Lecture 14
Neural Networks: Part II

GEOL 4397: Data analytics and machine learning for geoscientists

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UNIVERSITY of HOUSTON
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EARTH AND ATMOSPHERIC SCIENCES

Outline

- Vanishing gradients
  - What causes it?
  - Activation function
  - Xavier and He initialization
  - Batch normalization

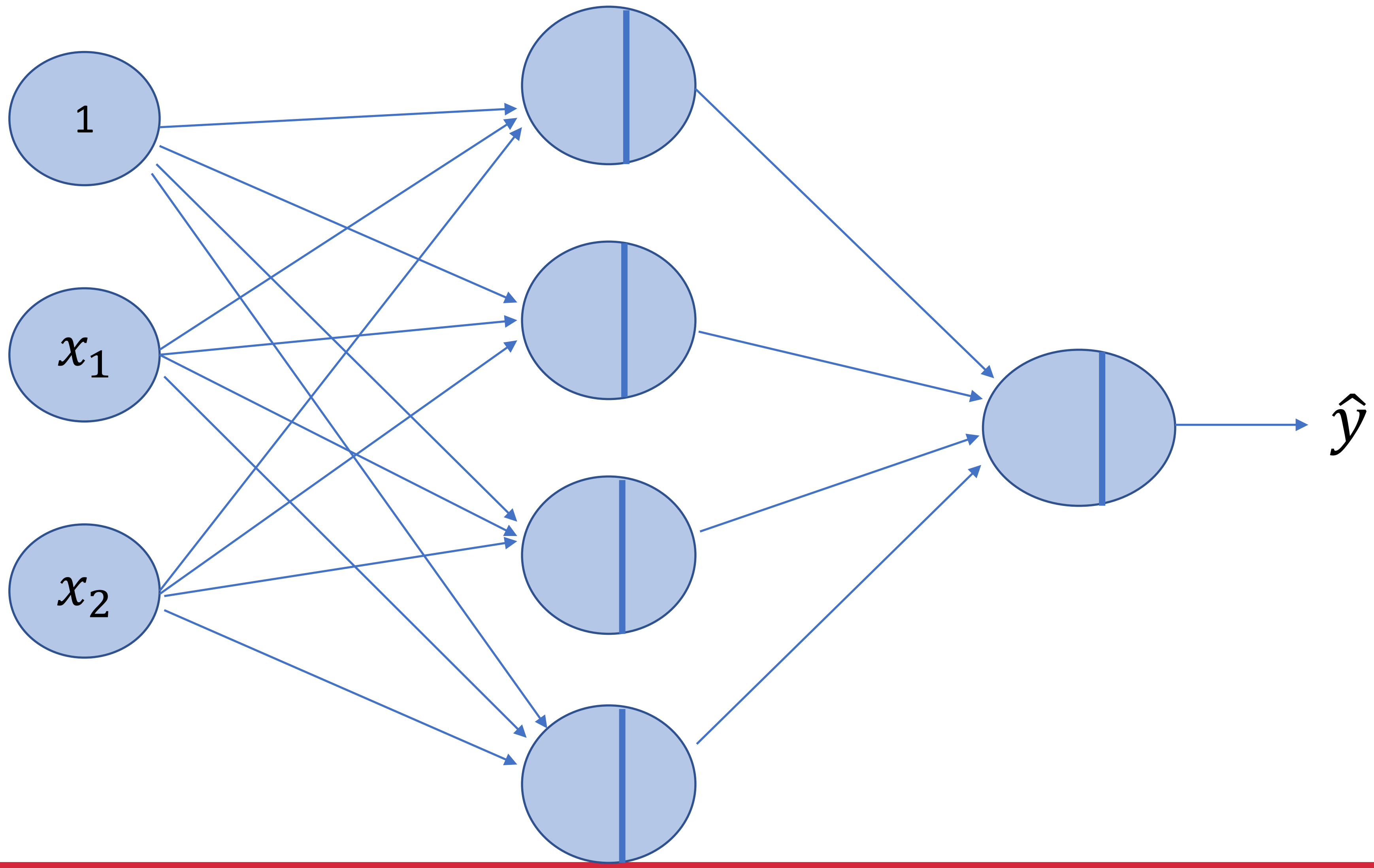
- Optimization algorithms

- Implementing DNN in TensorFlow

Acknowledgments

- Michael Nielsen for an excellent explanation of the vanishing gradients (http://neuralnetworksanddeeplearning.com/chap5.html)

A shallow neural network



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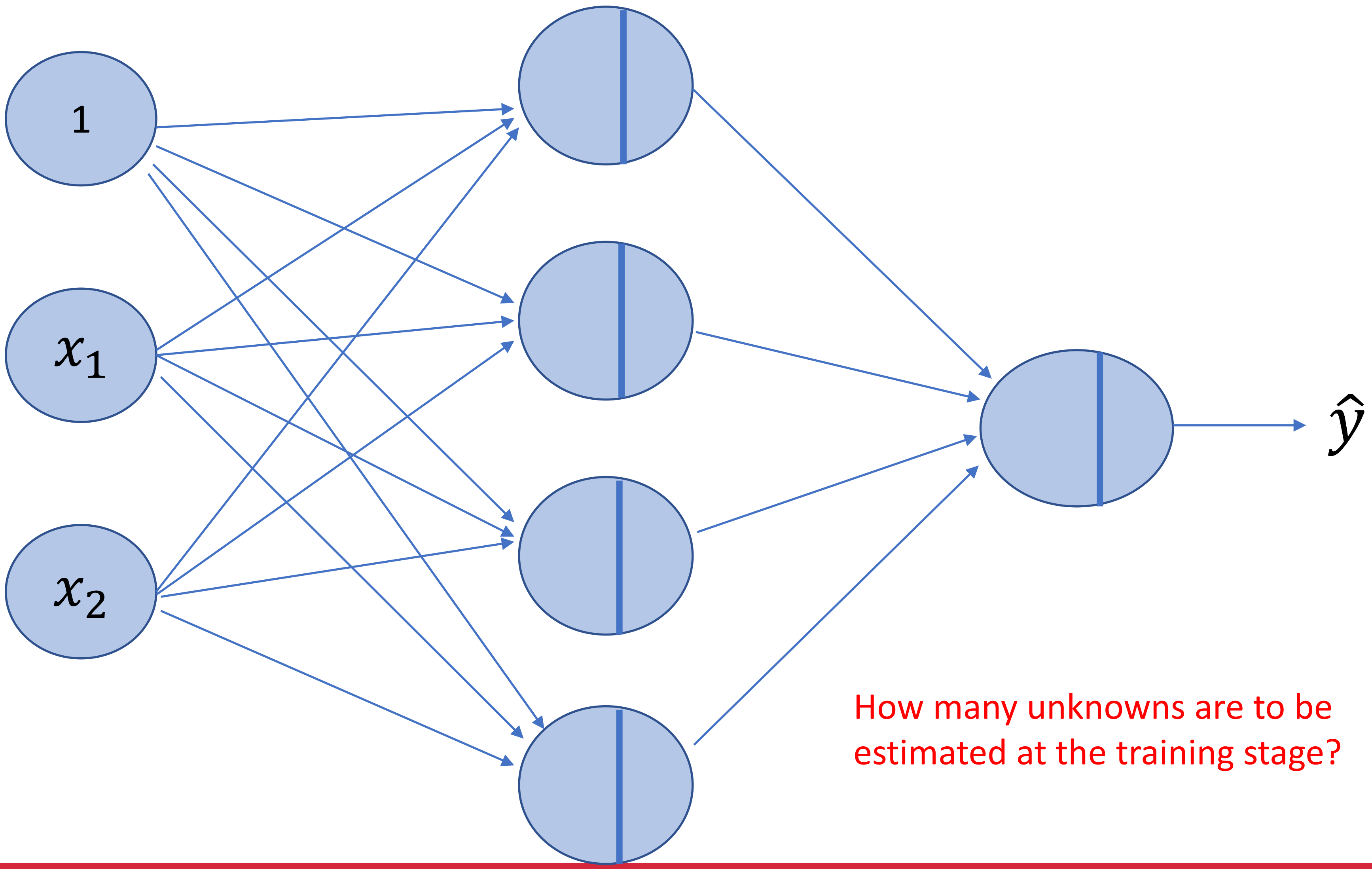
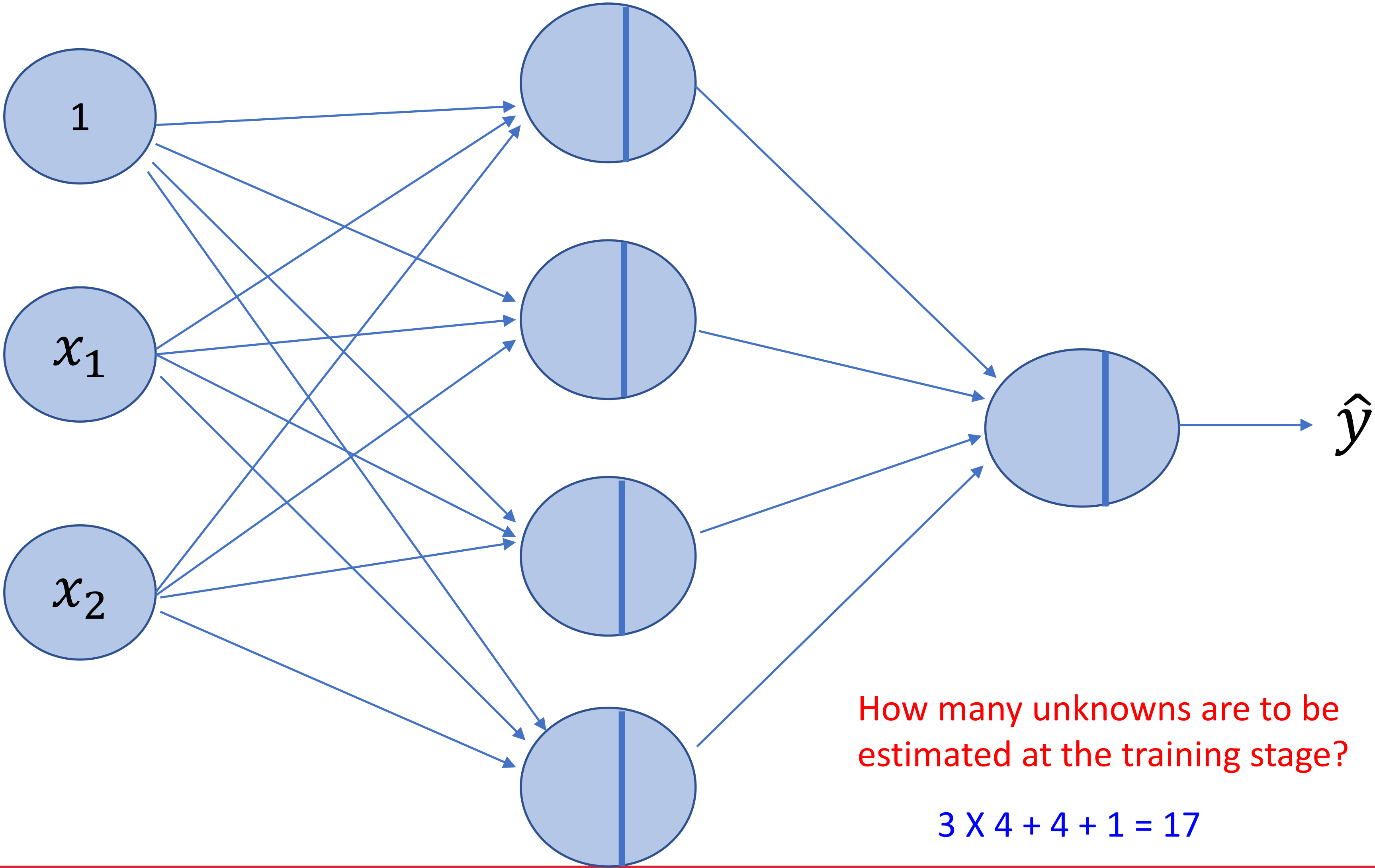


How many unknowns are to be estimated at the training stage?

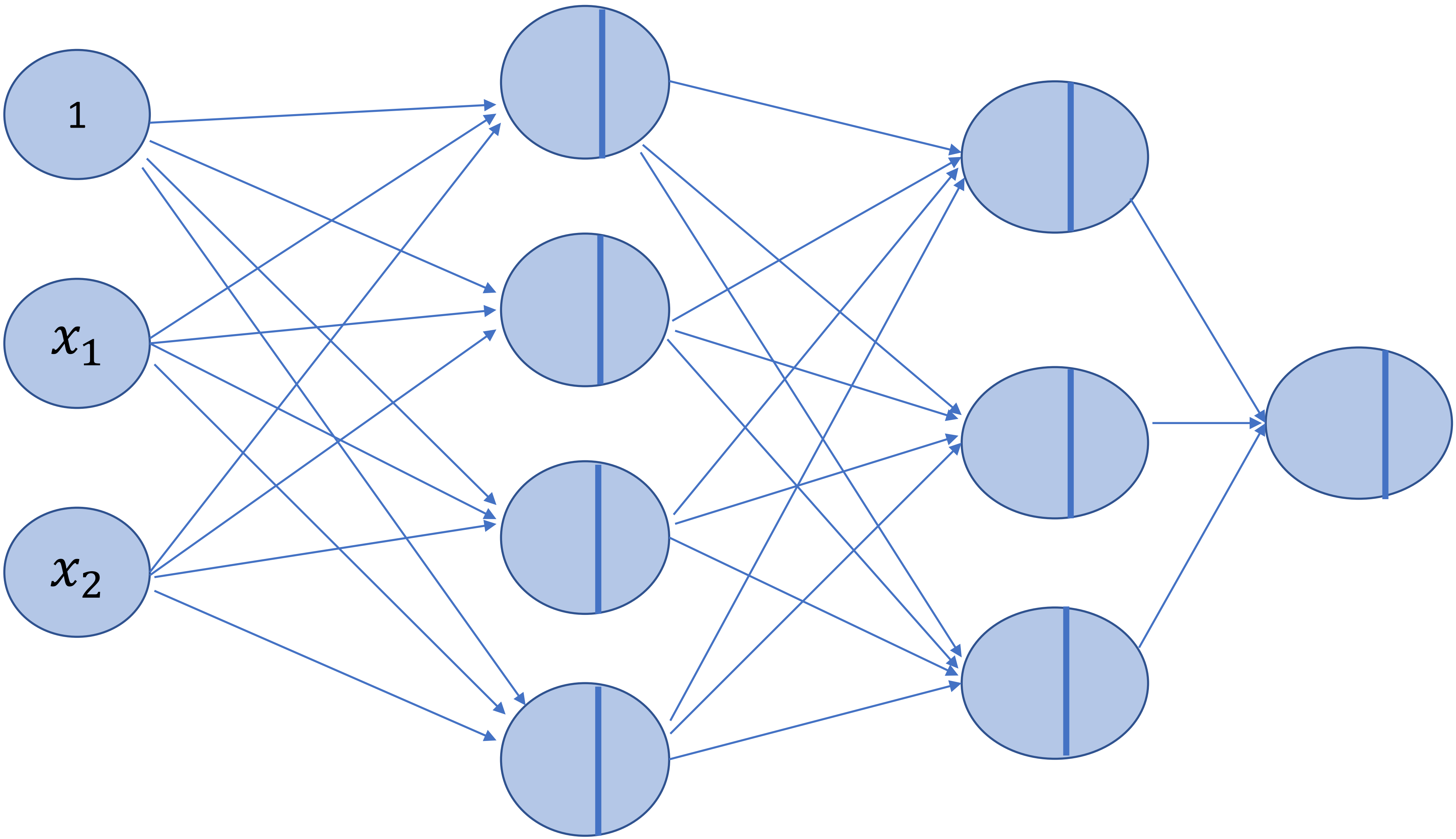
A shallow neural network



How many unknowns are to be estimated at the training stage?

3 X 4 + 4 + 1 = 17

A deep neural network



Another deep neural network

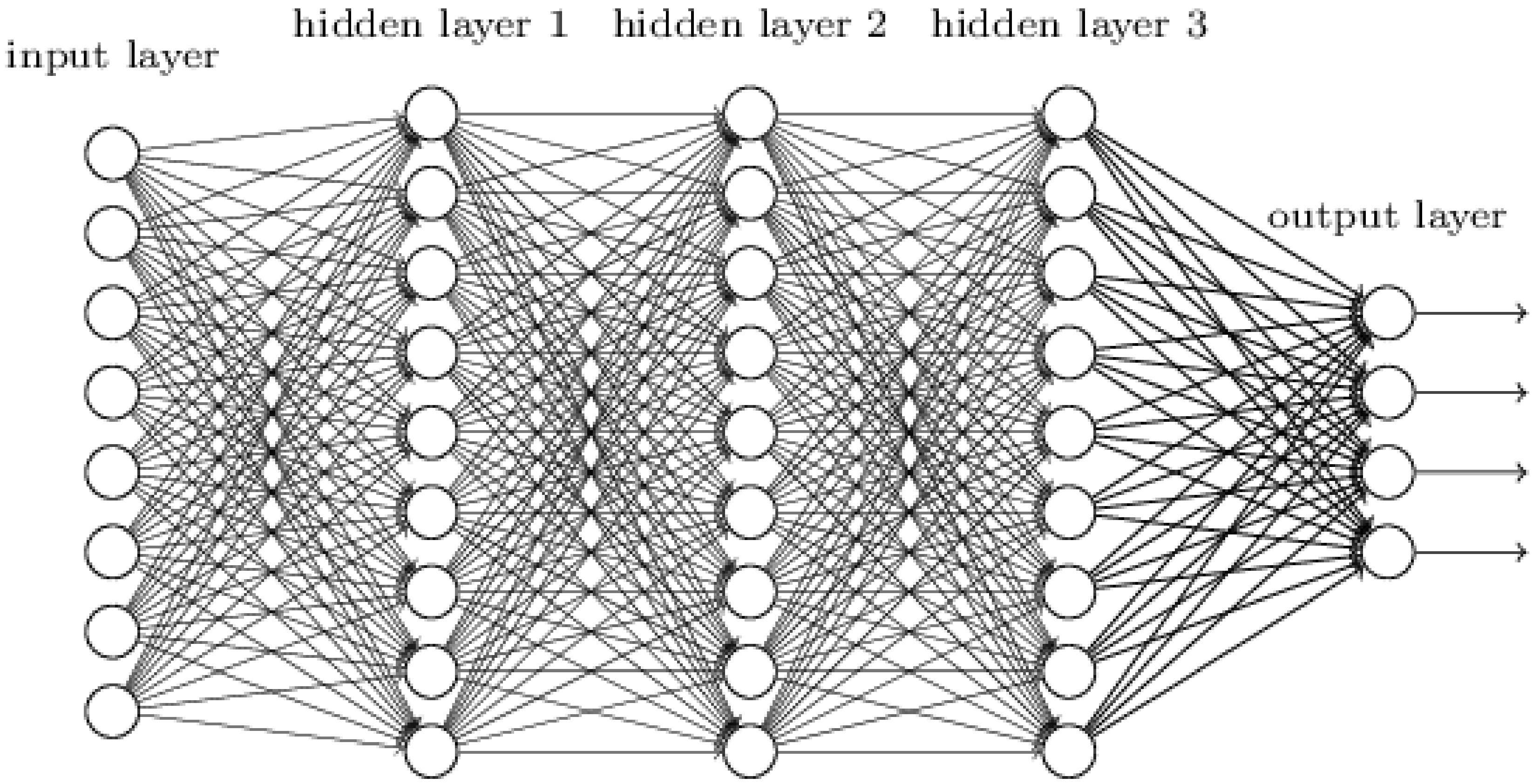
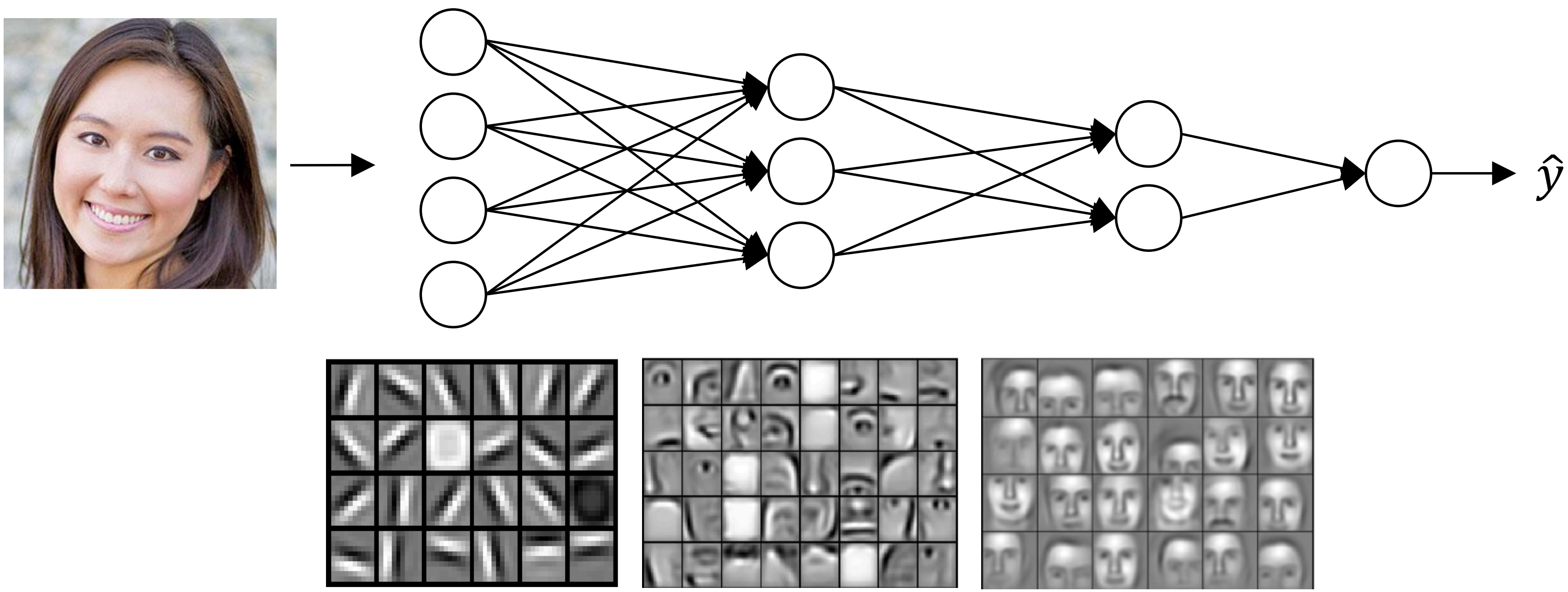


Image source: http://neuralnetworksanddeeplearning.com/chap5.html

Why deep representation?

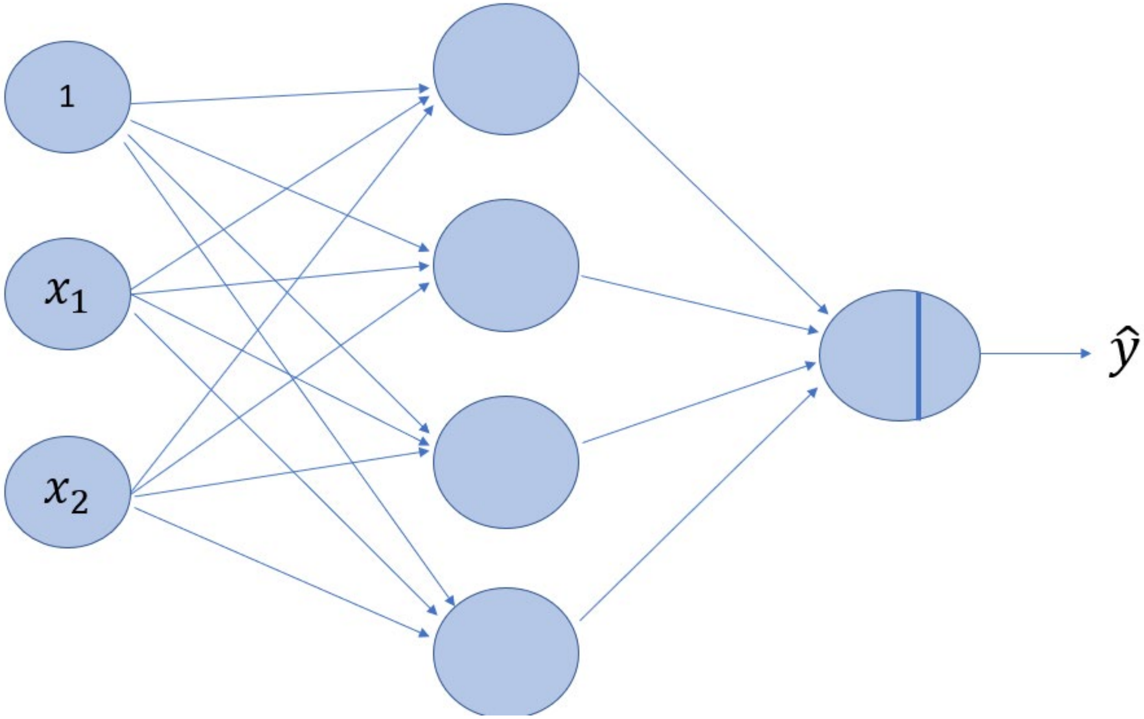


Credit: Andrew Ng

Forward propagation

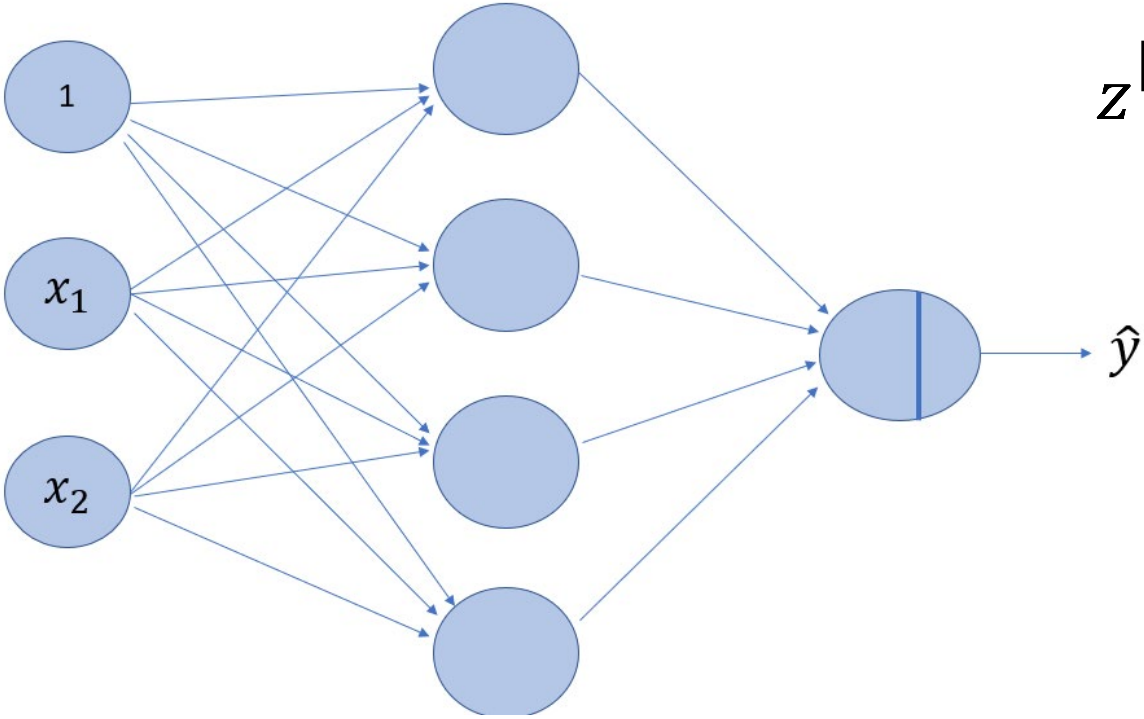
$$z^{[1]} = w^{[1]}x + b^{[1]}$$
$$a^{[1]} = g(z^{[1]})$$

$$z^{[2]} = w^{[2]}a^{[1]} + b^{[2]}$$
$$a^{[2]} = g(z^{[2]})$$



$$L = \frac{1}{2}||a^{[2]} - y||^2$$

A different representation



$$z^{[1]} = f_1(w^{[1]}, b^{[1]}, x)$$
$$a^{[1]} = g_1(z^{[1]})$$

$$z^{[2]} = f_2(w^{[2]}, b^{[2]}, a^{[1]})$$
$$a^{[2]} = g_2(z^{[2]})$$
$$L = l(a^{[2]})$$

Forward Propagation

$$
\left.\begin{array}{l} x \\ w^{[1]} \\ b^{[1]} \end{array}\right\} \rightarrow z^{[1]} = f_1(w^{[1]}, b^{[1]}) \rightarrow a^{[1]} = g_1(z^{[1]}) \rightarrow z^{[2]} = f_2(w^{[2]}, a^{[1]}, b^{[2]}) \rightarrow a^{[2]} = g_2(z^{[2]}) \rightarrow L(a^{[2]})
$$

Back Propagation

$$\frac{\partial L}{\partial w^{[1]}} = \frac{\partial L}{\partial g_2}\frac{\partial g_2}{\partial f_2}\frac{\partial f_2}{\partial g_1}\frac{\partial g_1}{\partial f_1}\frac{\partial f_1}{\partial w^{[1]}}$$

x, $w^{[1]}$, $b^{[1]}$

$$z^{[1]} = f_1(w^{[1]}, b^{[1]}) \longrightarrow a^{[1]} = g_1(z^{[1]}) \longrightarrow z^{[2]} = f_2(w^{[2]}, a^{[1]}, b^{[2]}) \longrightarrow a^{[2]} = g_2(z^{[2]}) \longrightarrow L(a^{[2]})$$

Gradient descent (for a 2-layer NN)

- Initialize $w^{[1]}, b^{[1]}, w^{[2]}, b^{[2]}$
- While (not converge):
-     compute $\frac{\partial L}{\partial w^{[1]}}, \frac{\partial L}{\partial b^{[1]}}, \frac{\partial L}{\partial w^{[2]}}, \frac{\partial L}{\partial b^{[2]}}$
-     $w^{[1]} = w^{[1]}\text{-}\alpha \frac{\partial L}{\partial w^{[1]}}$
-     $b^{[1]} = b^{[1]}\text{-}\alpha \frac{\partial L}{\partial b^{[1]}}$
-     $w^{[2]} = w^{[2]}\text{-}\alpha \frac{\partial L}{\partial w^{[2]}}$
-     $b^{[2]} = b^{[2]}\text{-}\alpha \frac{\partial L}{\partial b^{[2]}}$
- end

- Backpropagation works its way from the output layer to the input layer
- Computes the error gradients on the way

Aurelien Geron, 2017, Hands-on Machine Learning with Scikit-Learn & TensorFlow, pp 275-276

Vanishing gradients

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- Unfortunately, gradients often get smaller and smaller as we move backward through the layers
- This leaves the weights associated with shallower layers virtually unchanged, and makes learning at those layers much slower than deeper layers.
- This was a barrier to training deep NN for a long time.

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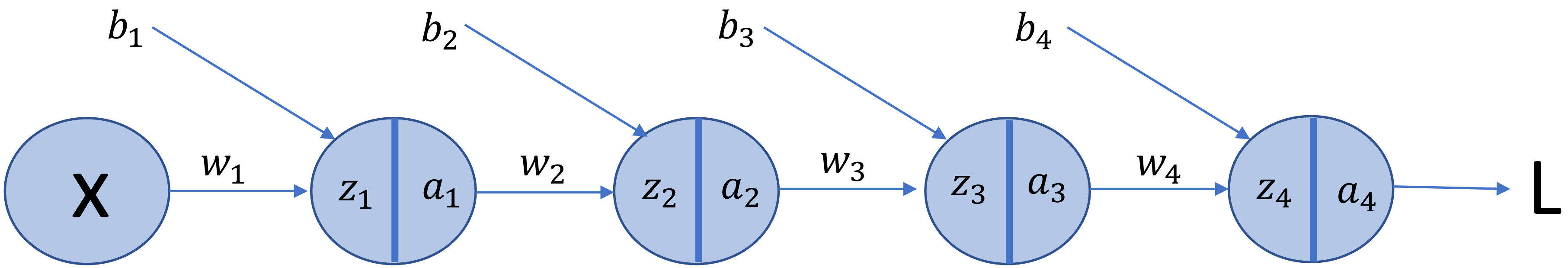
Understanding vanishing gradients

- Let us consider the simplest deep neural network



$$z_j = w_j a_{j-1} + b_j$$

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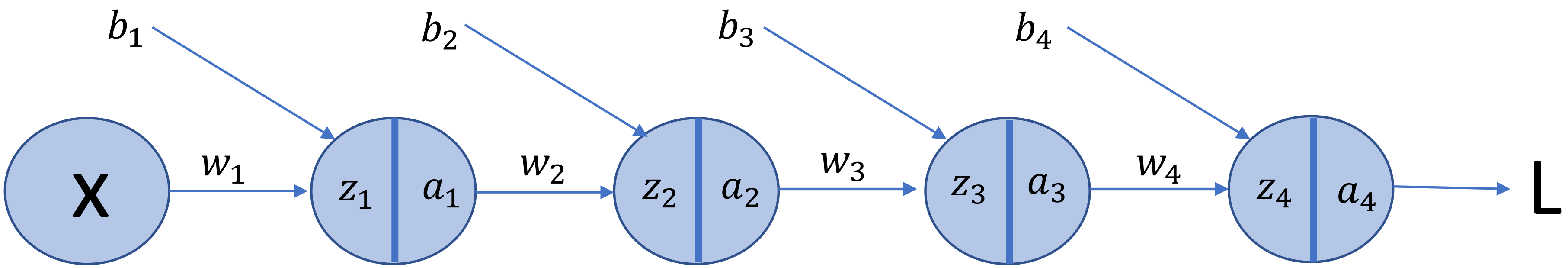

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Let us take a closer look at the gradient $\frac{\partial L}{\partial b_1}$

Understanding vanishing gradients

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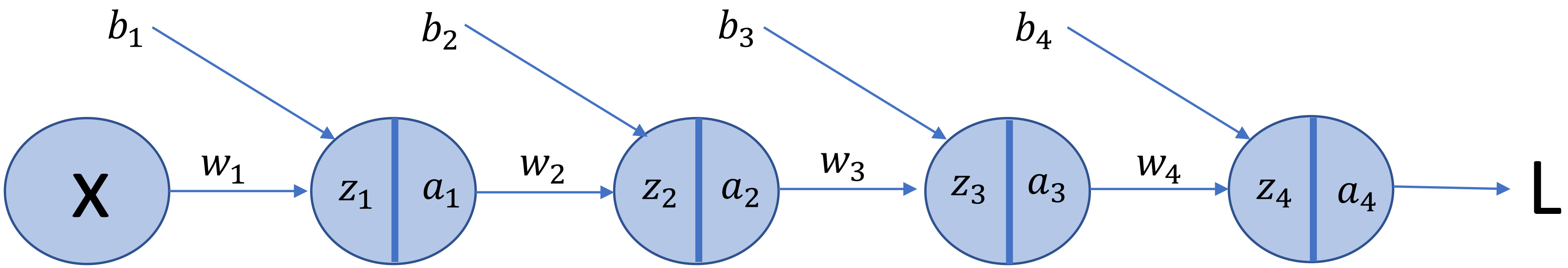

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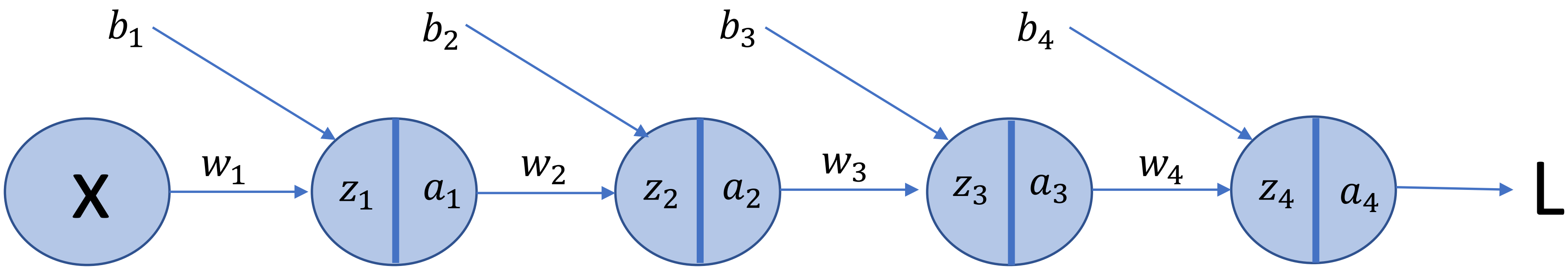

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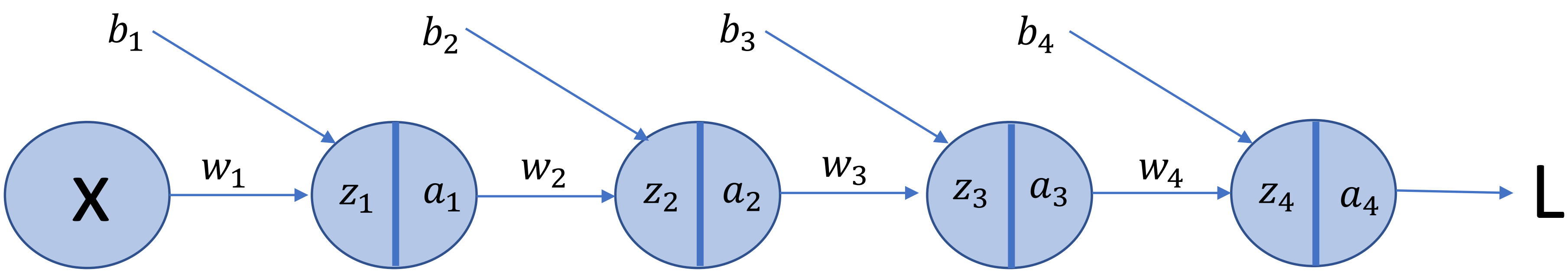

$$z_j = w_j a_{j-1} + b_j$$

$$a_j = g(z_j) \longrightarrow \frac{\partial a_j}{\partial z_j} = g'(z_j)$$

$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times \frac{\partial z_4}{\partial a_3} \times \frac{\partial a_3}{\partial z_3} \times \frac{\partial z_3}{\partial a_2} \times \frac{\partial a_2}{\partial z_2} \times \frac{\partial z_2}{\partial a_1} \times \frac{\partial a_1}{\partial z_1} \times \frac{\partial z_1}{\partial b_1}$$

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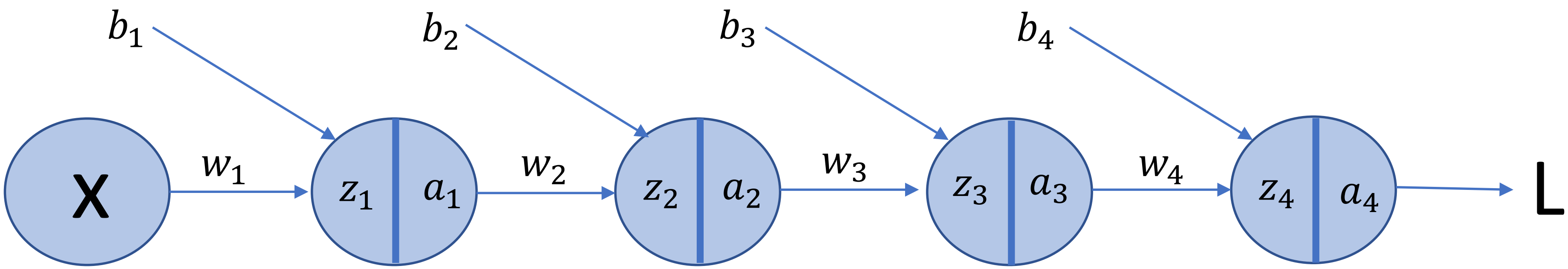

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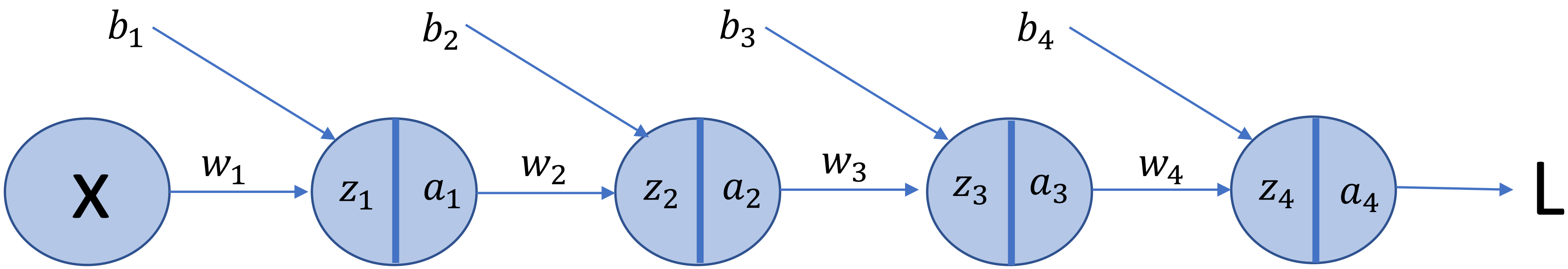

$$z_j = w_j a_{j-1} + b_j \Rightarrow \frac{\partial z_j}{\partial a_{j-1}} = w_j$$

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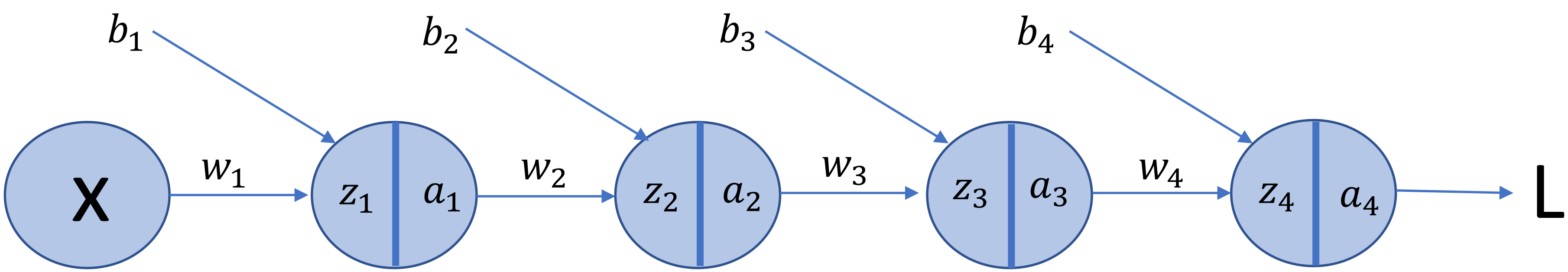

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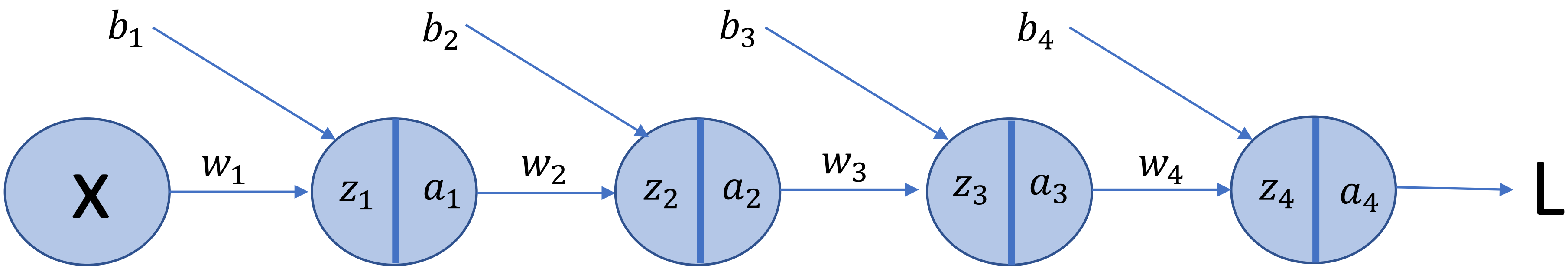

$$z_j = w_j a_{j-1} + b_j \Rightarrow \frac{\partial z_j}{\partial a_{j-1}} = w_j \qquad \frac{\partial z_1}{\partial b_1} = 1$$

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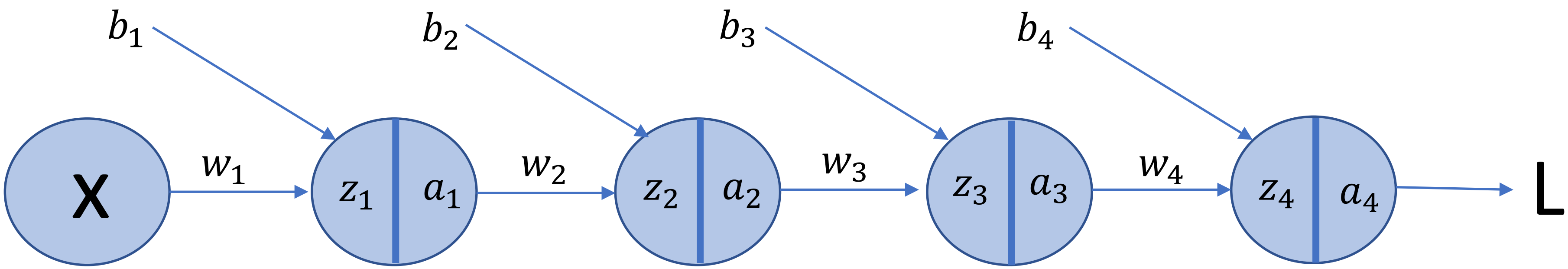

$$z_j = w_j a_{j-1} + b_j \quad \Rightarrow \quad \frac{\partial z_j}{\partial a_{j-1}} = w_j \qquad \frac{\partial z_1}{\partial b_1} = 1$$

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$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \times g'(z_4) \times w_4 \times g'(z_3) \times w_3 \times g'(z_2) \times w_2 \times g'(z_1)$$

Understanding vanishing gradients

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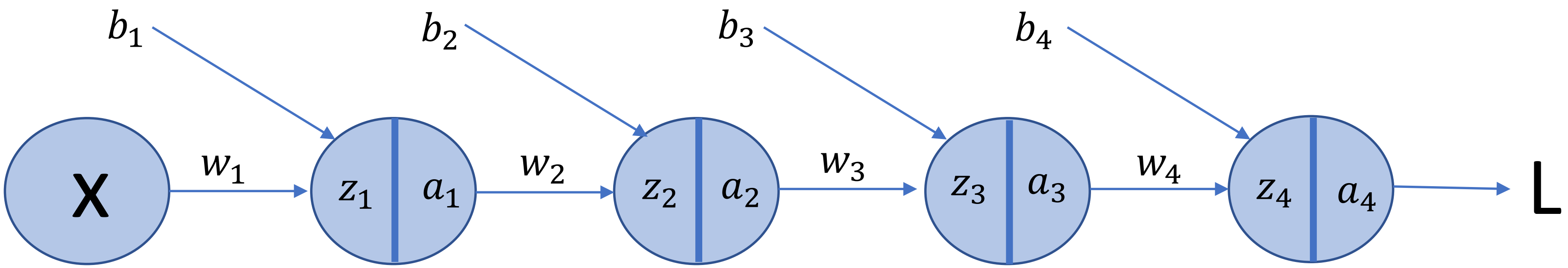
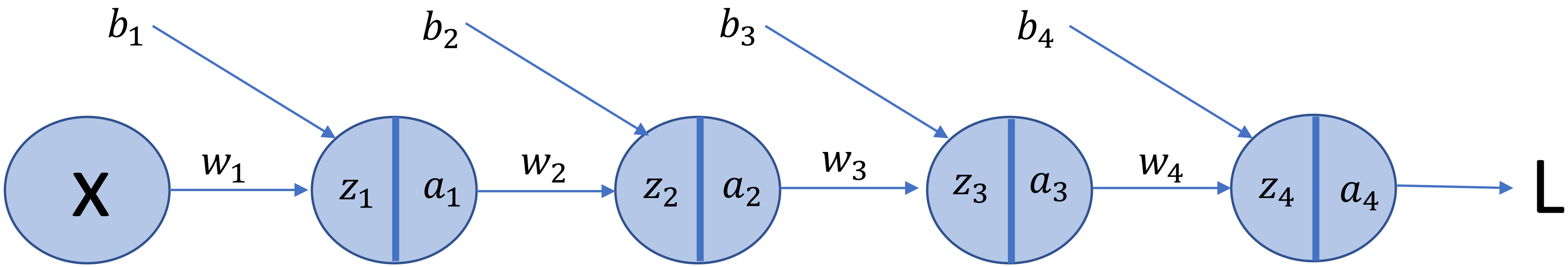


$\frac{\partial L}{\partial b_1}$ measures how much change would happen to the cost function if b_1 changes.

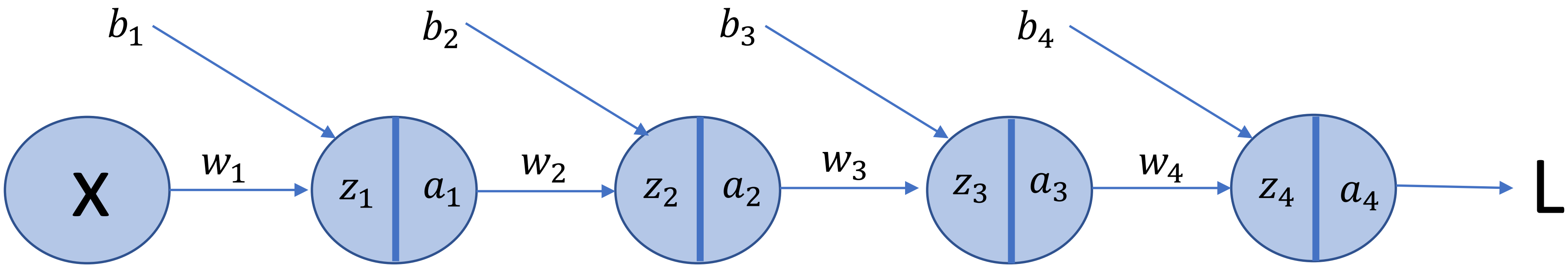
$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \times g'(z_4) \times w_4 \times g'(z_3) \times w_3 \times g'(z_2) \times w_2 \times g'(z_1)$$

Understanding vanishing gradients



$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \boxed{g'(z_4)\, w_4} \boxed{g'(z_3)\, w_3} \boxed{g'(z_2)\, w_2}\, g'(z_1)$$

Understanding vanishing gradients



$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \boxed{g'(z_4)\, w_4} \boxed{g'(z_3)\, w_3} \boxed{g'(z_2)\, w_2}\, g'(z_1)$$

Remember $g(z) = \frac{1}{1+e^{-z}}$

$$|g'(z_j)| \le \frac{1}{4}$$

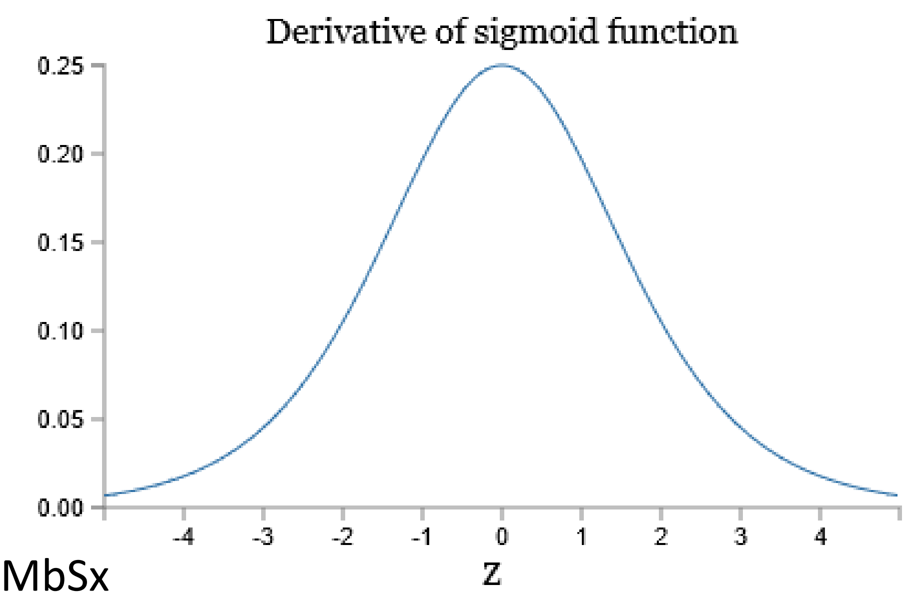
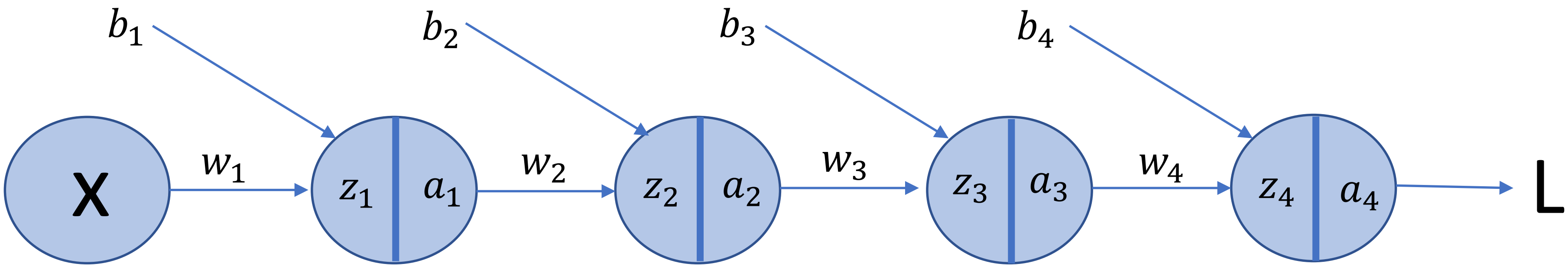


Image source: https://goo.gl/s3MbSx

Understanding vanishing gradients



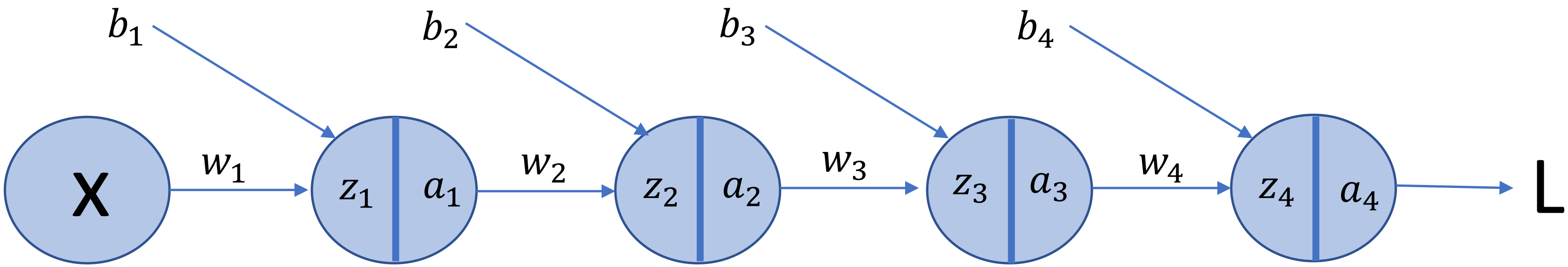
$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_4} \boxed{g'(z_4)\, w_4} \boxed{g'(z_3)\, w_3} \boxed{g'(z_2)\, w_2}\, g'(z_1)$$

Let us assume that the weights are randomly initialized using a Gaussian with mean 0 and standard deviation of 1. (very popular)

So, weights will usually satisfy $|w_j| < 1$

Therefore, $|g'(z_j)w_j| < \frac{1}{4}$

Understanding vanishing gradients



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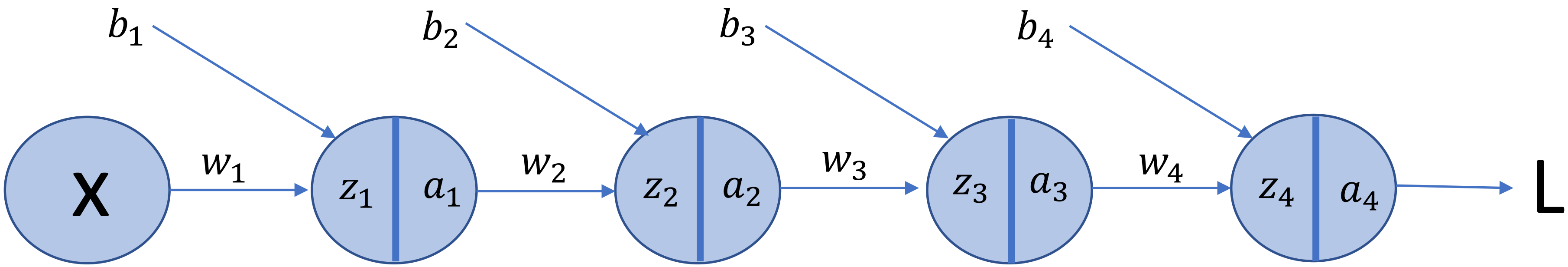
When we take a product of many such terms, the product will exponentially decrease: the more terms, the smaller the product.

$\frac{\partial L}{\partial b_1}$ becomes very very small for deep neural networks.

Therefore, $\left|g'(z_j)w_j\right| < \frac{1}{4}$

Understanding vanishing gradients



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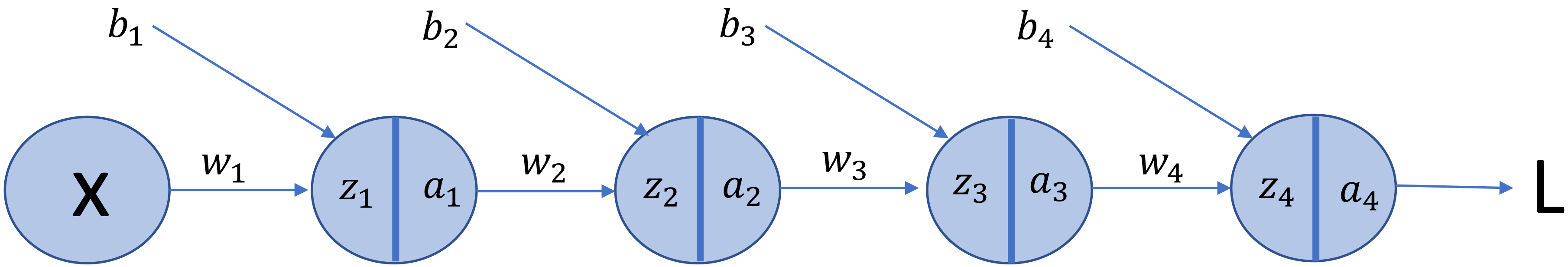
Vanishing gradients!!!

Understanding vanishing gradients



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<u>Vanishing gradients!!!</u>

Different layers in the network will learn at vastly different speeds.

Note

- The problem has been empirically observed for quite a while
- It was one of the reasons why deep NNs were mostly abandoned for a long time
- In 2010, a paper titled 'Understanding the difficulty of training deep feedforward neural networks' by Xavier Glorot and Yoshua Bengio shed some lights on it.

Observations

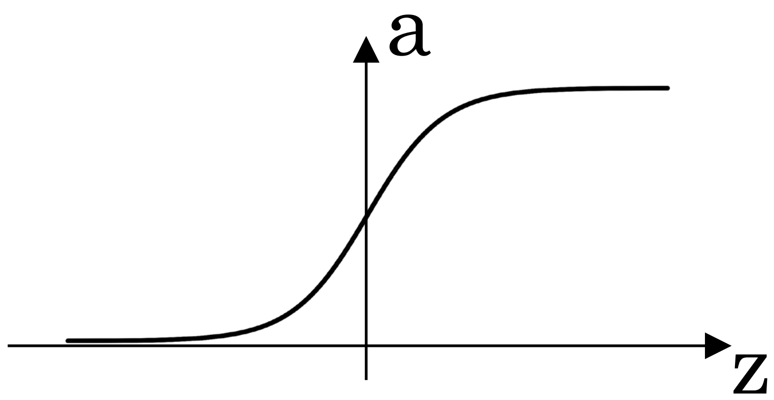
- It is the combination of logistic activation function and the weight initialization strategy that causes the vanishing gradient problem. (Glorot and Bengio, 2010).

Two strategies

- Use a different activation function
- Use a different initialization scheme

Activation function

- Sigmoid function

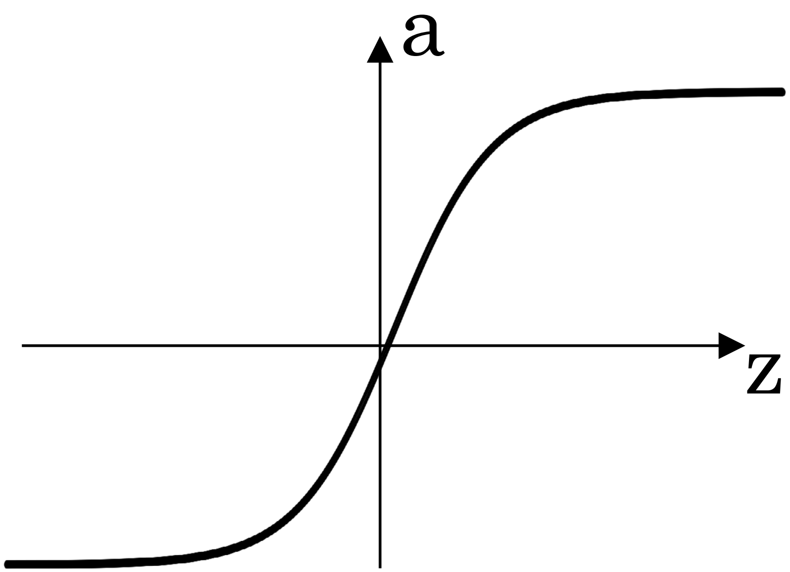


$$g(z) = \frac{1}{1 + e^{-z}}$$

Image credit: Andrew Ng

Activation function

- Tanh (hyperbolic tangent) function

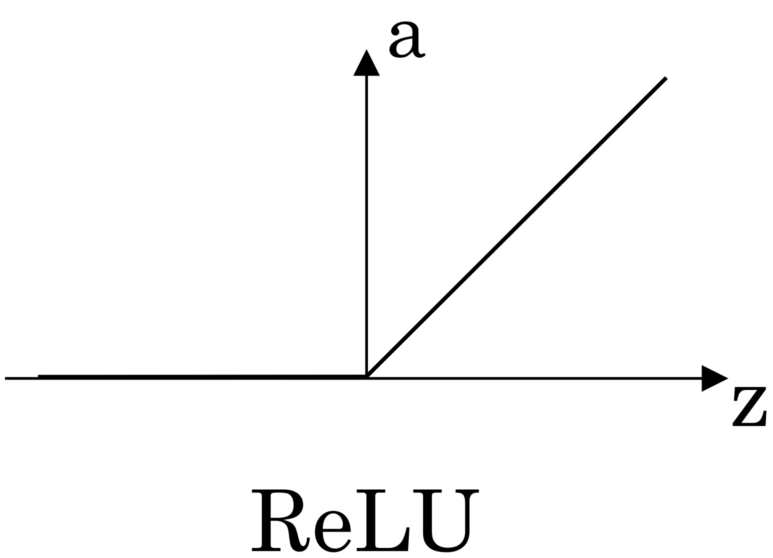


$$g(z) = \tanh(z)$$

Image credit: Andrew Ng

Activation function

- ReLU (rectified linear units) function



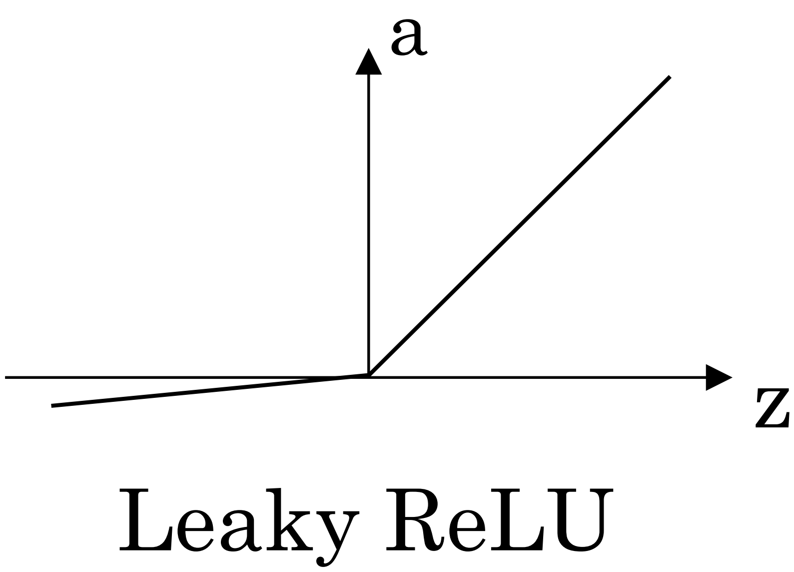
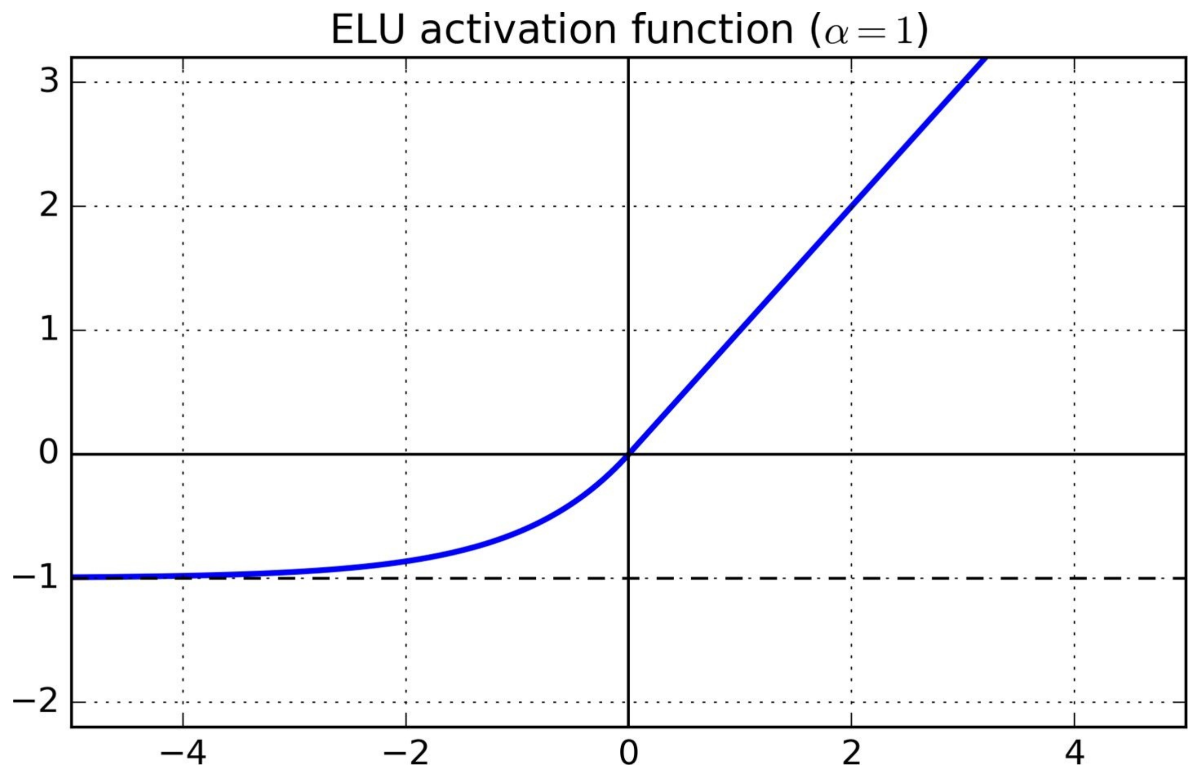


Image credit: Andrew Ng

Activation function

- ELU (exponential linear unit) function



Aurelien Geron, 2017, Hands-on Machine Learning with Scikit-Learn & TensorFlow, pp 280

Xavier and He initialization

Table 11-1. Initialization parameters for each type of activation function

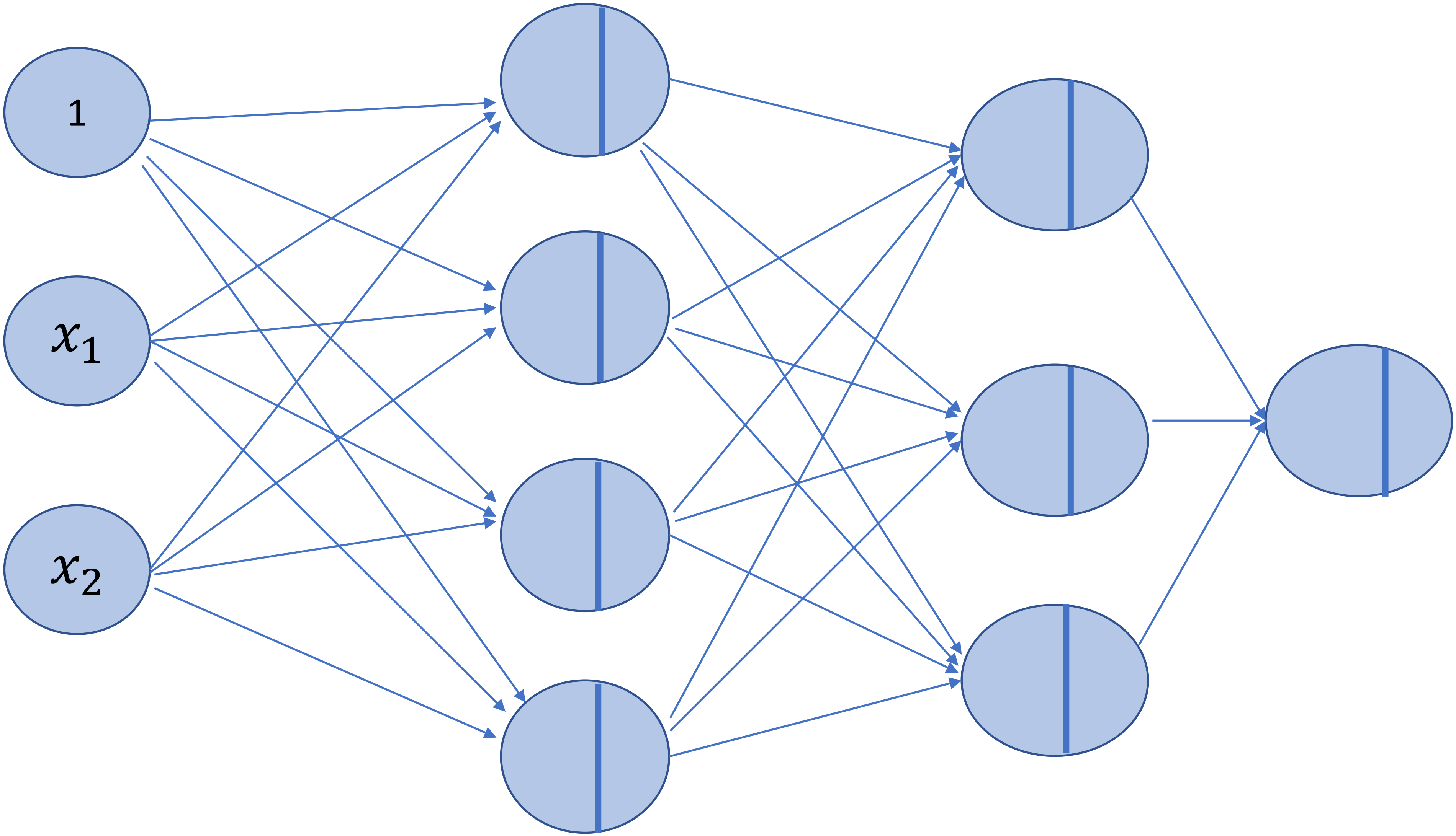
Activation function	Uniform distribution [–r, r]	Normal distribution
Xavier initialization (2010) Logistic	$r = \sqrt{\frac{6}{n_{\text{inputs}} + n_{\text{outputs}}}}$	$\sigma = \sqrt{\frac{2}{n_{\text{inputs}} + n_{\text{outputs}}}}$
Hyperbolic tangent	$r = 4\sqrt{\frac{6}{n_{\text{inputs}} + n_{\text{outputs}}}}$	$\sigma = 4\sqrt{\frac{2}{n_{\text{inputs}} + n_{\text{outputs}}}}$
He initialization (2015) ReLU (and its variants)	$r = \sqrt{2}\sqrt{\frac{6}{n_{\text{inputs}} + n_{\text{outputs}}}}$	$\sigma = \sqrt{2}\sqrt{\frac{2}{n_{\text{inputs}} + n_{\text{outputs}}}}$

Aurelien Geron, 2017, Hands-on Machine Learning with Scikit-Learn & TensorFlow, pp 278

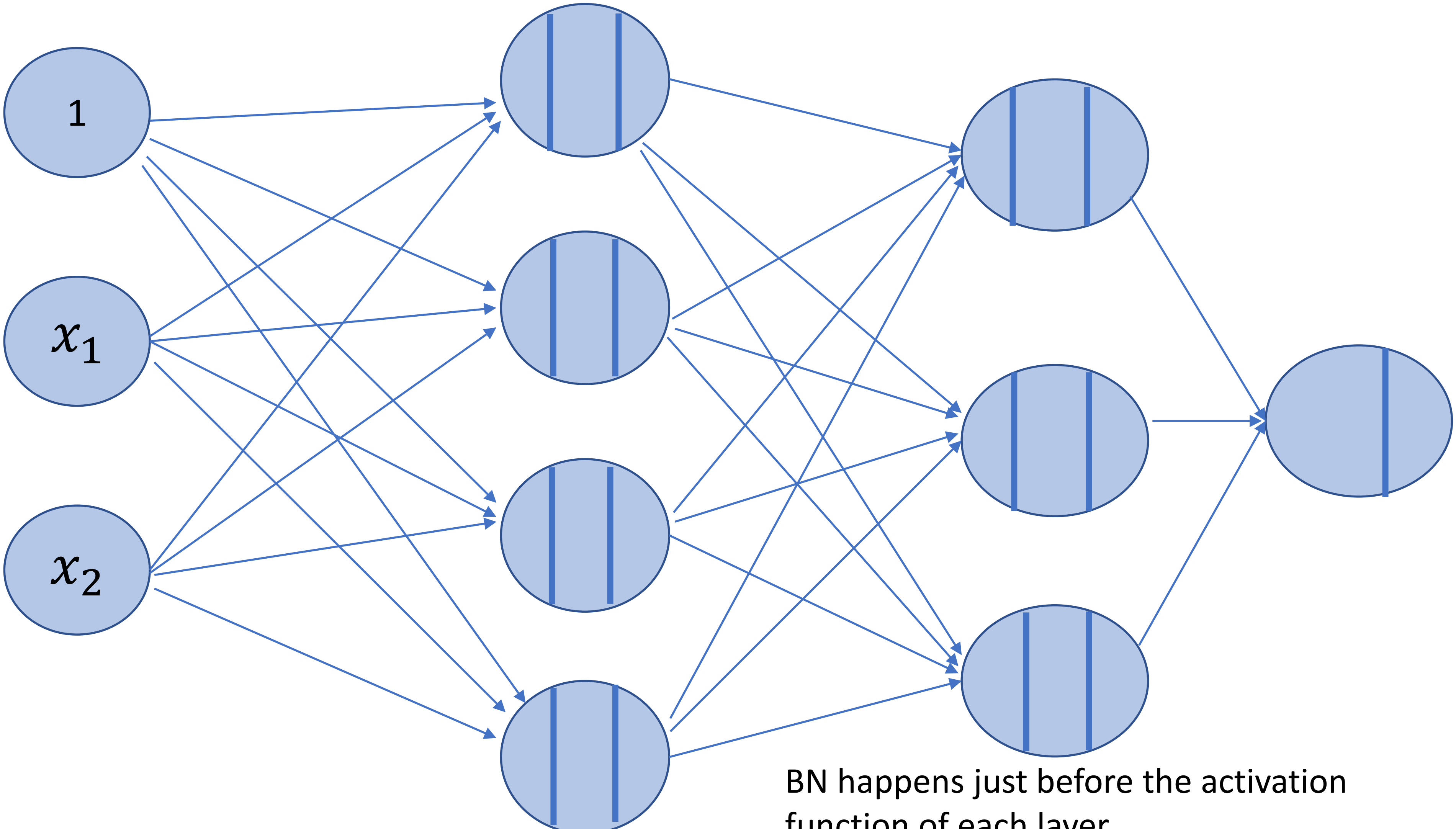
Batch normalization

- Another way of dealing with the vanishing gradient problem
- Proposed by Sergey Ioffe and Christian Szegedy in 2015.

A deep neural network w/o BN



A deep neural network w/ BN



BN happens just before the activation function of each layer

Batch normalization (Ioffe and Szegedy, 2015)

- Let us consider jth layer, suppose there are m neurons in this layers
- $\mu = \frac{1}{m}\sum_{i=1}^{m} z_i^{[j]}$
- $\sigma = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(z_i^{[j]} - \mu)^2}$
- $\hat{z}_i^{[j]} = \frac{z_i^{[j]}-\mu}{\sqrt{\sigma^2+\varepsilon}}$
- $\tilde{z}_i^{[j]} = \gamma\hat{z}_i^{[j]} + \beta$

γ and β are learned during training.

Optimization algorithms

- Mini-batch gradient descent
  - tf.train.GradientDescentOptimizer()
- Momentum Optimization
  - tf.train.MomentumOptimizer()
- RMSProp
  - tf.train.RMSPropOptimizer()
- Adam Optimization
  - tf.train.AdamOptimizer()

https://www.tensorflow.org/api_guides/python/train

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Training

`tf.train` provides a set of classes and functions that help train models.

Optimizers

The Optimizer base class provides methods to compute gradients for a loss and apply gradients to variables. A collection of subclasses implement classic optimization algorithms such as GradientDescent and Adagrad.

You never instantiate the Optimizer class itself, but instead instantiate one of the subclasses.

- `tf.train.Optimizer`
- `tf.train.GradientDescentOptimizer`
- `tf.train.AdadeltaOptimizer`
- `tf.train.AdagradOptimizer`
- `tf.train.AdagradDAOptimizer`
- `tf.train.MomentumOptimizer`
- `tf.train.AdamOptimizer`
- `tf.train.FtrlOptimizer`
- `tf.train.ProximalGradientDescentOptimizer`
- `tf.train.ProximalAdagradOptimizer`
- `tf.train.RMSPropOptimizer`

See `tf.contrib.opt` for more optimizers.

Implementing DNN in TensorFlow