矩阵导数

矩阵求导结果与布局有关，我们采用常见的分母布局。有关矩阵求导的更详细说明可以参考：

- https://zhuanlan.zhihu.com/p/107430410
- https://zhuanlan.zhihu.com/p/607077996?utm_id=0
- https://zhuanlan.zhihu.com/p/288541909?ivk_sa=1024320u
  矩阵求导中可能涉及向量化、逆向量化、Hadamard积、Kronecker积。可详参《矩阵分析与应用（清华大学出版社）》P100（Goodnotes中有）

常用矩阵函数的导数

■ 设 $A \in C^{n\times n}$

$$\frac{d}{dt}e^{At} = Ae^{At} = e^{At}A$$

$$\frac{d}{dt}\sin At = A\cos At = (\cos At)A$$

$$\frac{d}{dt}\cos At = -A\sin At = -(\sin At)A$$

1. 数量函数对矩阵变量的导数

数量函数例如行列式、二次型、内积、范数等

定义

❖ 定义：设 $f: C^{m\times n} \to F$，即：$\boldsymbol{X} \to \boldsymbol{f}(\boldsymbol{X})$，$\boldsymbol{f}(\boldsymbol{X}) \in \boldsymbol{F}$，记

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{pmatrix} \text{定义} \frac{df}{dX} = \left(\frac{\partial f}{\partial x_{ij}}\right)_{m\times n} = \begin{pmatrix} \frac{\partial f}{\partial x_{11}} & \cdots & \frac{\partial f}{\partial x_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial x_{m1}} & \cdots & \frac{\partial f}{\partial x_{mn}} \end{pmatrix}$$

例1：设 $x = [\xi_1 \quad \xi_2 \quad \cdots \quad \xi_n]^T$，n元函数

$y = f(\xi_1 \quad \xi_2 \quad \cdots \quad \xi_n)$ 计算 $\frac{df}{dx}$ 与 $\frac{df}{dx^T}$ 。

解：

$$\frac{df}{dx} = \begin{bmatrix} \frac{\partial f}{\partial \xi_1} \\ \frac{\partial f}{\partial \xi_2} \\ \vdots \\ \frac{\partial f}{\partial \xi_n} \end{bmatrix} = grad f \qquad \frac{df}{dx^T} = \begin{bmatrix} \frac{\partial f}{\partial \xi_1} & \frac{\partial f}{\partial \xi_2} & \cdots & \frac{\partial f}{\partial \xi_n} \end{bmatrix}$$

以向量为自变量的函数的导数——梯度向量

- 数量函数对向量变量的导数是一个向量
  例：$f(\mathbf{x}) = \mathbf{a}^T\mathbf{x} = \mathbf{x}^T\mathbf{a}$，则 $\frac{df}{d\mathbf{x}} = \mathbf{a}$
- 数量函数对矩阵变量的导数是一个矩阵
  例：$f(\mathbf{X}) = tr((AX))$，则 $\frac{df}{d\mathbf{X}} = \mathbf{A^T}$

- 复合函数的求导

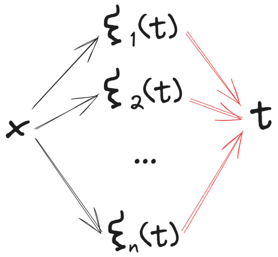
  例5：设 $x=(\xi_1,\xi_2,\cdots,\xi_n)^T$，一元函数 $y=f(\xi_1(t),\xi_2(t),\cdots,\xi_n(t))$

  计算 $\dfrac{df}{dt}$。

  解：$$\frac{df}{dt}=\frac{\partial f}{\partial \xi_1(t)}\frac{d\xi_1(t)}{dt}+\frac{\partial f}{\partial \xi_2(t)}\frac{d\xi_2(t)}{dt}+\cdots+\frac{\partial f}{\partial \xi_n(t)}\frac{d\xi_n(t)}{dt}$$

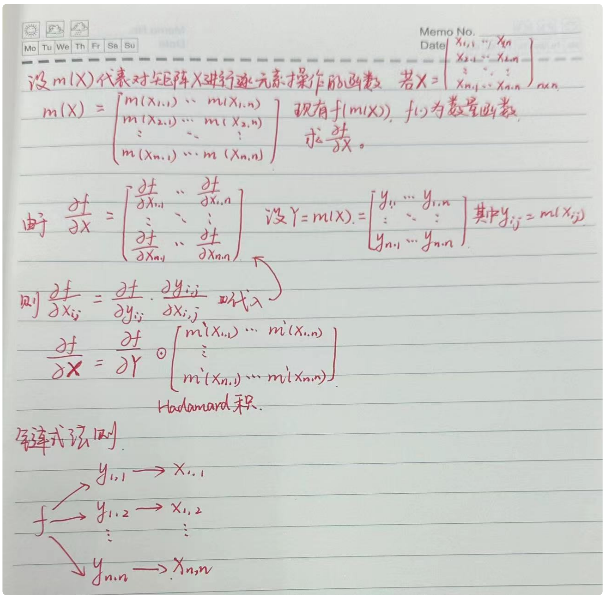
  $$=\begin{bmatrix}\dfrac{\partial f}{\partial \xi_1} & \dfrac{\partial f}{\partial \xi_2} & \cdots & \dfrac{\partial f}{\partial \xi_n}\end{bmatrix}\begin{bmatrix}\xi_1'(t)\\ \xi_2'(t)\\ \vdots \\ \xi_n'(t)\end{bmatrix}=\frac{df}{dx^{\mathrm{T}}}\frac{dx}{dt}$$

  本质上是链式法则



- 关于矩阵逐元素函数求导

  例如ReLU这样的激活函数



设 $m(X)$ 代表对矩阵X进行逐元素操作的函数 若 $X=\begin{pmatrix} x_{1,1} & \cdots & x_{1,n}\\ x_{2,1} & \cdots & x_{2,n}\\ \vdots & \ddots & \vdots\\ x_{n,1} & \cdots & x_{n,n}\end{pmatrix}_{n\times n}$

$m(X)=\begin{bmatrix} m(x_{1,1}) & \cdots & m(x_{1,n})\\ m(x_{2,1}) & \cdots & m(x_{2,n})\\ \vdots & \ddots & \vdots\\ m(x_{n,1}) & \cdots & m(x_{n,n})\end{bmatrix}$ 现有 $f(m(X))$，$f(\cdot)$ 为数量函数，求 $\frac{\partial f}{\partial X}$。

此时 $\frac{\partial f}{\partial X}=\begin{bmatrix}\frac{\partial f}{\partial x_{1,1}} & \cdots & \frac{\partial f}{\partial x_{1,n}}\\ \vdots & \ddots & \vdots\\ \frac{\partial f}{\partial x_{n,1}} & \cdots & \frac{\partial f}{\partial x_{n,n}}\end{bmatrix}$ 设 $Y=m(X)=\begin{bmatrix} y_{1,1} & \cdots & y_{1,n}\\ \vdots & \ddots & \vdots\\ y_{n,1} & \cdots & y_{n,n}\end{bmatrix}$ 其中 $y_{i,j}=m(x_{i,j})$

则 $\frac{\partial f}{\partial x_{i,j}}=\frac{\partial f}{\partial y_{i,j}}\cdot\frac{\partial y_{i,j}}{\partial x_{i,j}}$ 此代入

$\frac{\partial f}{\partial X}=\frac{\partial f}{\partial Y}\odot\begin{bmatrix} m'(x_{1,1}) & \cdots & m'(x_{1,n})\\ \vdots & & \\ m'(x_{n,1}) & \cdots & m'(x_{n,n})\end{bmatrix}$

Hadamard积.

链式法则.

$f\to y_{1,1}\longrightarrow x_{1,1}$

$f\to y_{1,2}\longrightarrow x_{1,2}$

$\vdots$

$f\to y_{n,n}\longrightarrow x_{n,n}$

2. 矩阵值函数对矩阵变量的导数

- 矩阵值函数 $F(X)$ 的定义 $F(X)=(f_{ij}(X))_{s\times t}$

  $f_{ij}: X\to f_{ij}(X)\quad (i=1,\cdots,s;\quad j=1,\cdots,t)\quad X=\begin{pmatrix}x_{11} & \cdots & x_{1n}\\ \vdots & \ddots & \vdots\\ x_{m1} & \cdots & x_{mn}\end{pmatrix}$

$$\frac{\partial F}{\partial x_{11}}=\begin{pmatrix}\frac{\partial f_{11}}{\partial x_{11}} & \cdots & \frac{\partial f_{1t}}{\partial x_{11}}\\ \vdots & \ddots & \vdots\\ \frac{\partial f_{s1}}{\partial x_{11}} & \cdots & \frac{\partial f_{st}}{\partial x_{11}}\end{pmatrix}$$

$$\frac{dF}{dX}=\begin{pmatrix}\frac{\partial F}{\partial x_{11}} & \cdots & \frac{\partial F}{\partial x_{1n}}\\ \vdots & \ddots & \vdots\\ \frac{\partial F}{\partial x_{m1}} & \cdots & \frac{\partial F}{\partial x_{mn}}\end{pmatrix}$$

$$\frac{\partial F}{\partial x_{ij}}=\begin{pmatrix}\frac{\partial f_{11}}{\partial x_{ij}} & \cdots & \frac{\partial f_{1t}}{\partial x_{ij}}\\ \vdots & \ddots & \vdots\\ \frac{\partial f_{s1}}{\partial x_{ij}} & \cdots & \frac{\partial f_{st}}{\partial x_{ij}}\end{pmatrix}$$

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总结：$F: s\times t$；$X: m\times n$，则 $\frac{\partial F}{\partial X}: ms\times nt$

例如：

- Hessens矩阵：

例1：设 $x=[\xi_1 \quad \xi_2 \quad \cdots \quad \xi_n]^T$，**n**元函数 $y=f(\xi_1 \quad \xi_2 \quad \cdots \quad \xi_n)$

计算 $\frac{df}{dx^T}\left(\frac{df}{dx}\right)$。

解：

$$\frac{df}{dx}=\begin{bmatrix}\frac{\partial f}{\partial \xi_1}\\ \frac{\partial f}{\partial \xi_2}\\ \vdots\\ \frac{\partial f}{\partial \xi_n}\end{bmatrix}$$

$$\frac{df}{dx^T}\left(\frac{df}{dx}\right)=\begin{bmatrix}\frac{\partial}{\partial \xi_1}\left(\frac{df}{dx}\right) & \frac{\partial}{\partial \xi_2}\left(\frac{df}{dx}\right) & \cdots & \frac{\partial}{\partial \xi_n}\left(\frac{df}{dx}\right)\end{bmatrix}$$

$$=\begin{bmatrix}\frac{\partial^2 f}{\partial \xi_1 \partial \xi_1} & \frac{\partial^2 f}{\partial \xi_2 \partial \xi_1} & \cdots & \frac{\partial^2 f}{\partial \xi_n \partial \xi_1}\\ \frac{\partial^2 f}{\partial \xi_1 \partial \xi_2} & \frac{\partial^2 f}{\partial \xi_2 \partial \xi_2} & \cdots & \frac{\partial^2 f}{\partial \xi_n \partial \xi_2}\\ \vdots & \vdots & \ddots & \vdots\\ \frac{\partial^2 f}{\partial \xi_1 \partial \xi_n} & \frac{\partial^2 f}{\partial \xi_2 \partial \xi_n} & \cdots & \frac{\partial^2 f}{\partial \xi_n \partial \xi_n}\end{bmatrix}$$

此矩阵被称为**Hessens**矩阵。

- Jacobi矩阵：

例2：设 $x=(\xi_1,\xi_2,\cdots,\xi_n)^T$，**n**元函数

$$f_j(x)=f_j(\xi_1,\xi_2,\cdots,\xi_n)$$

令 $\boldsymbol{F(x)=(f_1(x), f_2(x),\cdots, f_n(x))^T}$，计算 $\frac{dF}{dx^T}$ 。

解：

$$\frac{dF}{dx^T}=\begin{bmatrix}\frac{\partial F}{\partial \xi_1} & \frac{\partial F}{\partial \xi_2} & \cdots & \frac{\partial F}{\partial \xi_n}\end{bmatrix}=\begin{bmatrix}\frac{\partial f_1}{\partial \xi_1} & \frac{\partial f_1}{\partial \xi_2} & \cdots & \frac{\partial f_1}{\partial \xi_n}\\ \frac{\partial f_2}{\partial \xi_1} & \frac{\partial f_2}{\partial \xi_2} & \cdots & \frac{\partial f_2}{\partial \xi_n}\\ \vdots & \vdots & \ddots & \vdots\\ \frac{\partial f_n}{\partial \xi_1} & \frac{\partial f_n}{\partial \xi_2} & \cdots & \frac{\partial f_n}{\partial \xi_n}\end{bmatrix}$$

该式为非线性变换(映射) **$F:R^n \to R^n$** 的雅可比(**Jacobi**)式。

常用矩阵函数的导数

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- 设 $A\in C^{n\times n}$

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