

# Unconstrained Minimization of function (Example)

- Minimize

$$f(x_1, x_2, x_3) = (x_1)^2 + x_1(1 - x_2) + (x_2)^2 - x_2x_3 + (x_3)^2 + x_3$$

- Gradient

$$\nabla_X f^T = \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix}$$

# Unconstrained Minimization of function (Example)

- Set the gradient to null

$$\nabla_X f = 0 \Rightarrow \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

- Solving the 3 equations system with 3 unknowns

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$$

# Unconstrained Minimization of function (Example)

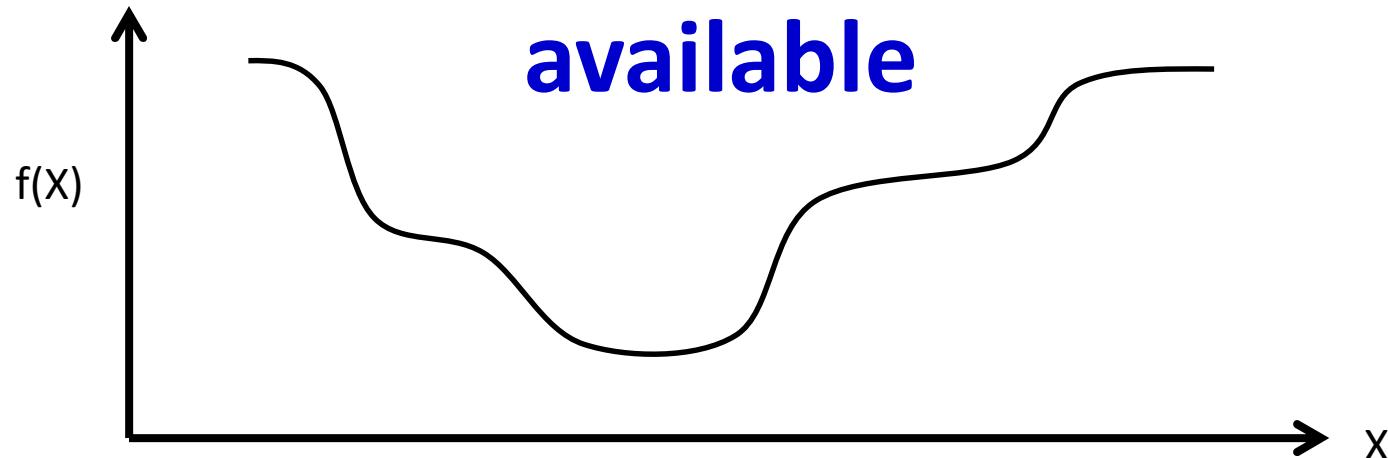
- Compute the Hessian matrix  $\nabla_X^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
- Evaluate the eigenvalues of the Hessian matrix

$$\lambda_1 = 3.414, \lambda_2 = 0.586, \lambda_3 = 2$$

- All the eigenvalues are positives  $\Rightarrow$  the Hessian matrix is positive definite

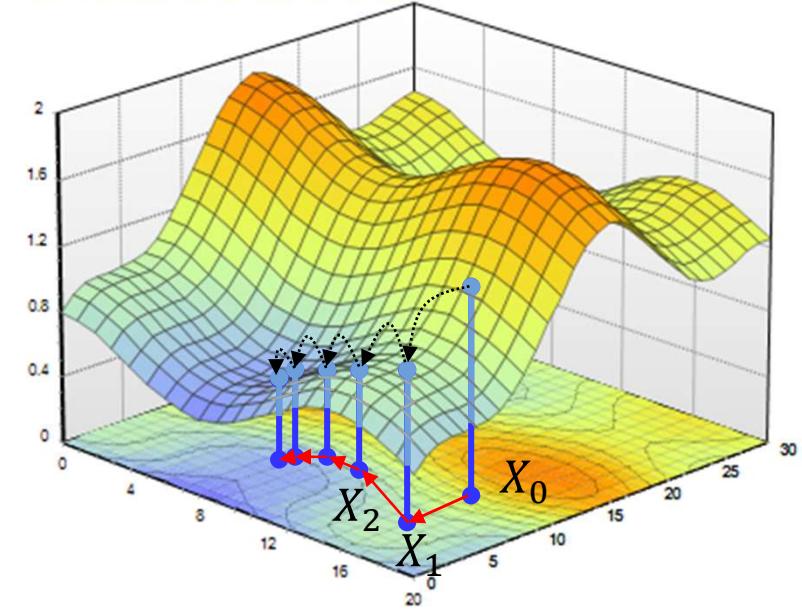
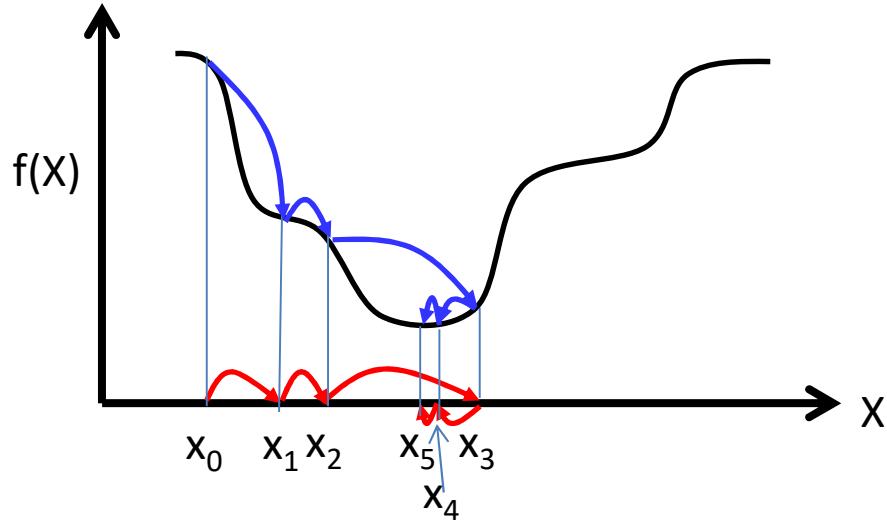
- The point  $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$  is a minimum

# Closed Form Solutions are not always available



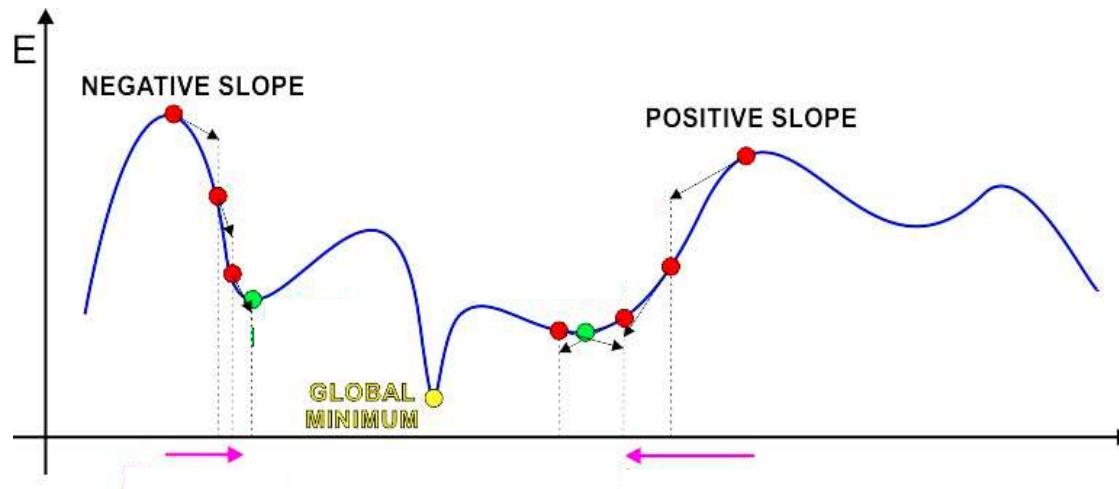
- Often it is not possible to simply solve  $\nabla_X f(X) = 0$ 
  - The function to minimize/maximize may have an intractable form
- In these situations, iterative solutions are used
  - Begin with a “guess” for the optimal  $X$  and refine it iteratively until the correct value is obtained

# Iterative solutions



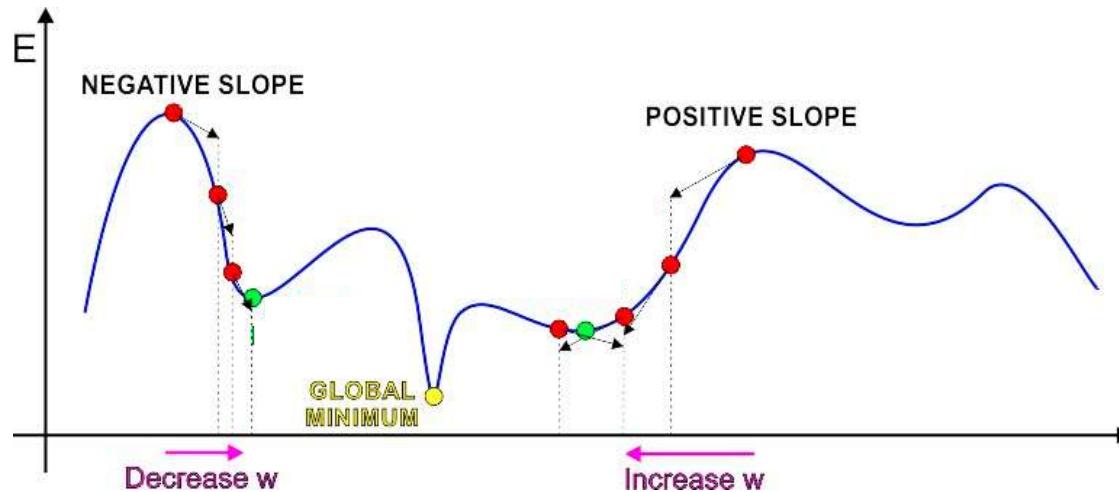
- Iterative solutions
  - Start from an initial guess  $X_0$  for the optimal  $X$
  - Update the guess towards a (hopefully) “better” value of  $f(X)$
  - Stop when  $f(X)$  no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

# The Approach of Gradient Descent



- Iterative solution:
  - Start at some point
  - Find direction in which to shift this point to decrease error
    - This can be found from the derivative of the function
      - A negative derivative → moving right decreases error
      - A positive derivative → moving left decreases error
  - Shift point in this direction

# The Approach of Gradient Descent



- Iterative solution: Trivial algorithm
  - Initialize  $x^0$
  - While  $f'(x^k) \neq 0$ 
$$x^{k+1} = x^k - \eta^k f'(x^k)$$
- $\eta^k$  is the “step size”

# Gradient descent/ascent (multivariate)

- The gradient descent/ascent method to find the minimum or maximum of a function  $f$  iteratively

- To find a *maximum* move *in the direction of the gradient*

$$x^{k+1} = x^k + \eta^k \nabla_x f(x^k)^T$$

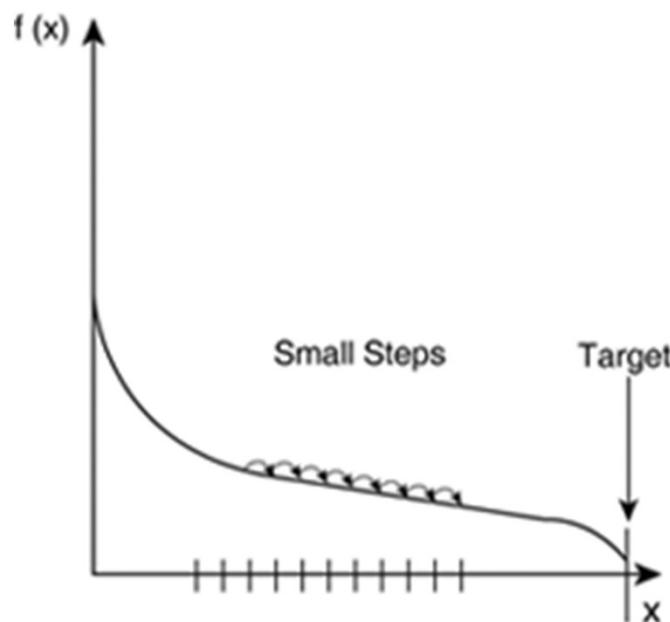
- To find a *minimum* move *exactly opposite the direction of the gradient*

$$x^{k+1} = x^k - \eta^k \nabla_x f(x^k)^T$$

- Many solutions to choosing step size  $\eta^k$

# 1. Fixed step size

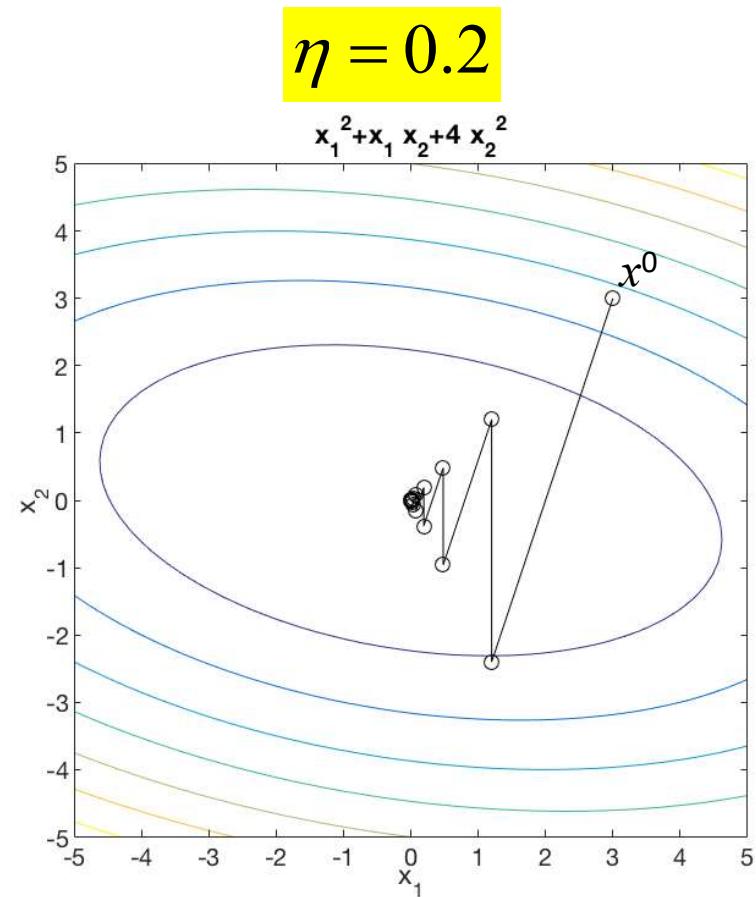
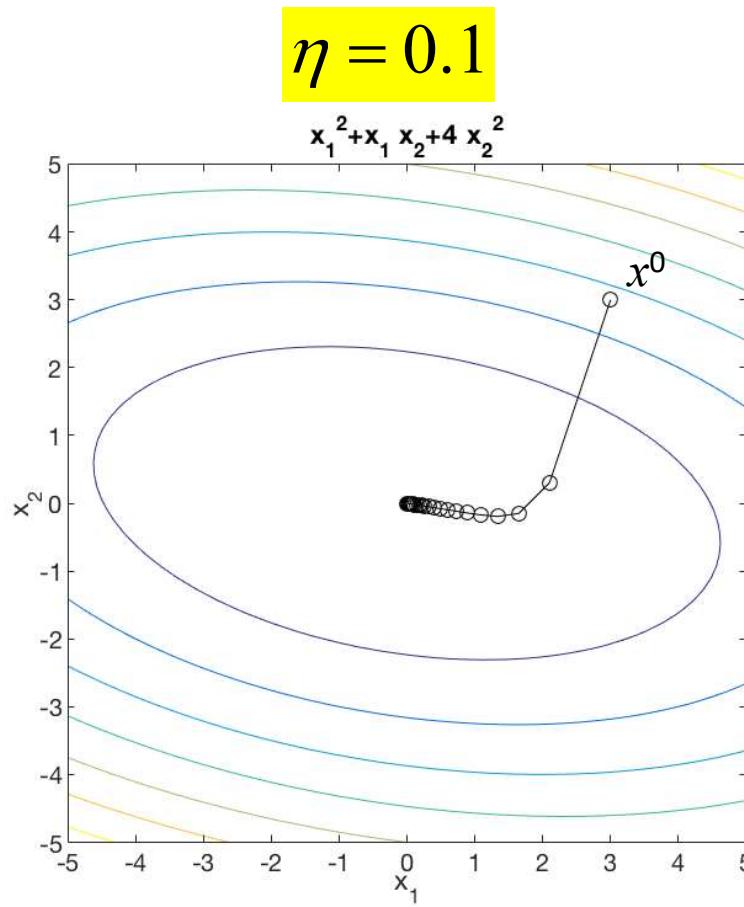
- Fixed step size
  - Use fixed value for  $\eta^k$



# Influence of step size example (constant step size)

$$f(x_1, x_2) = (x_1)^2 + x_1 x_2 + 4(x_2)^2$$

$$x^{initial} = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$



# What is the optimal step size?

- Step size is critical for fast optimization
- Will revisit this topic later
- For now, simply assume a potentially-iteration-dependent step size

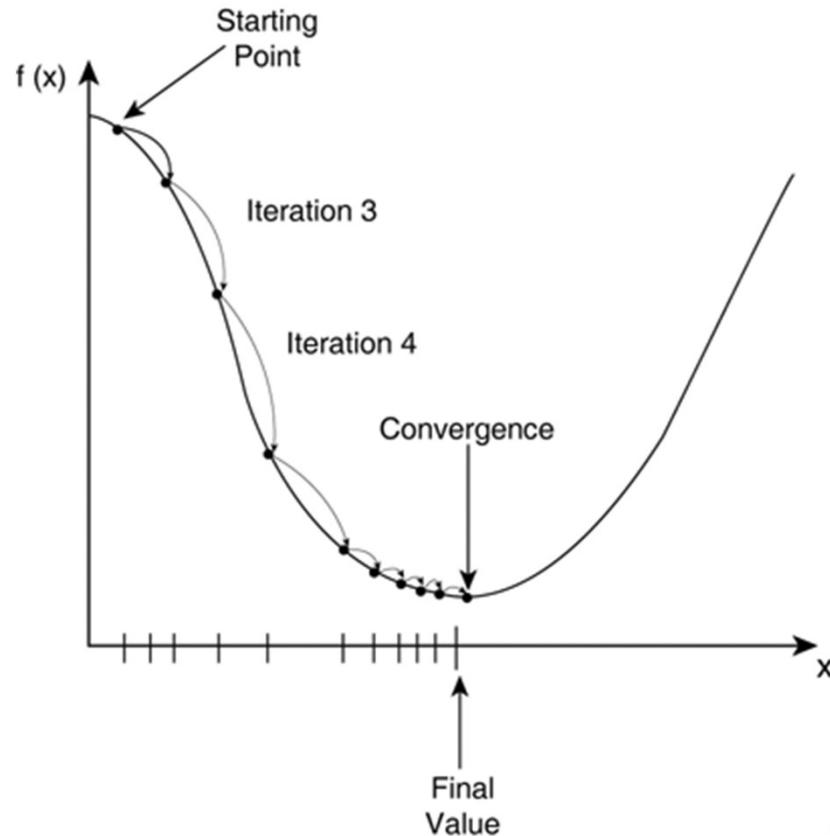
# Gradient descent convergence criteria

- The gradient descent algorithm converges when one of the following criteria is satisfied

$$|f(x^{k+1}) - f(x^k)| < \varepsilon_1$$

- Or

$$\|\nabla_x f(x^k)\| < \varepsilon_2$$



# Overall Gradient Descent Algorithm

- Initialize:
  - $x^0$
  - $k = 0$
- do
  - $x^{k+1} = x^k - \eta^k \nabla_x f(x^k)^T$
  - $k = k + 1$
- while  $|f(x^{k+1}) - f(x^k)| > \varepsilon$

# Problem Statement

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- Minimize the following function

$$Err(W) = \frac{1}{T} \sum_i \text{div}(f(X_i; W), d_i)$$

w.r.t  $W$

- This is problem of function minimization
  - An instance of optimization

# Problem Setup: Things to define

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- What are these input-output pairs?

$$Err(W) = \frac{1}{T} \sum_i div(f(X_i; W), d_i)$$

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What is  $f()$  and  
what are its  
parameters  $W$ ?

# Problem Setup: Things to define

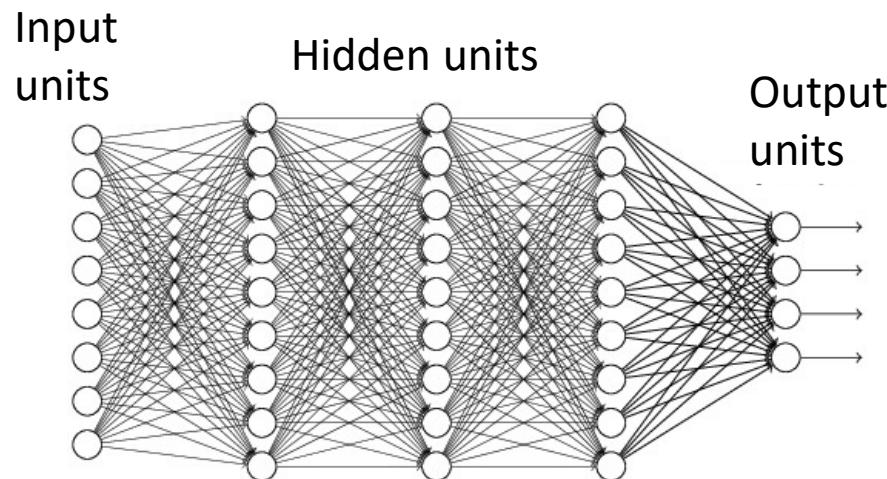
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What is the divergence  $\text{div}()$ ?

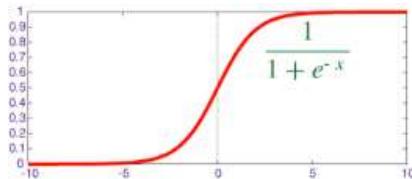
What is  $f()$  and what are its parameters  $W$ ?

# What is $f()$ ? Typical network



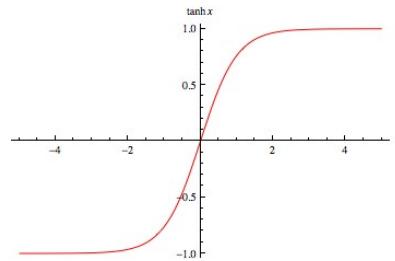
- Multi-layer perceptron
- A *directed* network with a set of inputs and outputs
  - No loops
- Generic terminology
  - We will refer to the inputs as the *input units*
    - **No neurons here – the “input units” are just the inputs**
  - We refer to the outputs as the output units
  - Intermediate units are “hidden” units

# Activations and their derivatives



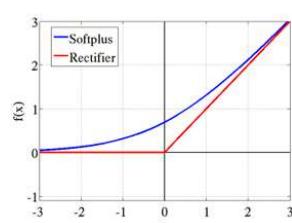
$$f(z) = \frac{1}{1 + \exp(-z)}$$

$$f'(z) = f(z)(1 - f(z))$$



$$f(z) = \tanh(z)$$

$$f'(z) = (1 - f^2(z))$$



$$f(z) = \begin{cases} 0, & z < 0 \\ z, & z \geq 0 \end{cases}$$

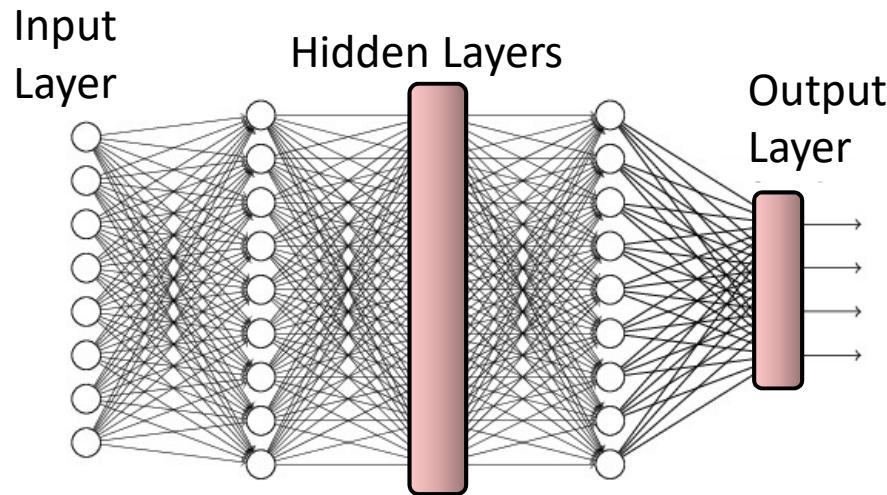
[\*]  $f'(z) = \begin{cases} 1, & z \geq 0 \\ 0, & z < 0 \end{cases}$

$$f(z) = \log(1 + \exp(z))$$

$$f'(z) = \frac{1}{1 + \exp(-z)}$$

- Some popular activation functions and their derivatives

# Vector Activations

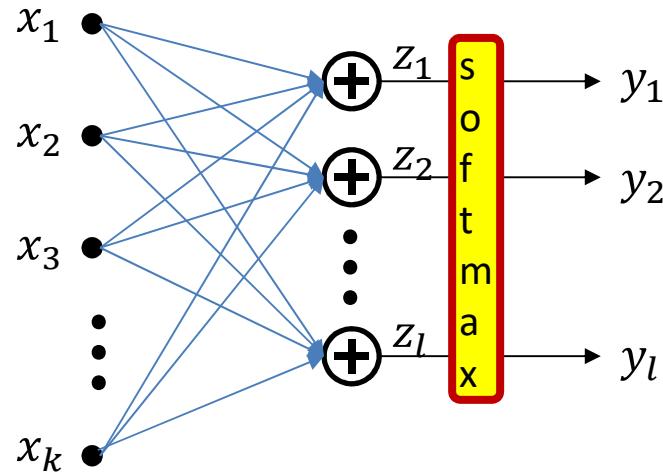


- We can also have neurons that have *multiple coupled* outputs

$$[y_1, y_2, \dots, y_l] = f(x_1, x_2, \dots, x_k; W)$$

- Function  $f()$  operates on set of inputs to produce set of outputs
- Modifying a single parameter in  $W$  will affect *all* outputs

# Vector activation example: Softmax



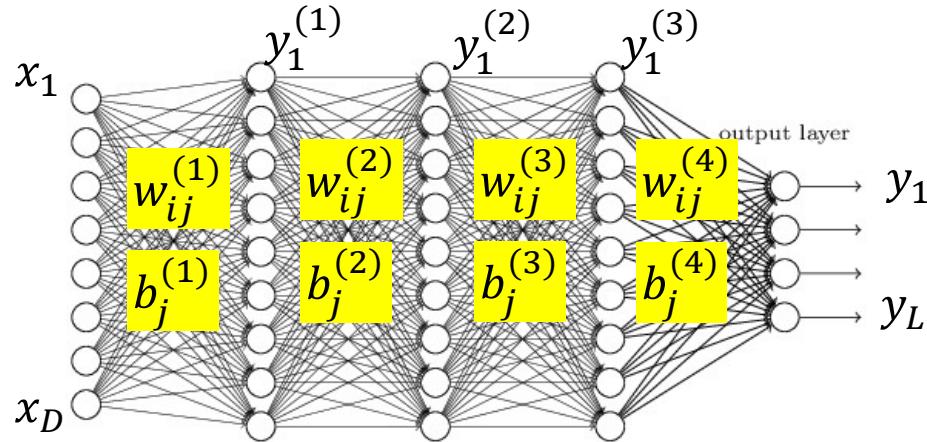
- Example: Softmax *vector* activation

$$z_i = \sum_j w_{ji} x_j + b_i$$

$$y = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Parameters are  
weights  $w_{ji}$   
and bias  $b_i$

# Notation



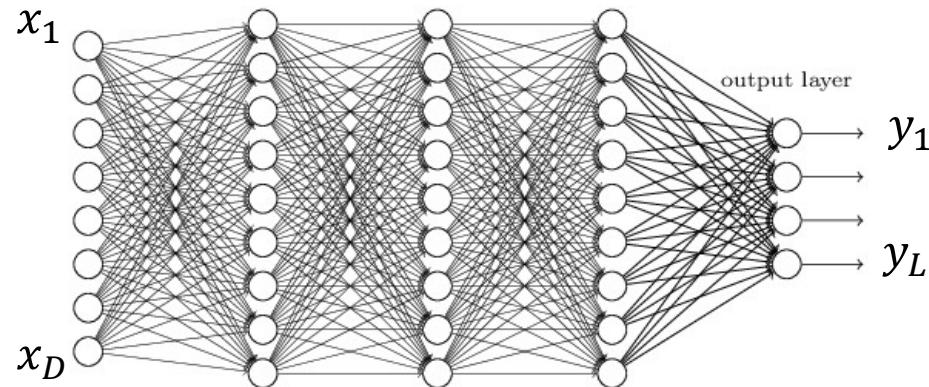
- The input layer is the  $0^{\text{th}}$  layer
- We will represent the output of the  $i$ -th perceptron of the  $k^{\text{th}}$  layer as  $y_i^{(k)}$ 
  - **Input to network:**  $y_i^{(0)} = x_i$
  - **Output of network:**  $y_i = y_i^{(N)}$
- We will represent the weight of the connection between the  $i$ -th unit of the  $k-1$ th layer and the  $j$ th unit of the  $k$ -th layer as  $w_{ij}^{(k)}$ 
  - The bias to the  $j$ th unit of the  $k$ -th layer is  $b_j^{(k)}$

# Problem Setup: Things to define

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- What are these input-output pairs?

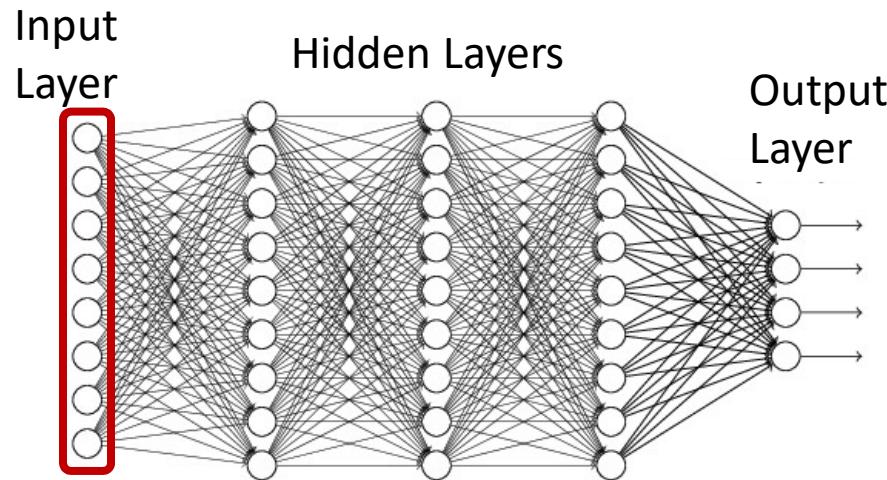
$$Err(W) = \frac{1}{T} \sum_i div(f(X_i; W), d_i)$$

# Vector notation



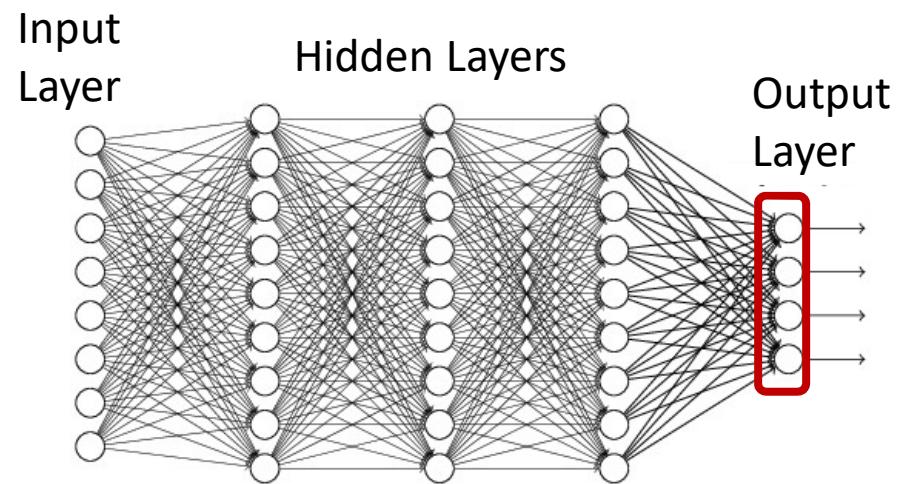
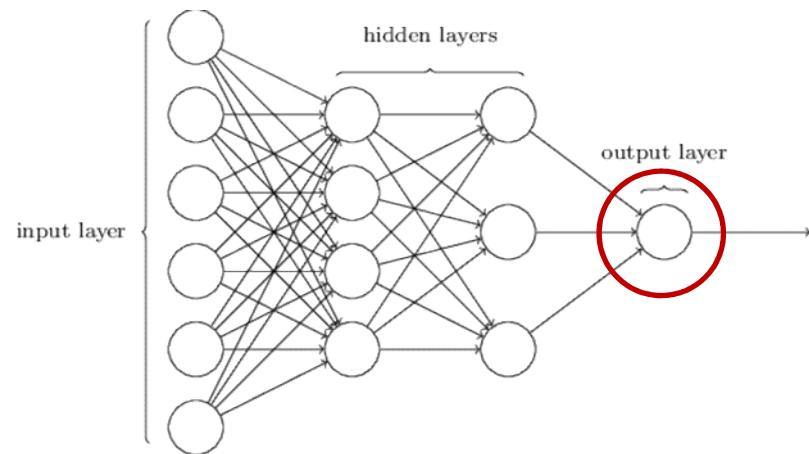
- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- $X_n = [x_{n1}, x_{n2}, \dots, x_{nD}]$  is the  $n$ th input vector
- $d_n = [d_{n1}, d_{n2}, \dots, d_{nL}]$  is the  $n$ th desired output
- $Y_n = [y_{n1}, y_{n2}, \dots, y_{nL}]$  is the  $n$ th vector of *actual* outputs of the network
- We will sometimes drop the first subscript when referring to a *specific* instance

# Representing the input



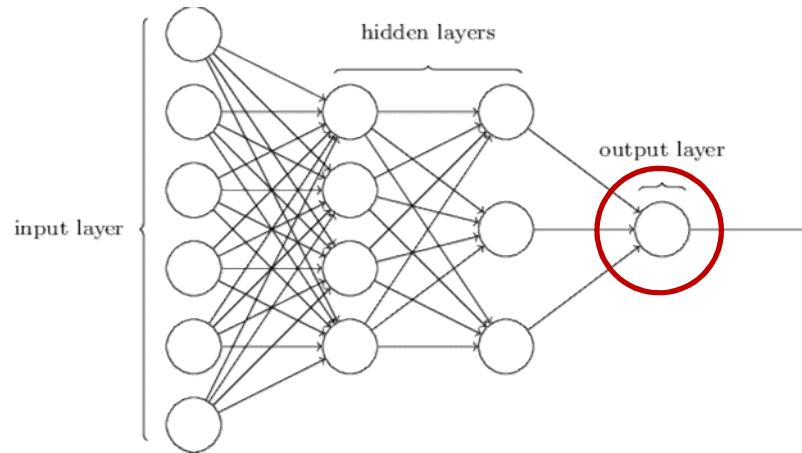
- Vectors of numbers
  - (or may even be just a scalar, if input layer is of size 1)
  - E.g. vector of pixel values
  - E.g. vector of speech features
  - E.g. real-valued vector representing text
    - We will see how this happens later in the course
  - Other real valued vectors

# Representing the output



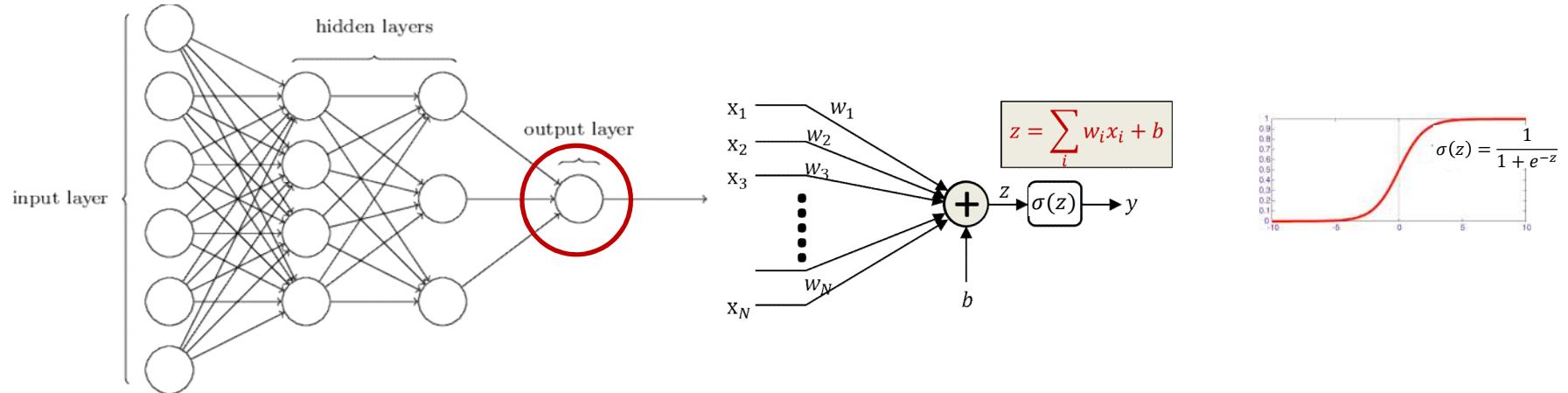
- If the desired *output* is real-valued, no special tricks are necessary
  - Scalar Output : single output neuron
    - $d$  = scalar (real value)
  - Vector Output : as many output neurons as the dimension of the desired output
    - $d = [d_1 \ d_2 \ \dots \ d_L]$  (vector of real values)

# Representing the output



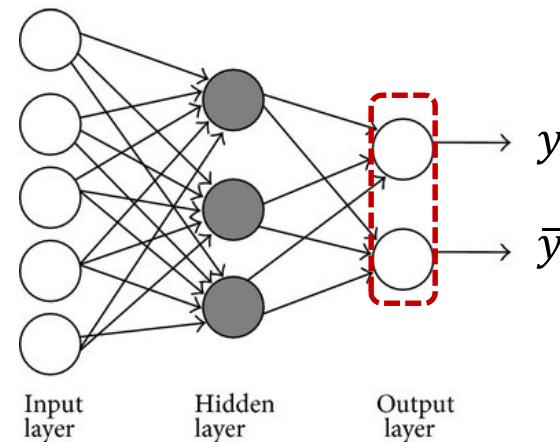
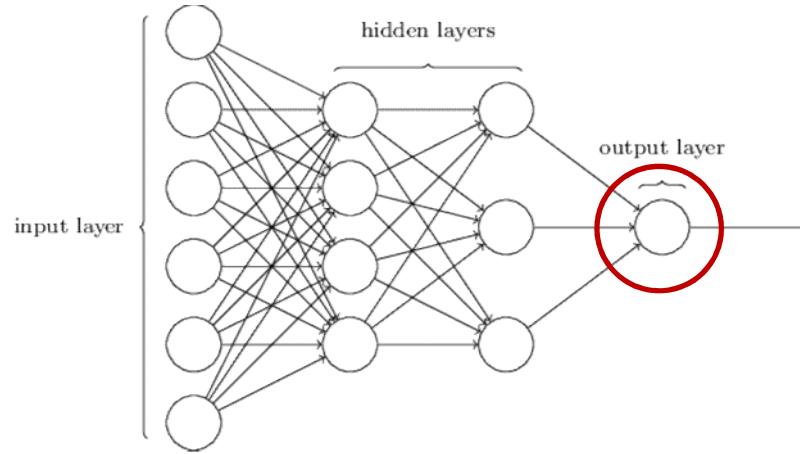
- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes it's a cat
  - 0 = No it's not a cat.

# Representing the output



- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
- Output activation: Typically a sigmoid
  - Viewed as the *probability*  $P(Y = 1|X)$  of class value 1
    - Indicating the fact that for actual data, in general a feature value  $X$  may occur for both classes, but with different probabilities
    - Is differentiable

# Representing the output

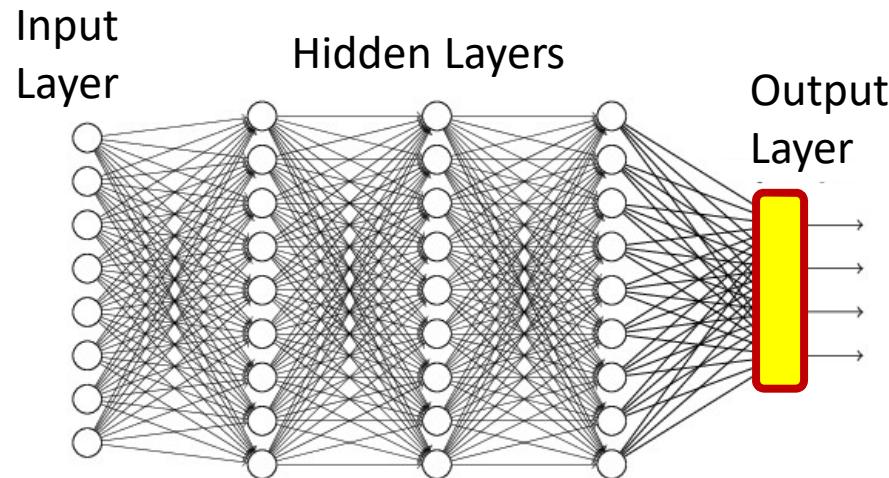


- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes it's a cat
  - 0 = No it's not a cat.
- Sometimes represented by *two independent* outputs, one representing the desired output, the other representing the *negation* of the desired output
  - Yes:  $\rightarrow [1 0]$
  - No:  $\rightarrow [0 1]$

# Multi-class output: One-hot representations

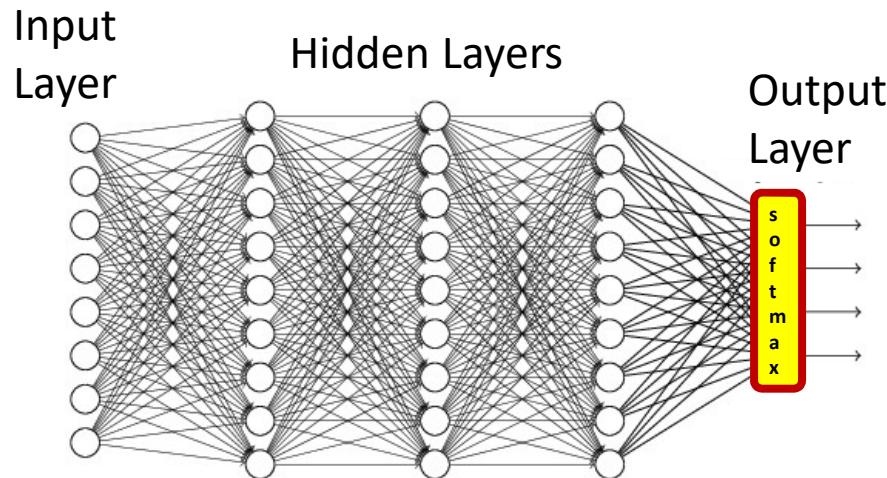
- Consider a network that must distinguish if an input is a cat, a dog, a camel, a hat, or a flower
- We can represent this set as the following vector:
$$[\text{cat } \text{dog } \text{camel } \text{hat } \text{flower}]^T$$
- For inputs of each of the five classes the desired output is:
  - cat:  $[1 \ 0 \ 0 \ 0 \ 0]^T$
  - dog:  $[0 \ 1 \ 0 \ 0 \ 0]^T$
  - camel:  $[0 \ 0 \ 1 \ 0 \ 0]^T$
  - hat:  $[0 \ 0 \ 0 \ 1 \ 0]^T$
  - flower:  $[0 \ 0 \ 0 \ 0 \ 1]^T$
- For an input of any class, we will have a five-dimensional vector output with four zeros and a single 1 at the position of that class
- This is a *one hot vector*

# Multi-class networks



- For a multi-class classifier with  $N$  classes, the one-hot representation will have  $N$  binary outputs
  - An  $N$ -dimensional binary vector
- The neural network's output too must ideally be binary ( $N-1$  zeros and a single 1 in the right place)
- More realistically, it will be a probability vector
  - $N$  probability values that sum to 1.

# Multi-class classification: Output



- Softmax *vector* activation is often used at the output of multi-class classifier nets

$$z_i = \sum_j w_{ji}^{(n)} y_j^{(n-1)}$$

$$y_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- This can be viewed as the probability  $y_i = P(\text{class} = i | X)$

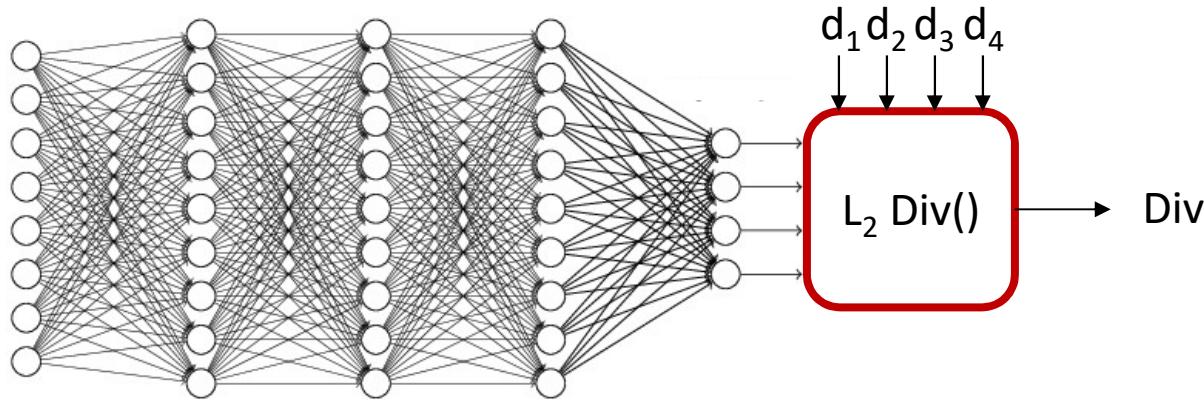
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What is the  
divergence  $\text{div}()$ ?

# Examples of divergence functions



- For real-valued output vectors, the (scaled)  $L_2$  divergence is popular

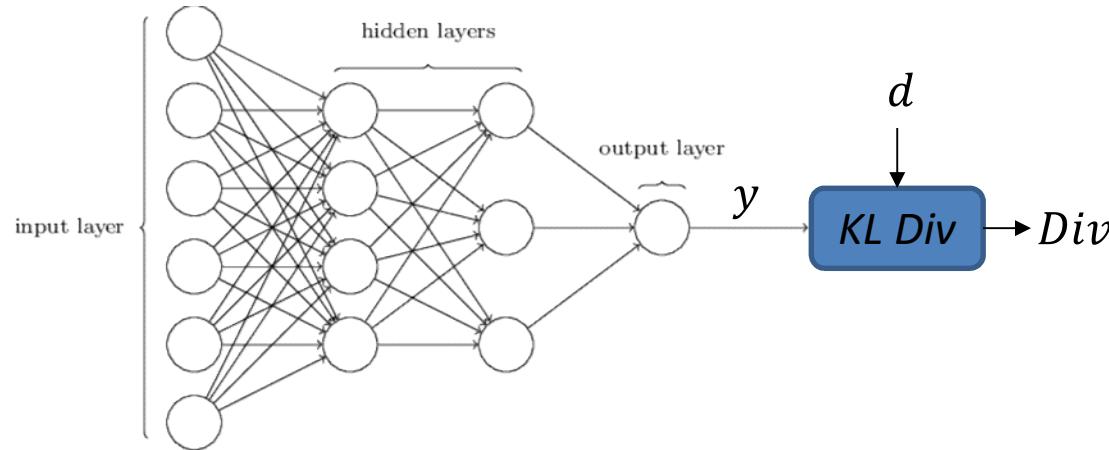
$$Div(Y, d) = \frac{1}{2} \|Y - d\|^2 = \frac{1}{2} \sum_i (y_i - d_i)^2$$

- Squared Euclidean distance between true and desired output
- Note: this is differentiable

$$\frac{dDiv(Y, d)}{dy_i} = (y_i - d_i)$$

$$\nabla_Y Div(Y, d) = [y_1 - d_1, y_2 - d_2, \dots]$$

# For binary classifier



- For binary classifier with scalar output,  $Y \in (0,1)$ ,  $d$  is 0/1, the cross entropy between the probability distribution  $[Y, 1 - Y]$  and the ideal output probability  $[d, 1 - d]$  is popular

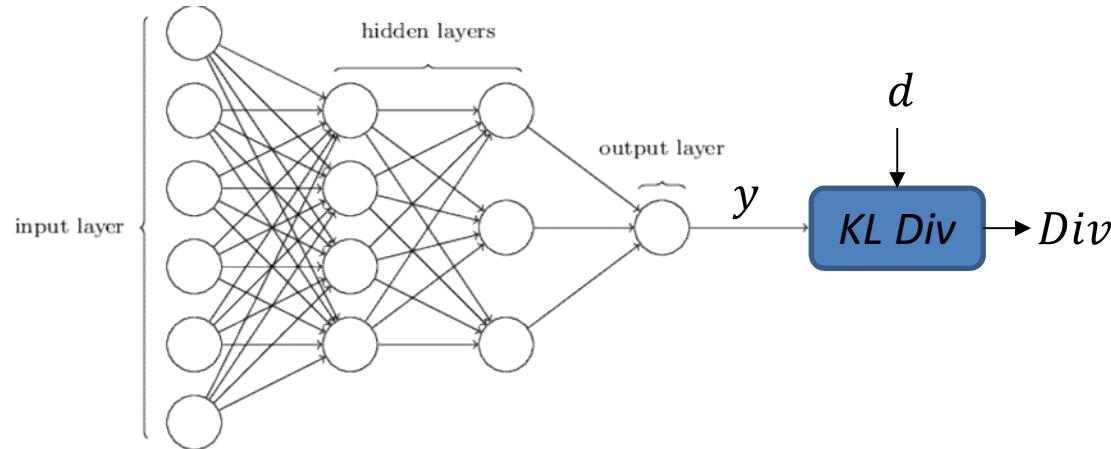
$$Div(Y, d) = -d \log Y - (1 - d) \log(1 - Y)$$

- Minimum when  $d = Y$

- Derivative

$$\frac{dDiv(Y, d)}{dY} = \begin{cases} -\frac{1}{Y} & \text{if } d = 1 \\ \frac{1}{1 - Y} & \text{if } d = 0 \end{cases}$$

# For binary classifier



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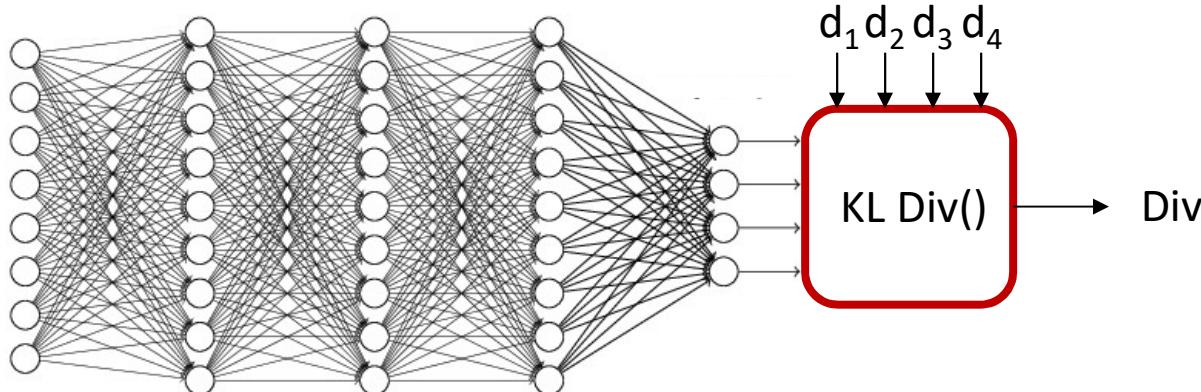
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Note: when  $y = d$  the derivative is *not* 0

*Even though div() = 0 (minimum) when  $y = d$*

# For multi-class classification



- Desired output  $d$  is a one hot vector  $[0 0 \dots 1 \dots 0 0 0]$  with the 1 in the  $c$ -th position (for class  $c$ )
- Actual output will be probability distribution  $[y_1, y_2, \dots]$
- The cross-entropy between the desired one-hot output and actual output:

$$Div(Y, d) = - \sum_i d_i \log y_i = - \log y_c$$

- Derivative

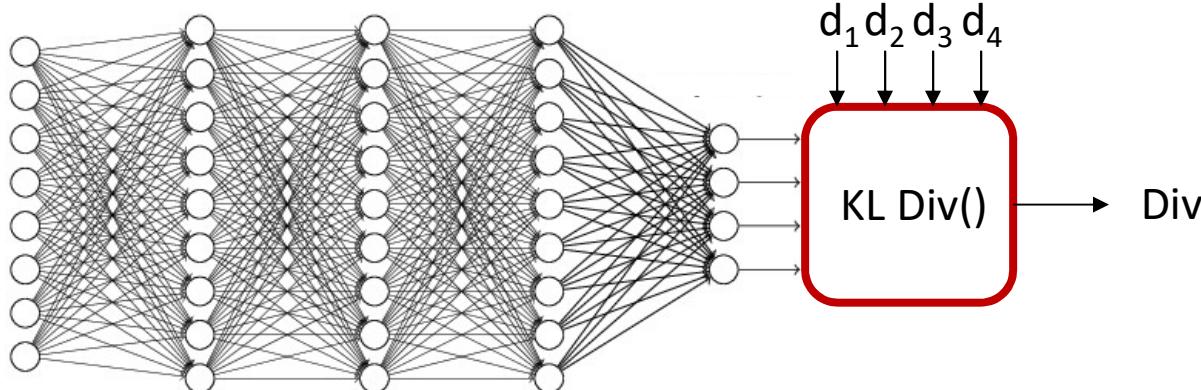
$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1}{y_c} & \text{for the } c\text{-th component} \\ 0 & \text{for remaining component} \end{cases}$$

$$\nabla_Y Div(Y, d) = \left[ 0 \ 0 \ \dots \frac{-1}{y_c} \dots \ 0 \ 0 \right]$$

If  $y_c < 1$ , the slope is negative w.r.t.  $y_c$

Indicates *increasing*  $y_c$  will *reduce* divergence

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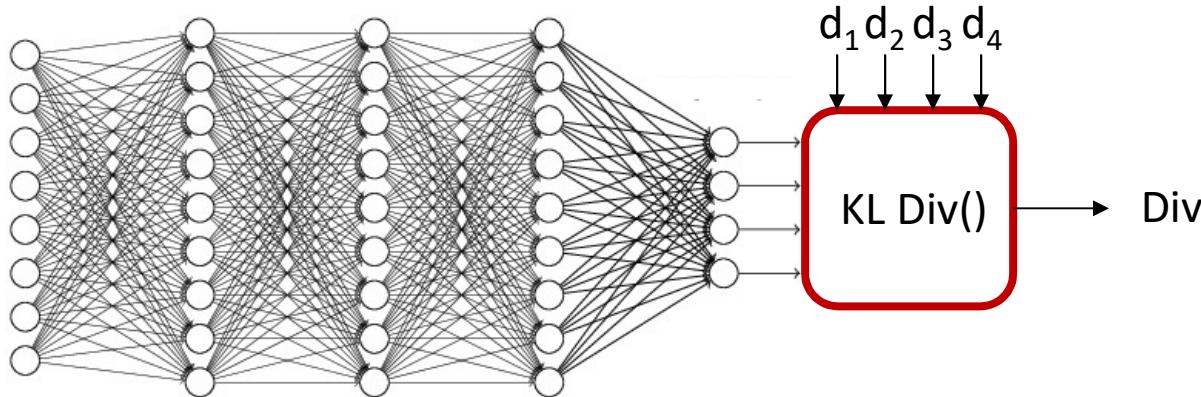
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Note: when  $y = d$  the derivative is *not* 0

*Even though div() = 0 (minimum) when  $y = d$*

# For multi-class classification



- It is sometimes useful to set the target output to  $[\epsilon \ \epsilon \dots (1 - (K - 1)\epsilon) \dots \epsilon \ \epsilon \ \epsilon]$  with the value  $1 - (K - 1)\epsilon$  in the  $c$ -th position (for class  $c$ ) and  $\epsilon$  elsewhere for some small  $\epsilon$ 
  - “Label smoothing” -- aids gradient descent
- The cross-entropy remains:

$$Div(Y, d) = - \sum_i d_i \log y_i$$

- Derivative

$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1 - (K - 1)\epsilon}{y_c} & \text{for the } c\text{-th component} \\ -\frac{\epsilon}{y_i} & \text{for remaining components} \end{cases}$$

# Training Neural Nets through Gradient Descent

Total training error:

$$Err = \frac{1}{T} \sum_t Div(\mathbf{Y}_t, \mathbf{d}_t)$$

- Gradient descent algorithm:
- Initialize all weights and biases  $\{w_{ij}^{(k)}\}$ 
  - Using the extended notation: the bias is also a weight
- Do:
  - For every layer  $k$  for all  $i, j$ , update:
    - $w_{i,j}^{(k)} = w_{i,j}^{(k)} - \eta \frac{dErr}{dw_{i,j}^{(k)}}$
- Until  $Err$  has converged

Assuming the bias is also represented as a weight

# The derivative

Total training error:

$$Err = \frac{1}{T} \sum_t Div(\mathbf{Y}_t, \mathbf{d}_t)$$

- Computing the derivative

Total derivative:

$$\frac{dErr}{dw_{i,j}^{(k)}} = \frac{1}{T} \sum_t \frac{dDiv(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$$

# Training by gradient descent

- Initialize all weights  $\{w_{ij}^{(k)}\}$
- Do:
  - For all  $i, j, k$ , initialize  $\frac{d\text{Err}}{dw_{i,j}^{(k)}} = 0$
  - For all  $t = 1:T$ 
    - For every layer  $k$  for all  $i, j$ :
      - Compute  $\frac{d\text{Div}(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$
      - $\frac{d\text{Err}}{dw_{i,j}^{(k)}} += \frac{d\text{Div}(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$
    - For every layer  $k$  for all  $i, j$ :
$$w_{i,j}^{(k)} = w_{i,j}^{(k)} - \frac{\eta}{T} \frac{d\text{Err}}{dw_{i,j}^{(k)}}$$
  - Until  $\text{Err}$  has converged

# The derivative

Total training error:

$$Err = \frac{1}{T} \sum_t Div(\mathbf{Y}_t, \mathbf{d}_t)$$

Total derivative:

$$\frac{dErr}{dw_{i,j}^{(k)}} = \frac{1}{T} \sum_t \frac{dDiv(\mathbf{Y}_t, \mathbf{d}_t)}{dw_{i,j}^{(k)}}$$

- So we must first figure out how to compute the derivative of divergences of individual training inputs

# Calculus Refresher: Chain rule

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

$$\frac{dy}{dx} = \frac{\partial f}{\partial g(x)} \frac{dg(x)}{dx}$$

Check - we can confirm that :  $\Delta y = \frac{dy}{dx} \Delta x$

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

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



# Calculus Refresher: Distributed Chain rule

$$y = f(g_1(x), g_2(x), \dots, g_M(x))$$

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

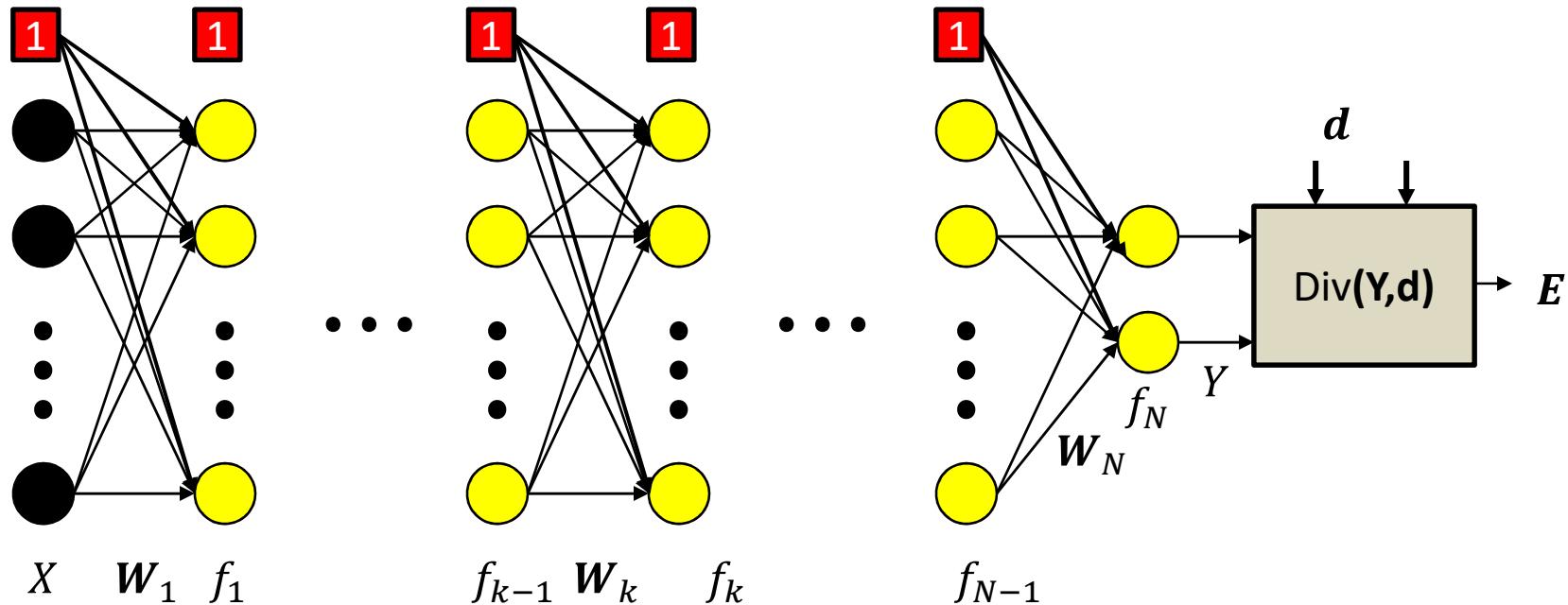
Check:  $\Delta y = \frac{dy}{dx} \Delta x$

$$\Delta y = \frac{\partial f}{\partial g_1(x)} \Delta g_1(x) + \frac{\partial f}{\partial g_2(x)} \Delta g_2(x) + \dots + \frac{\partial f}{\partial g_M(x)} \Delta g_M(x)$$

$$\Delta y = \frac{\partial f}{\partial g_1(x)} \frac{dg_1(x)}{dx} \Delta x + \frac{\partial f}{\partial g_2(x)} \frac{dg_2(x)}{dx} \Delta x + \dots + \frac{\partial f}{\partial g_M(x)} \frac{dg_M(x)}{dx} \Delta x$$

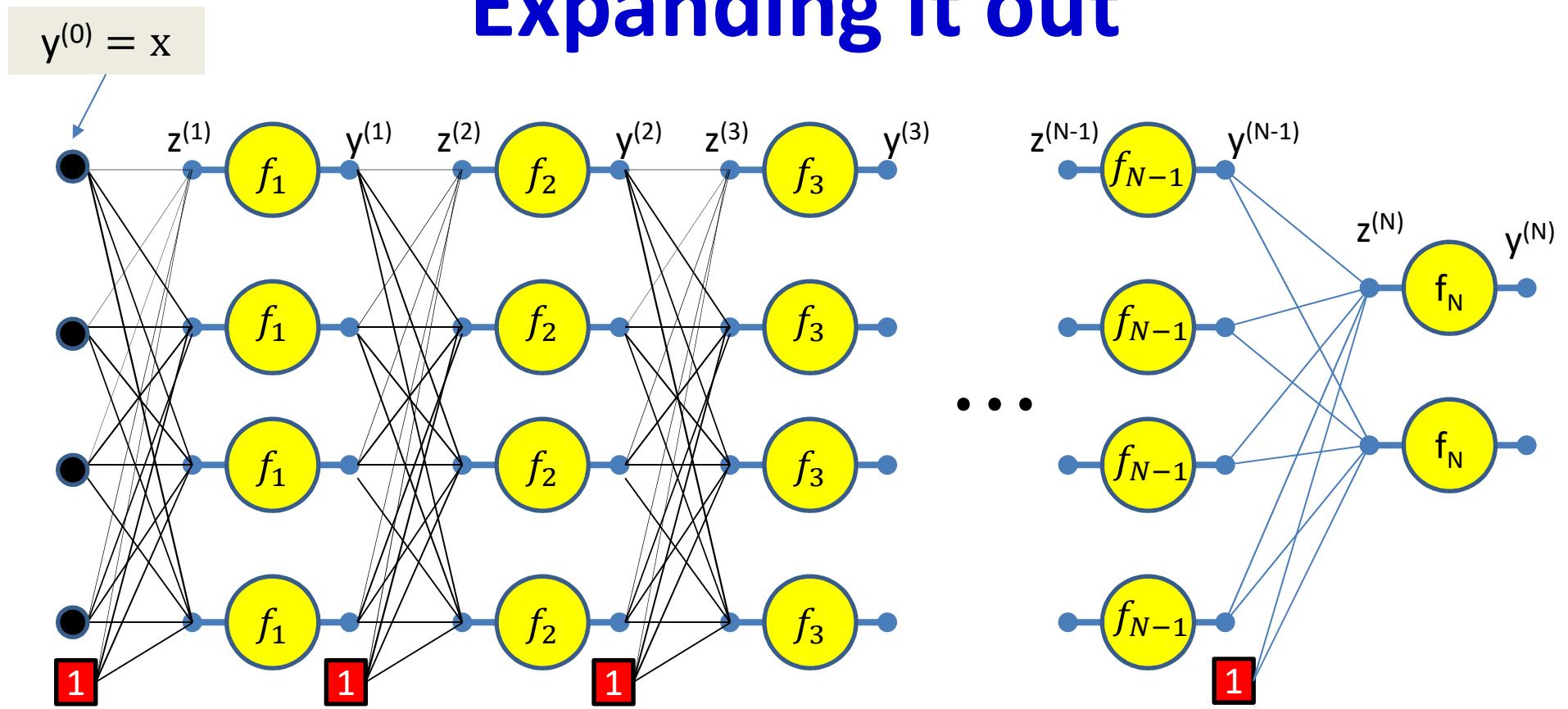
$$\Delta y = \left( \frac{\partial f}{\partial g_1(x)} \frac{dg_1(x)}{dx} + \frac{\partial f}{\partial g_2(x)} \frac{dg_2(x)}{dx} + \dots + \frac{\partial f}{\partial g_M(x)} \frac{dg_M(x)}{dx} \right) \Delta x$$

# BP: Scalar Formulation



- The network again

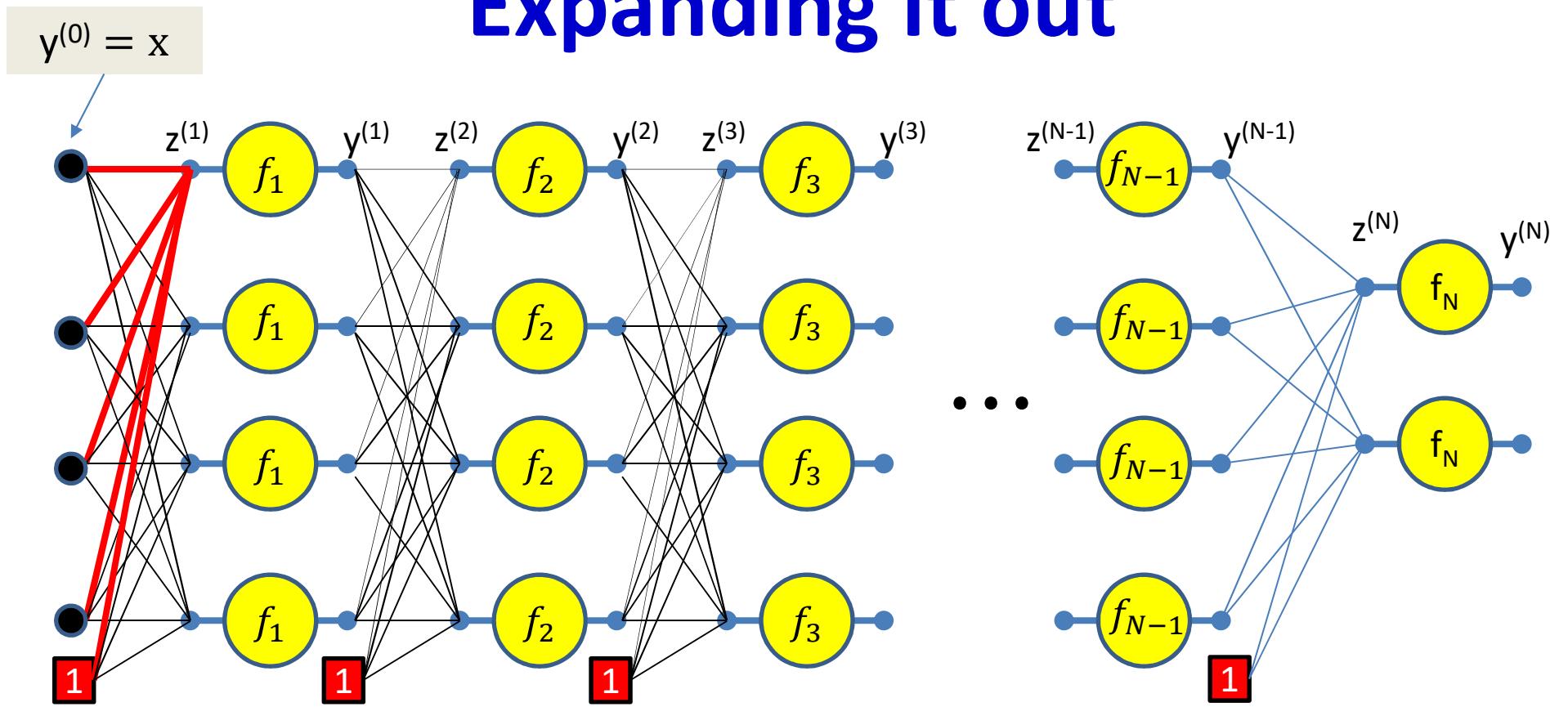
# Expanding it out



Setting  $y_i^{(0)} = x_i$  for notational convenience

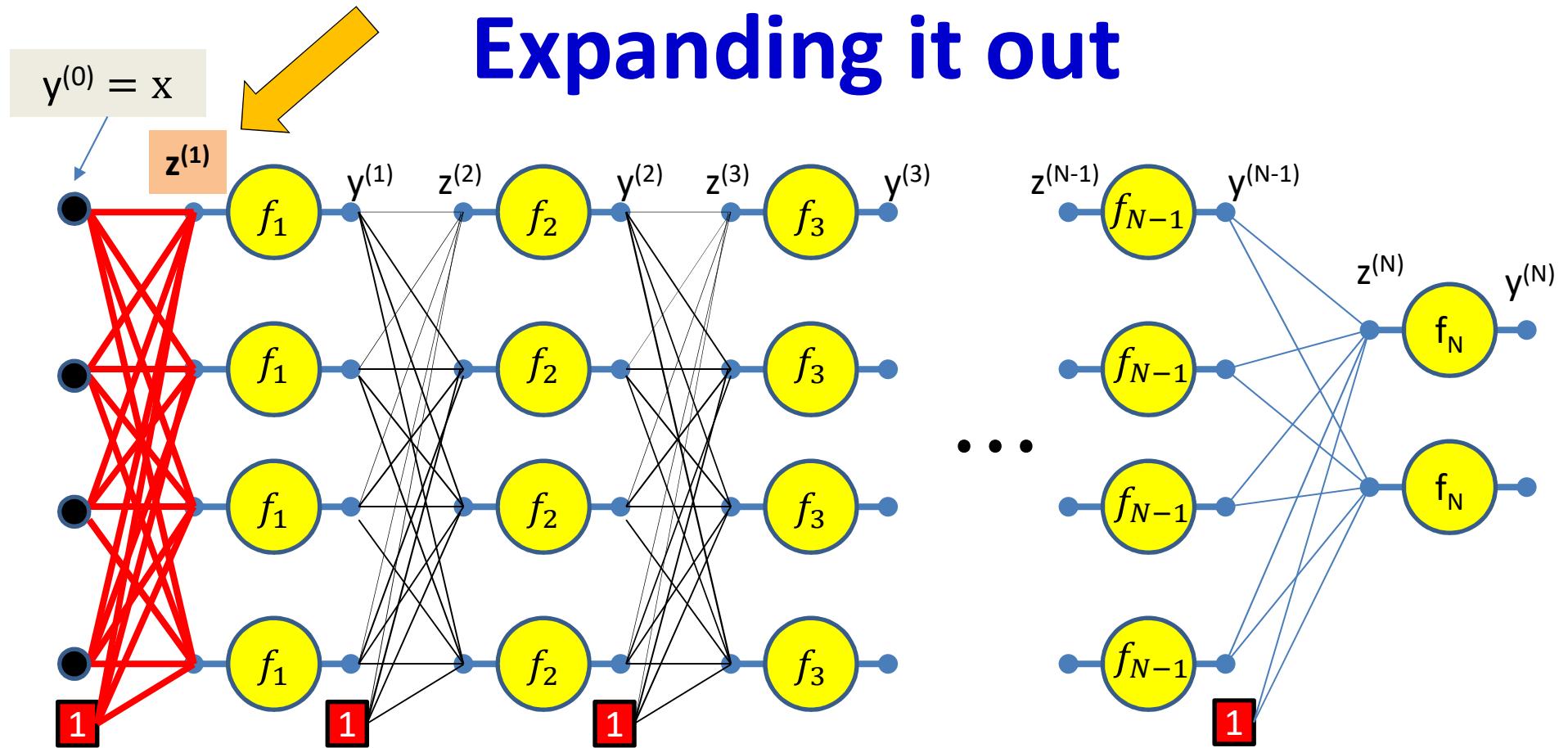
Assuming  $w_{0j}^{(k)} = b_j^{(k)}$  and  $y_0^{(k)} = 1$  -- assuming the bias is a weight and extending the output of every layer by a constant 1, to account for the biases

# Expanding it out

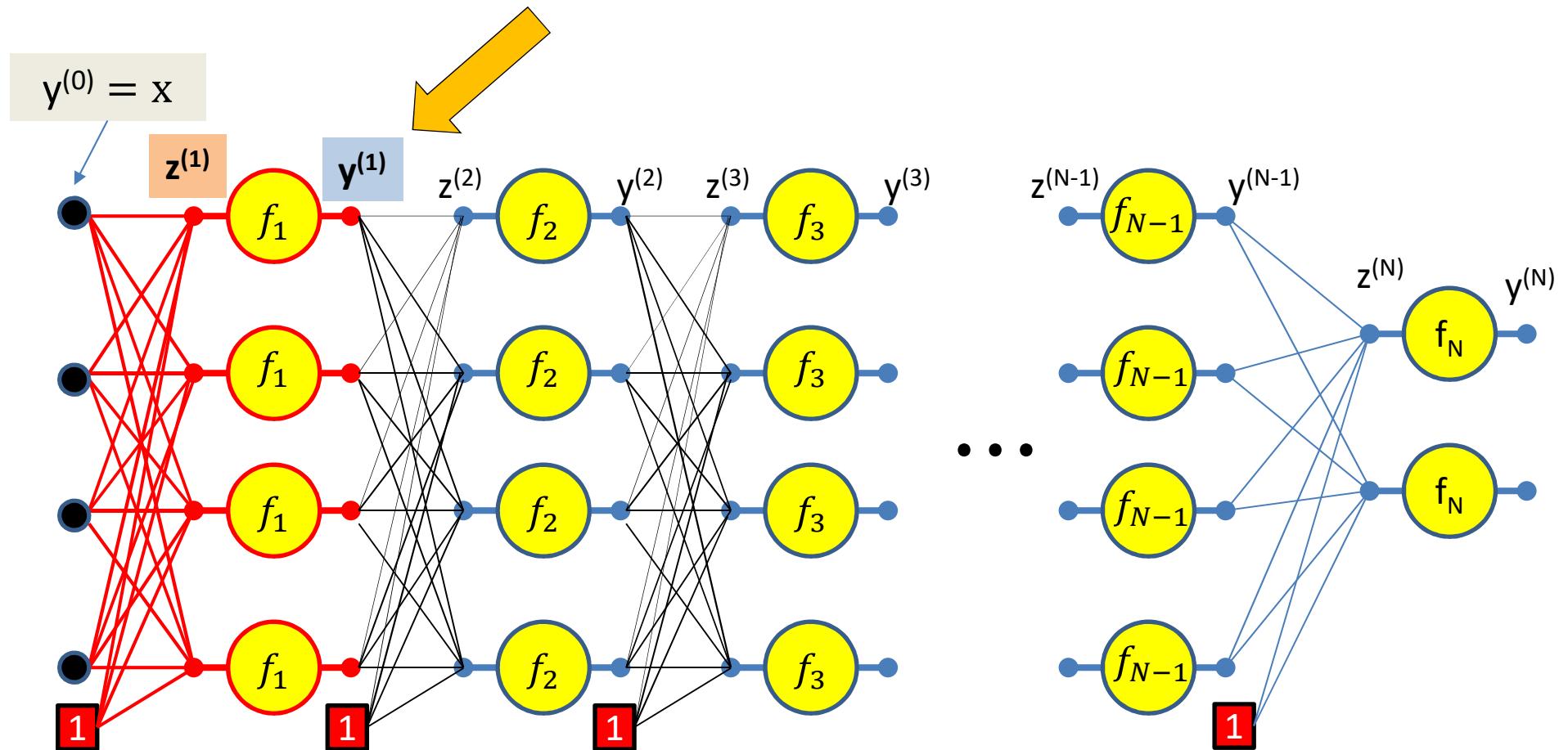


$$z_1^{(1)} = \sum_i w_{i1}^{(1)} y_i^{(0)}$$

# Expanding it out

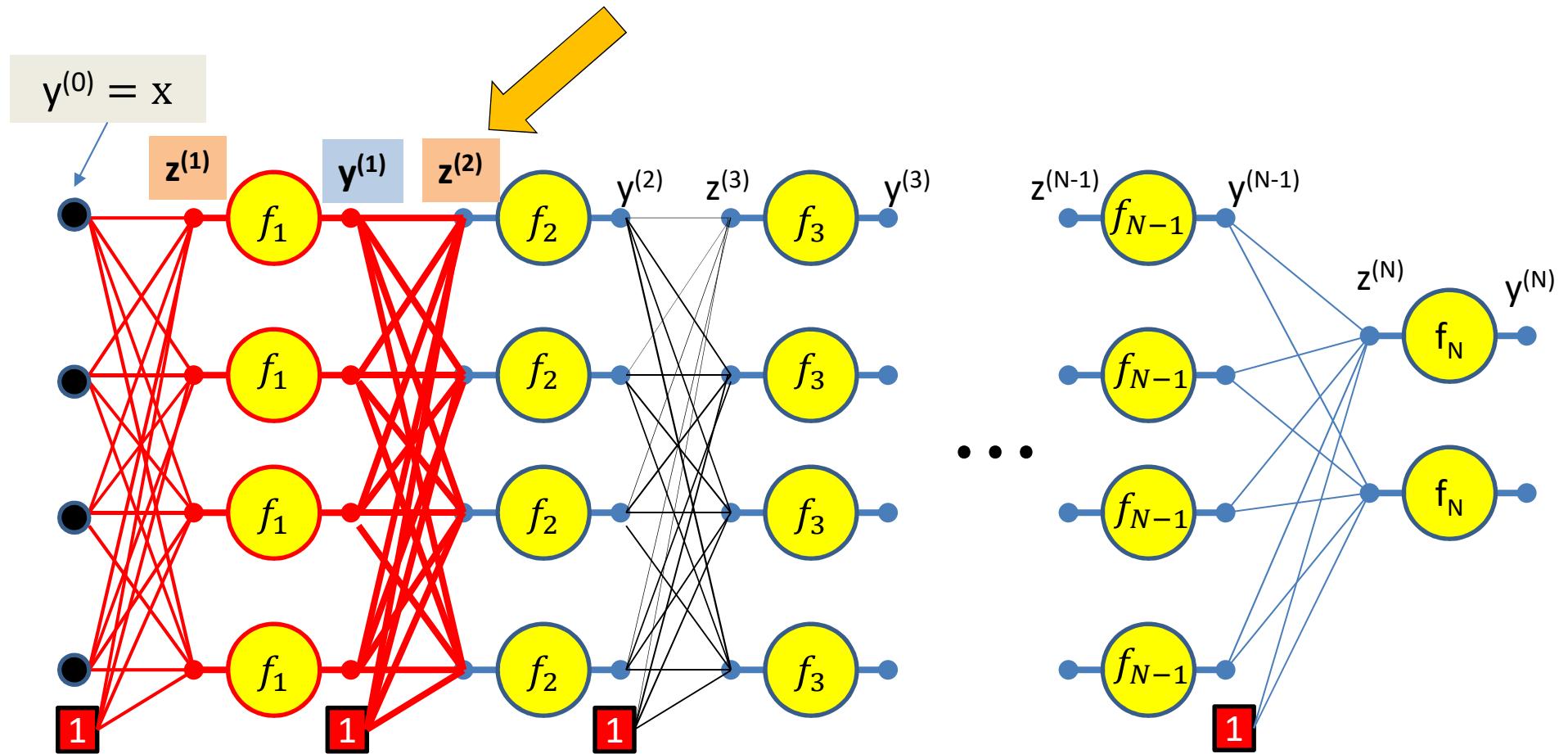


$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

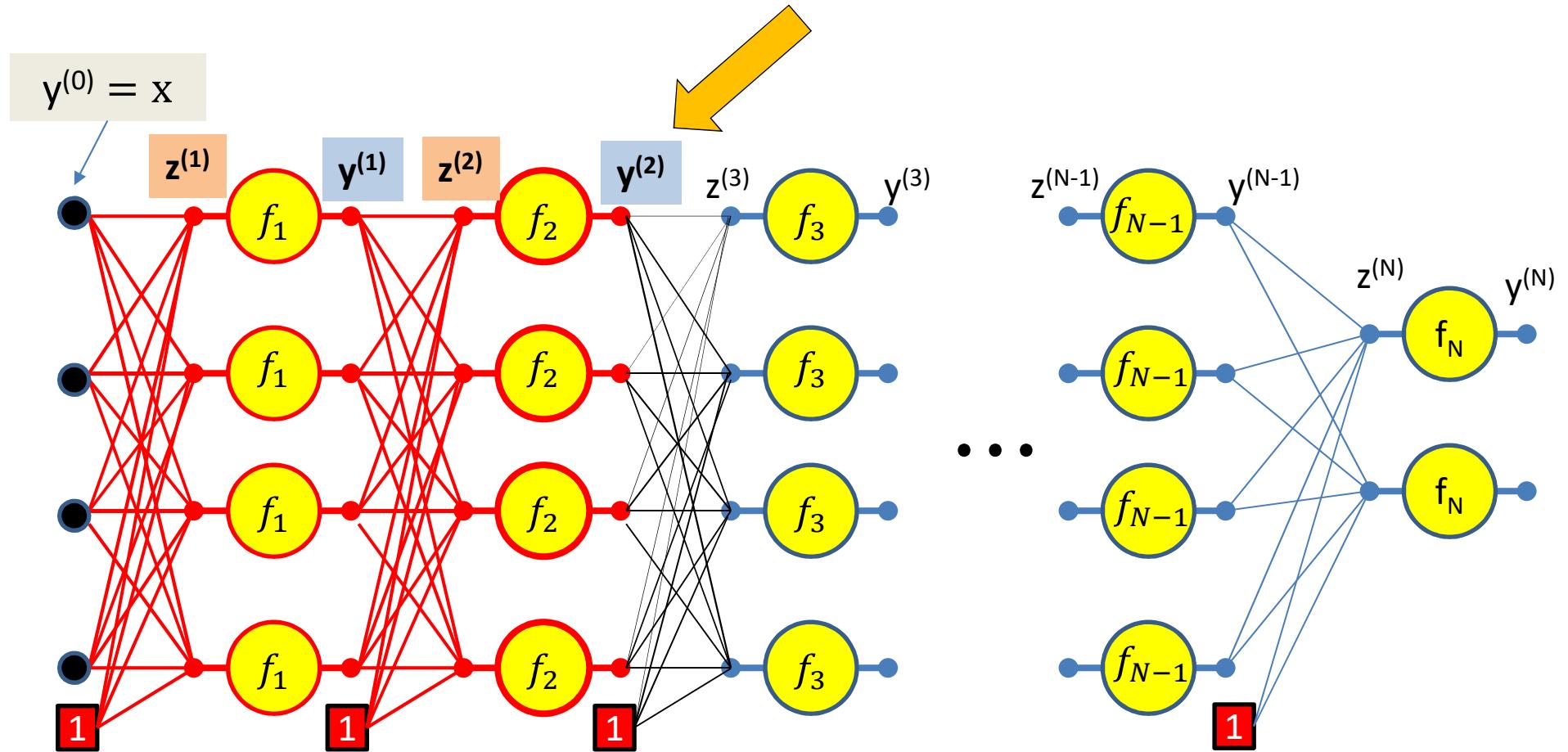
$$y_j^{(1)} = f_1(z_j^{(1)})$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1(z_j^{(1)})$$

$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

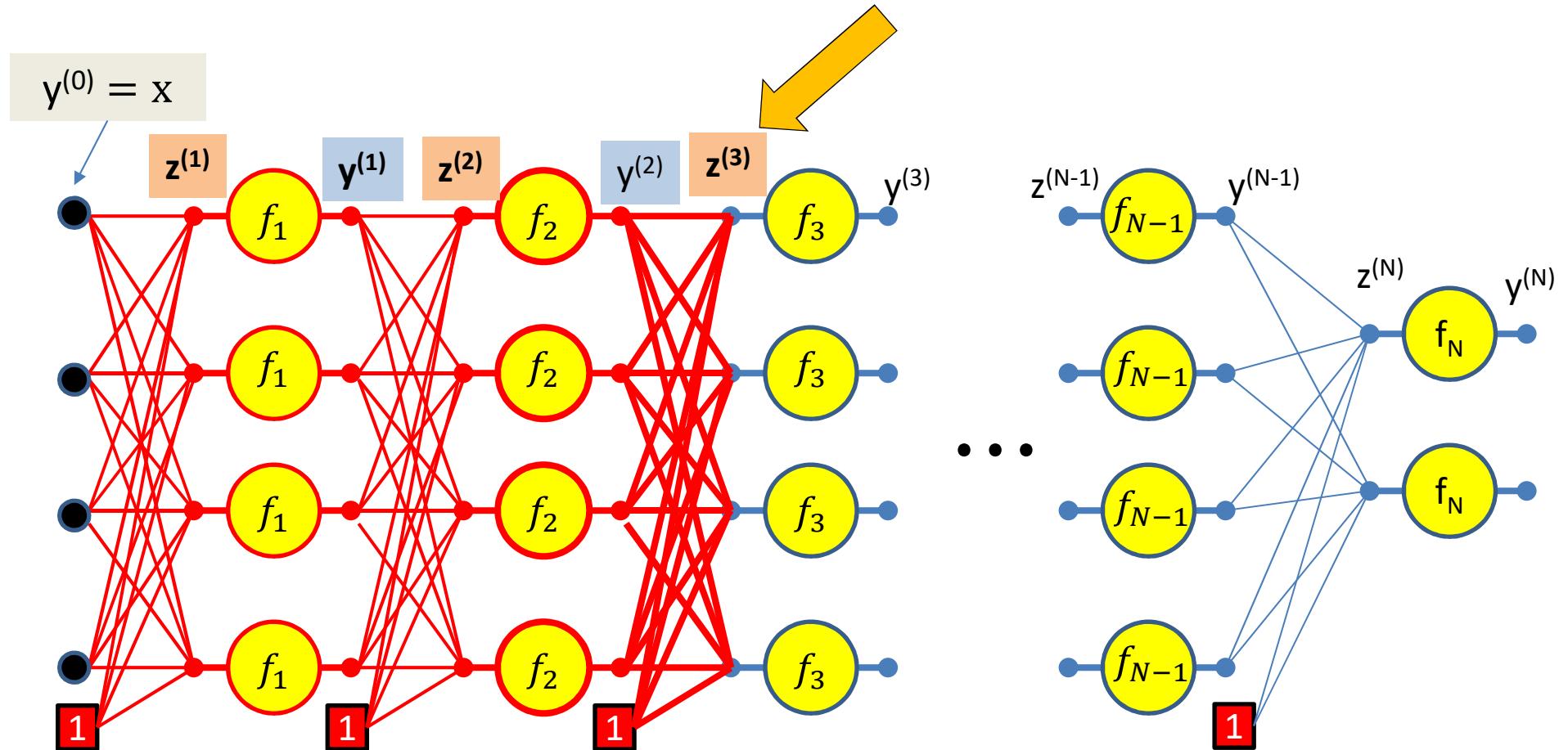


$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1(z_j^{(1)})$$

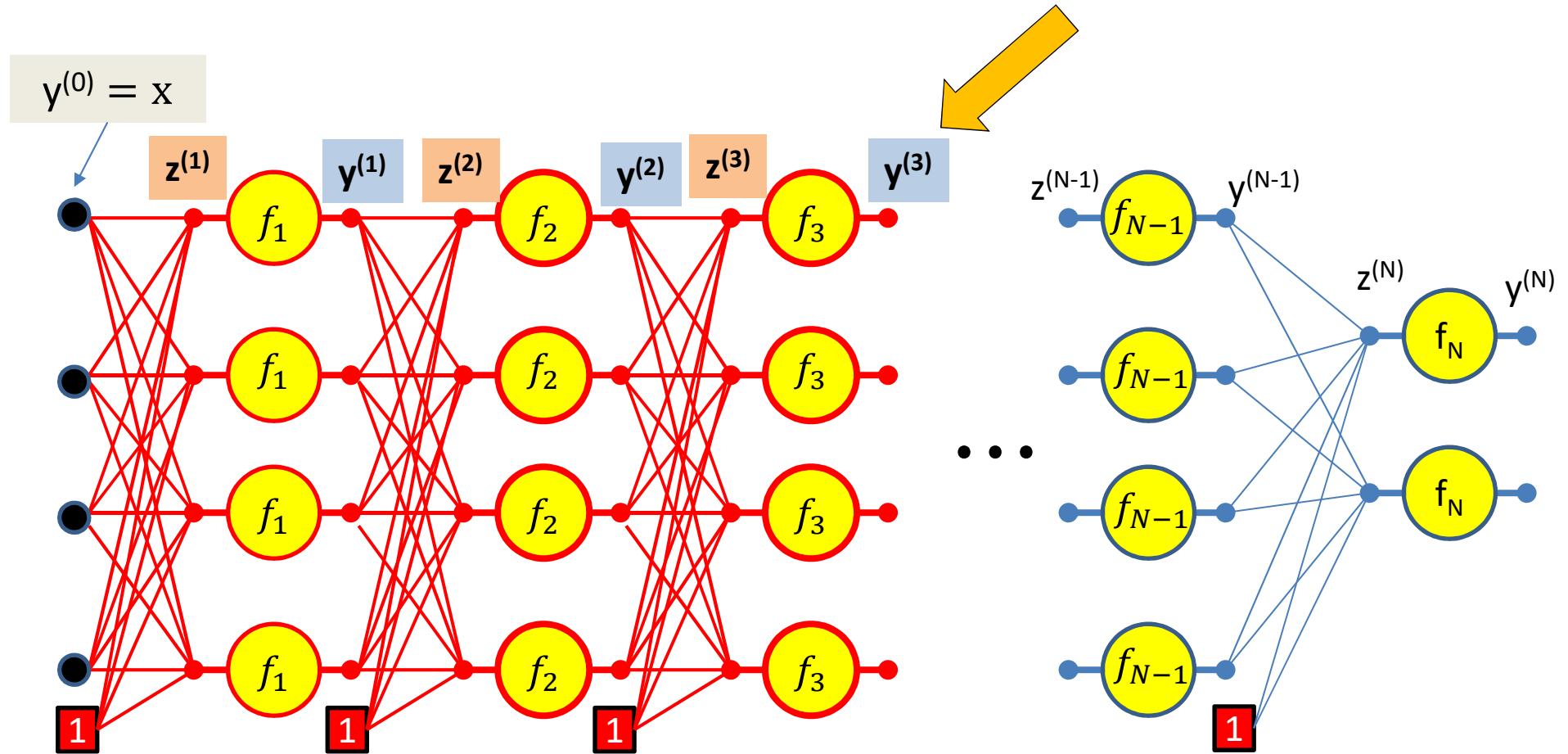
$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

$$y_j^{(2)} = f_2(z_j^{(2)})$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)} \quad y_j^{(1)} = f_1(z_j^{(1)}) \quad z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)} \quad y_j^{(2)} = f_2(z_j^{(2)})$$

$$z_j^{(3)} = \sum_i w_{ij}^{(3)} y_i^{(2)}$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1(z_j^{(1)})$$

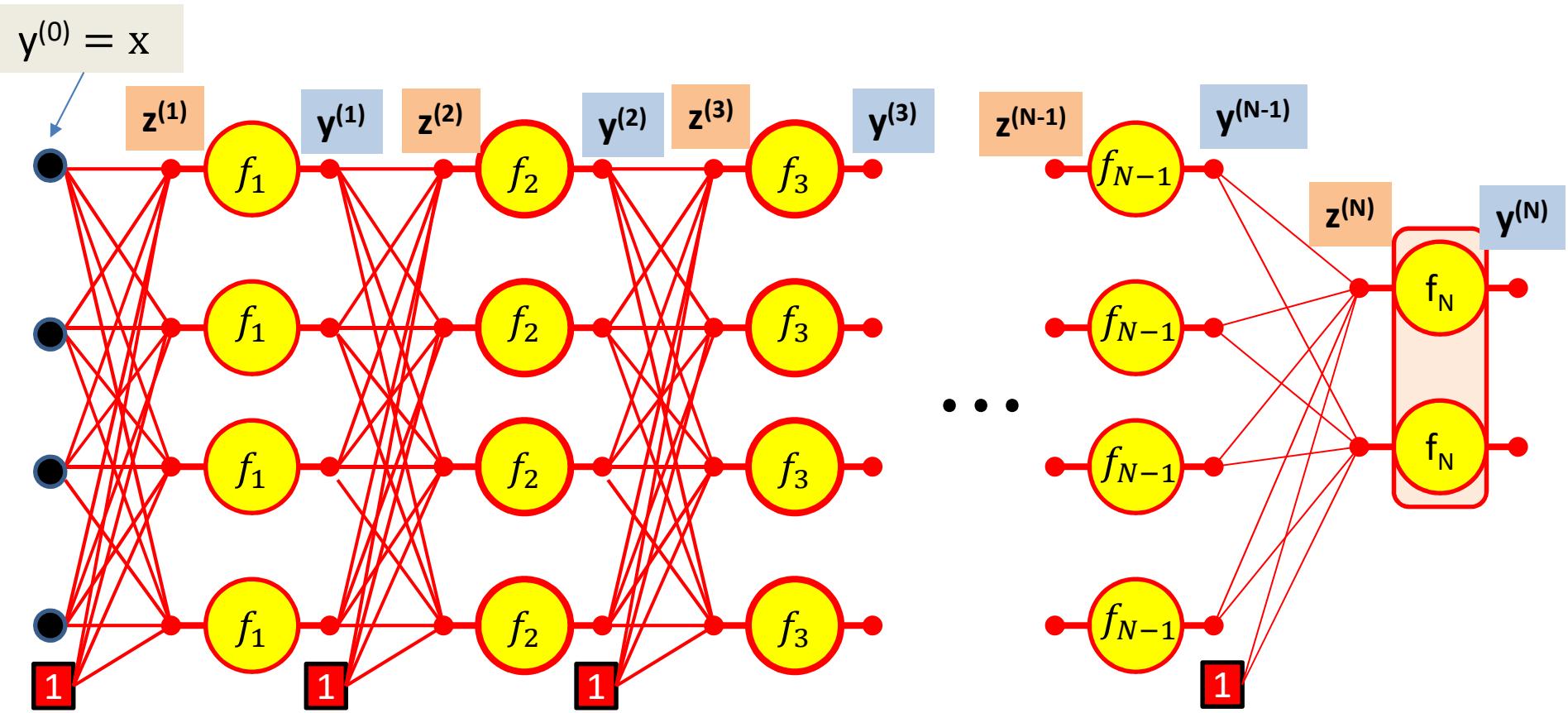
$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

$$y_j^{(2)} = f_2(z_j^{(2)})$$

$$z_j^{(3)} = \sum_i w_{ij}^{(3)} y_i^{(2)}$$

$$y_j^{(3)} = f_3(z_j^{(3)})$$

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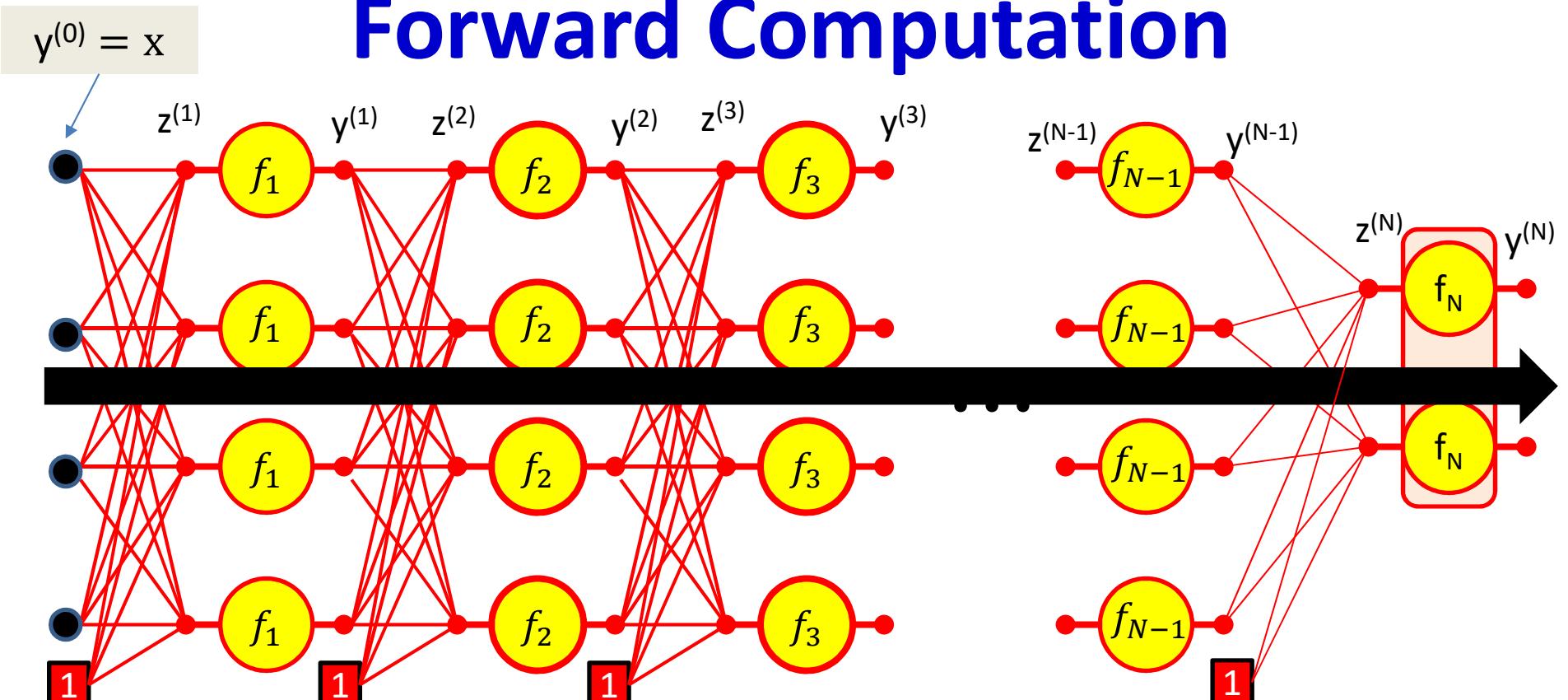


$$y_j^{(N-1)} = f_{N-1}(z_j^{(N-1)})$$

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

$$\mathbf{y}^{(N)} = f_N(\mathbf{z}^{(N)})$$

# Forward Computation



ITERATE FOR  $k = 1:N$

for  $j = 1:\text{layer-width}$

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

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

$$y_j^{(k)} = f_k(z_j^{(k)})$$

# Forward “Pass”

- Input:  $D$  dimensional vector  $\mathbf{x} = [x_j, j = 1 \dots D]$
- Set:
  - $D_0 = D$ , is the width of the 0<sup>th</sup> (input) layer
  - $y_j^{(0)} = x_j, j = 1 \dots D$ ;  $y_0^{(k=1 \dots N)} = x_0 = 1$
- For layer  $k = 1 \dots N$ 
  - For  $j = 1 \dots D_k$   $D_k$  is the size of the  $k$ th layer
    - $z_j^{(k)} = \sum_{i=0}^{D_{k-1}} w_{i,j}^{(k)} y_i^{(k-1)}$
    - $y_j^{(k)} = f_k(z_j^{(k)})$
- Output:
  - $Y = y_j^{(N)}, j = 1 \dots D_N$