矩阵求导（多元线性回归）

$$\bar{v} = X\bar{w} + \bar{b} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{pmatrix}_{n\times d} * \begin{pmatrix} w_1 \\ w_2 \\ \dots \\ w_d \end{pmatrix}_{d\times 1} + \begin{pmatrix} b \\ b \\ \dots \\ b \end{pmatrix}_{n\times 1} = \begin{pmatrix} \sum_{j=1}^{d} x_{1j} * w_j + b \\ \sum_{j=1}^{d} x_{2j} * w_j + b \\ \dots \\ \sum_{j=1}^{d} x_{nj} * w_j + b \end{pmatrix}_{n\times 1}$$

首先对X扩充一列：

$$X = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{pmatrix}_{n\times d} \Rightarrow \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} & 1 \\ x_{21} & x_{22} & \dots & x_{2d} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} & 1 \end{pmatrix}_{n\times (d+1)} = \begin{pmatrix} \bar{x}_1 & 1 \\ \bar{x}_2 & 1 \\ \dots & \dots \\ \bar{x}_n & 1 \end{pmatrix}_{n\times (d+1)}$$

扩充一列后的 X

b加入到 w 中，增加一行得到**新的** ：

$$\bar{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{pmatrix}_{d\times 1} \Rightarrow \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \\ b \end{pmatrix}_{(d+1)\times 1} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \\ w_{d+1} \end{pmatrix}_{(d+1)\times 1}$$

扩充w为更简单形式

这样的话：

$$\bar{v} = X\bar{w} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} & 1 \\ x_{21} & x_{22} & \dots & x_{2d} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} & 1 \end{pmatrix}_{n\times (d+1)} * \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \\ w_{d+1} \end{pmatrix}_{(d+1)\times 1} = \begin{pmatrix} \sum_{j=1}^{d+1} x_{1j} * w_j \\ \sum_{j=1}^{d+1} x_{2j} * w_j \\ \dots \\ \sum_{j=1}^{d+1} x_{nj} * w_j \end{pmatrix}_{n\times 1} = \begin{pmatrix} \sum_{j=1}^{d} x_{1j} * w_j + b \\ \sum_{j=1}^{d} x_{2j} * w_j + b \\ \dots \\ \sum_{j=1}^{d} x_{nj} * w_j + b \end{pmatrix}_{n\times 1}$$

和西瓜书格式一样了

求解目标也转化为通过loss关于新的 （包含以前的 w 和b）的导数为零的极值点：

$$\frac{1}{n}\frac{\partial||\bar{y}-\bar{v}||^2}{\partial\bar{w}}=0 \Rightarrow \frac{1}{n}\frac{\partial||\bar{y}-X\bar{w}||^2}{\partial\bar{w}}=0$$

$$loss=||\bar{y}-X\bar{w}||^2=(\bar{y}-X\bar{w})^T(\bar{y}-X\bar{w})$$

$[x_{i1},x_{i2},\ldots,x_{id}]$ 表示一个行向量，故 $[x_{i1},x_{i2},\ldots,x_{id}]^T$ 是一个列向量。

$$loss=||\bar{y}-X\bar{w}||^2=(\bar{y}-X\bar{w})^T(\bar{y}-X\bar{w})=(\bar{y}^T-\bar{w}^TX^T)(\bar{y}-X\bar{w})$$

$$\Rightarrow loss=\bar{y}^T\bar{y}-\bar{y}^TX\bar{w}-\bar{w}^TX^T\bar{y}+\bar{w}^TX^TX\bar{w}$$

$$\frac{\partial losss}{\partial\bar{w}}=\frac{\partial||\bar{y}-X\bar{w}||^2}{\partial\bar{w}}=\frac{\partial(\bar{y}^T\bar{y}-\bar{y}^TX\bar{w}-\bar{w}^TX^T\bar{y}+\bar{w}^TX^TX\bar{w})}{\partial\bar{w}}=0$$

$$\Rightarrow\frac{\partial\bar{y}^T\bar{y}}{\partial\bar{w}}-\frac{\partial\bar{y}^TX\bar{w}}{\partial\bar{w}}-\frac{\partial\bar{w}^TX^T\bar{y}}{\partial\bar{w}}+\frac{\partial\bar{w}^TX^TX\bar{w}}{\partial\bar{w}}=0$$

所以loss对 $\bar{w}$ 求导转化为了以上四个式子对 $\bar{w}$ 求导。

常用的矩阵求导公式(采用分子布局的矩阵求导公式)：

下面的式子中小写字母a表示标量a，带横线的小写字母 $\bar{a}$ 表示列向量，大写字母A表示矩阵， a，$\bar{a}$ 和A都不是x或 $\bar{x}$ 的函数。

需要记住 下面的求导公式，就像记住高中常见的求导公式一样。

(c1) $\frac{\partial\bar{a}}{\partial x}=\bar{0}$ ($\bar{0}$ 是与 $\bar{a}$ 相同规模的列向量)

(c2) $\frac{\partial a}{\partial\bar{x}}=\bar{0}^T$ ($\bar{0}^T$ 是与 $\bar{x}$ 相同规模的行向量)

(c3) $\frac{\partial a}{\partial X}=0^T$ (0^T 是与 X 相同规模的矩阵)

(c4) $\frac{\partial\bar{a}}{\partial\bar{x}}=0$ (0 是矩阵)

(c5) $\frac{\partial\bar{x}}{\partial\bar{x}}=I$ (I 是单位矩阵)

下面的几个最重要:

下面的式子中小写字母a表示标量a，带横线的小写字母 $\bar{a}$ 表示列向量，大写字母A表示矩阵，a，$\bar{a}$ 和A都不是x或 $\bar{x}$ 的函数。

(c6) $\frac{\partial \bar{a}^T \bar{x}}{\partial \bar{x}} = \frac{\partial \bar{x}^T \bar{a}}{\partial \bar{x}} = \bar{a}^T$

(c7) $\frac{\partial \bar{x}^T \bar{x}}{\partial \bar{x}} = 2\bar{x}^T$

(c8) $\frac{\partial (\bar{x}^T \bar{a})^2}{\partial \bar{x}} = 2\bar{x}^T \bar{a}\bar{a}^T$

(c9) $\frac{\partial A\bar{x}}{\partial \bar{x}} = A$

(c10) $\frac{\partial \bar{x}^T A}{\partial \bar{x}} = A^T$

(c11) $\frac{\partial \bar{x}^T A\bar{x}}{\partial \bar{x}} = \bar{x}^T (A + A^T)$

所以:

(1) $\frac{\partial \bar{y}^T \bar{y}}{\partial \bar{w}} = \bar{0}^T$ ，因为 $\bar{y}^T \bar{y}$ 和 $\bar{w}$ 无关

(2) $\frac{\partial \bar{y}^T X \bar{w}}{\partial \bar{w}} = ?$

根据公式（c6） $\frac{\partial \bar{a}^T \bar{x}}{\partial \bar{x}} = \frac{\partial \bar{x}^T \bar{a}}{\partial \bar{x}} = \bar{a}^T$

可知 $\bar{y}^T X$ 就是公式c6的 $\bar{a}^T$ ，故$\frac{\partial \bar{y}^T X \bar{w}}{\partial \bar{w}} = \frac{\partial (\bar{y}^T X) \bar{w}}{\partial \bar{w}} = \bar{y}^T X$

(3) $\frac{\partial \bar{w}^T X^T \bar{y}}{\partial \bar{w}} = ?$

根据公式（c6） $\frac{\partial \bar{a}^T \bar{x}}{\partial \bar{x}} = \frac{\partial \bar{x}^T \bar{a}}{\partial \bar{x}} = \bar{a}^T$

可知： $X^T \bar{y}$ 就是公式里的 $\bar{a}$ ， $\frac{\partial \bar{w}^T X^T \bar{y}}{\partial \bar{w}} = (X^T \bar{y})^T = \bar{y}^T X$

(4) $\frac{\partial \bar{w}^T X^T X \bar{w}}{\partial \bar{w}} = ?$

根据公式（c11): $\frac{\partial \bar{x}^T A \bar{x}}{\partial \bar{x}} = \bar{x}^T (A + A^T)$

可知 $X^T X$ 就是公式c11里的A：
$\frac{\partial \bar{w}^T X^T X \bar{w}}{\partial \bar{w}} = \bar{w}^T (X^T X + (X^T X)^T) = \bar{w}^T (X^T X + X^T X) = 2\bar{w}^T X^T X$

综上所述：

$$\frac{\partial loss s}{\partial \bar{w}} = \frac{\partial \bar{y}^T \bar{y}}{\partial \bar{w}} - \frac{\partial \bar{y}^T X \bar{w}}{\partial \bar{w}} - \frac{\partial \bar{w}^T X^T \bar{y}}{\partial \bar{w}} + \frac{\partial \bar{w}^T X^T X \bar{w}}{\partial \bar{w}} = 0$$

$$\Rightarrow \frac{\partial loss s}{\partial \bar{w}} = \bar{0}^T - \bar{y}^T X - \bar{y}^T X + 2\bar{w}^T X^T X = 2\bar{w}^T X^T X - 2\bar{y}^T X = 0$$

大功告成!

多元线性回归或者最小二乘法（最小平方法）的解为:

$$2\bar{w}^T X^T X - 2\bar{y}^T X = 0 \Rightarrow \bar{w}^T X^T X = \bar{y}^T X$$

等号两边同时转置得: $\bar{w}^T X^T X = \bar{y}^T X \Rightarrow X^T X \bar{w} = X^T \bar{y}$

所以可得: $\bar{w} = (X^T X)^{-1} X^T \bar{y}$ ，这就是多元线性回归的解。

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