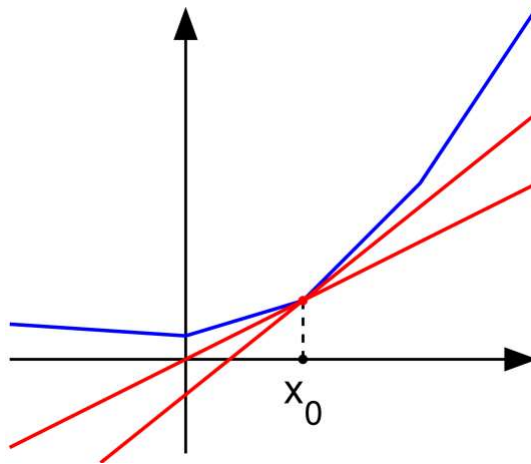
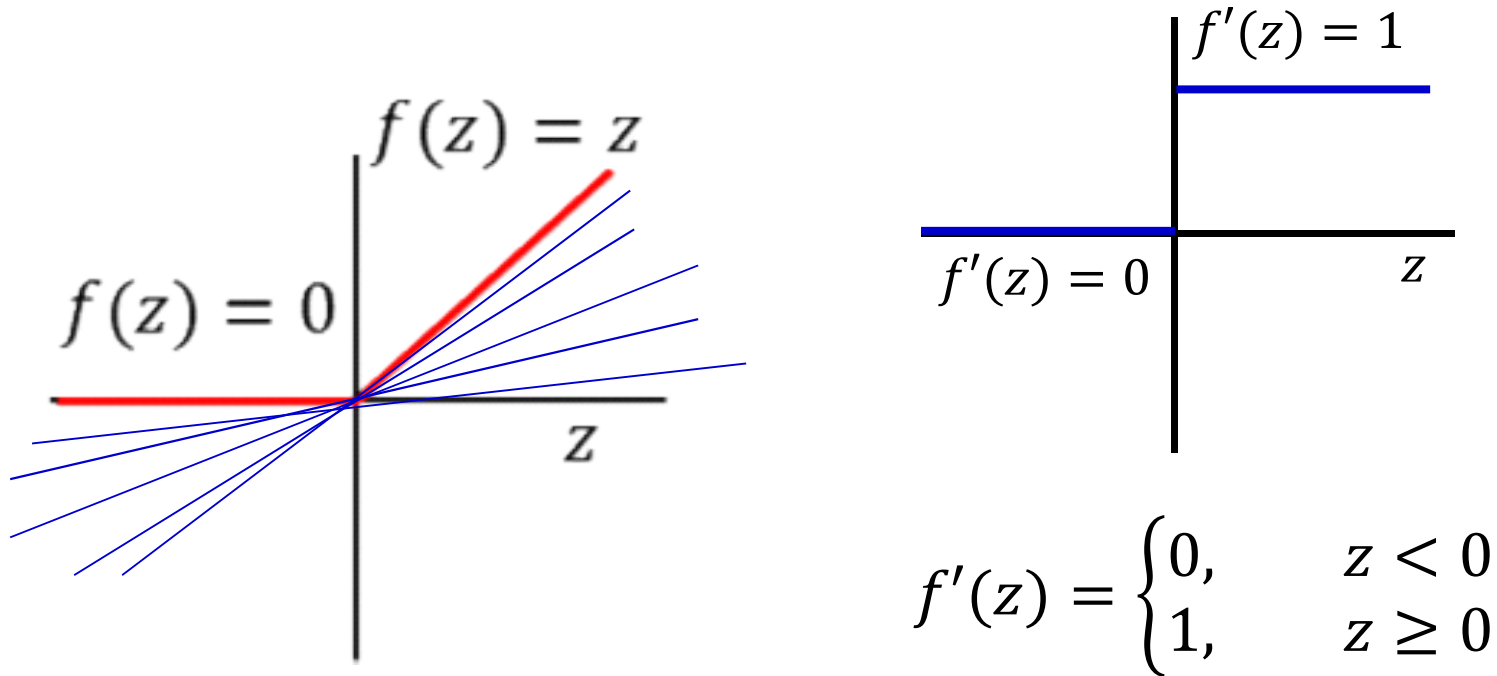


# The subgradient



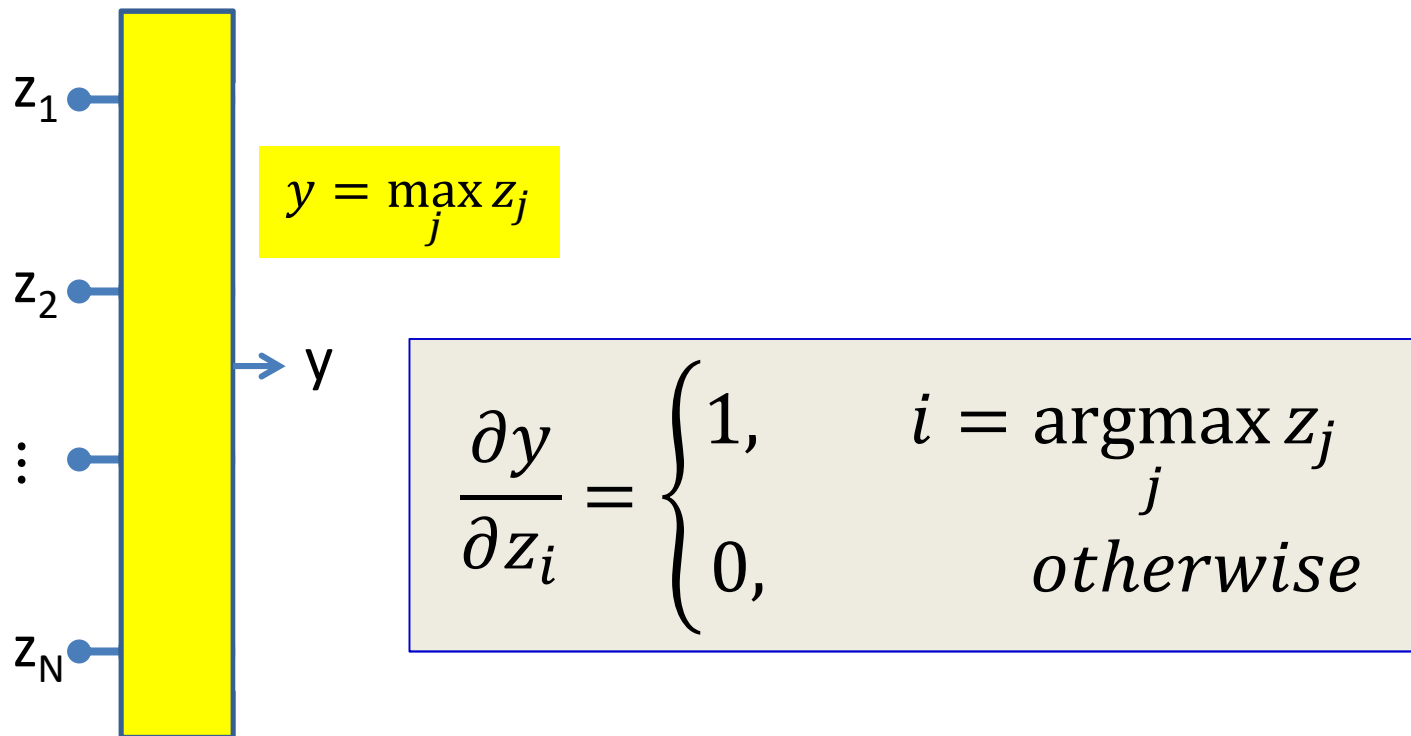
- A subgradient of a function  $f(x)$  at a point  $x_0$  is any vector  $v$  such that
$$(f(x) - f(x_0)) \geq v^T (x - x_0)$$
  - Any direction such that moving in that direction increases the function
- Guaranteed to exist only for convex functions
  - “bowl” shaped functions
  - For non-convex functions, the equivalent concept is a “quasi-secant”
- The subgradient is a direction in which the function is guaranteed to increase
- If the function is differentiable at  $x_0$ , the subgradient is the gradient
  - The gradient is not always the subgradient though

# Subgradients and the RELU



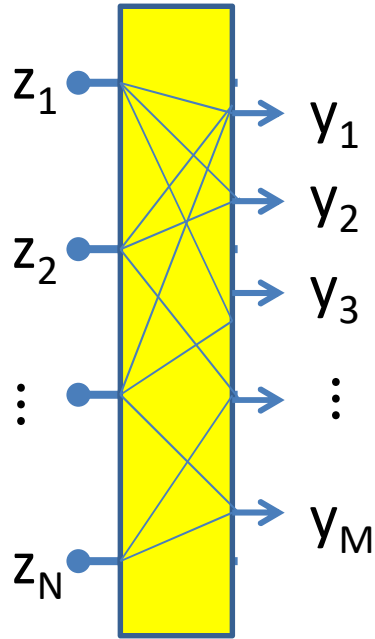
- Can use any subgradient
  - At the differentiable points on the curve, this is the same as the gradient
  - Typically, will use the equation given

# Subgradients and the Max



- Vector equivalent of subgradient
  - 1 w.r.t. the largest incoming input
    - Incremental changes in this input will change the output
  - 0 for the rest
    - Incremental changes to these inputs will not change the output

# Subgradients and the Max



$$y_i = \operatorname{argmax}_{l \in \mathcal{S}_j} z_l$$

$$\frac{\partial y_j}{\partial z_i} = \begin{cases} 1, & i = \operatorname{argmax}_{l \in \mathcal{S}_j} z_l \\ 0, & \text{otherwise} \end{cases}$$

- Multiple outputs, each selecting the max of a different subset of inputs
  - Will be seen in convolutional networks
- Gradient for any output:
  - 1 for the specific component that is maximum in corresponding input subset
  - 0 otherwise

# Backward Pass: Recap

- Output layer (N) :
  - For  $i = 1 \dots D_N$ 
    - $\frac{\partial Div}{\partial Y_i} = \frac{\partial Div(Y, d)}{\partial y_i^{(N)}}$
    - $\frac{\partial Div}{\partial z_i^{(N)}} = \frac{\partial Div}{\partial y_i^{(N)}} \frac{\partial y_i^{(N)}}{\partial z_i^{(N)}} \quad \text{OR} \quad \sum_j \frac{\partial Div}{\partial y_j^{(N)}} \frac{\partial y_j^{(N)}}{\partial z_i^{(N)}} \text{ (vector activation)}$
- For layer  $k = N - 1$  *downto* 0
  - For  $i = 1 \dots D_k$ 
    - $\frac{\partial Div}{\partial y_i^{(k)}} = \sum_j w_{ij}^{(k+1)} \frac{\partial Div}{\partial z_j^{(k+1)}}$
    - $\frac{\partial Div}{\partial z_i^{(k)}} = \frac{\partial Div}{\partial y_i^{(k)}} \frac{\partial y_i^{(k)}}{\partial z_i^{(k)}} \quad \text{OR} \quad \sum_j \frac{\partial Div}{\partial y_j^{(k)}} \frac{\partial y_j^{(k)}}{\partial z_i^{(k)}} \text{ (vector activation)}$
    - $\frac{\partial Div}{\partial w_{ji}^{(k+1)}} = y_j^{(k)} \frac{\partial Div}{\partial z_i^{(k+1)}} \text{ for } j = 1 \dots D_{k+1}$

These may be subgradients

# Overall Approach

- For each data instance
  - **Forward pass:** Pass instance forward through the net. Store all intermediate outputs of all computation
  - **Backward pass:** Sweep backward through the net, iteratively compute all derivatives w.r.t weights
- Actual loss is the sum of the divergence over all training instances

$$\mathbf{Loss} = \frac{1}{|\{X\}|} \sum_X \text{Div}(Y(X), d(X))$$

- Actual gradient is the sum or average of the derivatives computed for each training instance

$$\nabla_W \mathbf{Loss} = \frac{1}{|\{X\}|} \sum_X \nabla_W \text{Div}(Y(X), d(X)) \quad W \leftarrow W - \eta \nabla_W \mathbf{Loss}^T$$

# Training by BackProp

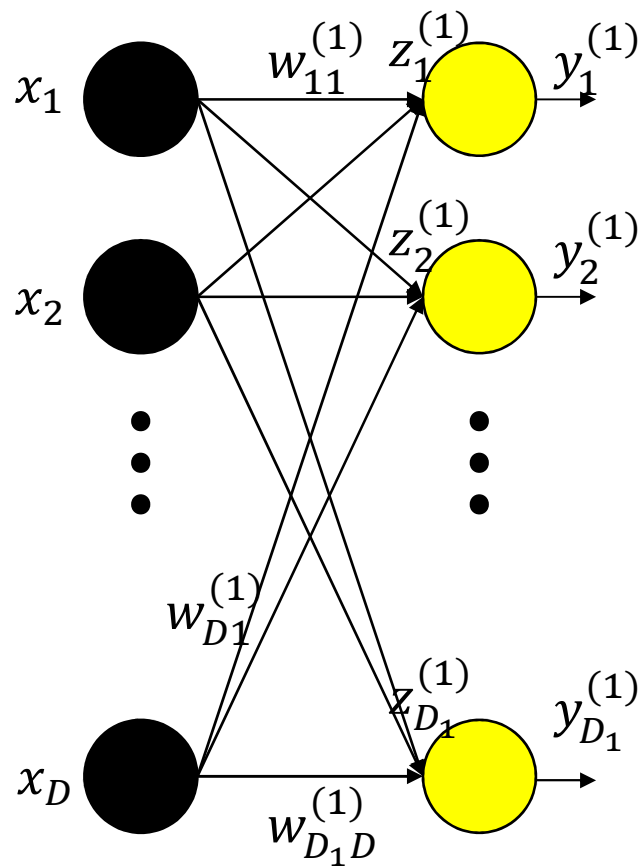
- Initialize weights  $\mathbf{W}^{(k)}$  for all layers  $k = 1 \dots K$
- Do:
  - Initialize  $Loss = 0$ ; For all  $i, j, k$ , initialize  $\frac{dLoss}{dw_{i,j}^{(k)}} = 0$
  - For all  $t = 1:T$  (Loop over training instances)
    - **Forward pass:** Compute
      - Output  $\mathbf{Y}_t$
      - $Loss += Div(\mathbf{Y}_t, \mathbf{d}_t)$
    - **Backward pass:** For all  $i, j, k$ :
      - Compute  $\frac{dDiv(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$
      - Compute  $\frac{dLoss}{dw_{i,j}^{(k)}} += \frac{dDiv(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$
  - For all  $i, j, k$ , update:
$$w_{i,j}^{(k)} = w_{i,j}^{(k)} - \frac{\eta}{T} \frac{dLoss}{dw_{i,j}^{(k)}}$$
- Until  $Loss$  has converged

# Vector formulation

- For layered networks it is generally simpler to think of the process in terms of vector operations
  - Simpler arithmetic
  - Fast matrix libraries make operations *much* faster
- We can restate the entire process in vector terms
  - On slides, please read
  - This is what is *actually* used in any real system
  - Will appear in quiz



# Vector formulation



$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix}$$

$$\mathbf{z}_k = \begin{bmatrix} z_1^{(k)} \\ z_2^{(k)} \\ \vdots \\ z_{D_k}^{(k)} \end{bmatrix}$$

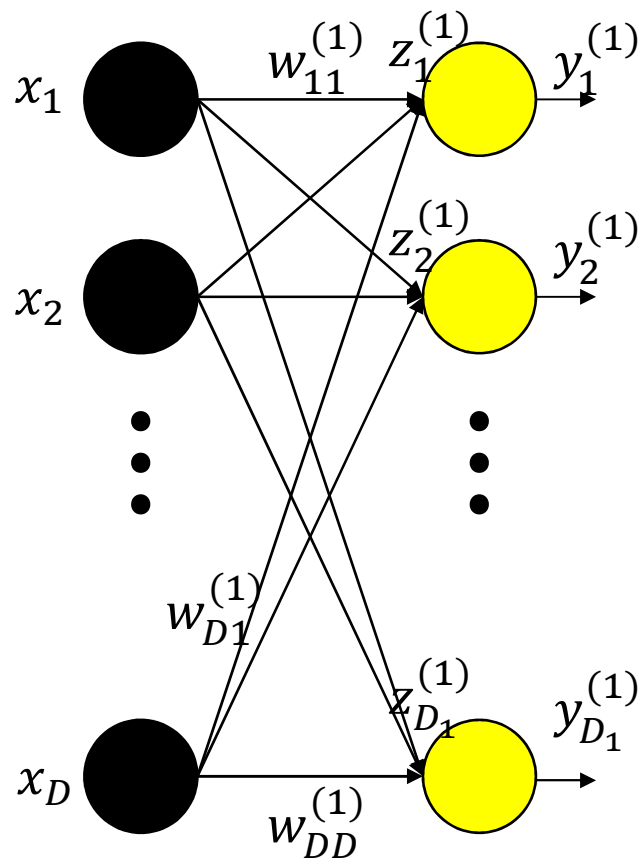
$$\mathbf{y}_k = \begin{bmatrix} y_1^{(k)} \\ y_2^{(k)} \\ \vdots \\ y_{D_k}^{(k)} \end{bmatrix}$$

$$\mathbf{W}_k = \begin{bmatrix} w_{11}^{(k)} & w_{21}^{(k)} & \vdots & w_{D_{k-1}1}^{(k)} \\ w_{12}^{(k)} & w_{22}^{(k)} & \vdots & w_{D_{k-1}2}^{(k)} \\ \dots & \dots & \ddots & \vdots \\ w_{1D_k}^{(k)} & w_{2D_k}^{(k)} & \dots & w_{D_{k-1}D_k}^{(k)} \end{bmatrix}$$

$$\mathbf{b}_k = \begin{bmatrix} b_1^{(k)} \\ b_2^{(k)} \\ \vdots \\ b_{D_{k+1}}^{(k)} \end{bmatrix}$$

- Arrange all inputs to the network in a vector  $\mathbf{x}$
- Arrange the *inputs* to neurons of the  $k$ th layer as a vector  $\mathbf{z}_k$
- Arrange the outputs of neurons in the  $k$ th layer as a vector  $\mathbf{y}_k$
- Arrange the weights to any layer as a matrix  $\mathbf{W}_k$ 
  - Similarly with biases

# Vector formulation



$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix}$$

$$\mathbf{z}_k = \begin{bmatrix} z_1^{(k)} \\ z_2^{(k)} \\ \vdots \\ z_{D_k}^{(k)} \end{bmatrix}$$

$$\mathbf{y}_k = \begin{bmatrix} y_1^{(k)} \\ y_2^{(k)} \\ \vdots \\ y_{D_k}^{(k)} \end{bmatrix}$$

$$\mathbf{W}_k = \begin{bmatrix} w_{11}^{(k)} & w_{21}^{(k)} & \vdots & w_{D_{k-1}1}^{(k)} \\ w_{12}^{(k)} & w_{22}^{(k)} & \vdots & w_{D_{k-1}2}^{(k)} \\ \dots & \dots & \ddots & \vdots \\ w_{1D_k}^{(k)} & w_{2D_k}^{(k)} & \dots & w_{D_{k-1}D_k}^{(k)} \end{bmatrix}$$

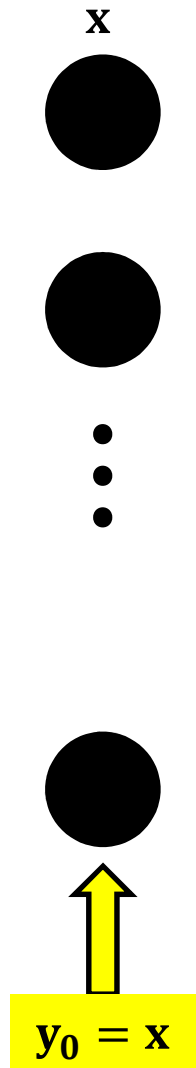
$$\mathbf{b}_k = \begin{bmatrix} b_1^{(k)} \\ b_2^{(k)} \\ \vdots \\ b_{D_{k+1}}^{(k)} \end{bmatrix}$$

- The computation of a single layer is easily expressed in matrix notation as (setting  $\mathbf{y}_0 = \mathbf{x}$ ):

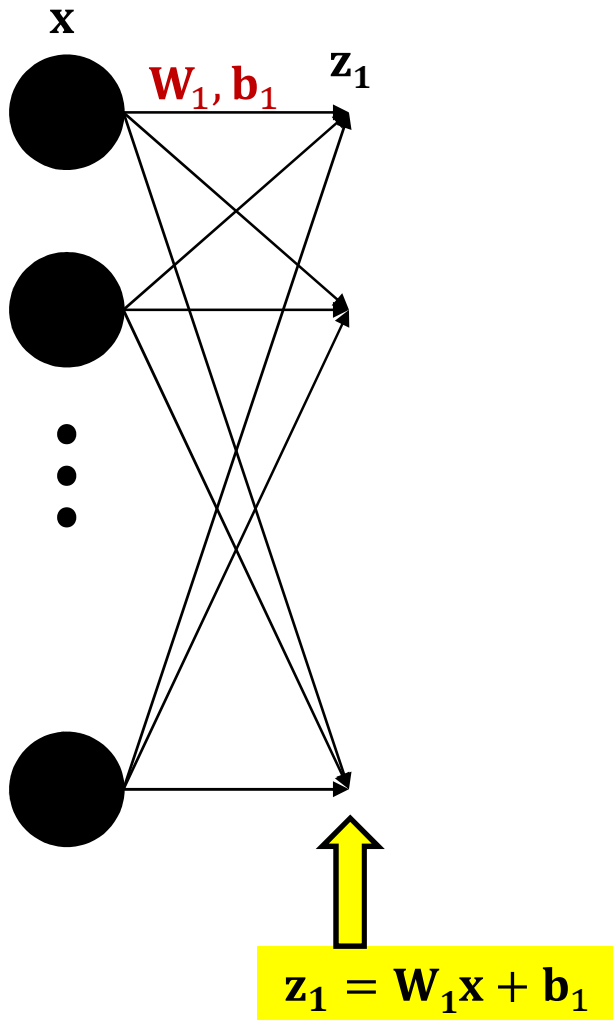
$$\mathbf{z}_k = \mathbf{W}_k \mathbf{y}_{k-1} + \mathbf{b}_k$$

$$\mathbf{y}_k = f_k(\mathbf{z}_k)$$

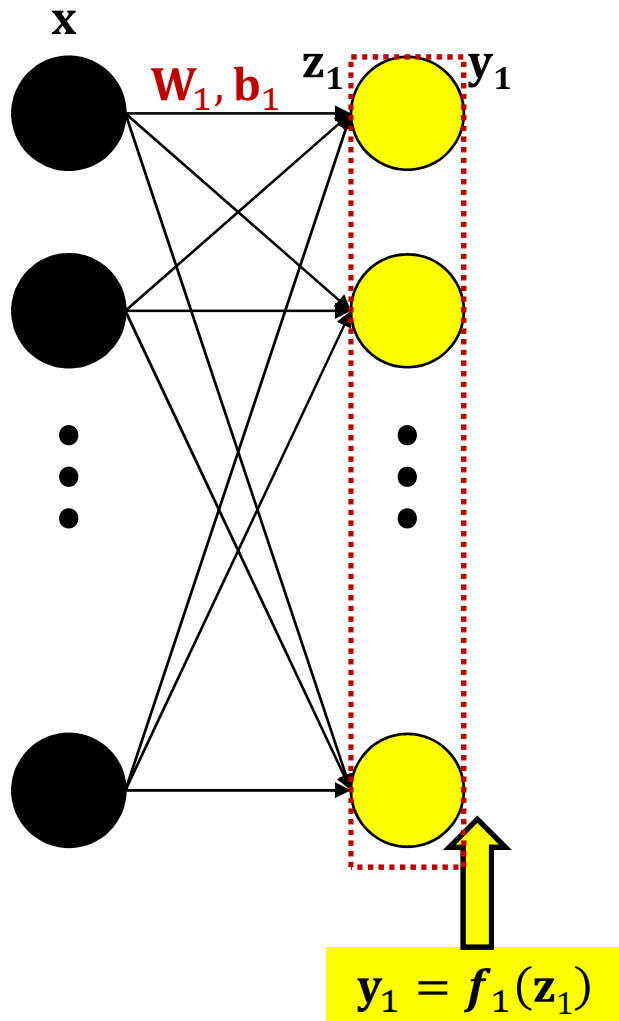
# The forward pass: Evaluating the network



# The forward pass



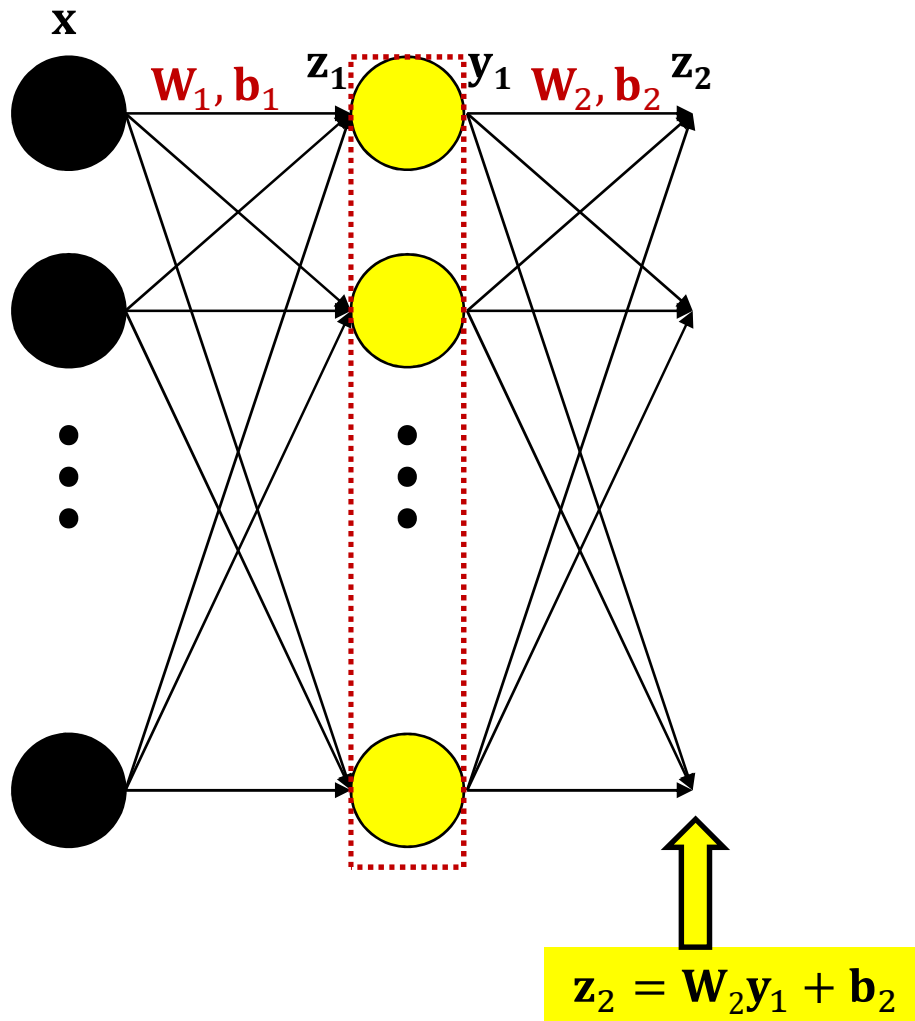
# The forward pass



The Complete computation

$$\mathbf{y}_1 = f_1(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1)$$

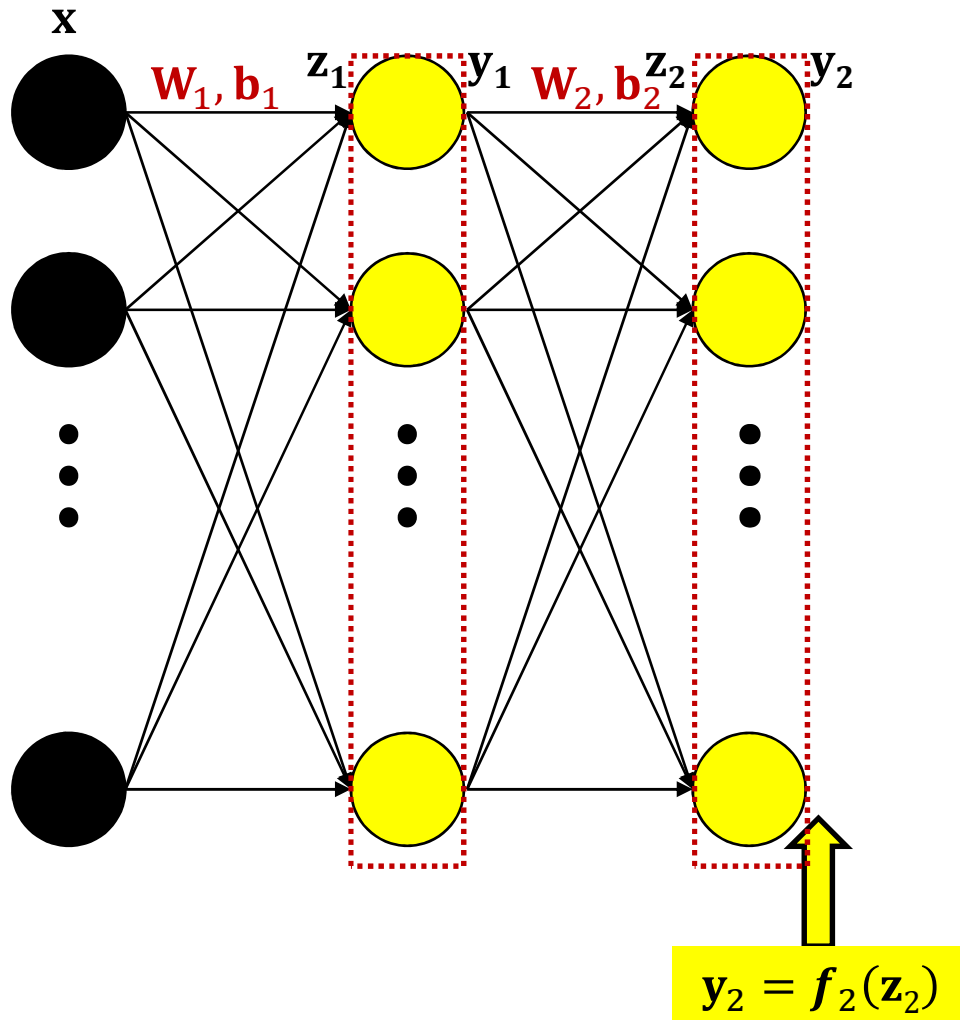
# The forward pass



The Complete computation

$$\mathbf{y}_1 = f_1(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1)$$

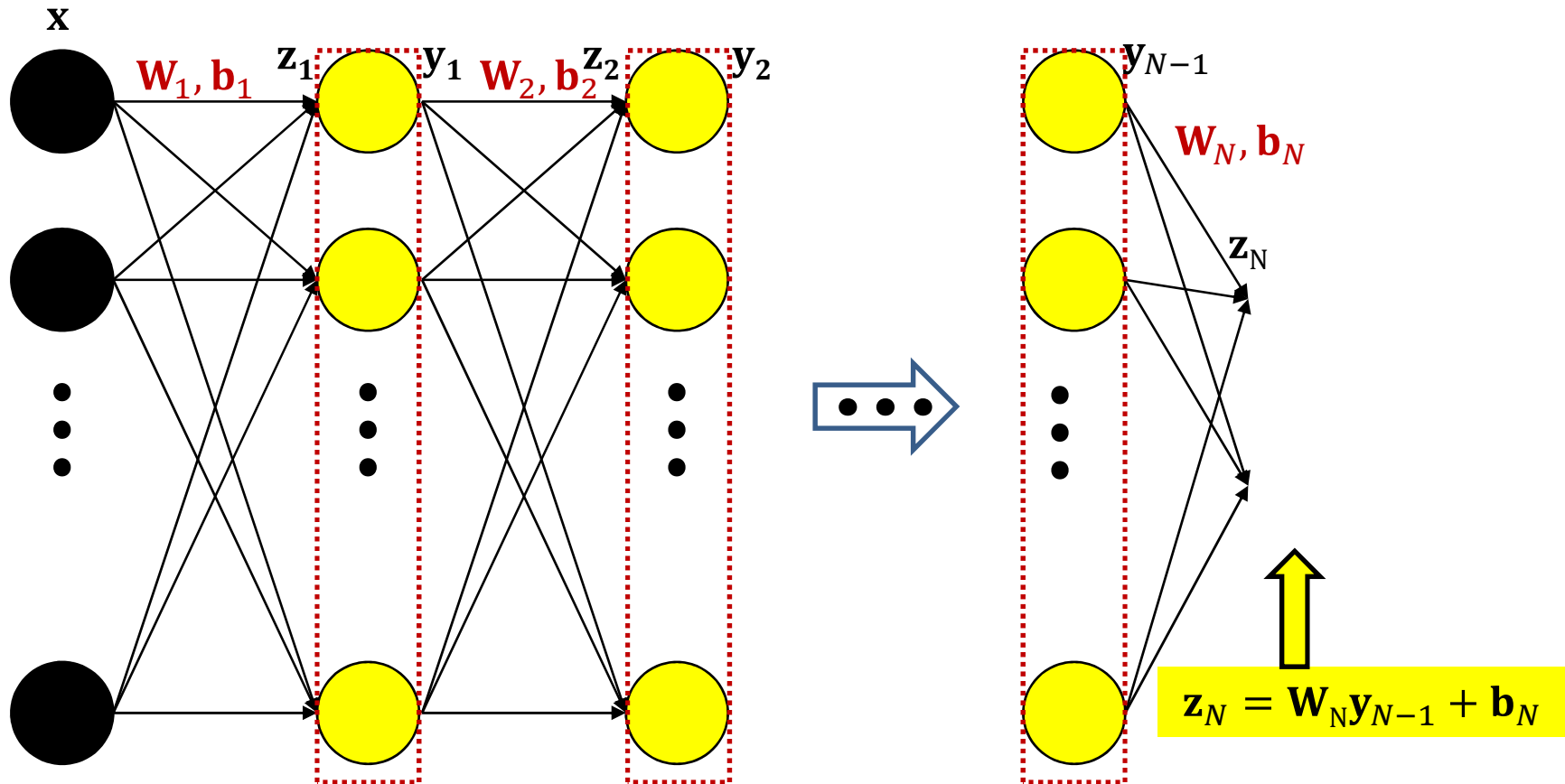
# The forward pass



The Complete computation

$$\mathbf{y}_2 = f_2(\mathbf{W}_2 f_1(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2)$$

# The forward pass

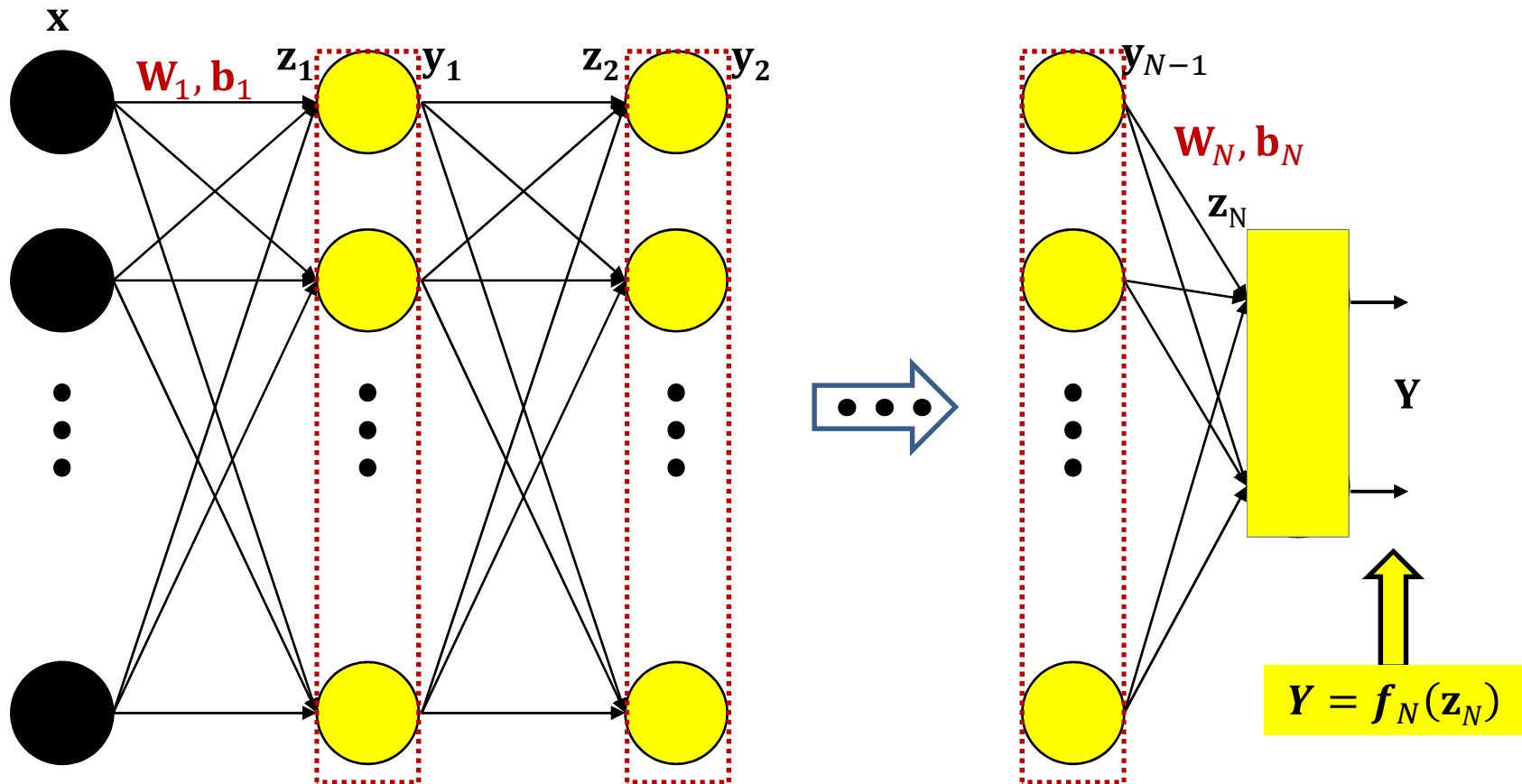


The Complete computation

$$y_2 = f_2(w_2 f_1(w_1 x + b_1) + b_2)$$



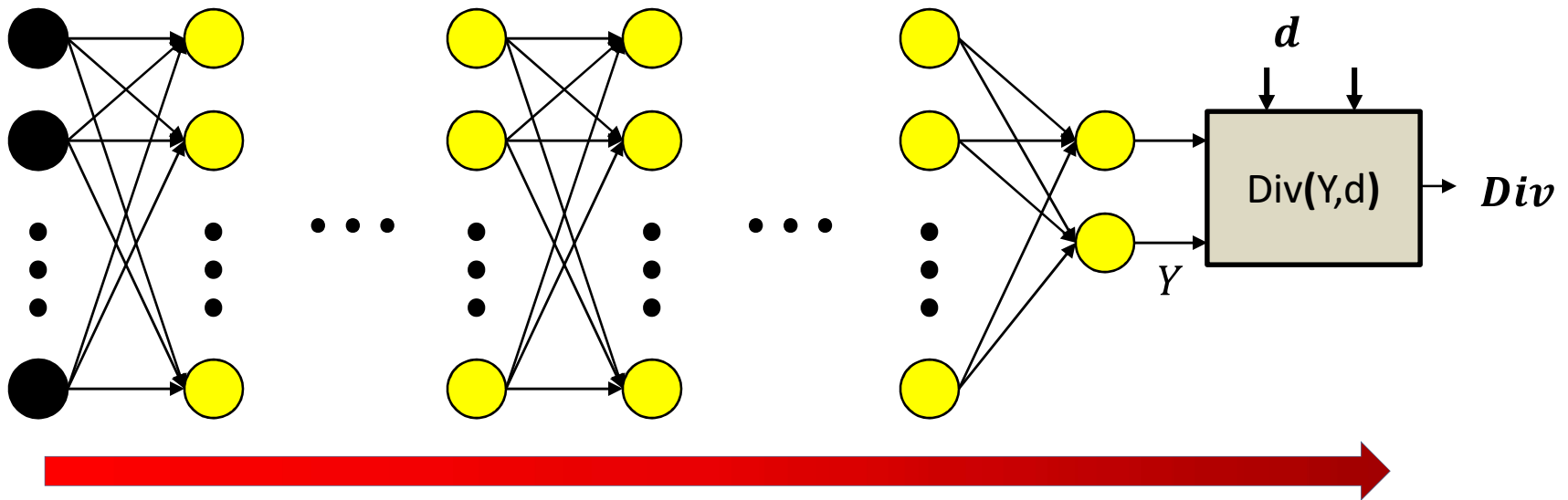
# The forward pass



The Complete computation

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

# Forward pass



## Forward pass:

Initialize

$$\mathbf{y}_0 = \mathbf{x}$$

For  $k = 1$  to  $N$ :

$$\mathbf{z}_k = \mathbf{W}_k \mathbf{y}_{k-1} + \mathbf{b}_k$$

$$\mathbf{y}_k = f_k(\mathbf{z}_k)$$

Output

$$\mathbf{Y} = \mathbf{y}_N$$

# The Forward Pass

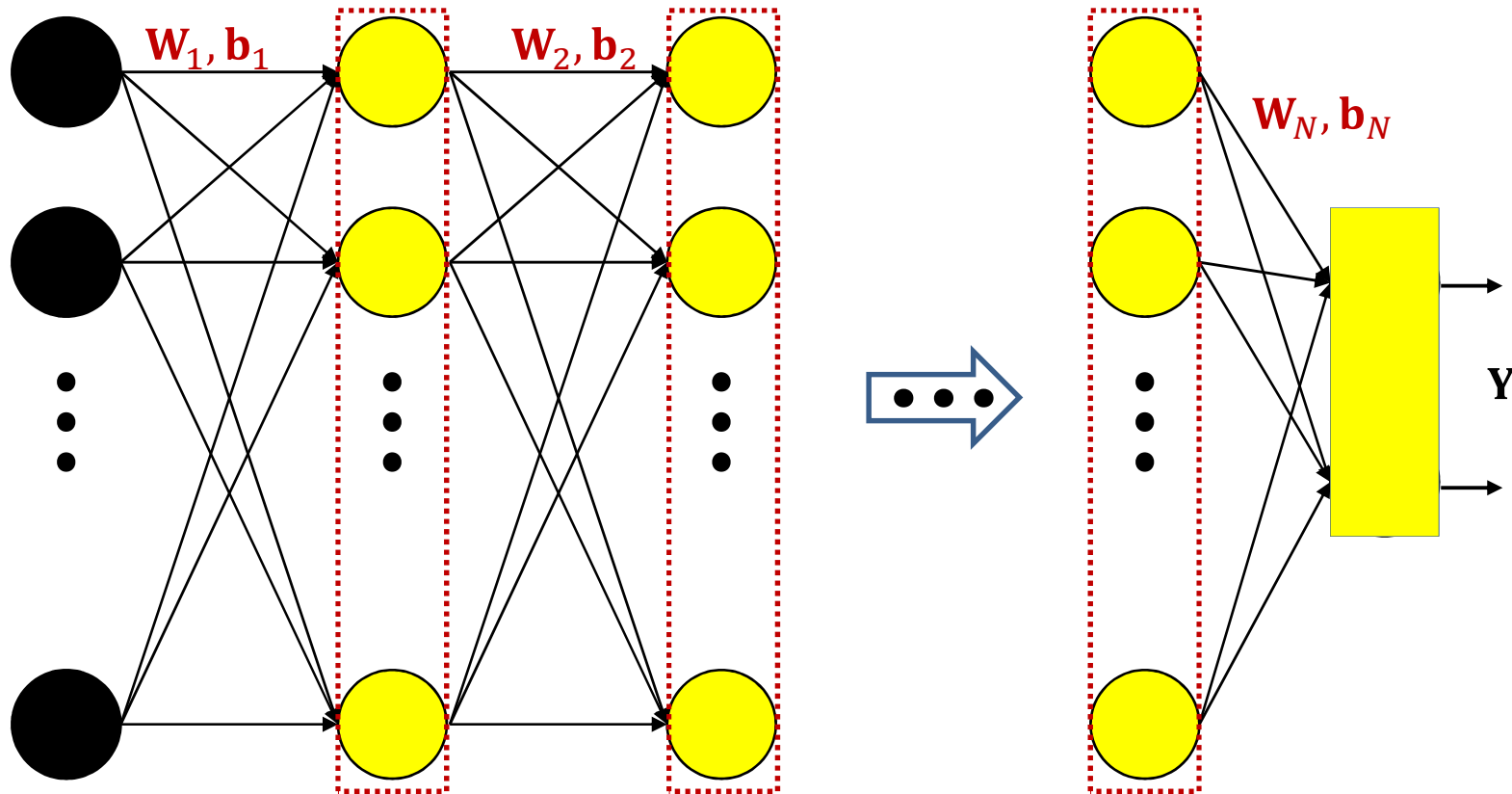
- Set  $\mathbf{y}_0 = \mathbf{x}$
- Recursion through layers:
  - For layer  $k = 1$  to  $N$ :

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

- Output:

$$\mathbf{Y} = \mathbf{y}_N$$

# The backward pass



- The network is a nested function

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

- The error for any  $\mathbf{x}$  is also a nested function

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

# Calculus recap 2: The Jacobian

- The derivative of a vector function w.r.t. vector input is called a *Jacobian*
- It is the matrix of partial derivatives given below

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = f \left( \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_D \end{bmatrix} \right)$$

Using vector notation

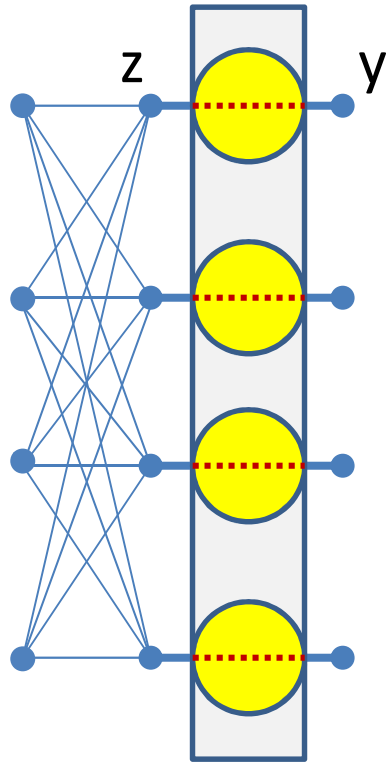
$$\mathbf{y} = f(\mathbf{z})$$

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

Check:

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

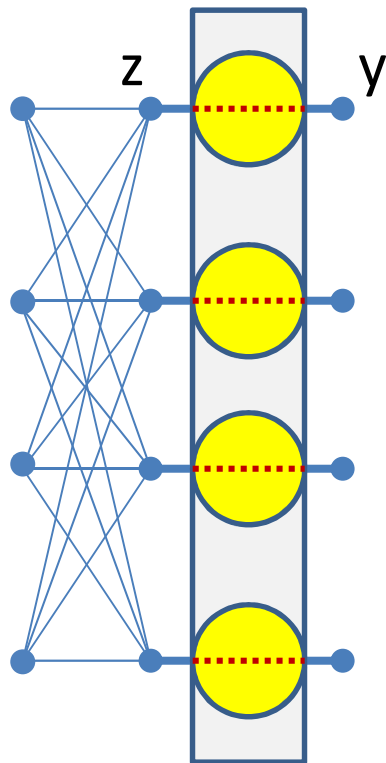
# Jacobians can describe the derivatives of neural activations w.r.t their input



$$J_y(\mathbf{z}) = \begin{bmatrix} \frac{dy_1}{dz_1} & 0 & \dots & 0 \\ 0 & \frac{dy_2}{dz_2} & \dots & 0 \\ \dots & \dots & \ddots & \dots \\ 0 & 0 & \dots & \frac{dy_D}{dz_D} \end{bmatrix}$$

- **For Scalar activations**
  - Number of outputs is identical to the number of inputs
- Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs
  - Not showing the superscript “(k)” in equations for brevity

# Jacobians can describe the derivatives of neural activations w.r.t their input

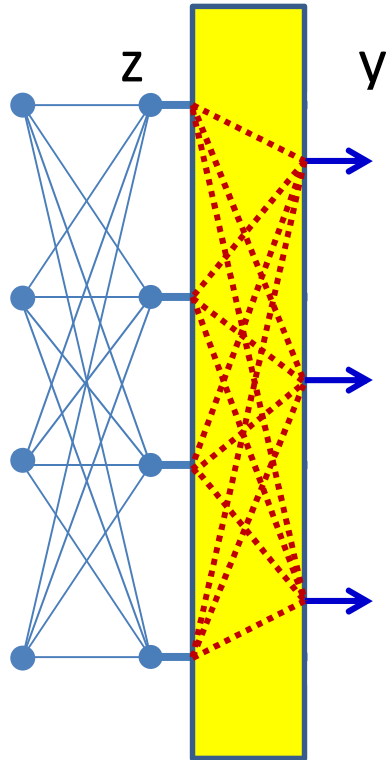


$$y_i = f(z_i)$$

$$J_{\mathbf{y}}(\mathbf{z}) = \begin{bmatrix} f'(z_1) & 0 & \dots & 0 \\ 0 & f'(z_2) & \dots & 0 \\ \dots & \dots & \ddots & \dots \\ 0 & 0 & \dots & f'(z_M) \end{bmatrix}$$

- **For scalar activations (shorthand notation):**
  - Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs

# For *Vector* activations



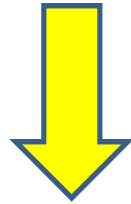
$$J_{\mathbf{y}}(\mathbf{z}) = \begin{bmatrix} \frac{\partial y_1}{\partial z_1} & \frac{\partial y_1}{\partial z_2} & \dots & \frac{\partial y_1}{\partial z_D} \\ \frac{\partial y_2}{\partial z_1} & \frac{\partial y_2}{\partial z_2} & \dots & \frac{\partial y_2}{\partial z_D} \\ \dots & \dots & \ddots & \dots \\ \frac{\partial y_M}{\partial z_1} & \frac{\partial y_M}{\partial z_2} & \dots & \frac{\partial y_M}{\partial z_D} \end{bmatrix}$$

- Jacobian is a full matrix
  - Entries are partial derivatives of individual outputs w.r.t individual inputs



# Special case: Affine functions

$$\mathbf{z} = \mathbf{W}\mathbf{y} + \mathbf{b}$$

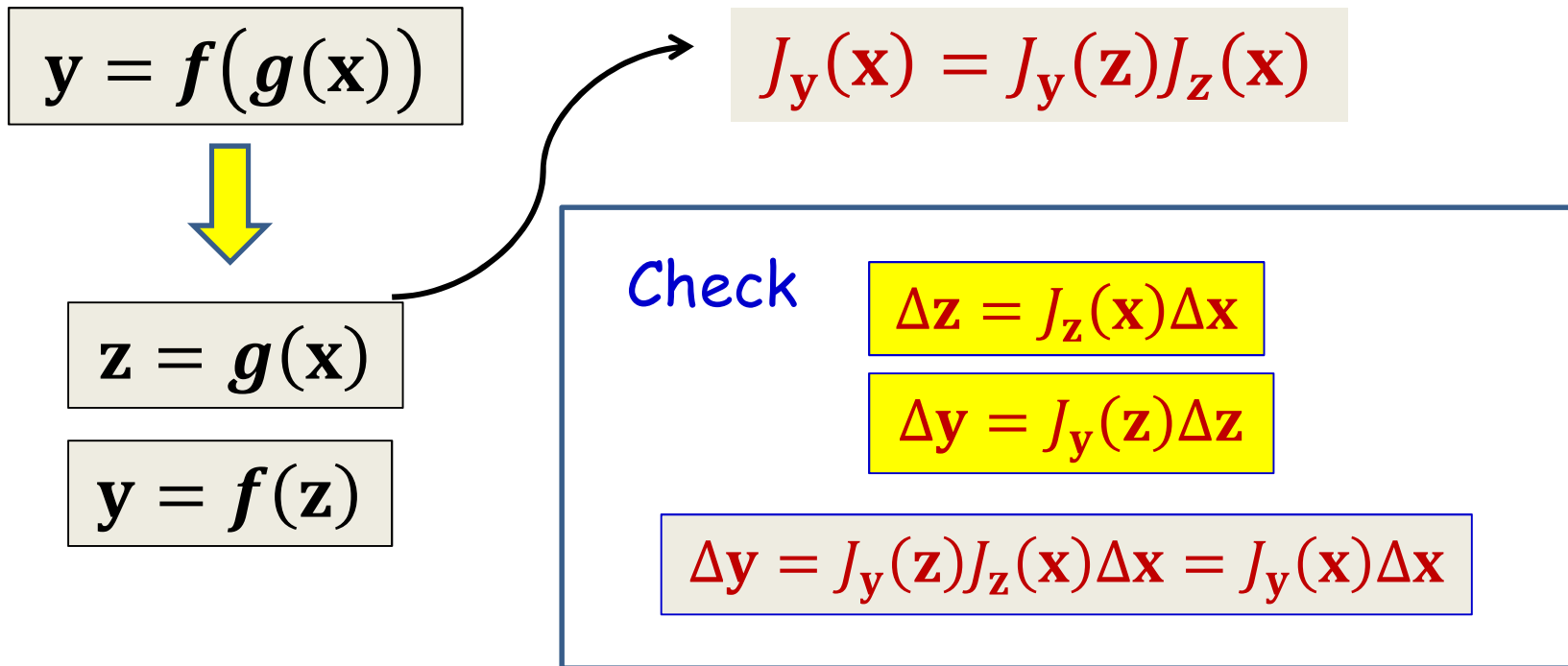


$$J_{\mathbf{z}}(\mathbf{y}) = \mathbf{W}$$

- Matrix  $\mathbf{W}$  and bias  $\mathbf{b}$  operating on vector  $\mathbf{y}$  to produce vector  $\mathbf{z}$
- The Jacobian of  $\mathbf{z}$  w.r.t  $\mathbf{y}$  is simply the matrix  $\mathbf{W}$

# Vector derivatives: Chain rule

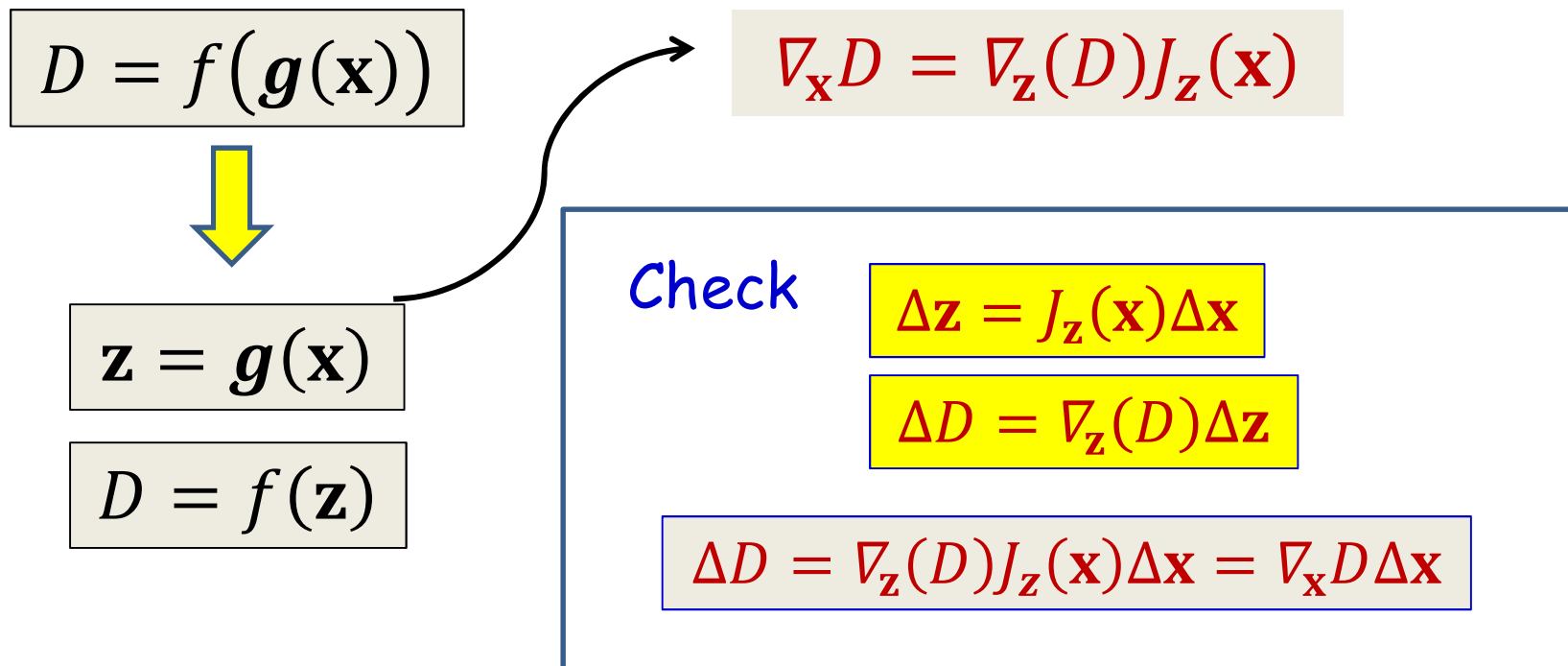
- We can define a chain rule for Jacobians
- **For vector functions of vector inputs:**



Note the order: The derivative of the outer function comes first

# Vector derivatives: Chain rule

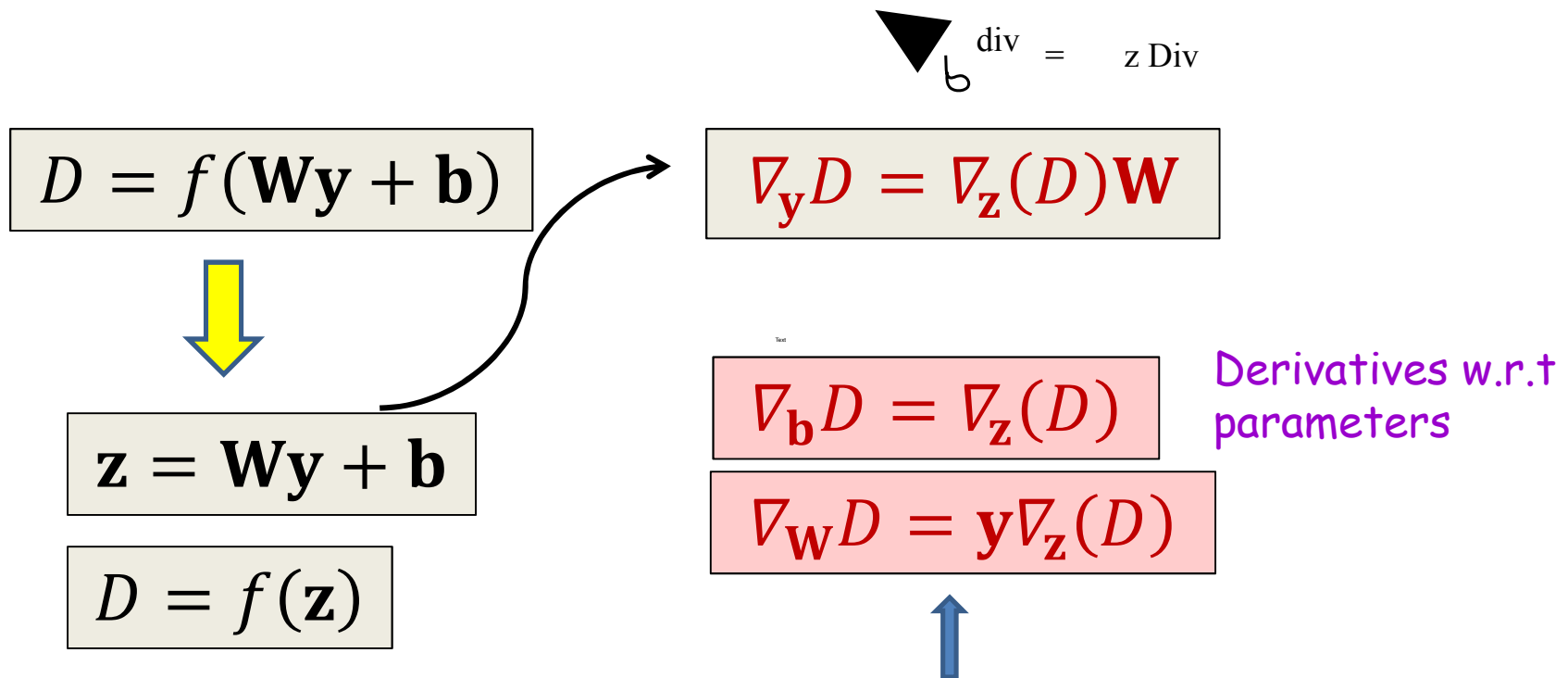
- *The chain rule can combine Jacobians and Gradients*
- **For scalar functions of vector inputs ( $g()$  is vector):**



Note the order: The derivative of the outer function comes first

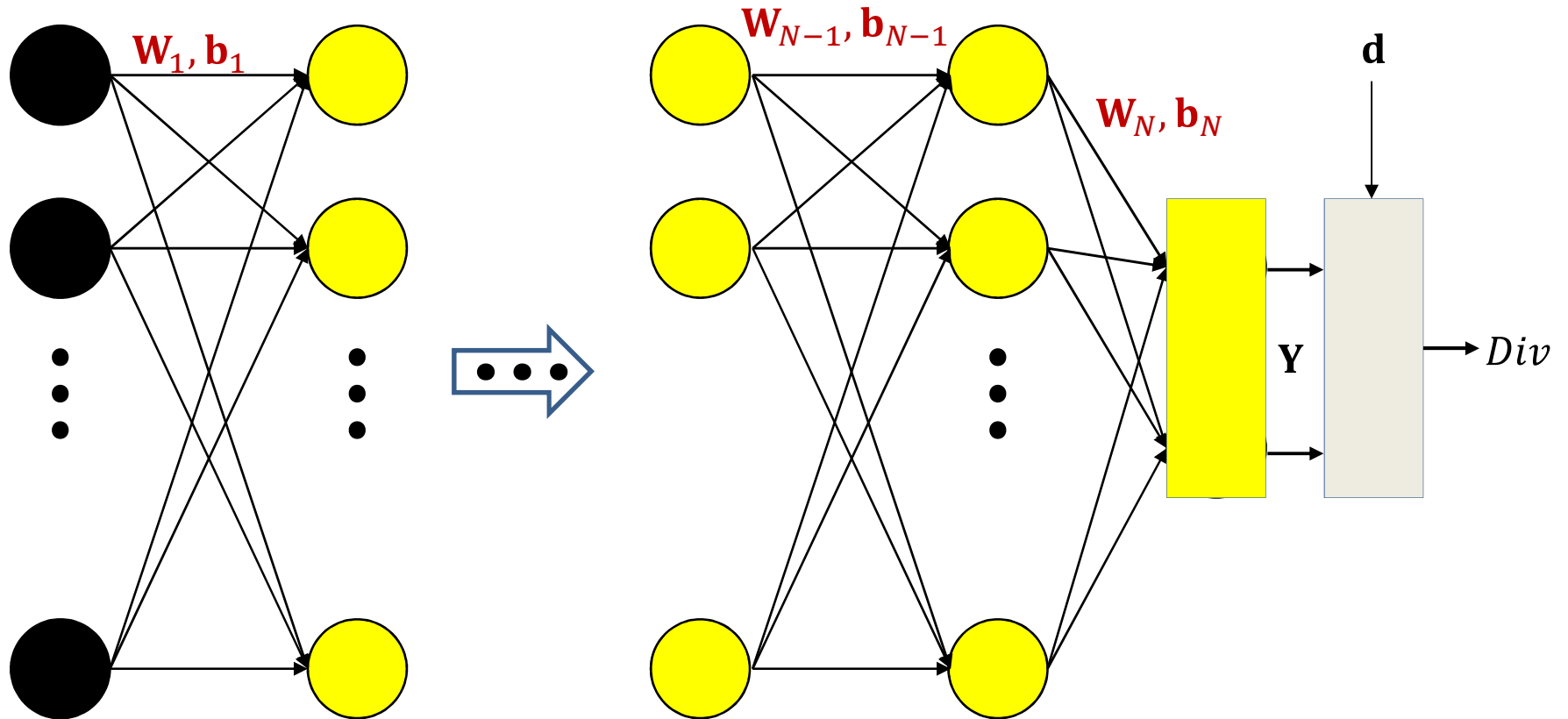
# Special Case

- Scalar functions of Affine functions



Note reversal of order. This is in fact a simplification of a product of tensor terms that occur in the *right* order

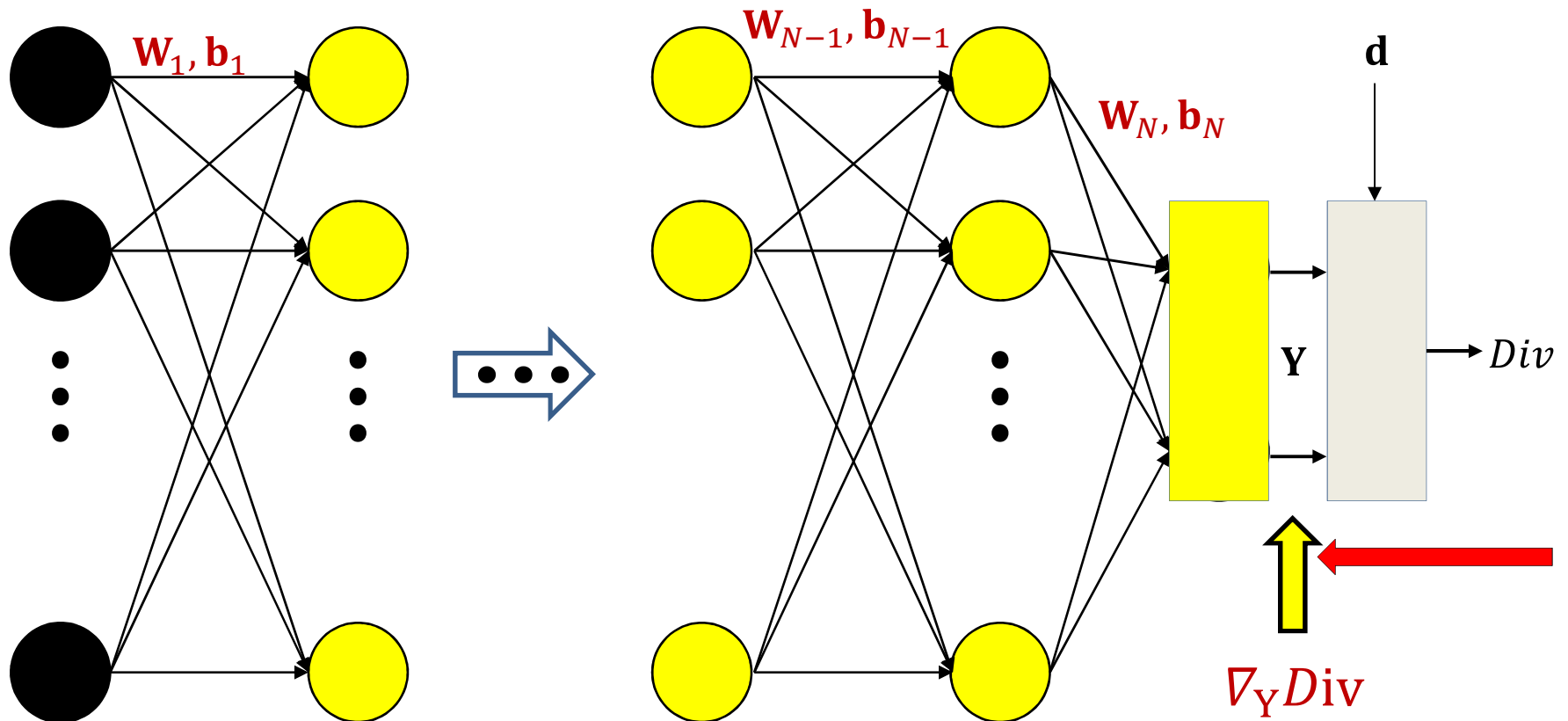
# The backward pass



In the following slides we will also be using the notation  $\nabla_{\mathbf{z}} \mathbf{Y}$  to represent the Jacobian  $J_{\mathbf{Y}}(\mathbf{z})$  to explicitly illustrate the chain rule

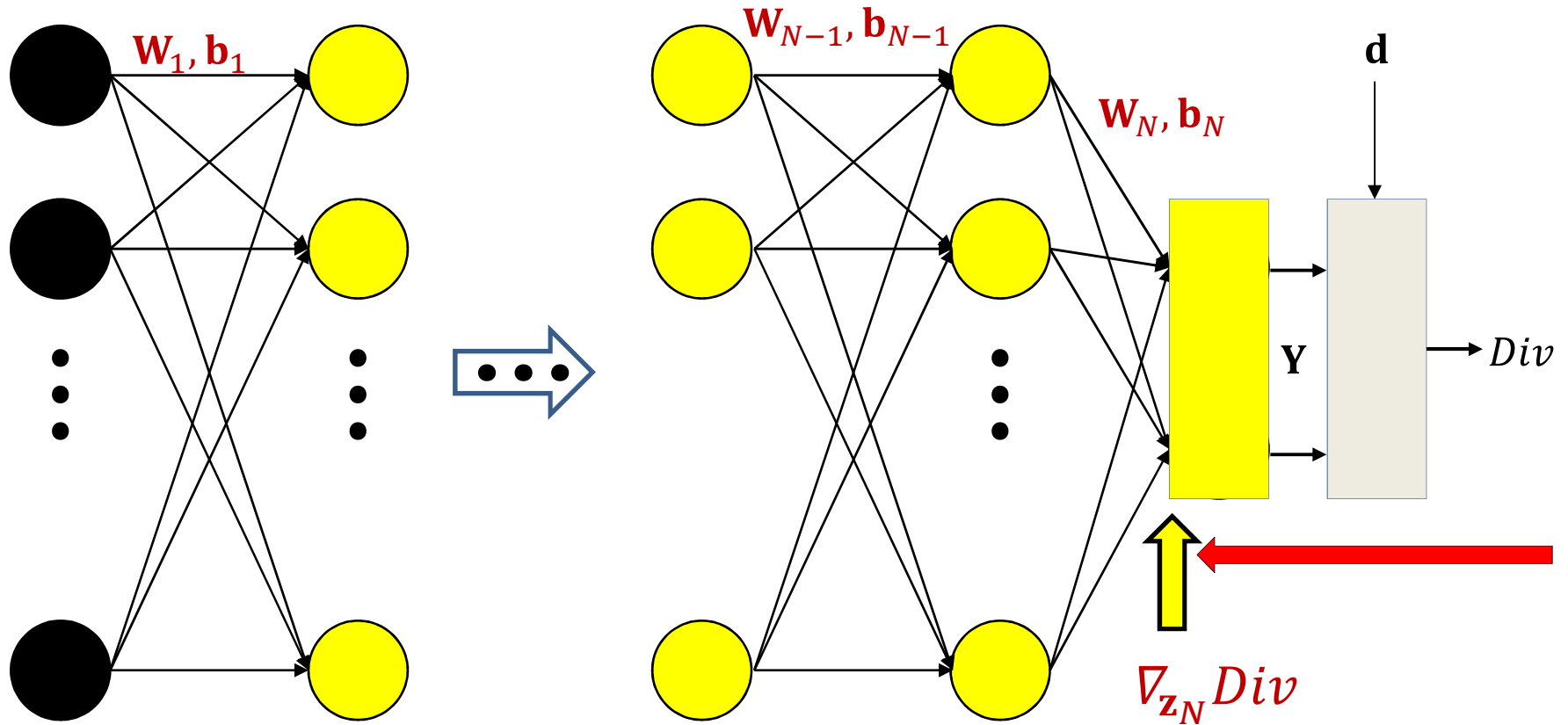
In general  $\nabla_{\mathbf{a}} \mathbf{b}$  represents a derivative of  $\mathbf{b}$  w.r.t.  $\mathbf{a}$  and could be a the transposed gradient (for scalar  $\mathbf{b}$ ) or a Jacobian (for vector  $\mathbf{b}$ )

# The backward pass



First compute the gradient of the divergence w.r.t.  $Y$ .  
The actual gradient depends on the divergence function.

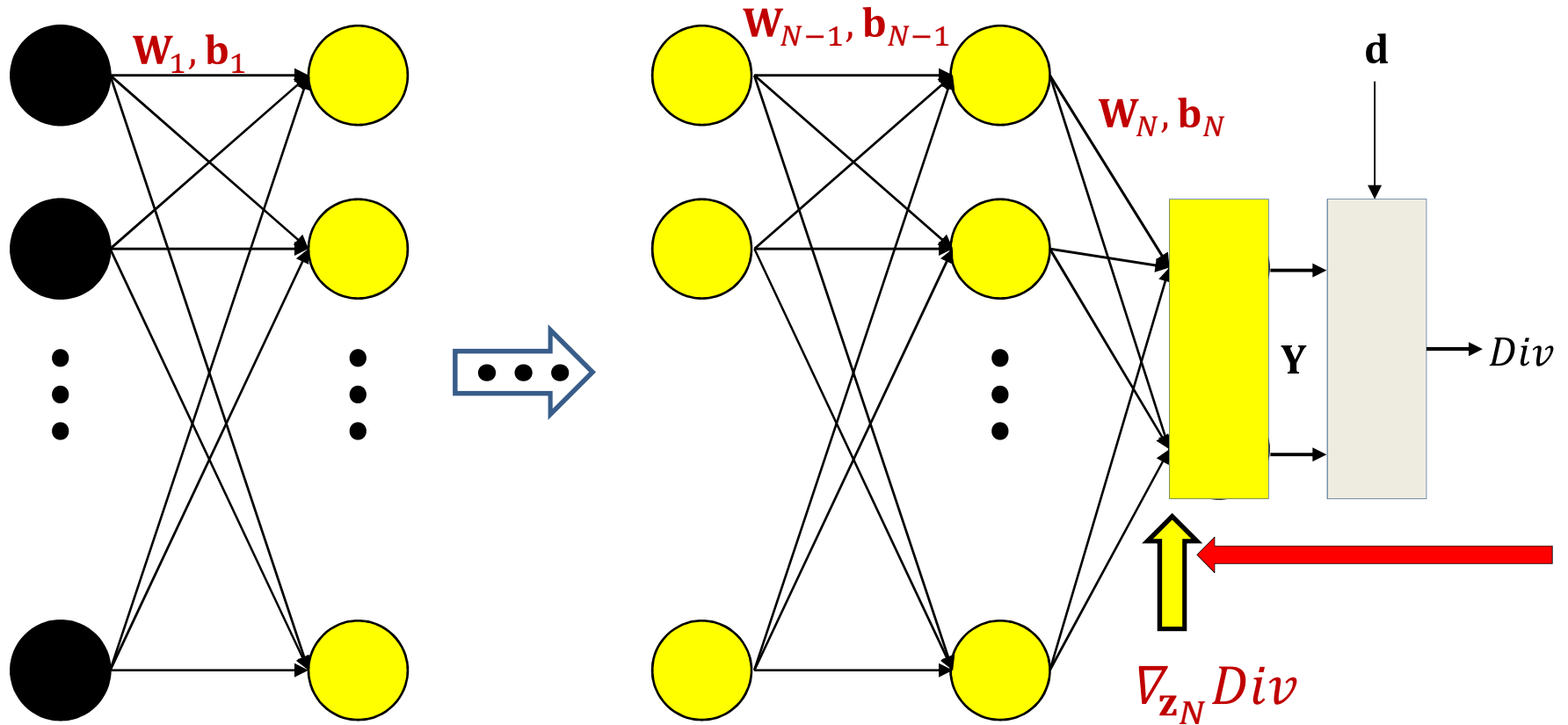
# The backward pass



$$\nabla_{z_N} Div = \nabla_Y Div \cdot \nabla_{z_N} Y$$

Already computed      New term

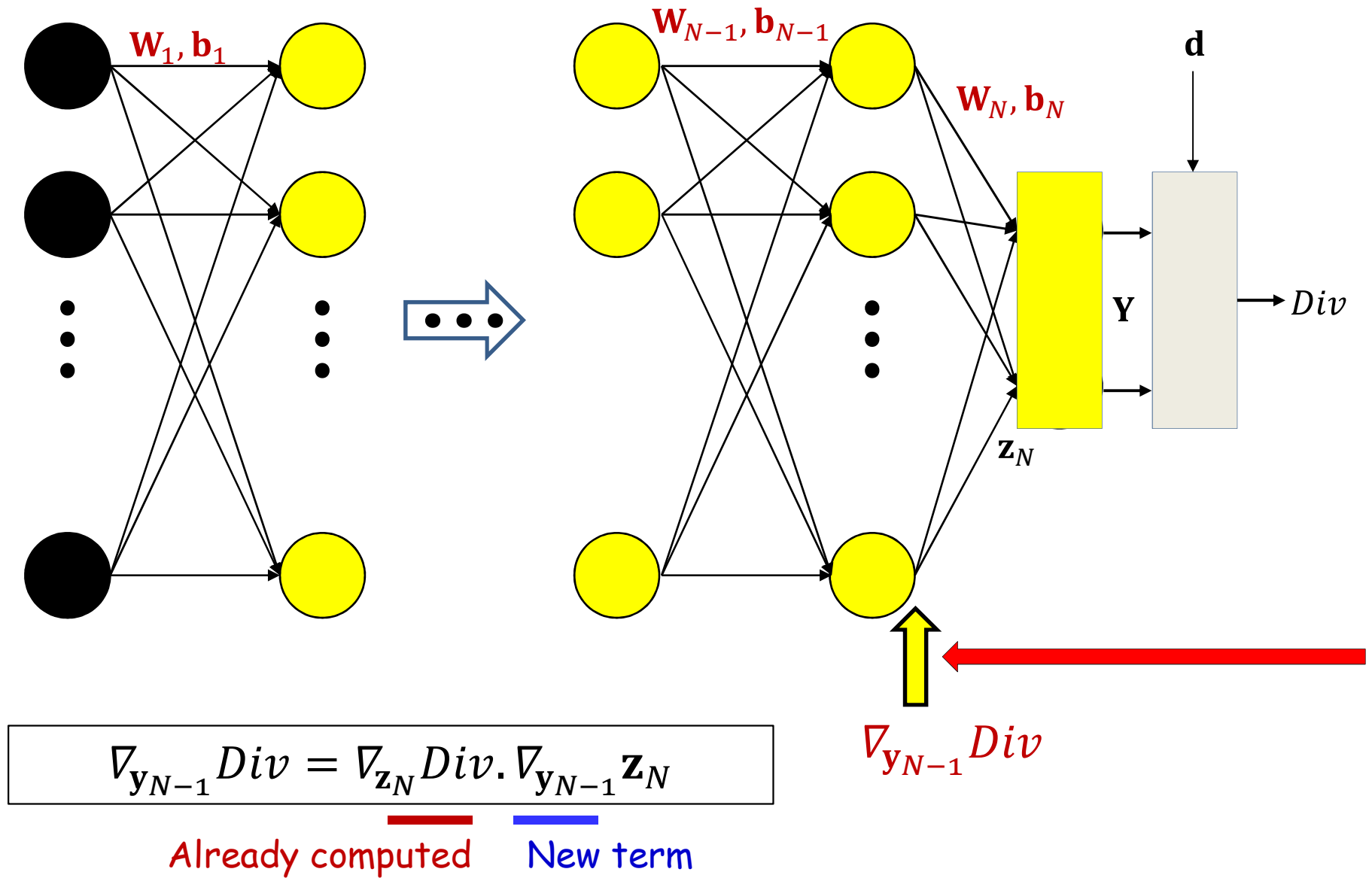
# The backward pass



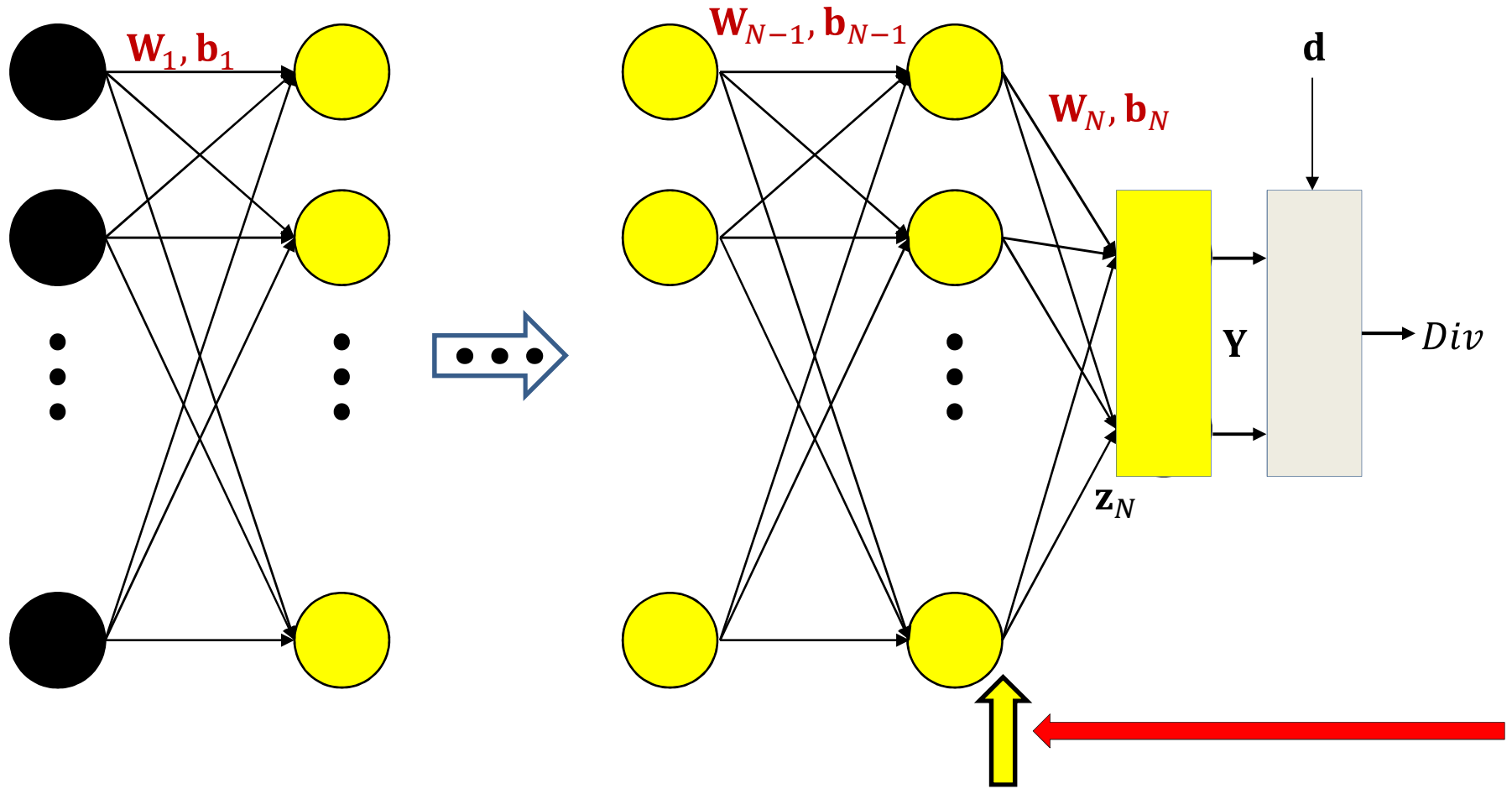
$$\nabla_{\mathbf{z}_N} Div = \underbrace{\nabla_Y Div}_{\text{Already computed}} \underbrace{J_Y(\mathbf{z}_N)}_{\text{New term}}$$



# The backward pass



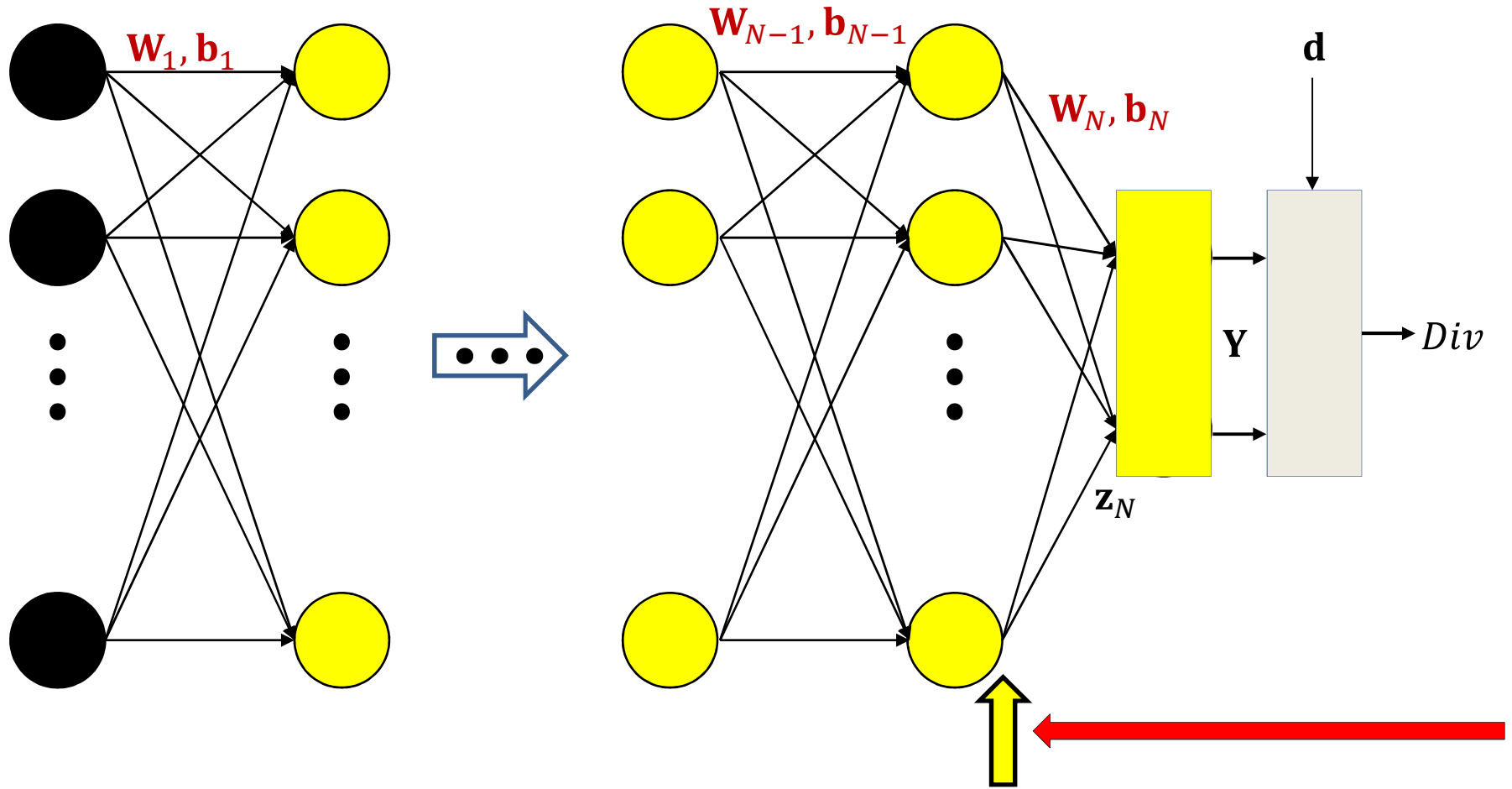
# The backward pass



$$\nabla_{y_{N-1}} Div = \underbrace{\nabla_{z_N} Div}_{\text{Already computed}} \underbrace{W_N}_{\text{New term}}$$

$$\nabla_{y_{N-1}} Div$$

# The backward pass

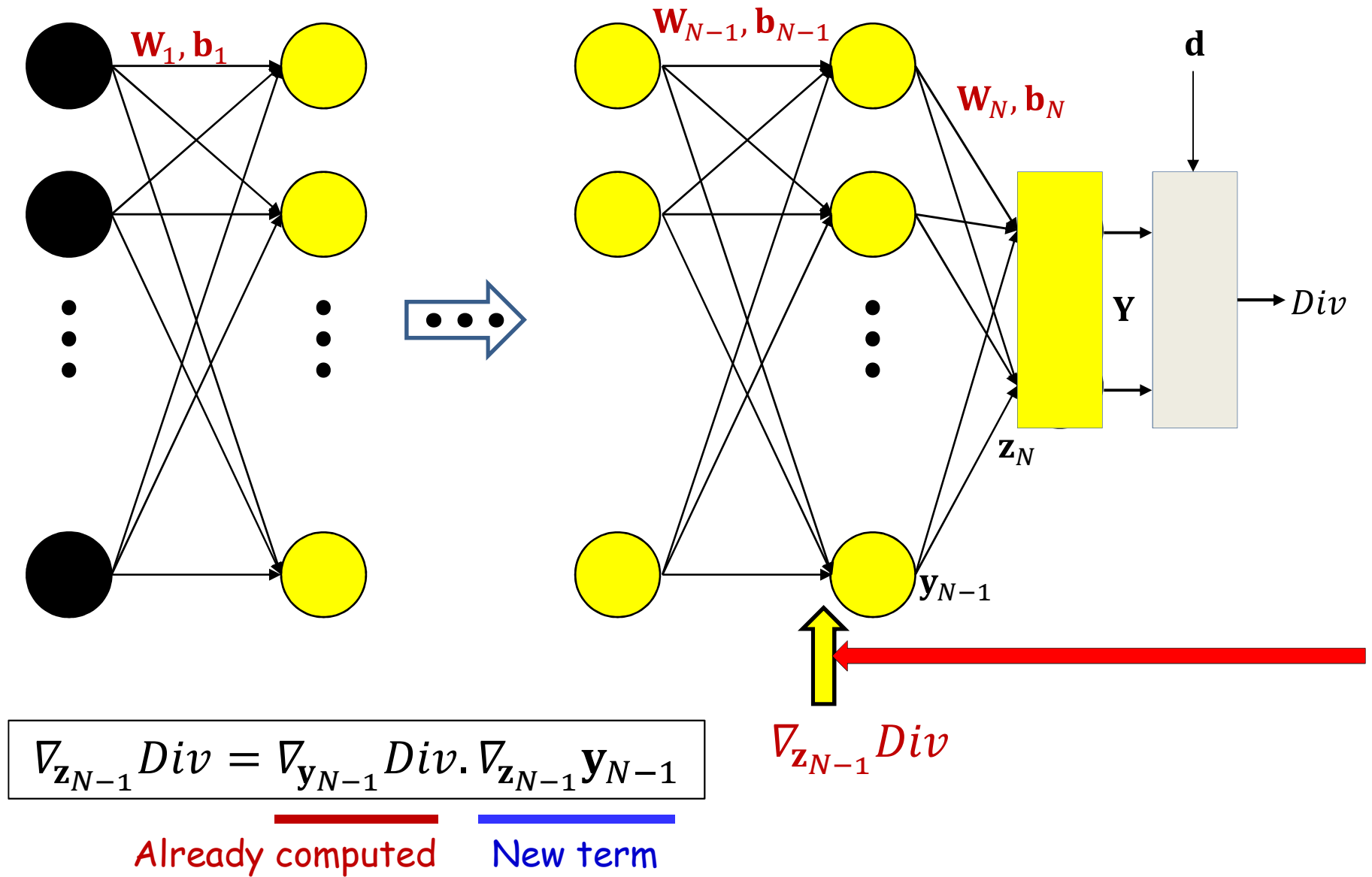


$$\nabla_{y_{N-1}} Div = \nabla_{z_N} Div W_N$$

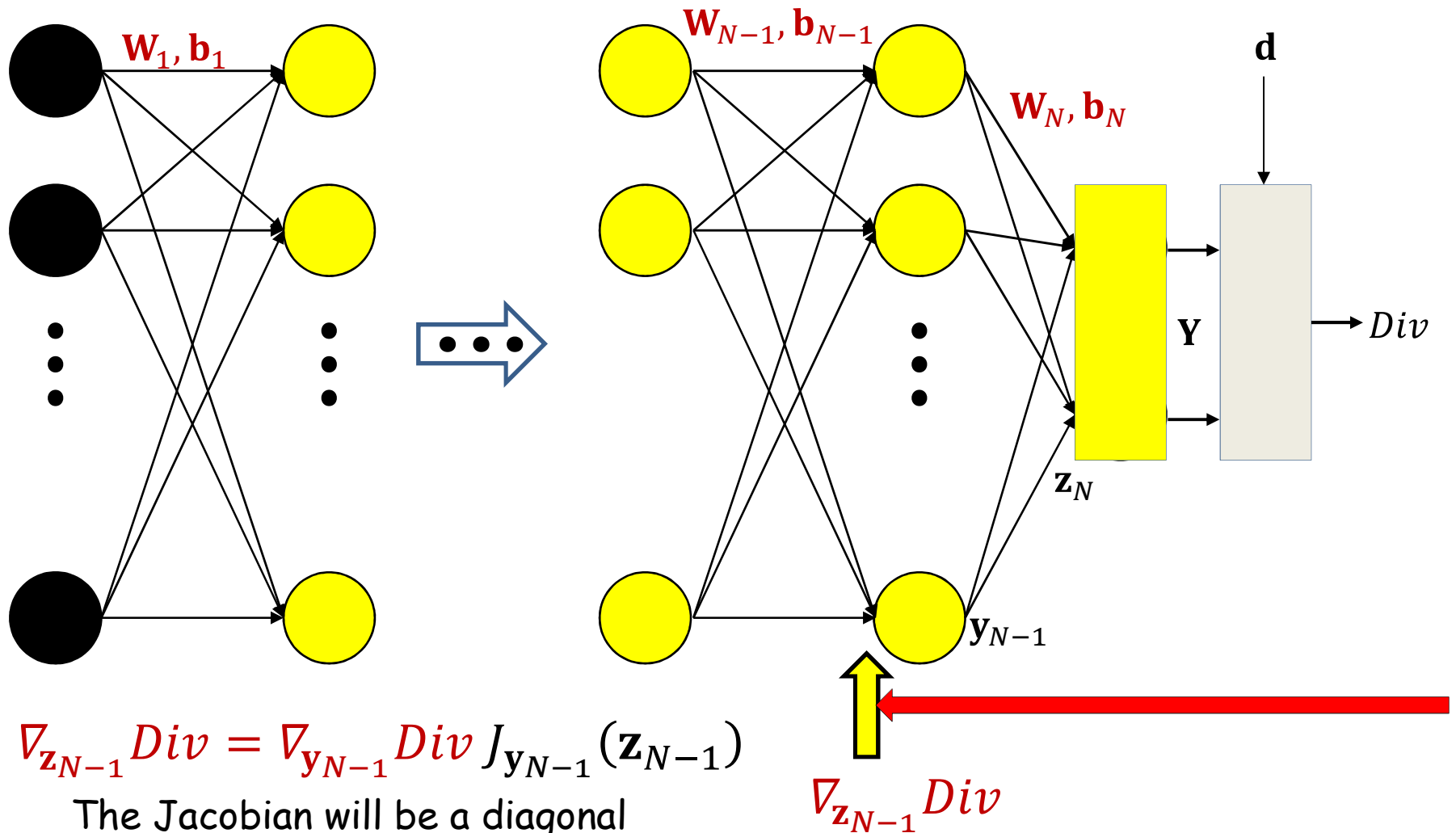
$$\nabla_{W_N} Div = y_{N-1} \nabla_{z_N} Div$$

$$\nabla_{b_N} Div = \nabla_{z_N} Div$$

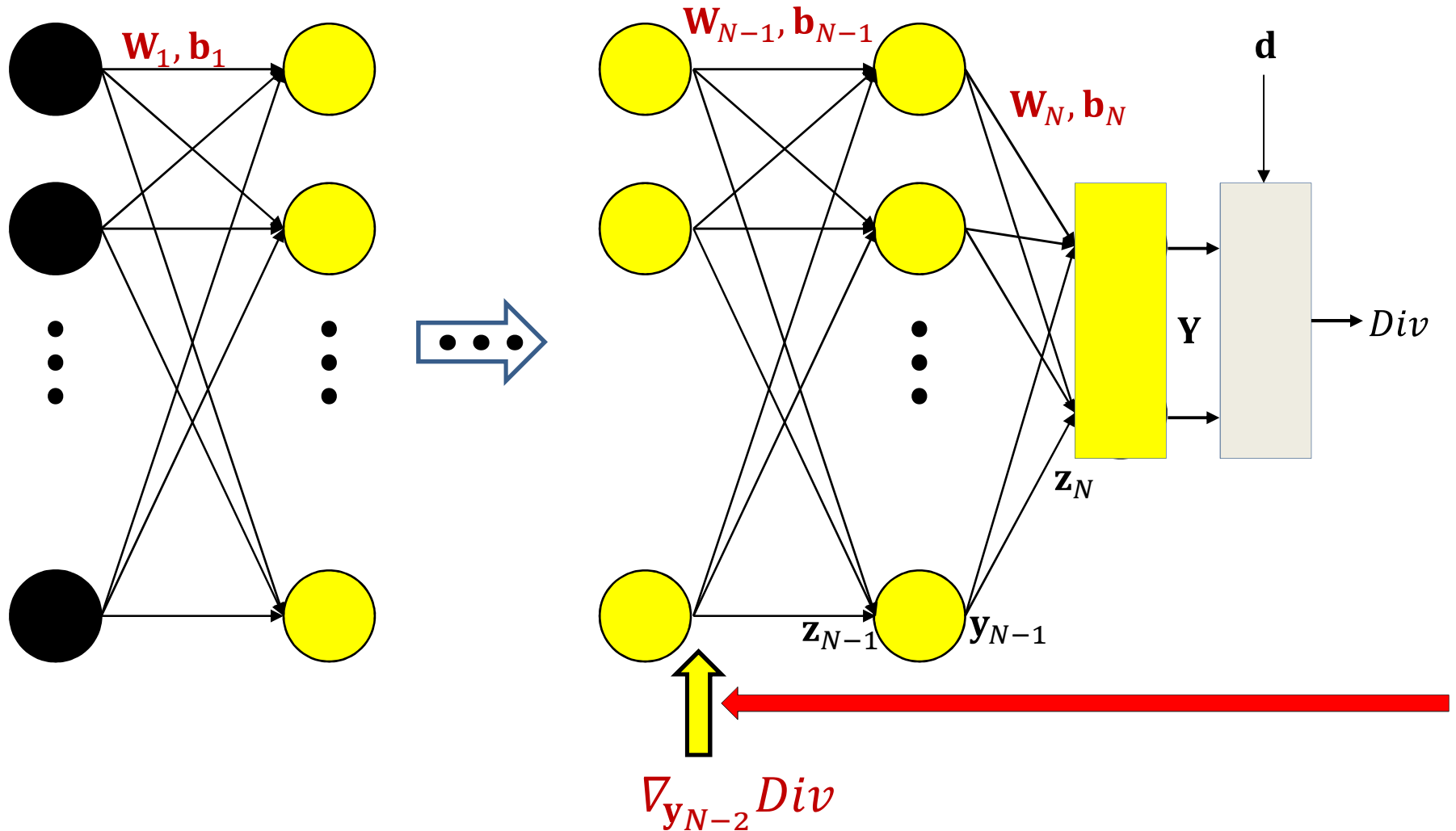
# The backward pass



# The backward pass

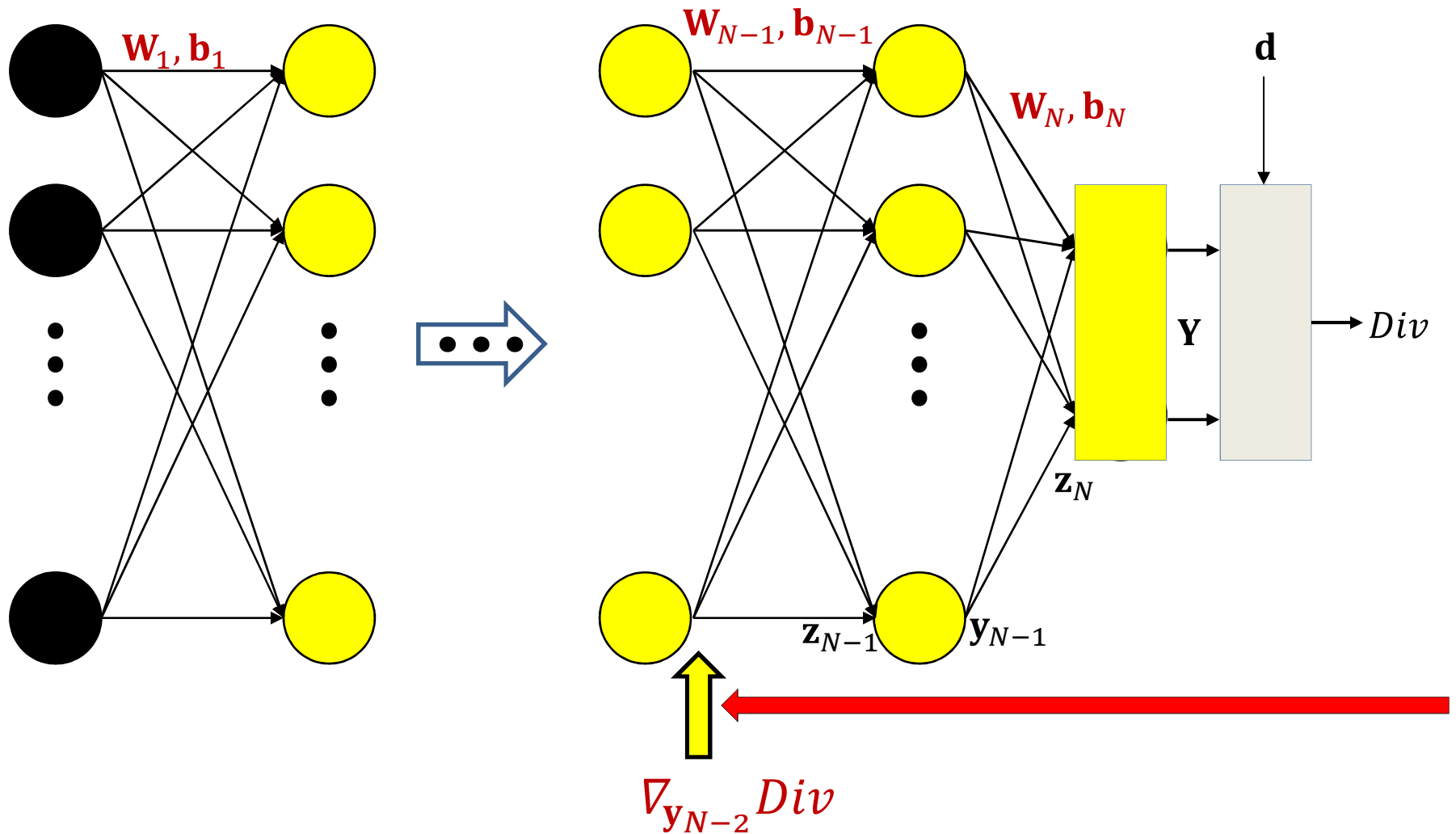


# The backward pass



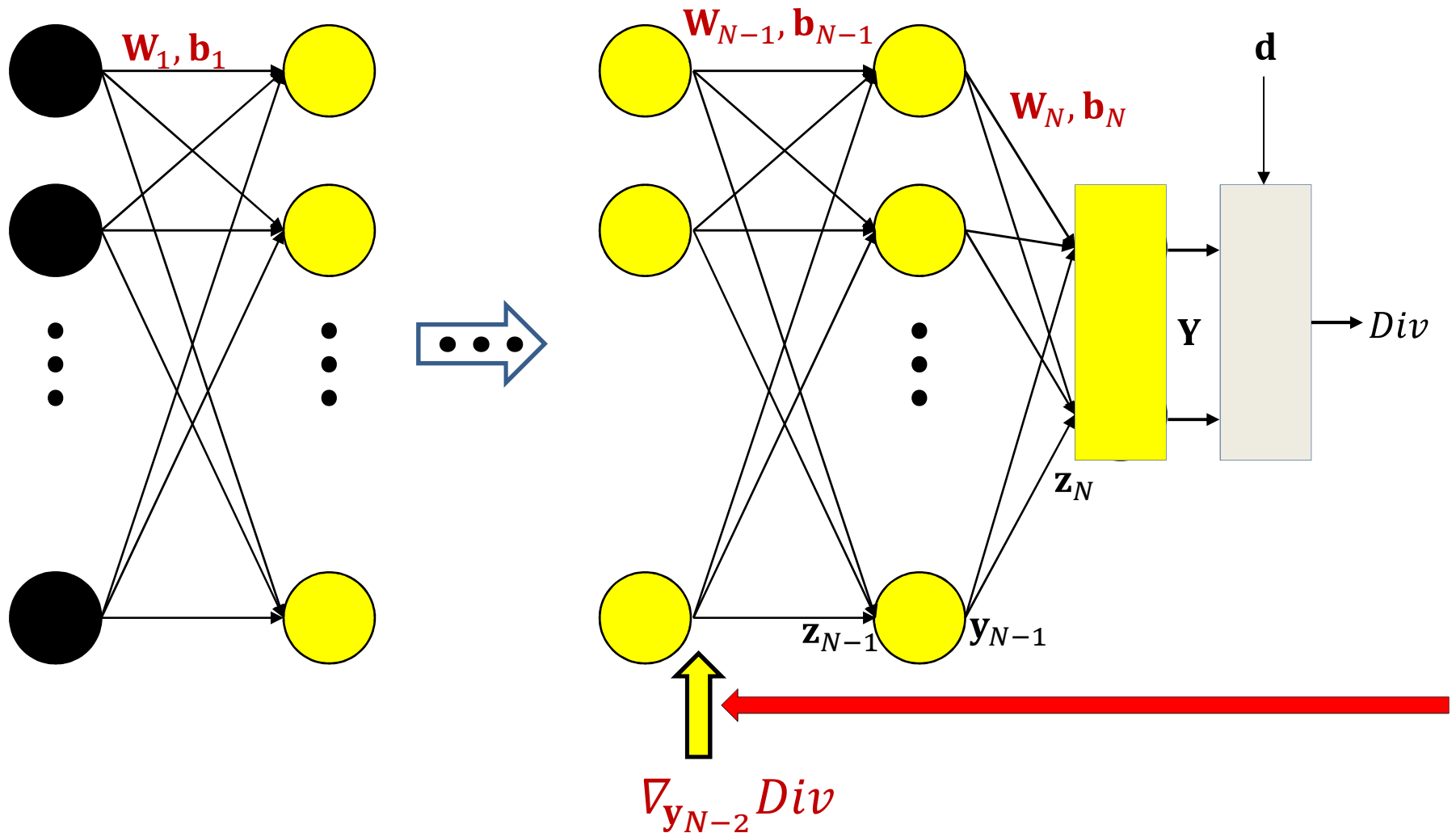
$$\nabla_{y_{N-2}} Div = \nabla_{z_{N-1}} Div \cdot \nabla_{y_{N-2}} z_{N-1}$$

# The backward pass



$$\nabla_{\mathbf{y}_{N-2}} \text{Div} = \nabla_{\mathbf{z}_{N-1}} \text{Div} \mathbf{W}_{N-1}$$

# The backward pass



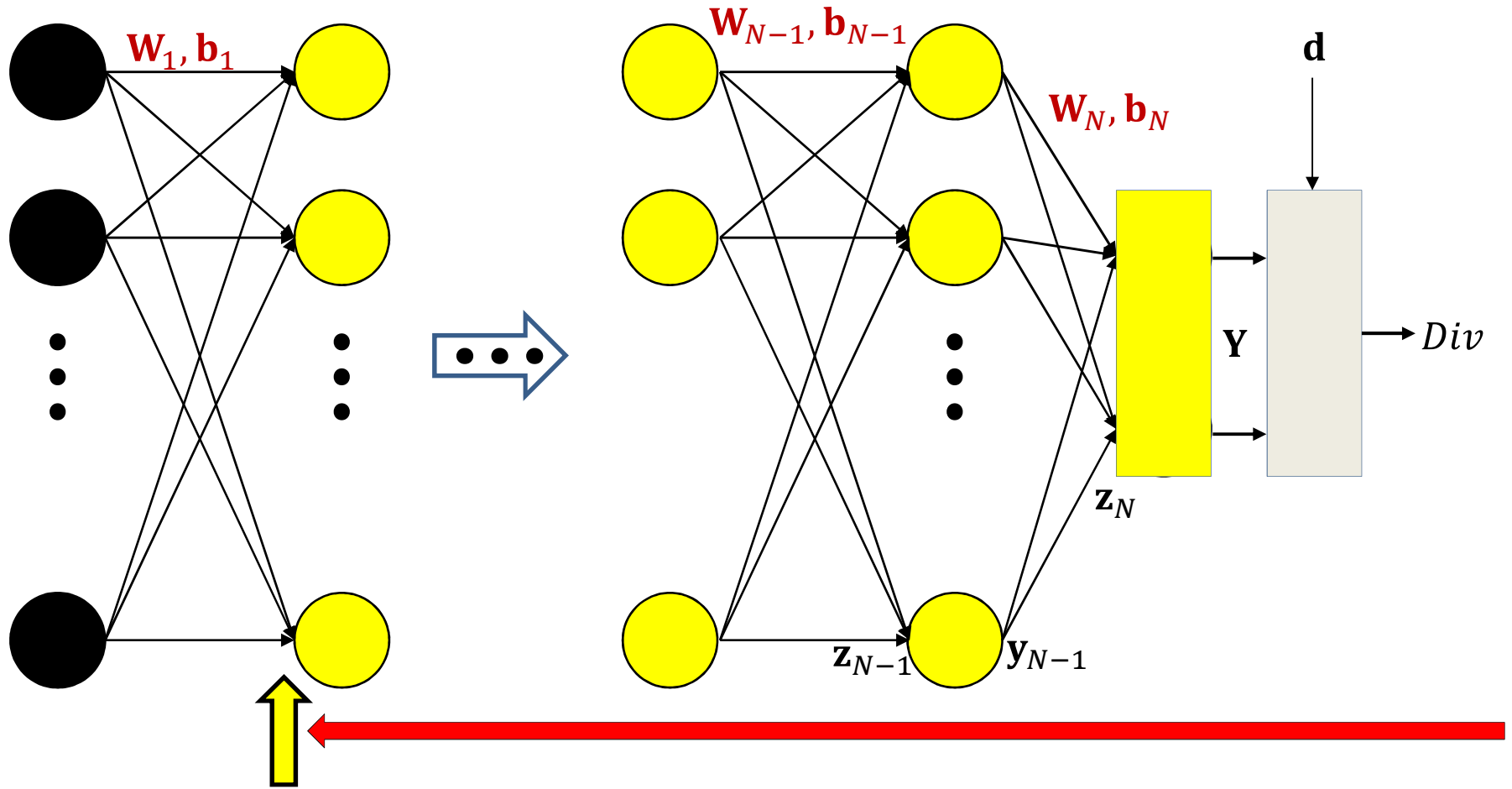
$$\nabla_{\mathbf{y}_{N-2}} Div = \nabla_{\mathbf{z}_{N-1}} Div \mathbf{W}_{N-1}$$

$$\nabla_{\mathbf{W}_{N-1}} Div = \mathbf{y}_{N-2} \nabla_{\mathbf{z}_{N-1}} Div$$

$$\nabla_{\mathbf{b}_{N-1}} Div = \nabla_{\mathbf{z}_{N-1}} Div$$

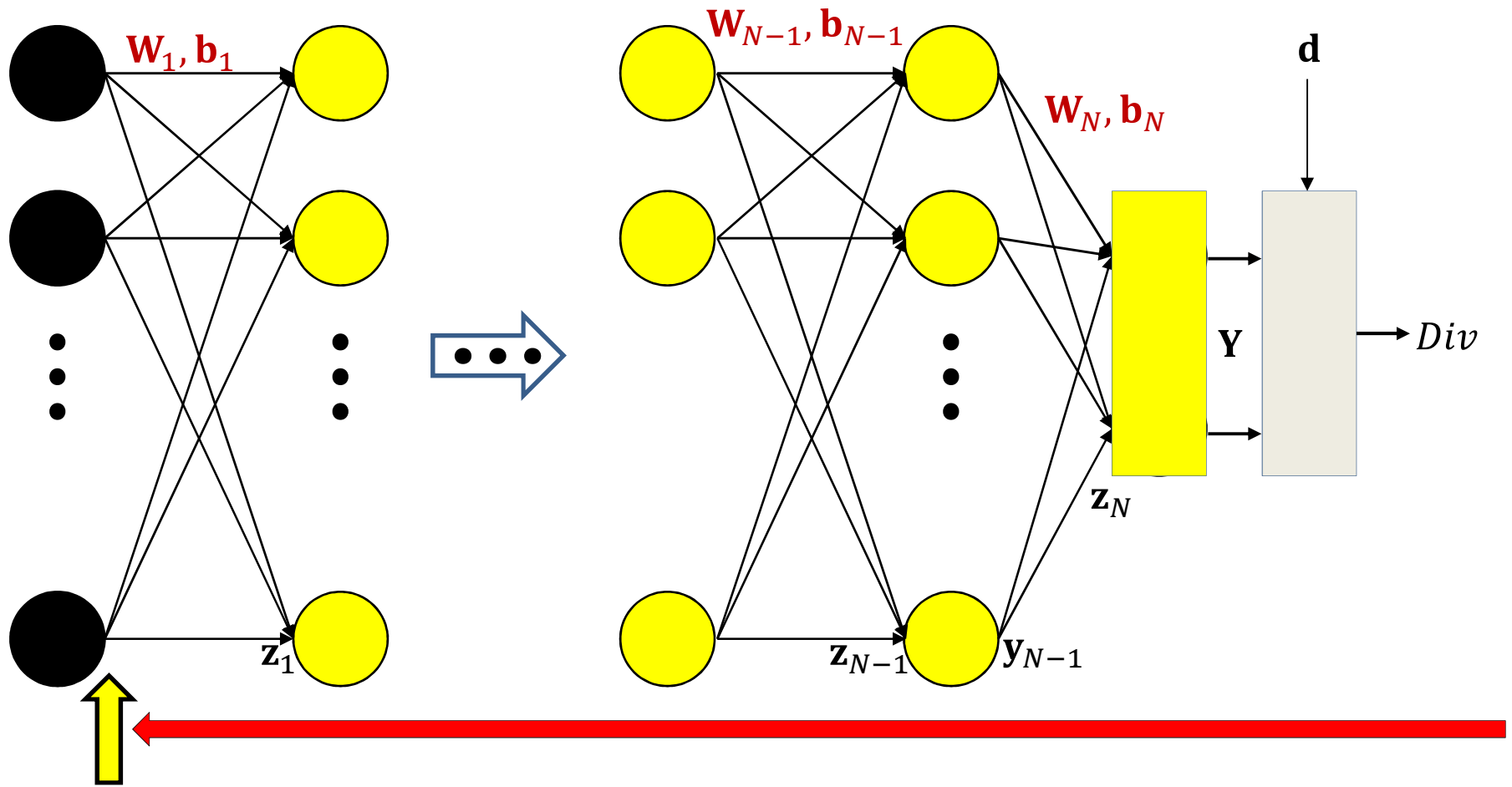


# The backward pass



$$\nabla_{z_1} Div = \nabla_{y_1} Div J_{y_1}(z_1)$$

# The backward pass



$$\nabla_{w_1} Div = x \nabla_{z_1} Div$$

$$\nabla_{b_1} Div = \nabla_{z_1} Div$$

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

# The Backward Pass

- Set  $\mathbf{y}_N = Y, \mathbf{y}_0 = \mathbf{x}$
- Initialize: Compute  $\nabla_{\mathbf{y}_N} Div = \nabla_Y Div$
- For layer  $k = N$  downto 1:
  - Compute  $J_{\mathbf{y}_k}(\mathbf{z}_k)$ 
    - Will require intermediate values computed in the forward pass
  - Backward recursion step:
$$\nabla_{\mathbf{z}_k} Div = \nabla_{\mathbf{y}_k} Div J_{\mathbf{y}_k}(\mathbf{z}_k)$$
$$\nabla_{\mathbf{y}_{k-1}} Div = \nabla_{\mathbf{z}_k} Div \mathbf{W}_k$$
  - Gradient computation:
$$\nabla_{\mathbf{W}_k} Div = \mathbf{y}_{k-1} \nabla_{\mathbf{z}_k} Div$$
$$\nabla_{\mathbf{b}_k} Div = \nabla_{\mathbf{z}_k} Div$$

# The Backward Pass

- Set  $\mathbf{y}_N = Y, \mathbf{y}_0 = \mathbf{x}$
- Initialize: Compute  $\nabla_{\mathbf{y}_N} Div = \nabla_Y Div$
- For layer  $k = N$  downto 1:
  - Compute  $J_{\mathbf{y}_k}(\mathbf{z}_k)$ 
    - Will require intermediate values computed in the forward pass
  - Backward recursion step: Note analogy to forward pass
$$\nabla_{\mathbf{z}_k} Div = \nabla_{\mathbf{y}_k} Div J_{\mathbf{y}_k}(\mathbf{z}_k)$$
$$\nabla_{\mathbf{y}_{k-1}} Div = \nabla_{\mathbf{z}_k} Div \mathbf{W}_k$$
  - Gradient computation:
$$\nabla_{\mathbf{W}_k} Div = \mathbf{y}_{k-1} \nabla_{\mathbf{z}_k} Div$$
$$\nabla_{\mathbf{b}_k} Div = \nabla_{\mathbf{z}_k} Div$$

# For comparison: The Forward Pass

- Set  $\mathbf{y}_0 = \mathbf{x}$
- For layer  $k = 1$  to  $N$  :
  - Forward recursion step:

$$\mathbf{z}_k = \mathbf{W}_k \mathbf{y}_{k-1} + \mathbf{b}_k$$

$$\mathbf{y}_k = \mathbf{f}_k(\mathbf{z}_k)$$

- Output:

$$\mathbf{Y} = \mathbf{y}_N$$

# Neural network training algorithm

- Initialize all weights and biases  $(\mathbf{W}_1, \mathbf{b}_1, \mathbf{W}_2, \mathbf{b}_2, \dots, \mathbf{W}_N, \mathbf{b}_N)$
- Do:

- $Loss = 0$

- For all  $k$ , initialize  $\nabla_{\mathbf{W}_k} Loss = 0, \nabla_{\mathbf{b}_k} Loss = 0$

- For all  $t = 1:T$  # Loop through training instances

- Forward pass : Compute

- Output  $\mathbf{Y}(\mathbf{X}_t)$

- Divergence  $Div(\mathbf{Y}_t, \mathbf{d}_t)$

- $Loss += Div(\mathbf{Y}_t, \mathbf{d}_t)$

- Backward pass: For all  $k$  compute:

- $\nabla_{\mathbf{y}_k} Div = \nabla_{\mathbf{z}_{k+1}} Div \mathbf{W}_{k+1}$

- $\nabla_{\mathbf{z}_k} Div = \nabla_{\mathbf{y}_k} Div J_{\mathbf{y}_k}(\mathbf{z}_k)$

- $\nabla_{\mathbf{W}_k} Div(\mathbf{Y}_t, \mathbf{d}_t) = \mathbf{y}_{k-1} \nabla_{\mathbf{z}_k} Div; \nabla_{\mathbf{b}_k} Div(\mathbf{Y}_t, \mathbf{d}_t) = \nabla_{\mathbf{z}_k} Div$

- $\nabla_{\mathbf{W}_k} Loss += \nabla_{\mathbf{W}_k} Div(\mathbf{Y}_t, \mathbf{d}_t); \nabla_{\mathbf{b}_k} Loss += \nabla_{\mathbf{b}_k} Div(\mathbf{Y}_t, \mathbf{d}_t)$

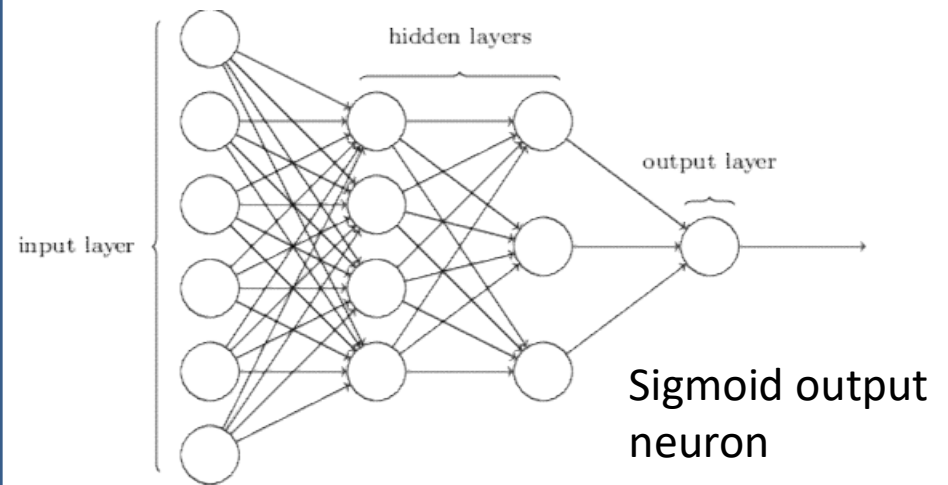
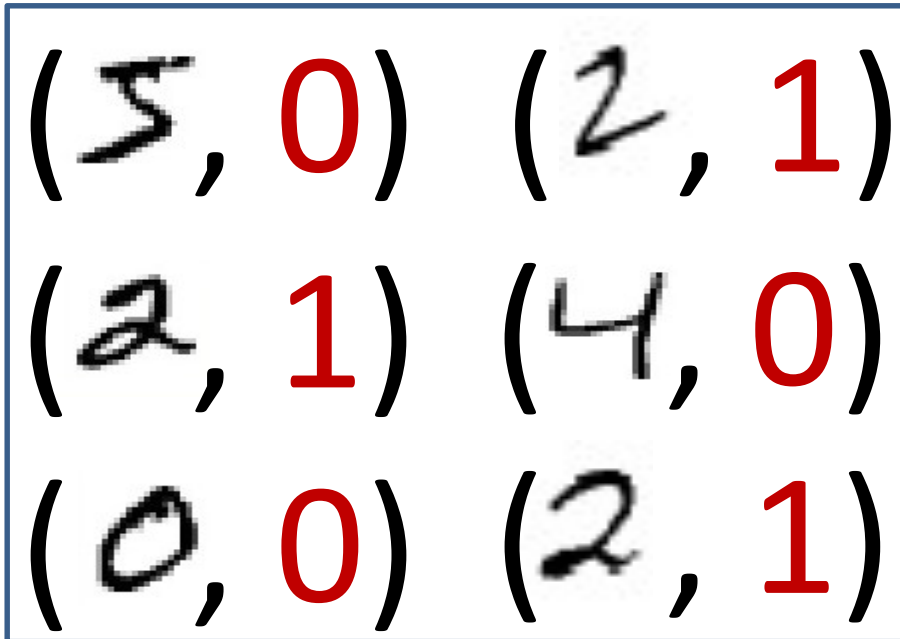
- For all  $k$ , update:

$$\mathbf{W}_k = \mathbf{W}_k - \frac{\eta}{T} (\nabla_{\mathbf{W}_k} Loss)^T; \quad \mathbf{b}_k = \mathbf{b}_k - \frac{\eta}{T} (\nabla_{\mathbf{b}_k} Loss)^T$$

- Until  $Loss$  has converged

# Setting up for digit recognition

Training data

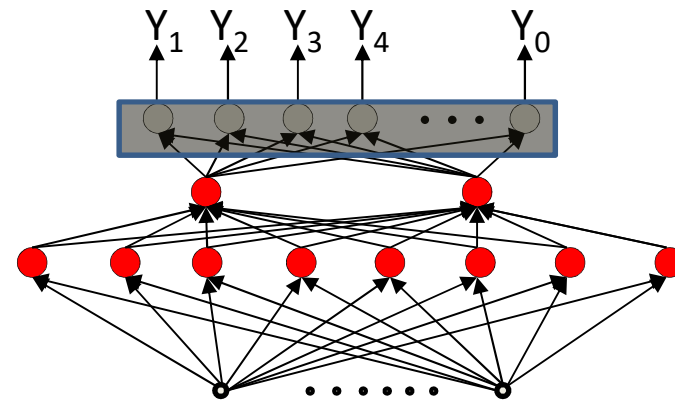


- Simple Problem: Recognizing “2” or “not 2”
- Single output with sigmoid activation
  - $Y \in (0,1)$
  - $d$  is either 0 or 1
- Use KL divergence
- Backpropagation to learn network parameters

# Recognizing the digit

Training data

(5, 5)	(2, 2)
(2, 2)	(4, 4)
(0, 0)	(2, 2)



- More complex problem: Recognizing digit
- Network with 10 (or 11) outputs
  - First ten outputs correspond to the ten digits
    - Optional 11th is for none of the above
- Softmax output layer:
  - Ideal output: One of the outputs goes to 1, the others go to 0
- Backpropagation with KL divergence to learn network



# Issues

- Convergence: How well does it learn
  - And how can we improve it
- How well will it generalize (outside training data)
- What does the output really mean?
- *Etc..*