$$\underset{m\times 1}{a^{l-1}} \xrightarrow{\underset{n\times m}{W^l}} \underset{n\times 1}{z^l} \xrightarrow{f_l} \underset{n\times 1}{a^l} \xrightarrow{\underset{p\times n}{W^{l+1}}} \underset{p\times 1}{z^{l+1}} \xrightarrow{f_{l+1}} \underset{p\times 1}{a^{l+1}} \qquad \underset{p\times 1}{y}$$

$$z^l = W^l a^{l-1} + b^l$$

$$a^l = f_l(z^l)$$

$$\mathrm{vec}(AXB) = (B^T \otimes A)\,\mathrm{vec}(X)$$

$$A(m\times n) \quad B(p\times q) \quad A\otimes B = [A_{ij}B]_{mp\times nq}$$

设已知：① $\nabla^2_{z^l} J = Q^l \in \mathbb{R}^{n\times n}$

$$\therefore \mathrm{vec}(d\nabla_{z^l} J) = Q^{lT}\,\mathrm{vec}(dz^l)$$

而 $\mathrm{vec}(dz^l) = (\nabla_{W^l} z^l)^T\,\mathrm{vec}(dW^l)$

$$\therefore \mathrm{vec}(d\nabla_{z^l} J) = Q^{lT}(\nabla_{W^l} z^l)^T\,\mathrm{vec}(dW^l) \quad \cdots\cdots ①$$

② $\nabla^2_{W^l} z^l = P^l \in \mathbb{R}^{mn\times mn^2}$

$$\therefore \mathrm{vec}(d\nabla_{W^l} z^l) = P^{lT}\,\mathrm{vec}(dW^l) \quad \cdots\cdots ②$$

$$\because \mathrm{vec}(dJ) = (\underset{n\times 1}{\underline{\nabla_{z^l} J}})^T\,\mathrm{vec}(dz^l)$$

而 $\mathrm{vec}(dz^l) = (\nabla_{W^l} z^l)^T\,\mathrm{vec}(dW^l)$

$$\therefore \mathrm{vec}(dJ) = (\nabla_{z^l} J)^T(\nabla_{W^l} z^l)^T\,\mathrm{vec}(dW^l)$$

故 $\underset{mn\times 1}{\nabla_{W^l} J} = \underset{mn\times n}{\nabla_{W^l} z^l} \cdot \underset{n\times 1}{\nabla_{z^l} J}$

$$\therefore \underset{mn\times 1}{d\nabla_{W^l} J} = d(\nabla_{W^l} z^l)\cdot \nabla_{z^l} J + \nabla_{W^l} z^l \cdot d(\nabla_{z^l} J)$$

$$\therefore \underset{mn\times 1}{\mathrm{vec}(d\nabla_{W^l} J)} = \mathrm{vec}\Big(\underset{mn\times mn}{I_{mn}} \cdot \underset{mn\times n}{d\nabla_{W^l} z^l} \cdot \underset{n\times 1}{\nabla_{z^l} J}\Big) + \mathrm{vec}\Big(\underset{mn\times n}{\nabla_{W^l} z^l} \cdot \underset{n\times 1}{d\nabla_{z^l} J} \cdot \underset{1\times 1}{I_1}\Big)$$

$$= \Big(\underset{1\times n}{\underline{(\nabla_{z^l} J)^T}} \otimes \underset{mn\times mn}{\underline{I_{mn}}}\Big)\,\underset{mn^2\times 1}{\mathrm{vec}(d\nabla_{W^l} z^l)} + \underset{mn\times n}{\nabla_{W^l} z^l}\,\underset{n\times 1}{\mathrm{vec}(d\nabla_{z^l} J)}$$

将①②代入 $= \big((\nabla_{z^l} J)^T \otimes I_{mn}\big) P^{lT}\,\mathrm{vec}(dW^l) + (\nabla_{W^l} z^l)\cdot Q^{lT}\cdot(\nabla_{W^l} z^l)^T\,\mathrm{vec}(dW^l)$

$$\therefore \underset{mn\times mn}{\nabla^2_{W^l} J} = \underset{mn\times mn^2}{P^l}\cdot(\underset{n\times 1}{\nabla_{z^l} J} \otimes \underset{mn\times mn}{I_{mn}}) + (\underset{mn\times n}{\nabla_{W^l} z^l})\,\underset{n\times n}{Q^l}\,(\underset{n\times mn}{\nabla_{W^l} z^l})^T$$

$$\underset{n\times 1}{\nabla_{b^l} J} = \underset{n\times n}{\nabla_{b^l} z^l} \cdot \underset{n\times 1}{\nabla_{z^l} J}$$

$$\therefore d\nabla_{b^l} J = d\nabla_{b^l} z^l \cdot \nabla_{z^l} J + \nabla_{b^l} z^l \cdot d\nabla_{z^l} J$$

$$\therefore \mathrm{vec}(d\nabla_{b^l} J) = \mathrm{vec}(\underset{n\times n}{I_n} \cdot \underset{n\times n}{d\nabla_{b^l} z^l} \cdot \underset{n\times 1}{\nabla_{z^l} J}) + \mathrm{vec}(\underset{n\times n}{\nabla_{b^l} z^l} \cdot \underset{n\times 1}{d\nabla_{z^l} J} \cdot \underset{1\times 1}{I_1})$$

$$= \underbrace{((\nabla_{z^l} J)^T \otimes I_n)\, \mathrm{vec}(d\nabla_{b^l} z^l)}_{=0} + \nabla_{b^l} z^l \cdot \mathrm{vec}(d\nabla_{z^l} J)$$

类①式 $= (\nabla_{b^l} z^l) \cdot Q^{l\,T} (\nabla_{b^l} z^l)^T \mathrm{vec}(db^l)$

$$\therefore \underset{n\times n}{\nabla^2_{b^l} J} = (\underset{n\times n}{\nabla_{b^l} z^l})\, \underset{n\times n}{Q^l}\, (\underset{n\times n}{\nabla_{b^l} z^l})^T$$

$$z^l = W^l a^{l-1} + b^l$$

$$\therefore dz^l = dW^l \cdot a^{l-1}$$

$$\therefore \mathrm{vec}(dz^l) = \mathrm{vec}(I_n \cdot dW^l \cdot a^{l-1})$$

$$= (a^{(l-1)T} \otimes I_n)\, \mathrm{vec}(dW^l)$$

$$\therefore \nabla_{W^l} z^l = \underset{m\times 1}{a^{l-1}} \otimes \underset{n\times n}{I_n} \quad \in \mathbb{R}^{mn\times n}$$

$$\therefore dz^l = db^l$$

$$\therefore \mathrm{vec}(dz^l) = \mathrm{vec}(db^l)$$

$$\therefore \nabla_{b^l} z^l = I_n \quad \in \mathbb{R}^{n\times n}$$

设 $l+1$ 是最后一层

$$\nabla^2_{z^{l+1}} J = Q^{l+1}$$

$$\nabla_{z^{l+1}} J = \delta^{l+1}$$

$$J = -y^T \ln a^{l+1} - (1-y)^T \ln(1-a^{l+1})$$

$$d\sigma(X) = \sigma'(X) \odot dX$$

$$dJ = (-y + a^{l+1})^T dz^{l+1}$$

$$\therefore \underset{1\times 1}{\mathrm{vec}(dJ)} = \mathrm{vec}\Big(\underset{1\times p}{(-y+a^{l+1})^T}\ \underset{p\times 1}{dz^{l+1}} \cdot \underset{1\times 1}{I_1}\Big)$$

$$= (-y + a^{l+1})^T \mathrm{vec}(dz^{l+1})$$

$$\therefore \nabla_{z^{l+1}} J = \delta^{l+1} = -y + a^{l+1}$$

$$d(\nabla_{z^{l+1}} J) = d(-y + a^{l+1}) = da^{l+1}$$

$$= \mathrm{diag}(a^{l+1} \odot (1-a^{l+1}))\, dz^{l+1}$$

$\because a^{l+1} = \mathrm{sigmoid}(z^{l+1})$ 简写为 $s(z^{l+1})$

$s' = s(1-s)$

$$\therefore \mathrm{vec}(d\nabla_{z^{l+1}} J) = \mathrm{vec}\big(\mathrm{diag}(a^{l+1} \odot (1-a^{l+1})) \cdot dz^{l+1} \cdot I_1\big)$$

$$= \mathrm{diag}(a^{l+1} \odot (1-a^{l+1})) \cdot \mathrm{vec}(dz^{l+1})$$

$$\therefore \underset{p\times p}{\nabla^2_{z^{l+1}} J} = \underset{p\times p}{Q^{l+1}} = \mathrm{diag}(a^{l+1} \odot (1-a^{l+1})) = \mathrm{diag}(a^{l+1}) - a^{l+1} \cdot a^{(l+1)T}$$

$$= \begin{pmatrix} a_1^{l+1}(1-a_1^{l+1}) & & & \\ & a_2^{l+1}(1-a_2^{l+1}) & & \\ & & \ddots & \\ & & & a_p^{l+1}(1-a_p^{l+1}) \end{pmatrix}_{p\times p}$$

$\underset{p\times p}{\nabla^2_{z^{l+1}} J = Q^{l+1}}$ 已知，现求 $\underset{n\times n}{Q^{l}} = \nabla^2_{z^l} J$

设已知 $\nabla_{z^{l+1}} J = \delta^{l+1}$

$\therefore \mathrm{vec}(dJ) = \delta^{(l+1)T} \mathrm{vec}(d z^{l+1})$ ...... ③

又 $z^{l+1} = W^{l+1} a^l + b^{l+1}$

$\therefore dz^{l+1} = W^{l+1} da^l$ 又 $a^l = f_l(z^l)$ $\therefore da^l = \mathrm{diag}(f_l'(z^l)) \cdot dz^l$

$\therefore dz^{l+1} = W^{l+1} \mathrm{diag}(f_l'(z^l))\, dz^l$ ...... ④

④代入③ $\mathrm{vec}(dJ) = \delta^{(l+1)T} \mathrm{vec}(\underline{W^{l+1} \cdot \mathrm{diag}(f_l'(z^l))}\, \underline{dz^l} \cdot \underline{I_1})$

$= \delta^{(l+1)T} W^{l+1} \mathrm{diag}(f_l'(z^l)) \cdot \mathrm{vec}(dz^l)$

$\therefore \nabla_{z^l} J = \delta^l = \mathrm{diag}(f_l'(z^l))\, W^{(l+1)T} \delta^{l+1}$

即 $\nabla_{z^l} J = \mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot \nabla_{z^{l+1}} J$

$\therefore \mathrm{vec}(d\nabla_{z^l} J) = \mathrm{vec}(d\,\mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot \nabla_{z^{l+1}} J)$ ← ∵ $f_l(\cdot)$ 若是 ReLU 这种 piecewise函数，$f_l'' = 0$.

$+ \mathrm{vec}(\underbrace{\mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T}}_{A} \cdot \underbrace{d\nabla_{z^{l+1}} J}_{X} \cdot \underbrace{I_1}_{B})$

$= \mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot \mathrm{vec}(d\nabla_{z^{l+1}} J)$

$= \mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot Q^{(l+1)T} \mathrm{vec}(dz^{l+1})$

代入④ $= \mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot Q^{(l+1)T} \cdot \mathrm{vec}(\underline{W^{l+1} \mathrm{diag}(f_l'(z^l))}\, \underline{dz^l} \cdot \underline{I_1})$

$= \mathrm{diag}(f_l'(z^l)) \cdot W^{(l+1)T} \cdot Q^{(l+1)T} W^{l+1} \cdot \mathrm{diag}(f_l'(z^l)) \cdot \mathrm{vec}(dz^l)$

$= Q^{lT} \mathrm{vec}(dz^l)$

$$\therefore \underset{n\times n}{Q^l} = \underset{n\times n}{\mathrm{diag}(f_l'(z^l))} \cdot \underset{n\times p}{W^{(l+1)T}} \cdot \underset{p\times p}{Q^{l+1}} \cdot \underset{p\times n}{W^{l+1}} \cdot \underset{n\times n}{\mathrm{diag}(f_l'(z^l))}$$