frac{\partial a}{\partial \mathbf{X}} = \mathbf{0}^\top$$

单变量微积分中常数标量乘的求导法则为

$$\frac{\partial a u}{\partial x} = a \frac{\partial u}{\partial x}$$

类似的这里有

$$\frac{\partial a \boldsymbol{u}}{\partial x} = a \frac{\partial \boldsymbol{u}}{\partial x}, \quad \frac{\partial a u}{\partial \boldsymbol{x}} = a \frac{\partial u}{\partial \boldsymbol{x}}, \quad \frac{\partial a \boldsymbol{u}}{\partial \boldsymbol{x}} = a \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}, \quad \frac{\partial a \mathbf{U}}{\partial x} = a \frac{\partial \mathbf{U}}{\partial x}, \quad \frac{\partial a u}{\partial \mathbf{X}} = a \frac{\partial u}{\partial \mathbf{X}}$$

单变量微积分中加法的求导法则为

$$\frac{\partial (u+v)}{\partial x} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial x}$$

类似的这里有

$$\begin{aligned}
&\frac{\partial (\boldsymbol{u}+\boldsymbol{v})}{\partial x} = \frac{\partial \boldsymbol{u}}{\partial x} + \frac{\partial \boldsymbol{v}}{\partial x}, \quad \frac{\partial (u+v)}{\partial \boldsymbol{x}} = \frac{\partial u}{\partial \boldsymbol{x}} + \frac{\partial v}{\partial \boldsymbol{x}}, \quad \frac{\partial (\boldsymbol{u}+\boldsymbol{v})}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}} + \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} \\
&\frac{\partial (\mathbf{U}+\mathbf{V})}{\partial x} = \frac{\partial \mathbf{U}}{\partial x} + \frac{\partial \mathbf{V}}{\partial x}, \quad \frac{\partial (u+v)}{\partial \mathbf{X}} = \frac{\partial u}{\partial \mathbf{X}} + \frac{\partial v}{\partial \mathbf{X}}
\end{aligned}$$

单变量微积分中乘法的求导法则为

$$\frac{\partial uv}{\partial x} = \frac{\partial u}{\partial x} v + u \frac{\partial v}{\partial x}$$

类似的这里有

$$\begin{aligned}
&\frac{\partial \boldsymbol{u}\boldsymbol{v}}{\partial x} = \frac{\partial \boldsymbol{u}}{\partial x} \boldsymbol{v} + \boldsymbol{u} \frac{\partial \boldsymbol{v}}{\partial x}, \quad \frac{\partial uv}{\partial \boldsymbol{x}} = \frac{\partial u}{\partial \boldsymbol{x}} v + u \frac{\partial v}{\partial \boldsymbol{x}} \\
&\frac{\partial \mathbf{U}\mathbf{V}}{\partial x} = \frac{\partial \mathbf{U}}{\partial x} \mathbf{V} + \mathbf{U} \frac{\partial \mathbf{V}}{\partial x}, \quad \frac{\partial uv}{\partial \mathbf{X}} = \frac{\partial u}{\partial \mathbf{X}} v + u \frac{\partial v}{\partial \mathbf{X}}
\end{aligned}$$

其中第二行是因为

$$\left[\frac{\partial \mathbf{U}\mathbf{V}}{\partial x}\right]_{ij} = \frac{\partial \sum_k u_{ik} v_{kj}}{\partial x} = \sum_k \frac{\partial u_{ik}}{\partial x} v_{kj} + \sum_k u_{ik} \frac{\partial v_{kj}}{\partial x} = \left[\frac{\partial \mathbf{U}}{\partial x}\mathbf{V}\right]_{ij} + \left[\mathbf{U}\frac{\partial \mathbf{V}}{\partial x}\right]_{ij}$$

$$\left[\frac{\partial uv}{\partial \mathbf{X}}\right]_{ij} = \frac{\partial uv}{\partial x_{ji}} = \frac{\partial u}{\partial x_{ji}} v + u \frac{\partial v}{\partial x_{ji}} = \left[\frac{\partial u}{\partial \mathbf{X}}\right]_{ij} v + u \left[\frac{\partial v}{\partial \mathbf{X}}\right]_{ij}$$

第一行可看作第二行的特例。$\partial \boldsymbol{uv}/\partial \boldsymbol{x}$ 有两种可能，一是 $\boldsymbol{uv}$ 为标量，即两者的内积，这里暂且不表，后文再讲；二是 $\boldsymbol{uv}$ 为矩阵，这属于我们不考虑的 ∂矩阵/∂向量 情形。

单变量微积分中有 $\partial x/\partial x = 1$，类似的这里有

$$\frac{\partial x_i}{\partial \boldsymbol{x}} = \boldsymbol{e}_i^\top, \quad \frac{\partial \boldsymbol{x}}{\partial x_i} = \boldsymbol{e}_i, \quad \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}} = \mathbf{I}, \quad \frac{\partial x_{ij}}{\partial \mathbf{X}} = \mathbf{E}_{ji}, \quad \frac{\partial \mathbf{X}}{\partial x_{ij}} = \mathbf{E}_{ij}$$

其中 $\mathbf{E}_{ij}$ 是 (i,j) 处为 1 其余为 0 的矩阵。

单变量微积分中的链式法则为

$$\frac{\partial g(u)}{\partial x} = \frac{\partial g(u)}{\partial u}\frac{\partial u}{\partial x}$$

类似的，

- 只涉及向量：设 $\boldsymbol{x} \in \mathbb{R}^n$，$\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}) \in \mathbb{R}^m$，$\boldsymbol{g} : \mathbb{R}^m \mapsto \mathbb{R}^l$，则

$$\underbrace{\frac{\partial \boldsymbol{g}(\boldsymbol{u})}{\partial \boldsymbol{x}}}_{l\times n} = \underbrace{\frac{\partial \boldsymbol{g}(\boldsymbol{u})}{\partial \boldsymbol{u}}}_{l\times m}\underbrace{\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}}_{m\times n}$$

  这是因为

$$\begin{aligned}\left[\frac{\partial \boldsymbol{g}(\boldsymbol{u})}{\partial \boldsymbol{x}}\right]_{ij} &= \frac{\partial [\boldsymbol{g}(\boldsymbol{u})]_i}{\partial x_j} = \sum_{k\in[m]} \frac{\partial [\boldsymbol{g}(\boldsymbol{u})]_i}{\partial u_k}\frac{\partial u_k}{\partial x_j} = \frac{\partial [\boldsymbol{g}(\boldsymbol{u})]_i}{\partial \boldsymbol{u}}\frac{\partial \boldsymbol{u}}{\partial x_j} \\ &= \left[\frac{\partial \boldsymbol{g}(\boldsymbol{u})}{\partial \boldsymbol{u}}\right]_{i,:}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}\right]_{:,j} = \left[\frac{\partial \boldsymbol{g}(\boldsymbol{u})}{\partial \boldsymbol{u}}\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}\right]_{i,j}\end{aligned}$$

  注意若 $n = m = l = 1$，就退化成了单变量的链式法则。

- 自变量是矩阵：设 $u = u(\mathbf{X})$，$g : \mathbb{R} \mapsto \mathbb{R}$，则

$$\frac{\partial g(u)}{\partial \mathbf{X}} = \frac{\partial g(u)}{\partial u}\frac{\partial u}{\partial \mathbf{X}}$$

  这是因为

$$\left[\frac{\partial g(u)}{\partial \mathbf{X}}\right]_{ij} = \frac{\partial g(u)}{\partial x_{ji}} = \frac{\partial g(u)}{\partial u}\frac{\partial u}{\partial x_{ji}} = \frac{\partial g(u)}{\partial u}\left[\frac{\partial u}{\partial \mathbf{X}}\right]_{ij}$$

- 中间变量是矩阵：设 $\mathbf{U} = \mathbf{U}(x) \in \mathbb{R}^{m\times n}$，$g : \mathbb{R}^{m\times n} \mapsto \mathbb{R}$，则

$$\frac{\partial g(\mathbf{U})}{\partial x} = \sum_p \sum_q \frac{\partial g(\mathbf{U})}{\partial u_{pq}}\frac{\partial u_{pq}}{\partial x} = \sum_q \sum_p \left[\frac{\partial g(\mathbf{U})}{\partial \mathbf{U}}\right]_{qp}\left[\frac{\partial \mathbf{U}}{\partial x}\right]_{pq} = \operatorname{tr}\left(\frac{\partial g(\mathbf{U})}{\partial \mathbf{U}}\frac{\partial \mathbf{U}}{\partial x}\right) \tag{1}$$

2 向量对标量求导

矩阵和向量的乘积是向量，若 $\mathbf{A}$ 与 $\boldsymbol{x}$ 无关，易知有

$$\left[\frac{\partial \mathbf{A}\boldsymbol{u}}{\partial x}\right]_i = \frac{\partial [\mathbf{A}\boldsymbol{u}]_i}{\partial x} = \frac{\partial \sum_k a_{ik}u_k}{\partial x} = \sum_k a_{ik}\frac{\partial u_k}{\partial x} = \left[\mathbf{A}\frac{\partial \boldsymbol{u}}{\partial x}\right]_i \Longrightarrow \frac{\partial \mathbf{A}\boldsymbol{u}}{\partial x} = \mathbf{A}\frac{\partial \boldsymbol{u}}{\partial x}$$

$$\left[\frac{\partial \boldsymbol{u}^\top \mathbf{A}}{\partial x}\right]_i = \frac{\partial [\boldsymbol{u}^\top \mathbf{A}]_i}{\partial x} = \frac{\partial [\mathbf{A}^\top \boldsymbol{u}]_i}{\partial x} = \left[\mathbf{A}^\top \frac{\partial \boldsymbol{u}}{\partial x}\right]_i \Longrightarrow \frac{\partial \boldsymbol{u}^\top \mathbf{A}}{\partial x} = \mathbf{A}^\top \frac{\partial \boldsymbol{u}}{\partial x}$$

向量的外积也是向量，记 $\boldsymbol{u} = [u_1(x); u_2(x); u_3(x)]$，$\boldsymbol{v} = [v_1(x); v_2(x); v_3(x)]$，则

$$\boldsymbol{u}^\top \times \boldsymbol{v} = \begin{bmatrix} u_2 v_3 - u_3 v_2 \\ u_3 v_1 - u_1 v_3 \\ u_1 v_2 - u_2 v_1 \end{bmatrix}$$

于是

$$\frac{\partial (\boldsymbol{u}^\top \times \boldsymbol{v})}{\partial x} = \begin{bmatrix} \frac{\partial u_2}{\partial x} v_3 - \frac{\partial u_3}{\partial x} v_2 + u_2 \frac{\partial v_3}{\partial x} - u_3 \frac{\partial v_2}{\partial x} \\ \frac{\partial u_3}{\partial x} v_1 - \frac{\partial u_1}{\partial x} v_3 + u_3 \frac{\partial v_1}{\partial x} - u_1 \frac{\partial v_3}{\partial x} \\ \frac{\partial u_1}{\partial x} v_2 - \frac{\partial u_2}{\partial x} v_1 + u_1 \frac{\partial v_2}{\partial x} - u_2 \frac{\partial v_1}{\partial x} \end{bmatrix} = \left(\frac{\partial \boldsymbol{u}}{\partial x}\right)^\top \times \boldsymbol{v} + \boldsymbol{u}^\top \times \frac{\partial \boldsymbol{v}}{\partial x}$$

3 标量对向量求导

二次型是标量，设 $\mathbf{A}$ 与 $\boldsymbol{x}$ 无关，易知有

$$\begin{aligned} \left[\frac{\partial \boldsymbol{u}^\top \mathbf{A} \boldsymbol{v}}{\partial \boldsymbol{x}}\right]_i &= \frac{\partial \boldsymbol{u}^\top \mathbf{A} \boldsymbol{v}}{\partial x_i} = \frac{\partial \sum_j \sum_k u_j a_{jk} v_k}{\partial x_i} = \sum_j \sum_k u_j a_{jk} \frac{\partial v_k}{\partial x_i} + \sum_j \sum_k \frac{\partial u_j}{\partial x_i} a_{jk} v_k \\ &= \boldsymbol{u}^\top \mathbf{A} \frac{\partial \boldsymbol{v}}{\partial x_i} + \boldsymbol{v}^\top \mathbf{A}^\top \frac{\partial \boldsymbol{u}}{\partial x_i} = \left[\boldsymbol{u}^\top \mathbf{A} \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}}\right]_i + \left[\boldsymbol{v}^\top \mathbf{A}^\top \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}\right]_i \\ &\Longrightarrow \frac{\partial \boldsymbol{u}^\top \mathbf{A} \boldsymbol{v}}{\partial \boldsymbol{x}} = \boldsymbol{u}^\top \mathbf{A} \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} + \boldsymbol{v}^\top \mathbf{A}^\top \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}} \end{aligned}$$

特别的，

- 取 $\mathbf{A} = \mathbf{I}$，则

$$\frac{\partial \boldsymbol{u}^\top \boldsymbol{v}}{\partial \boldsymbol{x}} = \boldsymbol{u}^\top \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} + \boldsymbol{v}^\top \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}$$

进一步若 $\boldsymbol{u} = \boldsymbol{a}$ 与 $\boldsymbol{x}$ 无关，则

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{v}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}}, \quad \frac{\partial \boldsymbol{a}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top, \quad \frac{\partial \boldsymbol{b}^\top \mathbf{A} \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{b}^\top \mathbf{A}$$

- 取 $\boldsymbol{u} = \boldsymbol{v} = \boldsymbol{x}$，则

$$\frac{\partial \boldsymbol{x}^\top \mathbf{A} \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top \mathbf{A} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}} + \boldsymbol{x}^\top \mathbf{A}^\top \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top (\mathbf{A} + \mathbf{A}^\top)$$

进一步若 $\mathbf{A} = \mathbf{I}$，则

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \frac{\partial \|\boldsymbol{x}\|^2}{\partial \boldsymbol{x}} = 2\boldsymbol{x}^\top$$

- 若 $\mathbf{A} = \boldsymbol{b}\boldsymbol{a}^\top$，则

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{b} \boldsymbol{a}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{a}^\top \boldsymbol{x} \boldsymbol{x}^\top \boldsymbol{b}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top (\boldsymbol{a}\boldsymbol{b}^\top + \boldsymbol{b}\boldsymbol{a}^\top)$$

- 更一般的有

$$\begin{aligned}\frac{\partial(\mathbf{A}\boldsymbol{x}+\boldsymbol{b})^\top\mathbf{C}(\mathbf{D}\boldsymbol{x}+\boldsymbol{e})}{\partial\boldsymbol{x}}&=\frac{\partial(\boldsymbol{x}^\top\mathbf{A}^\top\mathbf{C}\mathbf{D}\boldsymbol{x}+\boldsymbol{b}^\top\mathbf{C}\mathbf{D}\boldsymbol{x}+\boldsymbol{x}^\top\mathbf{A}^\top\mathbf{C}\boldsymbol{e}+\boldsymbol{b}^\top\boldsymbol{e})}{\partial\boldsymbol{x}}\\&=\boldsymbol{x}^\top(\mathbf{A}^\top\mathbf{C}\mathbf{D}+\mathbf{D}^\top\mathbf{C}^\top\mathbf{A})+\boldsymbol{b}^\top\mathbf{C}\mathbf{D}+\boldsymbol{e}^\top\mathbf{C}^\top\mathbf{A}\\&=(\mathbf{D}\boldsymbol{x}+\boldsymbol{e})^\top\mathbf{C}^\top\mathbf{A}+(\mathbf{A}\boldsymbol{x}+\boldsymbol{b})^\top\mathbf{C}\mathbf{D}\end{aligned}$$

范数也是标量，若 $\boldsymbol{a}$ 与 $\boldsymbol{x}$ 无关，则

$$\left[\frac{\partial\|\boldsymbol{x}-\boldsymbol{a}\|}{\partial\boldsymbol{x}}\right]_i=\frac{\partial\|\boldsymbol{x}-\boldsymbol{a}\|}{\partial x_i}=\frac{\partial\sqrt{\sum_j(x_j-a_j)^2}}{\partial x_i}=\frac{1}{2}\frac{2(x_i-a_i)}{\sqrt{\sum_j(x_j-a_j)^2}}=\frac{x_i-a_i}{\|\boldsymbol{x}-\boldsymbol{a}\|}$$
$$\Longrightarrow\frac{\partial\|\boldsymbol{x}-\boldsymbol{a}\|}{\partial\boldsymbol{x}}=\frac{(\boldsymbol{x}-\boldsymbol{a})^\top}{\|\boldsymbol{x}-\boldsymbol{a}\|}$$

4 向量对向量求导

若 $\mathbf{A}$ 与 $\boldsymbol{x}$ 无关，易知有

$$\left[\frac{\partial\mathbf{A}\boldsymbol{u}}{\partial\boldsymbol{x}}\right]_{ij}=\frac{\partial[\mathbf{A}\boldsymbol{u}]_i}{\partial x_j}=\frac{\partial\sum_k a_{ik}u_k}{\partial x_j}=\sum_k a_{ik}\frac{\partial u_k}{\partial x_j}=\left[\mathbf{A}\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}\right]_{ij}\Longrightarrow\frac{\partial\mathbf{A}\boldsymbol{u}}{\partial\boldsymbol{x}}=\mathbf{A}\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}$$
$$\left[\frac{\partial\boldsymbol{u}^\top\mathbf{A}}{\partial\boldsymbol{x}}\right]_{ij}=\frac{\partial[\boldsymbol{u}^\top\mathbf{A}]_i}{\partial x_j}=\frac{\partial[\mathbf{A}^\top\boldsymbol{u}]_i}{\partial x_j}=\left[\mathbf{A}^\top\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}\right]_{ij}\Longrightarrow\frac{\partial\boldsymbol{u}^\top\mathbf{A}}{\partial\boldsymbol{x}}=\mathbf{A}^\top\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}$$

特别的，若 $\boldsymbol{u}=\boldsymbol{x}$，则

$$\frac{\partial\mathbf{A}\boldsymbol{x}}{\partial\boldsymbol{x}}=\mathbf{A}\frac{\partial\boldsymbol{x}}{\partial\boldsymbol{x}}=\mathbf{A},\quad\frac{\partial\boldsymbol{x}^\top\mathbf{A}}{\partial\boldsymbol{x}}=\mathbf{A}^\top\frac{\partial\boldsymbol{x}}{\partial\boldsymbol{x}}=\mathbf{A}^\top$$

若 $v=v(\boldsymbol{x})$，则

$$\left[\frac{\partial v\boldsymbol{u}}{\partial\boldsymbol{x}}\right]_{ij}=\frac{\partial vu_i}{\partial x_j}=v\frac{\partial u_i}{\partial x_j}+u_i\frac{\partial v}{\partial x_j}=v\left[\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}\right]_{ij}+\left[\boldsymbol{u}\frac{\partial v}{\partial\boldsymbol{x}}\right]_{ij}\Longrightarrow\frac{\partial v\boldsymbol{u}}{\partial\boldsymbol{x}}=v\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{x}}+\boldsymbol{u}\frac{\partial v}{\partial\boldsymbol{x}}$$

注意第一项是标量乘以 Jacobian 矩阵，第二项是列向量乘以行向量。

5 矩阵对标量求导

若 $u=u(x)$，$\mathbf{V}=\mathbf{V}(x)$，则

$$\left[\frac{\partial u\mathbf{V}}{\partial x}\right]_{ij}=\frac{\partial uv_{ij}}{\partial x}=\frac{\partial u}{\partial x}v_{ij}+u\frac{\partial v_{ij}}{\partial x}=\frac{\partial u}{\partial x}[\mathbf{V}]_{ij}+u\left[\frac{\partial\mathbf{V}}{\partial x}\right]_{ij}\Longrightarrow\frac{\partial u\mathbf{V}}{\partial x}=\frac{\partial u}{\partial x}\mathbf{V}+u\frac{\partial\mathbf{V}}{\partial x}$$

若乘积求导法则中的 $\mathbf{U}$ 或 $\mathbf{V}$ 可继续分解为 x 相关项的乘积，例如 $\mathbf{V}\leftarrow\mathbf{V}\mathbf{W}$，则

$$\frac{\partial\mathbf{U}\mathbf{V}\mathbf{W}}{\partial x}=\frac{\partial\mathbf{U}}{\partial x}\mathbf{V}\mathbf{W}+\mathbf{U}\frac{\partial\mathbf{V}\mathbf{W}}{\partial x}=\frac{\partial\mathbf{U}}{\partial x}\mathbf{V}\mathbf{W}+\mathbf{U}\left(\frac{\partial\mathbf{V}}{\partial x}\mathbf{W}+\mathbf{V}\frac{\partial\mathbf{W}}{\partial x}\right)=\frac{\partial\mathbf{U}}{\partial x}\mathbf{V}\mathbf{W}+\mathbf{U}\frac{\partial\mathbf{V}}{\partial x}\mathbf{W}+\mathbf{U}\mathbf{V}\frac{\partial\mathbf{W}}{\partial x}\tag{2}$$

由此可知若 $\mathbf{A}$、$\mathbf{B}$ 与 x 无关，则

$$\frac{\partial \mathbf{AUB}}{\partial x} = \mathbf{A}\frac{\partial \mathbf{U}}{\partial x}\mathbf{B}$$

当 $\mathbf{U}$ 为方阵、n 为正整数时有

$$\frac{\partial \mathbf{U}^n}{\partial x} = \mathbf{U}^{n-1}\frac{\partial \mathbf{U}}{\partial x} + \mathbf{U}^{n-2}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U} + \cdots + \mathbf{U}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{n-2} + \frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{n-1} = \sum_{i\in[n]} \mathbf{U}^{i-1}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{n-i} \tag{3}$$

令乘积求导法则中的 $\mathbf{V} = \mathbf{U}^{-1}$ 可得

$$\mathbf{0} = \frac{\partial \mathbf{I}}{\partial x} = \frac{\partial \mathbf{U}\mathbf{U}^{-1}}{\partial x} = \mathbf{U}\frac{\partial \mathbf{U}^{-1}}{\partial x} + \frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1} \Longrightarrow \frac{\partial \mathbf{U}^{-1}}{\partial x} = -\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1} \tag{4}$$

进一步结合式 (2) 可得 Hessian 矩阵

$$\begin{aligned}
\frac{\partial^2 \mathbf{U}^{-1}}{\partial x \partial y} &= \frac{\partial}{\partial y}\left(-\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1}\right) = -\frac{\partial \mathbf{U}^{-1}}{\partial y}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1} - \mathbf{U}^{-1}\frac{\partial^2 \mathbf{U}}{\partial x \partial y}\mathbf{U}^{-1} - \mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x}\frac{\partial \mathbf{U}^{-1}}{\partial y} \\
&= \mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial y}\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1} - \mathbf{U}^{-1}\frac{\partial^2 \mathbf{U}}{\partial x \partial y}\mathbf{U}^{-1} + \mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial y}\mathbf{U}^{-1} \\
&= \mathbf{U}^{-1}\left(\frac{\partial \mathbf{U}}{\partial y}\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial x} - \frac{\partial^2 \mathbf{U}}{\partial x \partial y} + \frac{\partial \mathbf{U}}{\partial x}\mathbf{U}^{-1}\frac{\partial \mathbf{U}}{\partial y}\right)\mathbf{U}^{-1}
\end{aligned}$$

矩阵除了常规的乘积外，还有 Kronecker 积和 Hadamard 积。设 $\mathbf{U} \in \mathbb{R}^{m\times n}$，$\mathbf{V} \in \mathbb{R}^{p\times q}$，则

$$\begin{aligned}
\frac{\partial \mathbf{U} \otimes \mathbf{V}}{\partial x} &= \begin{bmatrix} \frac{\partial u_{11}\mathbf{V}}{\partial x} & \frac{\partial u_{12}\mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{1n}\mathbf{V}}{\partial x} \\ \frac{\partial u_{21}\mathbf{V}}{\partial x} & \frac{\partial u_{22}\mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{2n}\mathbf{V}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}\mathbf{V}}{\partial x} & \frac{\partial u_{m2}\mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{mn}\mathbf{V}}{\partial x} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial u_{11}}{\partial x}\mathbf{V} + u_{11}\frac{\partial \mathbf{V}}{\partial x} & \frac{\partial u_{12}}{\partial x}\mathbf{V} + u_{12}\frac{\partial \mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{1n}}{\partial x}\mathbf{V} + u_{1n}\frac{\partial \mathbf{V}}{\partial x} \\ \frac{\partial u_{21}}{\partial x}\mathbf{V} + u_{21}\frac{\partial \mathbf{V}}{\partial x} & \frac{\partial u_{22}}{\partial x}\mathbf{V} + u_{22}\frac{\partial \mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{2n}}{\partial x}\mathbf{V} + u_{2n}\frac{\partial \mathbf{V}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}}{\partial x}\mathbf{V} + u_{m1}\frac{\partial \mathbf{V}}{\partial x} & \frac{\partial u_{m2}}{\partial x}\mathbf{V} + u_{m2}\frac{\partial \mathbf{V}}{\partial x} & \cdots & \frac{\partial u_{mn}}{\partial x}\mathbf{V} + u_{mn}\frac{\partial \mathbf{V}}{\partial x} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial u_{11}}{\partial x}\mathbf{V} & \frac{\partial u_{12}}{\partial x}\mathbf{V} & \cdots & \frac{\partial u_{1n}}{\partial x}\mathbf{V} \\ \frac{\partial u_{21}}{\partial x}\mathbf{V} & \frac{\partial u_{22}}{\partial x}\mathbf{V} & \cdots & \frac{\partial u_{2n}}{\partial x}\mathbf{V} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}}{\partial x}\mathbf{V} & \frac{\partial u_{m2}}{\partial x}\mathbf{V} & \cdots & \frac{\partial u_{mn}}{\partial x}\mathbf{V} \end{bmatrix} + \begin{bmatrix} u_{11}\frac{\partial \mathbf{V}}{\partial x} & u_{12}\frac{\partial \mathbf{V}}{\partial x} & \cdots & u_{1n}\frac{\partial \mathbf{V}}{\partial x} \\ u_{21}\frac{\partial \mathbf{V}}{\partial x} & u_{22}\frac{\partial \mathbf{V}}{\partial x} & \cdots & u_{2n}\frac{\partial \mathbf{V}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ u_{m1}\frac{\partial \mathbf{V}}{\partial x} & u_{m2}\frac{\partial \mathbf{V}}{\partial x} & \cdots & u_{mn}\frac{\partial \mathbf{V}}{\partial x} \end{bmatrix} \\
&= \frac{\partial \mathbf{U}}{\partial x} \otimes \mathbf{V} + \mathbf{U} \otimes \frac{\partial \mathbf{V}}{\partial x}
\end{aligned}$$

设 $\mathbf{U}, \mathbf{V} \in \mathbb{R}^{m\times n}$，则

$$\frac{\partial \mathbf{U} \circ \mathbf{V}}{\partial x} = \begin{bmatrix} \frac{\partial u_{11}v_{11}}{\partial x} & \frac{\partial u_{12}v_{12}}{\partial x} & \cdots & \frac{\partial u_{1n}v_{1n}}{\partial x} \\ \frac{\partial u_{21}v_{21}}{\partial x} & \frac{\partial u_{22}v_{22}}{\partial x} & \cdots & \frac{\partial u_{2n}v_{2n}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}v_{m1}}{\partial x} & \frac{\partial u_{m2}v_{m2}}{\partial x} & \cdots & \frac{\partial u_{mn}v_{mn}}{\partial x} \end{bmatrix}$$

$$
\begin{aligned}
&= \begin{bmatrix} \frac{\partial u_{11}}{\partial x} v_{11} & \frac{\partial u_{12}}{\partial x} v_{12} & \cdots & \frac{\partial u_{1n}}{\partial x} v_{1n} \\ \frac{\partial u_{21}}{\partial x} v_{21} & \frac{\partial u_{22}}{\partial x} v_{22} & \cdots & \frac{\partial u_{2n}}{\partial x} v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial u_{m1}}{\partial x} v_{m1} & \frac{\partial u_{m2}}{\partial x} v_{m2} & \cdots & \frac{\partial u_{mn}}{\partial x} v_{mn} \end{bmatrix} + \begin{bmatrix} u_{11} \frac{\partial v_{11}}{\partial x} & u_{12} \frac{\partial v_{12}}{\partial x} & \cdots & u_{1n} \frac{\partial v_{1n}}{\partial x} \\ u_{21} \frac{\partial v_{21}}{\partial x} & u_{22} \frac{\partial v_{22}}{\partial x} & \cdots & u_{2n} \frac{\partial v_{2n}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ u_{m1} \frac{\partial v_{m1}}{\partial x} & u_{m2} \frac{\partial v_{m2}}{\partial x} & \cdots & u_{mn} \frac{\partial v_{mn}}{\partial x} \end{bmatrix} \\
&= \frac{\partial \mathbf{U}}{\partial x} \circ \mathbf{V} + \mathbf{U} \circ \frac{\partial \mathbf{V}}{\partial x}
\end{aligned}
$$

设多项式函数 $g(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$，则 $g'(x) = a_1 + 2a_2 x + 3a_3 x^2 + \cdots$，若 $\mathbf{A}$ 为与 x 无关的方阵，记

$$
\begin{aligned}
g(x\mathbf{A}) &= a_0 \mathbf{I} + a_1 x \mathbf{A} + a_2 x^2 \mathbf{A}^2 + a_3 x^3 \mathbf{A}^3 + \cdots \\
g'(x\mathbf{A}) &= a_1 \mathbf{I} + 2a_2 x \mathbf{A} + 3a_3 x^2 \mathbf{A}^2 + \cdots
\end{aligned}
$$

易知有

$$
\begin{aligned}
\frac{\partial g(x\mathbf{A})}{\partial x} &= a_1 \mathbf{A} + 2a_2 x \mathbf{A}^2 + 3a_3 x^2 \mathbf{A}^3 + \cdots \\
&= \mathbf{A}(a_1 \mathbf{I} + 2a_2 x \mathbf{A} + 3a_3 x^2 \mathbf{A}^2 + \cdots) = \mathbf{A} g'(x\mathbf{A}) \\
&= (a_1 \mathbf{I} + 2a_2 x \mathbf{A} + 3a_3 x^2 \mathbf{A}^2 + \cdots)\mathbf{A} = g'(x\mathbf{A})\mathbf{A}
\end{aligned}
$$

对于 e^x、$\ln x$、$\sin x$、$\cos x$，上式依然适用，例如

$$
\frac{\partial e^{x\mathbf{A}}}{\partial x} = \mathbf{A} e^{x\mathbf{A}} = e^{x\mathbf{A}} \mathbf{A}
$$

6 标量对矩阵求导

矩阵常见的标量函数有迹和行列式。

6.1 迹对矩阵求导

若 a 与 $\mathbf{X}$ 无关，$\mathbf{U} = \mathbf{U}(\mathbf{X})$，$\mathbf{V} = \mathbf{V}(\mathbf{X})$，则以下结论是显然的：

$$
\frac{\partial \operatorname{tr}(\mathbf{X})}{\partial \mathbf{X}} = \mathbf{I}, \quad \frac{\partial \operatorname{tr}(\mathbf{U} + \mathbf{V})}{\partial \mathbf{X}} = \frac{\partial \operatorname{tr}(\mathbf{U})}{\partial \mathbf{X}} + \frac{\partial \operatorname{tr}(\mathbf{V})}{\partial \mathbf{X}}, \quad \frac{\partial \operatorname{tr}(a\mathbf{U})}{\partial \mathbf{X}} = a \frac{\partial \operatorname{tr}(\mathbf{U})}{\partial \mathbf{X}}
$$

对于乘积有

$$
\begin{aligned}
\left[\frac{\partial \operatorname{tr}(\mathbf{UV})}{\partial \mathbf{X}}\right]_{ij} &= \frac{\partial \operatorname{tr}(\mathbf{UV})}{\partial x_{ji}} = \frac{\partial \sum_p \sum_q u_{pq} v_{qp}}{\partial x_{ji}} = \sum_p \sum_q \left(\frac{\partial u_{pq}}{\partial x_{ji}} v_{qp} + u_{pq} \frac{\partial v_{qp}}{\partial x_{ji}} \right) \\
&= \operatorname{tr}\left(\frac{\partial \mathbf{U}}{\partial x_{ji}} \mathbf{V} \right) + \operatorname{tr}\left(\mathbf{U} \frac{\partial \mathbf{V}}{\partial x_{ji}} \right) = \operatorname{tr}\left(\frac{\partial \mathbf{UV}}{\partial x_{ji}} \right)
\end{aligned}
$$

由此可知迹和求导的顺序可以交换。特别的，

- 取 $\mathbf{U}=\mathbf{A}$ 与 $\mathbf{X}$ 无关，$\mathbf{V}=\mathbf{X}$，则

$$\left[\frac{\partial \operatorname{tr}(\mathbf{AX})}{\partial \mathbf{X}}\right]_{ij}=\operatorname{tr}\left(\mathbf{A}\frac{\partial \mathbf{X}}{\partial x_{ji}}\right)=\operatorname{tr}(\mathbf{AE}_{ji})=a_{ij}\Longrightarrow \frac{\partial \operatorname{tr}(\mathbf{AX})}{\partial \mathbf{X}}=\frac{\partial \operatorname{tr}(\mathbf{XA})}{\partial \mathbf{X}}=\mathbf{A}$$

进一步若 $\mathbf{B}$ 与 $\mathbf{X}$ 也无关，则

$$\frac{\partial \operatorname{tr}(\mathbf{AXB})}{\partial \mathbf{X}}=\frac{\partial \operatorname{tr}(\mathbf{BAX})}{\partial \mathbf{X}}=\mathbf{BA}$$

- 取 $\mathbf{U}=\mathbf{A}$ 与 $\mathbf{X}$ 无关，$\mathbf{V}=\mathbf{X}^\top$，则

$$\frac{\partial \operatorname{tr}(\mathbf{AX}^\top)}{\partial \mathbf{X}}=\frac{\partial \operatorname{tr}(\mathbf{XA}^\top)}{\partial \mathbf{X}}=\mathbf{A}^\top$$

- 取 $\mathbf{U}=\mathbf{A}$ 与 $\mathbf{X}$ 无关，$\mathbf{V}=\mathbf{XX}^\top$，则

$$\begin{aligned}\left[\frac{\partial \operatorname{tr}(\mathbf{AXX}^\top)}{\partial \mathbf{X}}\right]_{ij}&=\operatorname{tr}\left(\mathbf{A}\frac{\partial \mathbf{XX}^\top}{\partial x_{ji}}\right)=\operatorname{tr}\left(\mathbf{A}\frac{\partial \mathbf{X}}{\partial x_{ji}}\mathbf{X}^\top\right)+\operatorname{tr}\left(\mathbf{AX}\frac{\partial \mathbf{X}^\top}{\partial x_{ji}}\right)\\&=\operatorname{tr}(\mathbf{AE}_{ji}\mathbf{X}^\top)+\operatorname{tr}(\mathbf{AXE}_{ij})\\&=[\mathbf{X}^\top\mathbf{A}]_{ij}+[\mathbf{AX}]_{ji}\end{aligned}$$

从而

$$\frac{\partial \operatorname{tr}(\mathbf{AXX}^\top)}{\partial \mathbf{X}}=\frac{\partial \operatorname{tr}(\mathbf{X}^\top\mathbf{AX})}{\partial \mathbf{X}}=\mathbf{X}^\top\mathbf{A}+\mathbf{X}^\top\mathbf{A}^\top=\mathbf{X}^\top(\mathbf{A}+\mathbf{A}^\top)$$

- 取 $\mathbf{U}=\mathbf{A}$ 与 $\mathbf{X}$ 无关，$\mathbf{V}=\mathbf{X}^{-1}$，结合式 (4) 可得

$$\begin{aligned}\left[\frac{\partial \operatorname{tr}(\mathbf{AX}^{-1})}{\partial \mathbf{X}}\right]_{ij}&=\operatorname{tr}\left(\mathbf{A}\frac{\partial \mathbf{X}^{-1}}{\partial x_{ji}}\right)=\operatorname{tr}\left(-\mathbf{AX}^{-1}\frac{\partial \mathbf{X}}{\partial x_{ji}}\mathbf{X}^{-1}\right)=-\operatorname{tr}\left(\mathbf{X}^{-1}\mathbf{AX}^{-1}\mathbf{E}_{ji}\right)=-[\mathbf{X}^{-1}\mathbf{AX}^{-1}]_{ij}\\&\Longrightarrow \frac{\partial \operatorname{tr}(\mathbf{AX}^{-1})}{\partial \mathbf{X}}=\frac{\partial \operatorname{tr}(\mathbf{X}^{-1}\mathbf{A})}{\partial \mathbf{X}}=-\mathbf{X}^{-1}\mathbf{AX}^{-1}\end{aligned}$$

- 取 $\mathbf{U}=\mathbf{AXB}$，$\mathbf{V}=\mathbf{X}^\top\mathbf{C}$，其中 $\mathbf{A}$、$\mathbf{B}$、$\mathbf{C}$ 与 $\mathbf{X}$ 无关，则

$$\begin{aligned}\left[\frac{\partial \operatorname{tr}(\mathbf{AXBX}^\top\mathbf{C})}{\partial \mathbf{X}}\right]_{ij}&=\operatorname{tr}\left(\frac{\partial \mathbf{AXB}}{\partial x_{ji}}\mathbf{X}^\top\mathbf{C}\right)+\operatorname{tr}\left(\mathbf{AXB}\frac{\partial \mathbf{X}^\top\mathbf{C}}{\partial x_{ji}}\right)\\&=\operatorname{tr}\left(\mathbf{AE}_{ji}\mathbf{BX}^\top\mathbf{C}\right)+\operatorname{tr}\left(\mathbf{AXBE}_{ij}\mathbf{C}\right)\\&=[\mathbf{BX}^\top\mathbf{CA}]_{ij}+[\mathbf{CAXB}]_{ji}\\&\Longrightarrow \frac{\partial \operatorname{tr}(\mathbf{AXBX}^\top\mathbf{C})}{\partial \mathbf{X}}=\mathbf{BX}^\top\mathbf{CA}+\mathbf{B}^\top\mathbf{X}^\top\mathbf{A}^\top\mathbf{C}^\top\end{aligned}$$

- 取 $\mathbf{U}=\mathbf{A}$ 与 $\mathbf{X}$ 无关，$\mathbf{V}=\mathbf{X}^n$，其中 n 是正整数，结合式 (3) 可得

$$\begin{aligned}\left[\frac{\partial \operatorname{tr}(\mathbf{AX}^n)}{\partial \mathbf{X}}\right]_{ij}&=\operatorname{tr}\left(\mathbf{A}\frac{\partial \mathbf{X}^n}{\partial x_{ji}}\right)=\operatorname{tr}\left(\mathbf{A}\sum_{k\in[n]}\mathbf{X}^{k-1}\frac{\partial \mathbf{X}}{\partial x_{ji}}\mathbf{X}^{n-k}\right)=\sum_{k\in[n]}\operatorname{tr}\left(\mathbf{AX}^{k-1}\frac{\partial \mathbf{X}}{\partial x_{ji}}\mathbf{X}^{n-k}\right)\\&=\sum_{k\in[n]}\operatorname{tr}(\mathbf{X}^{n-k}\mathbf{AX}^{k-1}\mathbf{E}_{ji})=\sum_{k\in[n]}[\mathbf{X}^{n-k}\mathbf{AX}^{k-1}]_{ij}\end{aligned}$$

$$\Longrightarrow \frac{\partial \mathrm{tr}(\mathbf{A}\mathbf{X}^n)}{\partial \mathbf{X}} = \sum_{k\in[n]} \mathbf{X}^{n-k}\mathbf{A}\mathbf{X}^{k-1}$$

进一步若 $\mathbf{A}=\mathbf{I}$，则

$$\frac{\partial \mathrm{tr}(\mathbf{X}^n)}{\partial \mathbf{X}} = \sum_{k\in[n]} \mathbf{X}^{n-k}\mathbf{X}^{k-1} = \sum_{k\in[n]} \mathbf{X}^{n-1} = n\mathbf{X}^{n-1}$$

不难发现形式上和单变量的求导公式 $\partial x^n/\partial x = nx^{n-1}$ 是一样的。类似的记

$$\begin{aligned} e^{\mathbf{X}} &= \mathbf{I} + \mathbf{X} + \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^3}{3!} + \cdots \\ \sin \mathbf{X} &= \mathbf{X} - \frac{\mathbf{X}^3}{3!} + \frac{\mathbf{X}^5}{5!} - \cdots \\ \cos \mathbf{X} &= \mathbf{I} - \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^4}{4!} - \frac{\mathbf{X}^6}{6!} + \cdots \end{aligned}$$

结合式 (3) 可得

$$\begin{aligned} \frac{\partial \mathrm{tr}(e^{\mathbf{X}})}{\partial \mathbf{X}} &= \frac{\partial}{\partial \mathbf{X}} \mathrm{tr} \left(\mathbf{I} + \mathbf{X} + \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^3}{3!} + \cdots \right) \\ &= \frac{\partial \mathrm{tr}(\mathbf{I})}{\partial \mathbf{X}} + \frac{\partial \mathrm{tr}(\mathbf{X})}{\partial \mathbf{X}} + \frac{1}{2!}\frac{\partial \mathrm{tr}(\mathbf{X}^2)}{\partial \mathbf{X}} + \frac{1}{3!}\frac{\partial \mathrm{tr}(\mathbf{X}^3)}{\partial \mathbf{X}} + \cdots \\ &= \mathbf{I} + \mathbf{X} + \frac{\mathbf{X}^2}{2!} + \cdots = e^{\mathbf{X}} \end{aligned}$$

以及

$$\begin{aligned} \frac{\partial \mathrm{tr}(\sin \mathbf{X})}{\partial \mathbf{X}} &= \frac{\partial}{\partial \mathbf{X}} \mathrm{tr} \left(\mathbf{X} - \frac{\mathbf{X}^3}{3!} + \frac{\mathbf{X}^5}{5!} - \cdots \right) \\ &= \frac{1}{1!}\frac{\partial \mathrm{tr}(\mathbf{X})}{\partial \mathbf{X}} - \frac{1}{3!}\frac{\partial \mathrm{tr}(\mathbf{X}^3)}{\partial \mathbf{X}} + \frac{1}{5!}\frac{\partial \mathrm{tr}(\mathbf{X}^5)}{\partial \mathbf{X}} - \cdots \\ &= \mathbf{I} - \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^4}{4!} - \cdots = \cos \mathbf{X} \\ \frac{\partial \mathrm{tr}(\cos \mathbf{X})}{\partial \mathbf{X}} &= \frac{\partial}{\partial \mathbf{X}} \mathrm{tr} \left(\mathbf{I} - \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^4}{4!} - \frac{\mathbf{X}^6}{6!} + \cdots \right) \\ &= \frac{\partial \mathrm{tr}(\mathbf{I})}{\partial \mathbf{X}} - \frac{1}{2!}\frac{\partial \mathrm{tr}(\mathbf{X}^2)}{\partial \mathbf{X}} + \frac{1}{4!}\frac{\partial \mathrm{tr}(\mathbf{X}^4)}{\partial \mathbf{X}} - \frac{1}{6!}\frac{\partial \mathrm{tr}(\mathbf{X}^6)}{\partial \mathbf{X}} + \cdots \\ &= -\mathbf{X} + \frac{\mathbf{X}^3}{3!} - \frac{\mathbf{X}^5}{5!} + \cdots = -\sin \mathbf{X} \end{aligned}$$

均与单变量的求导公式一样。

6.2 行列式对矩阵求导

设 $\mathbf{X} \in \mathbb{R}^{m\times n}$、$\mathbf{A} \in \mathbb{R}^{l\times m}$、$\mathbf{B} \in \mathbb{R}^{n\times l}$、$\mathbf{Y} = \mathbf{A}\mathbf{X}\mathbf{B} \in \mathbb{R}^{l\times l}$，$\mathbf{A}$、$\mathbf{B}$ 与 $\mathbf{X}$ 无关，结合式 (1) 易知

$$\left[\frac{\partial |\mathbf{A}\mathbf{X}\mathbf{B}|}{\partial \mathbf{X}}\right]_{ij} = \frac{\partial |\mathbf{Y}|}{\partial x_{ji}} = \sum_p \sum_q \frac{\partial |\mathbf{Y}|}{\partial y_{pq}} \frac{\partial y_{pq}}{\partial x_{ji}} = \mathrm{tr}\left(\frac{\partial |\mathbf{Y}|}{\partial \mathbf{Y}} \frac{\partial \mathbf{Y}}{\partial x_{ji}}\right)$$

其中第二项

$$\frac{\partial \mathbf{Y}}{\partial x_{ji}} = \frac{\partial \mathbf{AXB}}{\partial x_{ji}} = \mathbf{A}\frac{\partial \mathbf{X}}{\partial x_{ji}}\mathbf{B} = \mathbf{A}\mathbf{E}_{ji}\mathbf{B}$$

记 y_{ji} 有一个微小增量 ϵ 后的矩阵为 $\mathbf{Y}(y_{ji}+\epsilon)$，根据第 j 行 Laplace 展开易知

$$|\mathbf{Y}(y_{ji}+\epsilon)| - |\mathbf{Y}| = \epsilon C_{ji}$$

其中 C_{ji} 是关于 y_{ji} 的代数余子式，因此

$$\left[\frac{\partial |\mathbf{Y}|}{\partial \mathbf{Y}}\right]_{ij} = \frac{\partial |\mathbf{Y}|}{\partial y_{ji}} = \lim_{\epsilon\to 0}\frac{|\mathbf{Y}(y_{ji}+\epsilon)| - |\mathbf{Y}|}{\epsilon} = C_{ji}$$

故第一项

$$\frac{\partial |\mathbf{Y}|}{\partial \mathbf{Y}} = \begin{bmatrix} C_{11} & C_{21} & \cdots & C_{n1} \\ C_{12} & C_{22} & \cdots & C_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ C_{1n} & C_{2n} & \cdots & C_{nn} \end{bmatrix} = \mathbf{Y}^*$$

代入可得

$$\left[\frac{\partial |\mathbf{AXB}|}{\partial \mathbf{X}}\right]_{ij} = \operatorname{tr}\left(\frac{\partial |\mathbf{Y}|}{\partial \mathbf{Y}}\frac{\partial \mathbf{Y}}{\partial x_{ji}}\right) = \operatorname{tr}(\mathbf{Y}^*\mathbf{A}\mathbf{E}_{ji}\mathbf{B}) = [\mathbf{B}\mathbf{Y}^*\mathbf{A}]_{ij}$$
$$\Longrightarrow \frac{\partial |\mathbf{AXB}|}{\partial \mathbf{X}} = \mathbf{B}(\mathbf{AXB})^*\mathbf{A}$$

若 $\mathbf{X}$、$\mathbf{A}$、$\mathbf{B}$ 均为可逆方阵，则 $\mathbf{Y} = \mathbf{AXB}$ 亦为可逆方阵，于是

$$\frac{\partial |\mathbf{AXB}|}{\partial \mathbf{X}} = \mathbf{B}(\mathbf{AXB})^*\mathbf{A} = \mathbf{B}|\mathbf{AXB}|(\mathbf{AXB})^{-1}\mathbf{A} = |\mathbf{AXB}|\mathbf{X}^{-1} \tag{5}$$

进一步若 $\mathbf{A} = \mathbf{B} = \mathbf{I}$，则

$$\frac{\partial |\mathbf{X}|}{\partial \mathbf{X}} = \mathbf{X}^* = |\mathbf{X}|\mathbf{X}^{-1}$$

由此可得

$$\frac{\partial |\mathbf{X}^n|}{\partial \mathbf{X}} = \frac{\partial |\mathbf{X}|^n}{\partial \mathbf{X}} = n|\mathbf{X}|^{n-1}\mathbf{X}^* = n|\mathbf{X}|^n\mathbf{X}^{-1} = n|\mathbf{X}^n|\mathbf{X}^{-1}$$

若 a 与 $\mathbf{X}$ 无关，则

$$\frac{\partial \ln |a\mathbf{X}|}{\partial \mathbf{X}} = \frac{\partial \ln a^m |\mathbf{X}|}{\partial \mathbf{X}} = \frac{\partial \ln a^m}{\partial \mathbf{X}} + \frac{\partial \ln |\mathbf{X}|}{\partial \mathbf{X}} = \frac{1}{|\mathbf{X}|}\frac{\partial |\mathbf{X}|}{\partial \mathbf{X}} = \frac{\mathbf{X}^*}{|\mathbf{X}|} = \mathbf{X}^{-1}$$

设 $\mathbf{X} \in \mathbb{R}^{m\times n}$、$\mathbf{A} \in \mathbb{R}^{m\times m}$、$\mathbf{Y} = \mathbf{X}^\top\mathbf{A}\mathbf{X} \in \mathbb{R}^{n\times n}$ 可逆，$\mathbf{A}$ 与 $\mathbf{X}$ 无关，易知有

$$\begin{aligned}\left[\frac{\partial |\mathbf{X}^\top\mathbf{A}\mathbf{X}|}{\partial \mathbf{X}}\right]_{ij} &= \operatorname{tr}\left(\mathbf{Y}^*\frac{\partial \mathbf{X}^\top\mathbf{A}\mathbf{X}}{\partial x_{ji}}\right) = \operatorname{tr}\left(\mathbf{Y}^*\frac{\partial \mathbf{X}^\top}{\partial x_{ji}}\mathbf{A}\mathbf{X}\right) + \operatorname{tr}\left(\mathbf{Y}^*\mathbf{X}^\top\mathbf{A}\frac{\partial \mathbf{X}}{\partial x_{ji}}\right) \\ &= \operatorname{tr}(\mathbf{Y}^*\mathbf{E}_{ij}\mathbf{A}\mathbf{X}) + \operatorname{tr}(\mathbf{Y}^*\mathbf{X}^\top\mathbf{A}\mathbf{E}_{ji}) = [\mathbf{A}\mathbf{X}\mathbf{Y}^*]_{ji} + [\mathbf{Y}^*\mathbf{X}^\top\mathbf{A}]_{ij}\end{aligned}$$

于是

$$
\begin{aligned}
\frac{\partial|\mathbf{X}^\top\mathbf{A}\mathbf{X}|}{\partial\mathbf{X}} &= (\mathbf{A}\mathbf{X}\mathbf{Y}^*)^\top + \mathbf{Y}^*\mathbf{X}^\top\mathbf{A} = (\mathbf{A}\mathbf{X}|\mathbf{X}^\top\mathbf{A}\mathbf{X}|(\mathbf{X}^\top\mathbf{A}\mathbf{X})^{-1})^\top + |\mathbf{X}^\top\mathbf{A}\mathbf{X}|(\mathbf{X}^\top\mathbf{A}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A} \\
&= |\mathbf{X}^\top\mathbf{A}\mathbf{X}|(\mathbf{X}^\top\mathbf{A}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A}^\top + |\mathbf{X}^\top\mathbf{A}\mathbf{X}|(\mathbf{X}^\top\mathbf{A}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A} \\
&= |\mathbf{X}^\top\mathbf{A}\mathbf{X}|((\mathbf{X}^\top\mathbf{A}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A}^\top + (\mathbf{X}^\top\mathbf{A}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A})
\end{aligned}
$$

若 $\mathbf{A}$ 对称，则

$$
\frac{\partial|\mathbf{X}^\top\mathbf{A}\mathbf{X}|}{\partial\mathbf{X}} = 2|\mathbf{X}^\top\mathbf{A}\mathbf{X}|(\mathbf{X}^\top\mathbf{A}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{A}
$$

- 若 $\mathbf{X}$、$\mathbf{A}$ 是方阵，则其均可逆，于是

$$
\frac{\partial|\mathbf{X}^\top\mathbf{A}\mathbf{X}|}{\partial\mathbf{X}} = 2|\mathbf{X}^\top||\mathbf{A}||\mathbf{X}|\mathbf{X}^{-1}\mathbf{A}^{-1}\mathbf{X}^{-\top}\mathbf{X}^\top\mathbf{A} = 2|\mathbf{X}|^2|\mathbf{A}|\mathbf{X}^{-1}
$$

- 若 $\mathbf{A} = \mathbf{I}$，则

$$
\frac{\partial|\mathbf{X}^\top\mathbf{X}|}{\partial\mathbf{X}} = 2|\mathbf{X}^\top\mathbf{X}|(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top = 2|\mathbf{X}^\top\mathbf{X}|\mathbf{X}^\dagger
$$

  以及

$$
\frac{\partial\ln|\mathbf{X}^\top\mathbf{X}|}{\partial\mathbf{X}} = \frac{1}{|\mathbf{X}^\top\mathbf{X}|}\frac{\partial|\mathbf{X}^\top\mathbf{X}|}{\partial\mathbf{X}} = 2\mathbf{X}^\dagger
$$