Neural Networks: Backpropagation

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Jacobian matrix

- Two functions $f(x, y)$, $g(x, y)$ with two parameters x, y

$$
\begin{aligned}
f(x, y) &= 3x^2 y \\
g(x, y) &= 5xy + y^3
\end{aligned}
$$

- **Jacobian matrix** (numerator layout):

$$
\begin{aligned}
J &= \begin{bmatrix} \nabla f(x, y) \\ \nabla g(x, y) \end{bmatrix} = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} & \frac{\partial f(x,y)}{\partial y} \\ \frac{\partial g(x,y)}{\partial x} & \frac{\partial g(x,y)}{\partial y} \end{bmatrix} \\
&= \begin{bmatrix} 6yx & 3x^2 \\ 5y & 5x + 3y^2 \end{bmatrix}
\end{aligned}
$$

- **Jacobian matrix** (denominator layout):

$$
J^T = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} & \frac{\partial g(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} & \frac{\partial g(x,y)}{\partial y} \end{bmatrix}
$$

Jacobian: Generalization

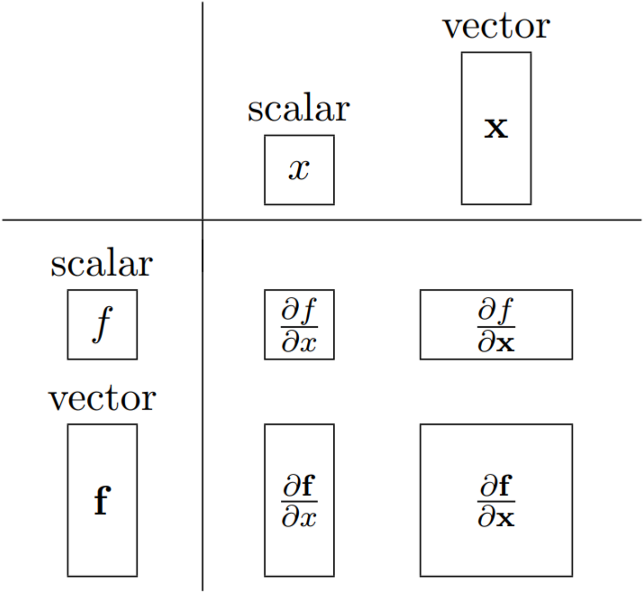
- $\mathbf{y} = \mathbf{f}(\mathbf{x})$: a vector of m scalar-valued functions that each takes a vector $\mathbf{x}$

$$\begin{aligned} y_1 &= f_1(\mathbf{x}) \\ &\vdots \\ y_m &= f_m(\mathbf{x}) \end{aligned}$$

- Jacobian matrix: has m rows for m equations.

$$\begin{aligned} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} &= \begin{bmatrix} \nabla f_1(\mathbf{x}) \\ \cdots \\ \nabla f_m(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial \mathbf{x}} f_1(\mathbf{x}) \\ \cdots \\ \frac{\partial}{\partial \mathbf{x}} f_m(\mathbf{x}) \end{bmatrix} \\ &= \begin{bmatrix} \frac{\partial}{\partial x_1} f_1(\mathbf{x}) & \cdots & \frac{\partial}{\partial x_n} f_1(\mathbf{x}) \\ \vdots & \cdots & \vdots \\ \frac{\partial}{\partial x_1} f_m(\mathbf{x}) & \cdots & \frac{\partial}{\partial x_n} f_m(\mathbf{x}) \end{bmatrix} \end{aligned}$$

Jacobian: Generalization



Vector chain rule

- Jacobian is the multiplication of two other Jacobians

$$
\begin{aligned}
\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{x})) &= \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{x}} \\
&= \begin{bmatrix} \frac{\partial f_1}{\partial g_1} & \cdots & \frac{\partial f_1}{\partial g_k} \\ \vdots & \cdots & \vdots \\ \frac{\partial f_m}{\partial g_1} & \cdots & \frac{\partial f_m}{\partial g_k} \end{bmatrix} \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \vdots & \cdots & \vdots \\ \frac{\partial g_k}{\partial x_1} & \cdots & \frac{\partial g_k}{\partial x_n} \end{bmatrix}
\end{aligned}
$$

Vector chain rule: Example

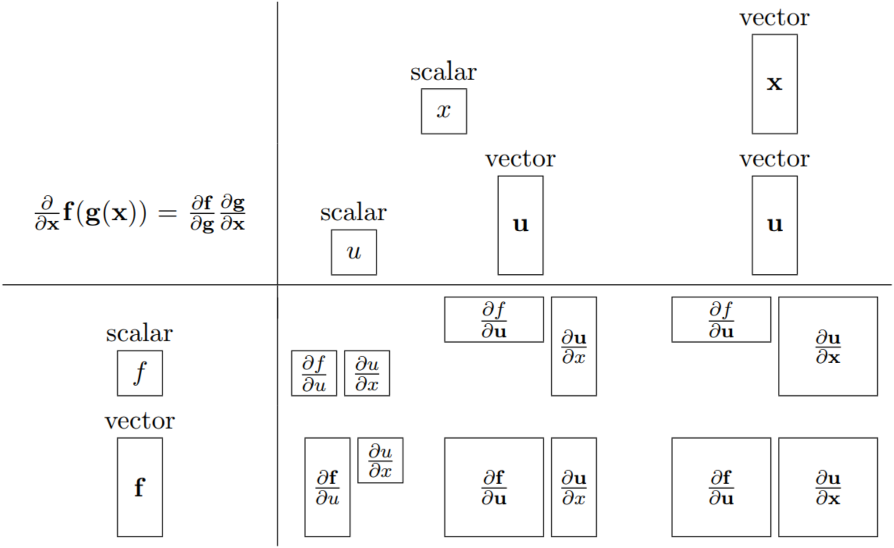
- $\mathbf{y} = \mathbf{f}(x)$

$$\mathbf{y} = \begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = \begin{bmatrix} ln(x^2) \\ sin(3x) \end{bmatrix}$$

- $\mathbf{y} = \mathbf{f}(\mathbf{g}(x))$: introduce two intermediate variables g_1, g_2:

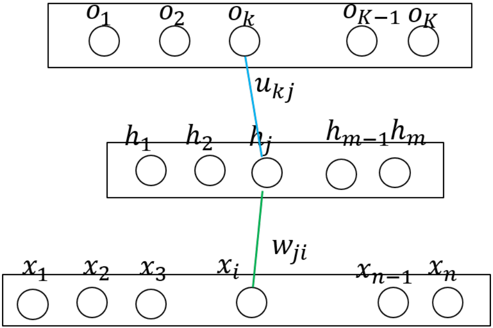
$$\begin{aligned} \mathbf{g} &= \begin{bmatrix} g_1(x) \\ g_2(x) \end{bmatrix} = \begin{bmatrix} x^2 \\ 3x \end{bmatrix} \\ \mathbf{y} &= \begin{bmatrix} f_1(\mathbf{g}) \\ f_2(\mathbf{g}) \end{bmatrix} = \begin{bmatrix} ln(g_1) \\ sin(g_2) \end{bmatrix} \end{aligned} \tag{1}$$

Jacobian: Generalization

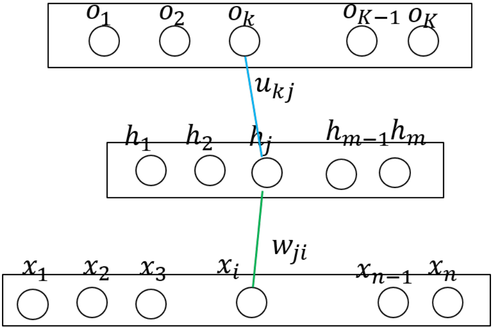


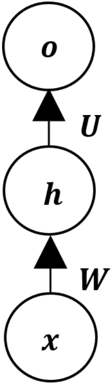
MLP with single hidden layer: Notation

- For simplicity, a network has single hidden layer only
  - o_k: k-th output unit, h_j: j-th hidden unit, x_i: i-th input
  - u_{kj}: weight b/w j-th hidden and k-th output
  - w_{ji}: weight b/w i-th input and j-th hidden
    - Bias terms are also contained in weights



MLP with single hidden layer: Matrix notation



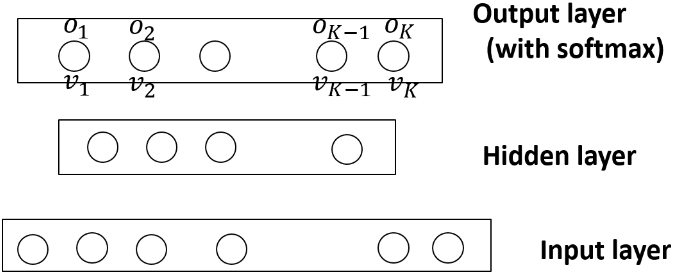


$$
\begin{aligned}
\mathbf{h} &= max(\mathbf{Wx}, 0) \\
\mathbf{o} &= softmax(\mathbf{Uh})
\end{aligned}
$$

Typical Setting for Classification

- K: the number of labels
- Input layer: Input values (raw features)
- Output layer: **Scores** of labels
- **Softmax** layer: $\mathbf{o} = softmax(\mathbf{v})$

$$o_k = \frac{exp(v_k)}{\sum_i exp(v_i)} = \frac{exp(v_k)}{Z}$$



Learning as Optimization

- Training data: $\mathcal{T} := \{(\mathbf{x}_i, y_i), \cdots, (\mathbf{x}_N, y_N)\}$
  - $\mathbf{x}_i$: i-th input feature vector
  - y_i (or $\mathbf{y}_i$): i-th target label
- Parameter: $\boldsymbol{\theta} := \{\mathbf{W}, \mathbf{U}\}$
  - Weight matrices: Input-to-hidden, and hidden-to-output
- Objective function (= Loss function)
  - Take Negative Log-likelihood (NLL) as Empirical risk

$$J(\boldsymbol{\theta}) = Loss(\mathcal{T}, \boldsymbol{\theta}) = -\sum_{(\mathbf{x},y)\in\mathcal{T}} logP\left(y|\mathbf{x}\right)$$

- Training process
  - Known as Empirical risk minimization

$$\boldsymbol{\theta}^* = argmin_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

Optimization by Gradient Method

- Gradient Descent:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \frac{\partial J}{\partial \boldsymbol{\theta}}$$
$$\frac{\partial J}{\partial \boldsymbol{\theta}} = \mathop{\mathbb{E}}_{(\mathbf{x},y)} [-logP(y|\mathbf{x})]$$

- Batch algorithm
  - Expectations over the training set are required
  - But, computing expectations exactly is very expensive, as it evaluates on every example in the entire dataset
- **Minibatch** algorithm
  - In practice, we compute these expectations by randomly sampling a small number of examples from the dataset, then taking the average over only those examples
  - Using exact gradient using large examples does not significantly reduce the estimation error: Slow convergence

Stochastic Gradient Method

1. Randomly a minibatch of m samples $\{(\mathbf{x}, y)\}$ from training data
2. Define NLL for $\{(\mathbf{x}_i, y_i)\}$

$$J(\boldsymbol{\theta}) = \sum_{1 \leq i \leq m} log\left(y_i | \mathbf{x}_i\right)$$

3. Compute derivatives $\frac{\partial J}{\partial \mathbf{W}}$ for $\mathbf{W} \in \boldsymbol{\theta}$
4. Update weight matrix for $\mathbf{W} \in \boldsymbol{\theta}$:

$$\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J}{\partial \mathbf{W}}$$

Iterate the above procedure until stopping criteria is satisfied

Logistic regression for binary classification

- $(\mathbf{x}, y)$: a training example for binary classification where $y \in \{0, 1\}$
- Logistic regression function:

$$o(\mathbf{x}) = \sigma\left(\mathbf{w}^T\mathbf{x} + b\right)$$

  which is rewritten to:

$$\begin{aligned} z &= \mathbf{w}^T\mathbf{x} + b \\ o &= \sigma(z) \end{aligned}$$

- J: the log-likelihood on $(\mathbf{x}, y)$

$$J = y log(o) + (1 - y) log(1 - o)$$

$$\frac{\partial J}{\partial o} = \frac{y}{o} - \frac{1 - y}{1 - o}$$

Logistic regression: Deriv J wrt $\mathbf{w}$

$$\begin{aligned} \frac{\partial z}{\partial \mathbf{w}} &= \mathbf{x}^T \\ \frac{\partial o}{\partial z} &= \sigma(z)(1-\sigma(z)) = o(1-o) \end{aligned}$$

All together lead to:

$$\begin{aligned} \frac{\partial J}{\partial \mathbf{w}} &= \frac{\partial J}{\partial o}\frac{\partial o}{\partial z}\frac{\partial z}{\partial \mathbf{w}} \\ &= \left(\frac{y}{o} - \frac{1-y}{1-o}\right) \cdot o(1-o)\mathbf{x}^T \\ &= (y-o)\mathbf{x}^T \end{aligned}$$

Logistic regression for multi-class classification

- K: the number of labels
- $(\mathbf{x}, k)$: a training example where $k \in \{1, \cdots, K\}$
- Logistic regression function:

$$\mathbf{o}(\mathbf{x}) = softmax(\mathbf{W}\mathbf{x} + b)$$

which is rewritten to:

$$\begin{aligned} \mathbf{z} &= \mathbf{W}\mathbf{x} + \mathbf{b} \\ \mathbf{o} &= softmax(\mathbf{z}) \end{aligned}$$

where $softmax(\mathbf{z}) = exp(\mathbf{z}) / \sum_i exp(\mathbf{z}_i) = exp(\mathbf{z})/Z$

- J: the log-likelihood on $(\mathbf{x}, k)$

$$J = \mathbf{y}^T log(\mathbf{o})$$

where $\mathbf{y}$ is one-hot encoding for target label.

$$\mathbf{y} = [0 \cdots 1 \cdots 0]^T$$

where $y_i = \mathcal{I}(i = k)$ where k is the target label.

$$
\begin{aligned}
\frac{\partial J}{\partial \mathbf{o}} &= \left[0 \cdots \frac{1}{o_k} \cdots 0\right] \\
\frac{\partial \mathbf{o}}{\partial \mathbf{z}} &= \left[\frac{\partial o_j}{\partial z_i}\right]_{ij} = \left[\frac{exp(z_j)\left(\mathcal{I}(i=j) \cdot \sum_k exp(z_k) - exp(z_i)\right)}{\left(\sum_k exp(z_k)\right)^2}\right]_{ij} \\
&= \left[\frac{exp(z_j)\left(\mathcal{I}(i=j) \cdot Z - exp(z_i)\right)}{(Z)^2}\right]_{ij} = \left[o_j \cdot \mathcal{I}(i=j) - o_i o_j\right]_{ij}
\end{aligned}
$$

Thus, we have:

$$
\begin{aligned}
\frac{\partial J}{\partial \mathbf{z}} &= \frac{\partial J}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial \mathbf{z}} \\
&= \left[0 \cdots \frac{1}{o_k} \cdots 0\right] \left[\frac{exp(z_j)\left(\mathcal{I}(i=j) \cdot Z - exp(z_i)\right)}{(Z)^2}\right]_{ij} \\
&= \left[\ \mathcal{I}(1=k) - o_1 \quad \cdots \quad 1 - o_k \quad \cdots \quad \mathcal{I}(K=k) - o_K\ \right]
\end{aligned}
$$

Given $\mathbf{z} = \mathbf{W}\mathbf{x} + \mathbf{b}$,

$$\frac{\partial z_i}{\partial \mathbf{W}_{i*}} = \mathbf{x}^T$$

where $\mathbf{W}_{i*}$ is i-th row vector of $\mathbf{W}$.

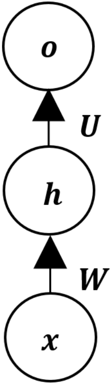
$$\frac{\partial J}{\partial \mathbf{W}_{i*}} = \frac{\partial J}{\partial z_i}\frac{\partial z_i}{\partial \mathbf{W}_{i*}} = \left(\mathcal{I}(i = k) - o_i\right)\mathbf{x}^T$$

Finally, this leads to:

$$\begin{aligned}\frac{\partial J}{\partial \mathbf{W}} &:= \begin{bmatrix} \frac{\partial J}{\partial \mathbf{W}_{1*}} \\ \vdots \\ \frac{\partial J}{\partial \mathbf{W}_{K*}} \end{bmatrix} = \begin{bmatrix} \left(\mathcal{I}(1 = k) - o_1\right)\mathbf{x}^T \\ \vdots \\ \left(\mathcal{I}(K = k) - o_K\right)\mathbf{x}^T \end{bmatrix} \\ &= \begin{bmatrix} \left(\mathcal{I}(1 = k) - o_1\right) \\ \vdots \\ \left(\mathcal{I}(K = k) - o_K\right) \end{bmatrix}\mathbf{x}^T = \frac{\partial J}{\partial \mathbf{z}}^T\mathbf{x}^T\end{aligned}$$

MLP with single hidden layer: Log-likelihood

$$\mathbf{h} = max(\mathbf{Wx}, 0)$$
$$\mathbf{o} = softmax(\mathbf{Uh})$$



- J: the log-likelihood on single example $(\mathbf{x}, \mathbf{y})$

$$J = \mathbf{y}^T log(\mathbf{o})$$

- $\mathbf{y}$: one-hot encoding for target label.

$$\mathbf{y} = [0 \cdots 1 \cdots 0]^T$$

where $y_i = \mathcal{I}(i = k)$ where k is a target label.

Derivative of J wrt Output layer

$$\begin{aligned}
\mathbf{v} &= \mathbf{Uh} \\
\mathbf{o} &= softmax(\mathbf{v}) = \frac{exp(\mathbf{v})}{\sum_i exp\left(v_i\right)} = \frac{exp(\mathbf{v})}{Z} \\
J &= \mathbf{y}^T log\left(\mathbf{o}\right)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial J}{\partial \mathbf{o}} &= \left[0 \cdots \frac{1}{o_k} \cdots 0\right] \\
\frac{\partial \mathbf{o}}{\partial \mathbf{v}} &= \left[\frac{\partial o_j}{\partial v_i}\right]_{ij} = \left[\frac{exp(v_j)\left(\mathcal{I}(i=j)\cdot\sum_k exp(v_k) - exp(v_i)\right)}{\left(\sum_k exp(v_k)\right)^2}\right]_{ij} \\
&= \left[\frac{exp(v_j)\left(\mathcal{I}(i=j)\cdot Z - exp(v_i)\right)}{(Z)^2}\right]_{ij}
\end{aligned}$$

Derivative of J wrt Output layer (Cont.)

$$
\begin{aligned}
\frac{\partial J}{\partial \mathbf{v}} &= \frac{\partial J}{\partial \mathbf{o}}\frac{\partial \mathbf{o}}{\partial \mathbf{v}} \\
&= \left[0 \cdots \frac{1}{o_k} \cdots 0\right]\left[\frac{exp(v_j)\left(\mathcal{I}(i=j)\cdot Z - exp(v_i)\right)}{(Z)^2}\right]_{ij} \\
&= \left[0 \cdots \frac{Z}{exp(v_k)} \cdots 0\right]\left[\frac{exp(v_j)\left(\mathcal{I}(i=j)\cdot Z - exp(v_i)\right)}{(Z)^2}\right]_{ij} \\
&= \left[\begin{array}{ccccc} -\frac{exp(v_1)}{Z} & \cdots & 1-\frac{exp(v_k)}{Z} & \cdots & -\frac{exp(v_K)}{Z} \end{array}\right] \\
&= \left[\begin{array}{ccccc} -o_1 & \cdots & 1-o_k & \cdots & -o_K \end{array}\right]
\end{aligned}
$$

- Let $\boldsymbol{\delta}^{(o)}$ be the error signal for output layer:

$$
\boldsymbol{\delta}^{(o)} := \frac{\partial J}{\partial \mathbf{v}} = \left[\begin{array}{ccccc} -o_1 & \cdots & 1-o_k & \cdots & -o_K \end{array}\right]
$$

Here, note that $\boldsymbol{\delta}^{(o)}$ is a **row vector**.

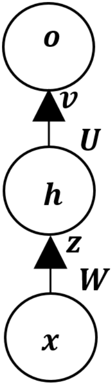
Error propagation to hidden layer

- Hidden-to-output: $\mathbf{v} = \mathbf{U}\mathbf{h}$

$$\frac{\partial \mathbf{v}}{\partial \mathbf{h}} = \mathbf{U}$$

- Let $\boldsymbol{\delta}^{(h)}$ be the error signal for hidden layer

$$\begin{aligned}\boldsymbol{\delta}^{(h)} &:= \frac{\partial J}{\partial \mathbf{h}} = \frac{\partial J}{\partial \mathbf{v}}\frac{\partial \mathbf{v}}{\partial \mathbf{h}} \\ &= \boldsymbol{\delta}^{(o)}\mathbf{U}\end{aligned}$$



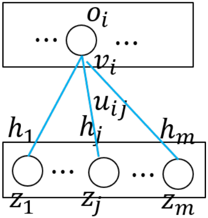
Deriv of J wrt hidden-output weight matrix $\mathbf{U}$

- Hidden-to-output: $\mathbf{v} = \mathbf{U}\mathbf{h}$

$$v_i = \mathbf{U}_{i*}\mathbf{h} = \sum_j u_{ij} \cdot h_j$$

$$\frac{\partial v_i}{\partial \mathbf{U}_{i*}} = \mathbf{h}^T$$

where $\mathbf{U}_{i*}$ is i-th row vector of $\mathbf{U}$.



$$\frac{\partial J}{\partial \mathbf{U}_{i*}} = \frac{\partial J}{\partial v_i}\frac{\partial v_i}{\partial \mathbf{U}_{i*}} = \delta_i^{(o)}\mathbf{h}^T$$

$$\frac{\partial J}{\partial \mathbf{U}} := \begin{bmatrix} \frac{\partial J}{\partial \mathbf{U}_{1*}} \\ \vdots \\ \frac{\partial J}{\partial \mathbf{U}_{K*}} \end{bmatrix} = \begin{bmatrix} \delta_1^{(o)} \\ \vdots \\ \delta_K^{(o)} \end{bmatrix} \mathbf{h}^T = \boldsymbol{\delta}^{(o)\,T}\mathbf{h}^T$$

Error prop to input layer

- Input-to-hidden layer: $\mathbf{z} = \mathbf{W}\mathbf{x} \quad \mathbf{h} = max(\mathbf{z}, 0)$

$$\frac{\partial \mathbf{h}}{\partial \mathbf{z}} = \begin{bmatrix} \mathcal{I}(z_1 > 0) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathcal{I}(z_m > 0) \end{bmatrix} = diag\left(\mathcal{I}(z_i > 0)\right)$$

$$\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \mathbf{W}$$

- Let $\boldsymbol{\delta}^{(z)}$ be the error signal for the pre-activated hidden layer

$$\boldsymbol{\delta}^{(z)} := \frac{\partial \mathbf{J}}{\partial \mathbf{z}} = \frac{\partial \mathbf{J}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{z}} = \boldsymbol{\delta}^{(h)} diag\left(\mathcal{I}(z_i > 0)\right)$$

- Let $\boldsymbol{\delta}^{(x)}$ be the error signal for input layer

$$\boldsymbol{\delta}^{(x)} := \frac{\partial \mathbf{J}}{\partial \mathbf{x}} = \frac{\partial \mathbf{J}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \boldsymbol{\delta}^{(h)} diag\left(\mathcal{I}(z_i > 0)\right) \mathbf{W}$$

Deriv of J wrt input-hidden weight matrix $\mathbf{W}$

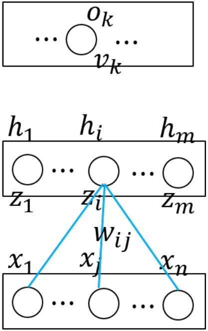
- Input-to-hidden layer: $\mathbf{z} = \mathbf{W}\mathbf{x}$

$$
\begin{aligned}
z_i &= \mathbf{W}_{i*}\mathbf{x} = \sum_j w_{ij} \cdot x_j \\
\frac{\partial z_i}{\partial \mathbf{W}_{i*}} &= \mathbf{x}^T
\end{aligned}
$$

where $\mathbf{W}_{i*}$ is i-th row vector of $\mathbf{W}$.

$$
\frac{\partial J}{\partial \mathbf{W}_{i*}} = \frac{\partial J}{\partial z_i}\frac{\partial z_i}{\partial \mathbf{W}_{i*}} = \delta_i^{(z)}\mathbf{x}^T
$$

$$
\frac{\partial J}{\partial \mathbf{W}} := \begin{bmatrix} \frac{\partial J}{\partial \mathbf{W}_{1*}} \\ \vdots \\ \frac{\partial J}{\partial \mathbf{W}_{m*}} \end{bmatrix} = \begin{bmatrix} \delta_1^{(z)} \\ \vdots \\ \delta_m^{(z)} \end{bmatrix} \mathbf{x}^T = \boldsymbol{\delta}^{(z)\,T}\mathbf{x}^T
$$



Discussion

- Here, error messages such as $\boldsymbol{\delta}^{(o)}$, $\boldsymbol{\delta}^{(h)}$ are row vectors
- But, we can define $\boldsymbol{\delta}^{(o)}$, $\boldsymbol{\delta}^{(h)}$ as column vectors and derive backprop again.
- In this case, only the slight modification on error prop is necessary