不能随意交换相乘的顺序

1. 加减法：$d(X\pm Y)=dX\pm dY$　乘法 $d(XY)=(dX)Y+XdY$

转置：$d(X^T)=(dX)^T$　迹：$d\,tr(X)=tr(dX)$

2. 逆：$dX^{-1}=-X^{-1}dXX^{-1}$

Why? 对 $XX^{-1}=I$ 两边求导 $\Rightarrow dXX^{-1}+XdX^{-1}=0\Rightarrow XdX^{-1}=-dXX^{-1}$

3. 行列式：$d|X|=tr(X^*dX)$　X^* 表示 X 的伴随矩阵，由 $X^{-1}=\frac{X^*}{|X|}$

$=|X|tr(X^{-1}dX)$　证明从略

4. 逐元素乘法：$d(X\odot Y)=dX\odot Y+X\odot dY$，$\odot$ 表示尺寸相同的矩阵逐元素相乘

5. 逐元素函数：$d\sigma(X)=\sigma'(X)\odot dX$，$\sigma(X)=[\sigma(X_{ij})]$ 是逐元素标量函数运算，$\sigma'(X)=[\sigma'(X_{ij})]$ 是逐元素求导数，如

$$X=\begin{bmatrix}X_{11} & X_{12}\\ X_{21} & X_{22}\end{bmatrix}\quad d\sin X=\begin{bmatrix}\cos X_{11}dX_{11} & \cos X_{12}dX_{12}\\ \cos X_{21}dX_{21} & \cos X_{22}dX_{22}\end{bmatrix}$$

$$=\cos X\odot dX$$

迹技巧：对角线元素之和

1、标量套上迹　$a=tr(a)$　Why? 我们有 trace trick，方便我们化简处理

2、转置　$tr(A^T)=tr(A)$

3、线性　$tr(A\pm B)=tr(A)\pm tr(B)$

A、B 尺寸相同 $tr(AB)=tr(BA)=\sum_{ij}A_{ij}B_{ij}$

4、矩阵乘法/逐元素乘法交换：$tr(A^T(B\odot C))=tr((A\odot B)^TC)$

其中A、B、C尺寸相同. 由于 B⊙C对角线元素为 $b_{ii}c_{ii}$, 则由 $tr(A^TD)$ $D=B\odot C$

可知 等号左右值相同且都等于 $\sum_{ij} A_{ij}B_{ij}C_{ij}$.

求导一般操作: 先对f表达式两边微分 ⇒套迹 ⇒tr( )括号里化成 $\square^T dX$

最后与 $df = tr(\frac{\partial f}{\partial X}^T dX)$ 比较即可

求微分时保留初始顺序

1、已知 $\frac{\partial f}{\partial Y}$, $Y=AXB$, 问 $\frac{\partial f}{\partial X}$?

↳ $df = tr(\frac{\partial f}{\partial Y}^T dY)$

$= tr(\frac{\partial f}{\partial Y}^T [(dA)XB + A(dX)B + AXdB])$

$= tr(\frac{\partial f}{\partial Y}^T A(dX)B) = tr(B\frac{\partial f}{\partial Y}^T A\,dX)$

$B\frac{\partial f}{\partial Y}^T A = (\frac{\partial f}{\partial X})^T$

故 $\frac{\partial f}{\partial X} = A^T \frac{\partial f}{\partial Y} B^T$

Ex1. $f = a^TXb$, 求 $\frac{\partial f}{\partial X}$. $a:(m,1)$ $X:(m,n)$ $b:(n\times1)$

$df = a^TdXb = tr(a^TdXb) = tr(ba^TdX)$ $\quad \frac{\partial f}{\partial X} = ab^T$

Ex2. $f = a^Te^{Xb}$, 求 $\frac{\partial f}{\partial X}$. $a:(m,1)$ $X:(m,n)$ $b:(n\times1)$ e为按元素求指数.

$df = a^T de^{Xb} = a^T[e^{Xb}\odot(dXb)]$

$de^{Xb} = e^{Xb}\odot d(Xb)$ (把Xb看成整体)

$= e^{Xb}\odot(dXb)$

$= tr(a^T(e^{Xb}\odot(dXb))) = tr([a\odot e^{Xb}]^T(dXb))$

$= tr(b[a\odot e^{Xb}]^T dX)$ $\quad \frac{\partial f}{\partial X} = [a\odot e^{Xb}]b^T$

Ex3: $f = tr(Y^T M Y)$, $Y = \sigma(WX)$, 求 $\frac{\partial f}{\partial X}$. 其中 $W(l,m)$, $X:(m,n)$.

$Y(l,n)$, $M(l,l)$ 对称阵, σ 是逐元素函数, f 是标量

$$df = tr((dY)^T M Y + Y^T M (dY))$$

$$= tr((dY)^T M Y) + tr(Y^T M (dY))$$

转置 ↓

$$= tr(Y^T M^T dY) + tr(Y^T M dY)$$

$$= tr(2Y^T M dY)$$

目标: 先求 $\frac{\partial f}{\partial Y}$ 再求 $\frac{\partial f}{\partial X}$

$$\frac{\partial f}{\partial Y} = 2M^T Y = 2MY$$

$$df = tr\left(\frac{\partial f}{\partial Y}^T dY\right) = tr\left(\frac{\partial f}{\partial Y}^T (\sigma'(WX) \odot d(WX))\right)$$

$$= tr\left(\left[\frac{\partial f}{\partial Y} \odot \sigma'(WX)\right]^T W dX\right)$$

$$\frac{\partial f}{\partial X} = W^T([2M\sigma(WX)] \odot \sigma'(WX))$$

▲ 多元线性回归:

$l = \|X\omega - y\|^2$, 求 ω 的最小二乘估计, 即求 $\frac{\partial l}{\partial \omega}$ 的零点 ⇓ 极小值点

$y(m,1)$ $X(m,n)$ $\omega(n,1)$

$l = (X\omega - y)^T (X\omega - y)$ 向量内积 $\langle\alpha, \beta\rangle = \langle\beta, \alpha\rangle$

$$dl = (Xd\omega)^T (X\omega - y) + (X\omega - y)^T (Xd\omega)$$

$$= (X\omega - y)^T (Xd\omega)$$

$$= 2(X\omega - y)^T (Xd\omega) = tr(2(X\omega - y)^T X d\omega)$$

$$\frac{\partial l}{\partial \omega} = 2X^T(X\omega - y) = 0 \Rightarrow \omega = (X^T X)^{-1} X^T y$$