Learning the network

11-785 Introduction to Deep Learning

– lecture 5 –

TAVE Research DL001
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01. Computing the derivative

02. Computing the gradient

03. Special cases

04. Vector formulation

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01. Computing the derivative

- Total training loss

$$Loss = \frac{1}{T}\sum_t Div(Y_t, d_t)$$

- Total derivative

$$\frac{dLoss}{dw_{ij}^{(k)}} = \frac{1}{T}\sum_t \frac{dDiv(Y_t, d_t)}{dw_{ij}^{(k)}}$$

Want!

✓ Chain Rule

– For any nested function $y = f(g(x))$

$$z = g(x) \Rightarrow \Delta z = \frac{dg(x)}{dx}\Delta x$$

$$y = f(z) \Rightarrow \Delta y = \frac{df}{dz}\Delta z = \frac{df}{dg(x)}\frac{dg(x)}{dx}\Delta x$$

- Distributed Chain rule

$$y = f(g_1(x), g_1(x), \dots, g_M(x))$$

Let $z_i = g_i(x)$

$$\Delta y = \frac{\partial f}{\partial z_1}\Delta z_1 + \frac{\partial f}{\partial z_2}\Delta z_2 + \cdots + \frac{\partial f}{\partial z_M}\Delta z_M$$

$$\Delta y = \frac{\partial f}{\partial z_1}\frac{dz_1}{dx}\Delta x + \frac{\partial f}{\partial z_2}\frac{dz_2}{dx}\Delta x + \cdots + \frac{\partial f}{\partial z_M}\frac{dz_M}{dx}\Delta x$$

$$\boxed{\frac{dy}{dx} = \frac{\partial f}{\partial g_1(x)}\frac{dg_1(x)}{dx} + \frac{\partial f}{\partial g_2(x)}\frac{dg_2(x)}{dx} + \cdots + \frac{\partial f}{\partial g_M(x)}\frac{dg_M(x)}{dx}}$$

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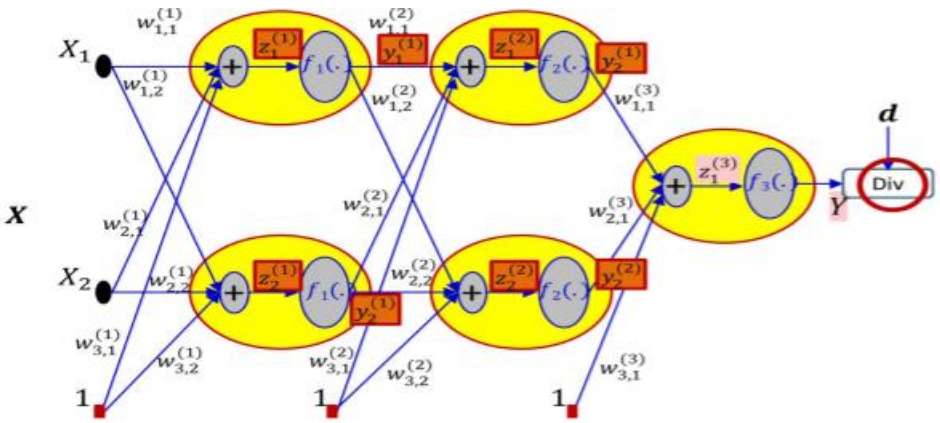
02. Computing the gradient

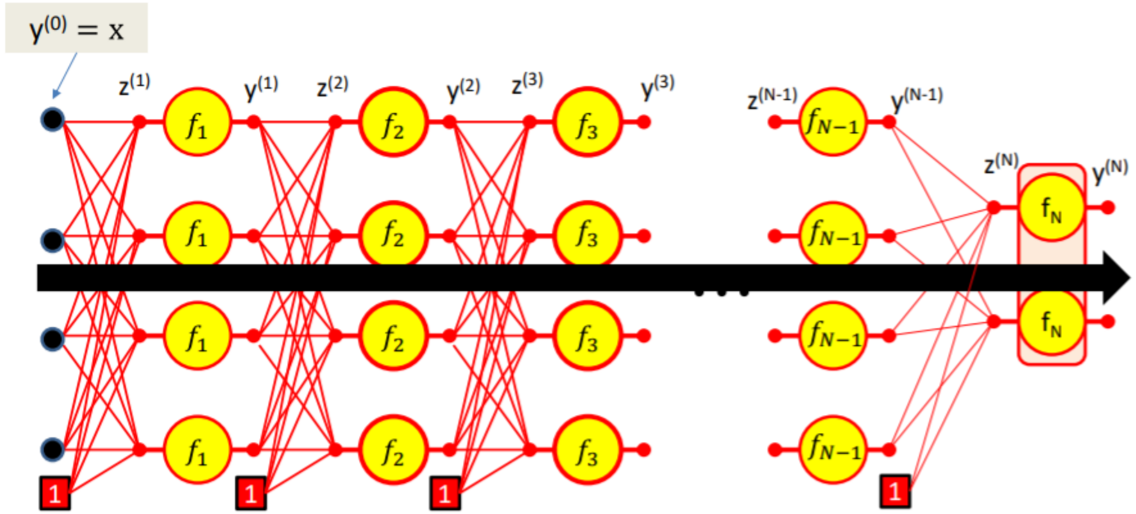
- computation of the derivative $\frac{dDiv(Y,d)}{dw_{ij}^{(k)}}$



✓ requires **intermediate and final output values** of the network in response to the input

- **The forward pass**

: the process of computing the output from an input as the forward pass



ITERATE FOR k = 1:N

for j = 1:layer-width

$$y_i^{(0)} = x_i$$

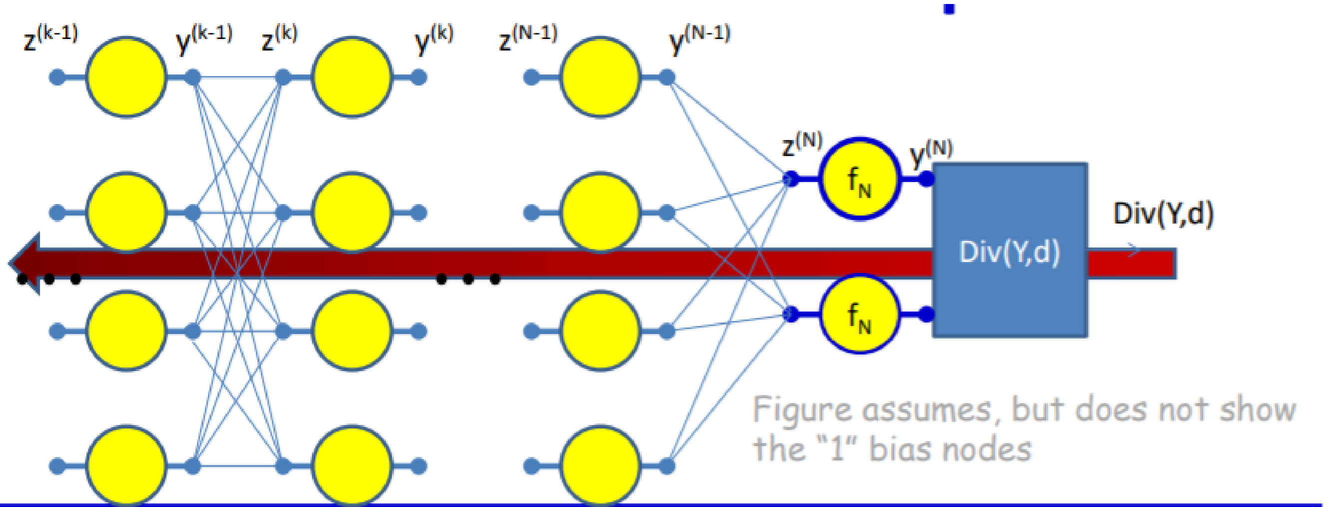
$$z_j^{(k)} = \sum_i w_{ij}^{(k)} y_i^{(k-1)}$$

$$y_j^{(k)} = f_k\left(z_j^{(k)}\right)$$

02. Computing the gradient

- The backward pass

: the process of computing the gradient from an output as the backward pass



Initialize: Gradient w.r.t network output

$$\frac{\partial Div}{\partial y_i^{(N)}} = \frac{\partial Div(Y,d)}{\partial y_i}$$

$$\frac{\partial Div}{\partial z_i^{(N)}} = f_k'\left(z_i^{(N)}\right)\frac{\partial Div}{\partial y_i^{(N)}}$$

$For\ k\ =\ N-1..0$

$For\ i\ =\ 1{:}\ layer\ width$

$$\frac{\partial Div}{\partial y_i^{(k)}} = \sum_j w_{ij}^{(k+1)}\frac{\partial Div}{\partial z_j^{(k+1)}}$$

$$\frac{\partial Div}{\partial z_i^{(k)}} = f_k'\left(z_i^{(k)}\right)\frac{\partial Div}{\partial y_i^{(k)}}$$

$$\forall j\ \frac{\partial Div}{\partial w_{ij}^{(k+1)}} = y_i^{(k)}\frac{\partial Div}{\partial z_j^{(k+1)}}$$

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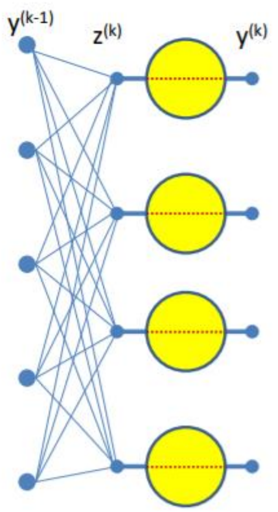
03. Special cases

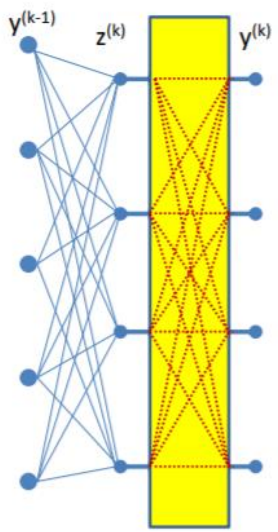
- Case 1. Vector activation



< Scalar activation >

- Each z_i
- influences one y_i

$$\frac{\partial Div}{\partial z_i^{(k)}} = \frac{\partial Div}{\partial y_i^{(k)}} \frac{dy_i^{(k)}}{dz_i^{(k)}}$$



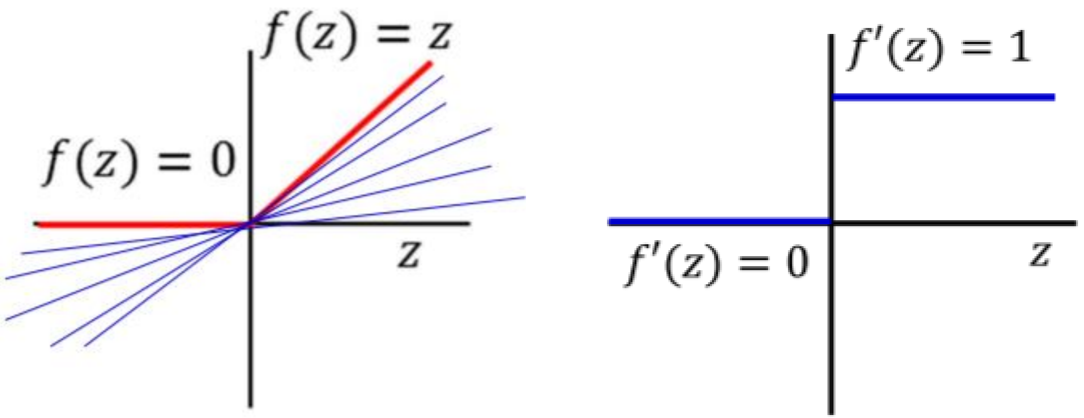
< Vector activation >

- Each z_i
- influences all, $y_1, \dots, y_M$

$$\frac{\partial Div}{\partial z_i^{(k)}} = \sum_i \frac{\partial Div}{\partial y_i^{(k)}} \frac{dy_i^{(k)}}{dz_i^{(k)}}$$

- Case 2. Non-differentiable activations

- ReLU



✓ At the differentiable points, we can use any sub-gradients

- Max

$$y = \max_j z_j \Rightarrow \frac{\partial y}{\partial z_i} = \begin{cases} 1, i = argmax_j z_j \\ 0, \quad otherwise \end{cases}$$

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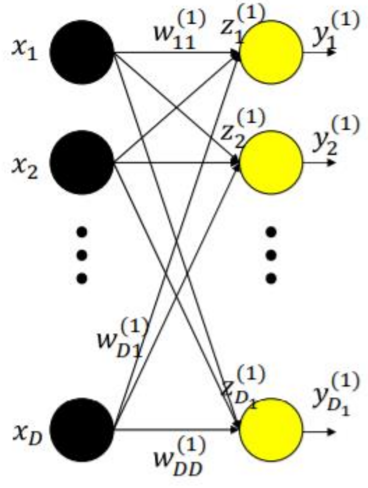
- Vector formulation

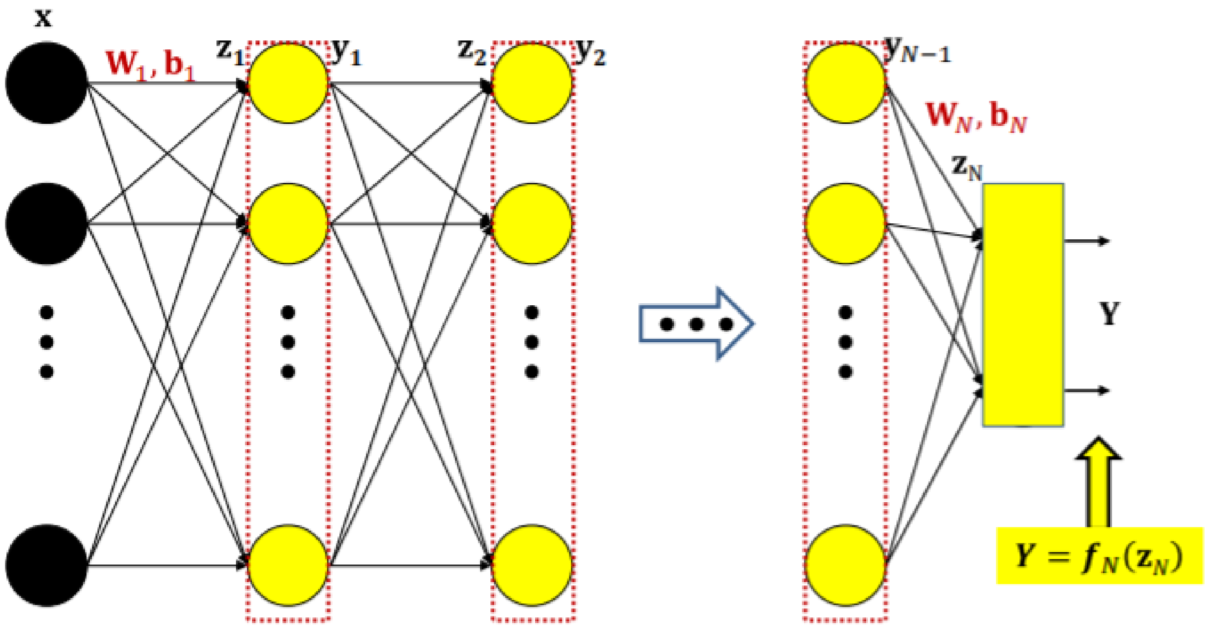


$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix} \qquad \mathbf{z}_k = \begin{bmatrix} z_1^{(k)} \\ z_2^{(k)} \\ \vdots \\ z_{D_k}^{(k)} \end{bmatrix} \qquad \mathbf{y}_k = \begin{bmatrix} y_1^{(k)} \\ y_2^{(k)} \\ \vdots \\ y_{D_k}^{(k)} \end{bmatrix}$$

$$\mathbf{W}_k = \begin{bmatrix} w_{11}^{(k)} & w_{21}^{(k)} & \vdots & w_{D_{k-1}1}^{(k)} \\ w_{12}^{(k)} & w_{22}^{(k)} & \vdots & w_{D_{k-1}2}^{(k)} \\ \cdots & \cdots & \ddots & \vdots \\ w_{1D_k}^{(k)} & w_{2D_k}^{(k)} & \cdots & w_{D_{k-1}D_k}^{(k)} \end{bmatrix} \qquad \mathbf{b}_k = \begin{bmatrix} b_1^{(k)} \\ b_2^{(k)} \\ \vdots \\ b_{D_{k+1}}^{(k)} \end{bmatrix}$$

$$\boxed{\mathbf{z}_k = \mathbf{W}_k \mathbf{y}_{k-1} + \mathbf{b}_k} \qquad \boxed{\mathbf{y}_k = \boldsymbol{f}_k(\mathbf{z}_k)}$$

- The forward pass



The Complete computation

$$Y = f_N(\mathbf{W}_N f_{N-1}(\dots f_2(\mathbf{W}_2 f_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2) \dots) + \mathbf{b}_N)$$

$$Div(Y, d) = Div(f_N(\mathbf{W}_N f_{N-1}(\dots f_2(\mathbf{W}_2 f_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2) \dots) + \mathbf{b}_N), d)$$

04. Vector formulation

- The Jacobian
  - The distributed chain rule

$$y = f\big(g_1(x), g_1(x), \dots, g_M(x)\big)$$

$$\downarrow$$

$$\Delta y = \frac{\partial f}{\partial z_1}\Delta z_1 + \frac{\partial f}{\partial z_2}\Delta z_2 + \cdots + \frac{\partial f}{\partial z_M}\Delta z_M$$

✓ What if y is a **vector**?

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = f\left(\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_D \end{bmatrix}\right) \longrightarrow J_{\mathbf{y}}(\mathbf{z}) = \begin{bmatrix} \frac{\partial y_1}{\partial z_1} & \frac{\partial y_1}{\partial z_2} & \cdots & \frac{\partial y_1}{\partial z_D} \\ \frac{\partial y_2}{\partial z_1} & \frac{\partial y_2}{\partial z_2} & \cdots & \frac{\partial y_2}{\partial z_D} \\ \cdots & \cdots & \ddots & \cdots \\ \frac{\partial y_M}{\partial z_1} & \frac{\partial y_M}{\partial z_2} & \cdots & \frac{\partial y_M}{\partial z_D} \end{bmatrix}$$

$$\Delta \mathbf{y} = J_{\mathbf{y}}(\mathbf{z})\Delta \mathbf{z}$$

- Chain rule
  - For vector functions of vector inputs

$$\boldsymbol{y} = \boldsymbol{f}\big(\mathbf{z}(\boldsymbol{x})\big) \;\rightarrow\; J_{\boldsymbol{y}}(\boldsymbol{x}) = J_{\boldsymbol{y}}(\mathbf{z}) J_{\mathbf{z}}(\boldsymbol{x})$$

  - For scalar functions of vector inputs

$$D = f\big(\mathbf{z}(\boldsymbol{x})\big) \;\rightarrow\; \nabla_{\boldsymbol{x}} D = \nabla_{\mathbf{z}}(D) J_{\mathbf{z}}(\boldsymbol{x})$$

$$(\because \Delta D = \nabla_{\mathbf{z}}(D)\Delta\mathbf{z}, \qquad \Delta\mathbf{z} = J_{\mathbf{z}}(x)\Delta x)$$

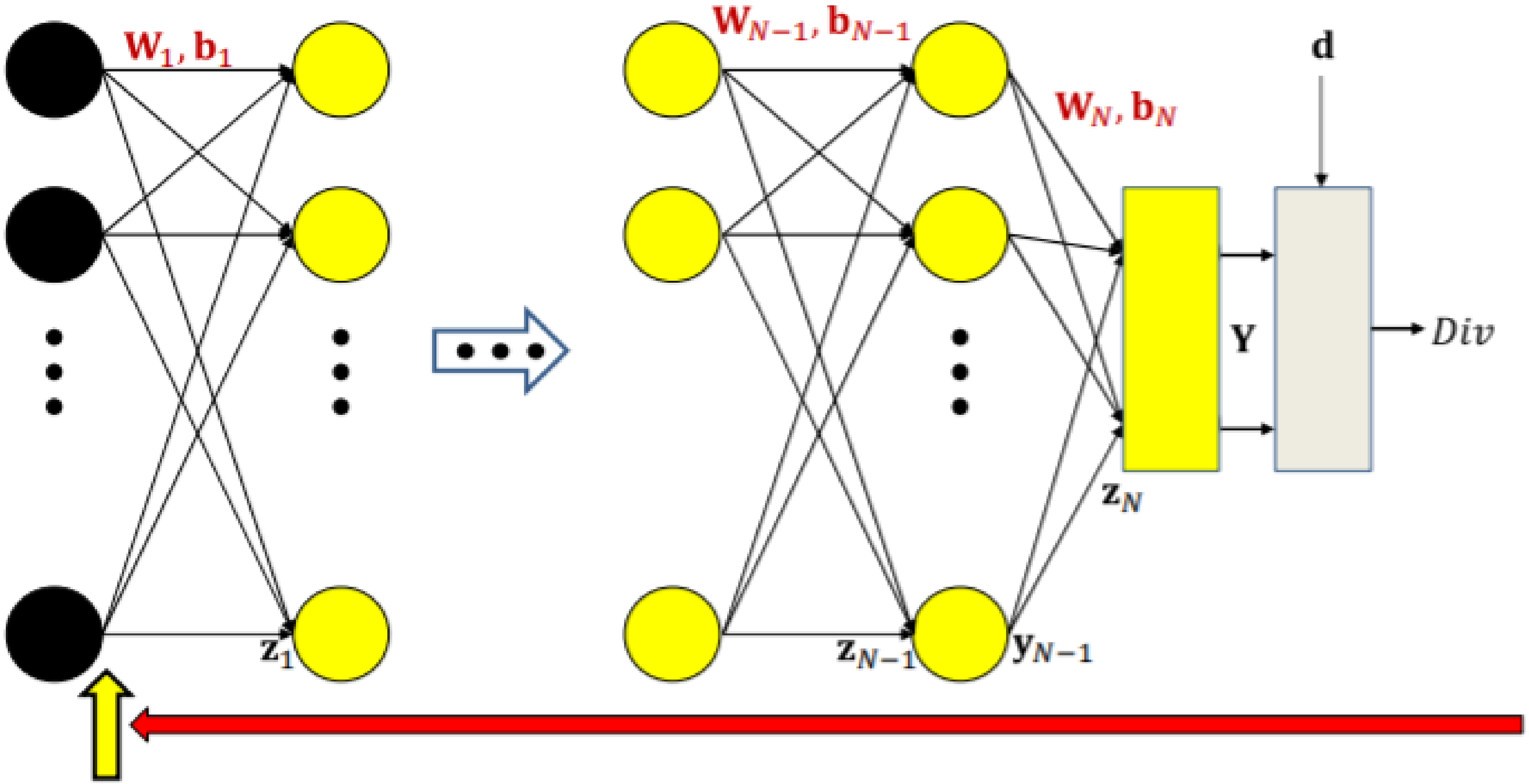
  - Affine functions

$$z = Wy + b \;\rightarrow\; J_z(y) = W$$

$$(\because W(y + \Delta y) + b = (Wy + b) + W\Delta y)$$
$$= z + \Delta \mathbf{z}$$

04. Vector formulation

- The backward pass



$$\nabla_{\mathbf{W}_1} Div = \mathbf{x} \nabla_{\mathbf{z}_1} Div$$

$$\nabla_{\mathbf{b}_1} Div = \nabla_{\mathbf{z}_1} Div$$

In some problems we will also want to compute the derivative w.r.t. the input

Thank you