Neural Networks: Feedforward

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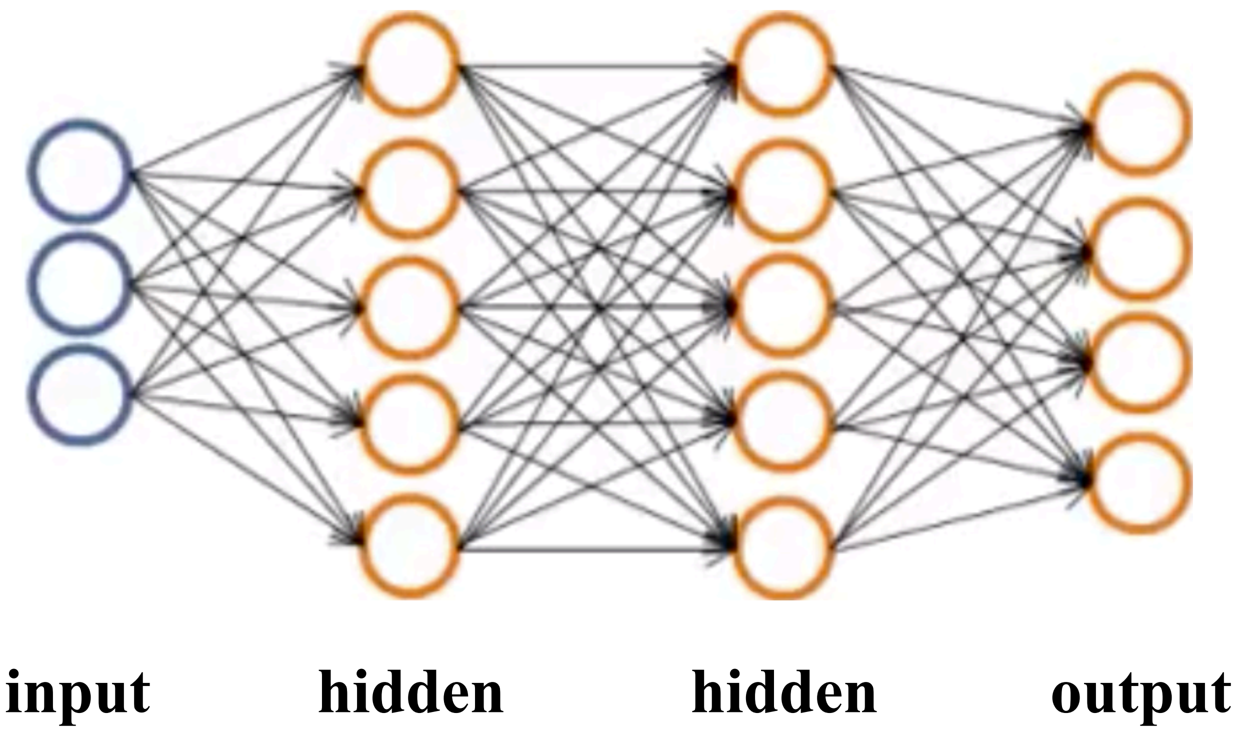
Recap

- Given a dataset $(\boldsymbol{x}^{(i)}, y^{(i)})$, the goal of neural network is to find intermediate features that will best predict each $y^{(i)}$ from the corresponding $\boldsymbol{x}^{(i)}$.
- Neural networks are sometime called 'black boxes' since it is difficult to understand the 'meaning' of induced intermediate features.



Neural Network's Notation

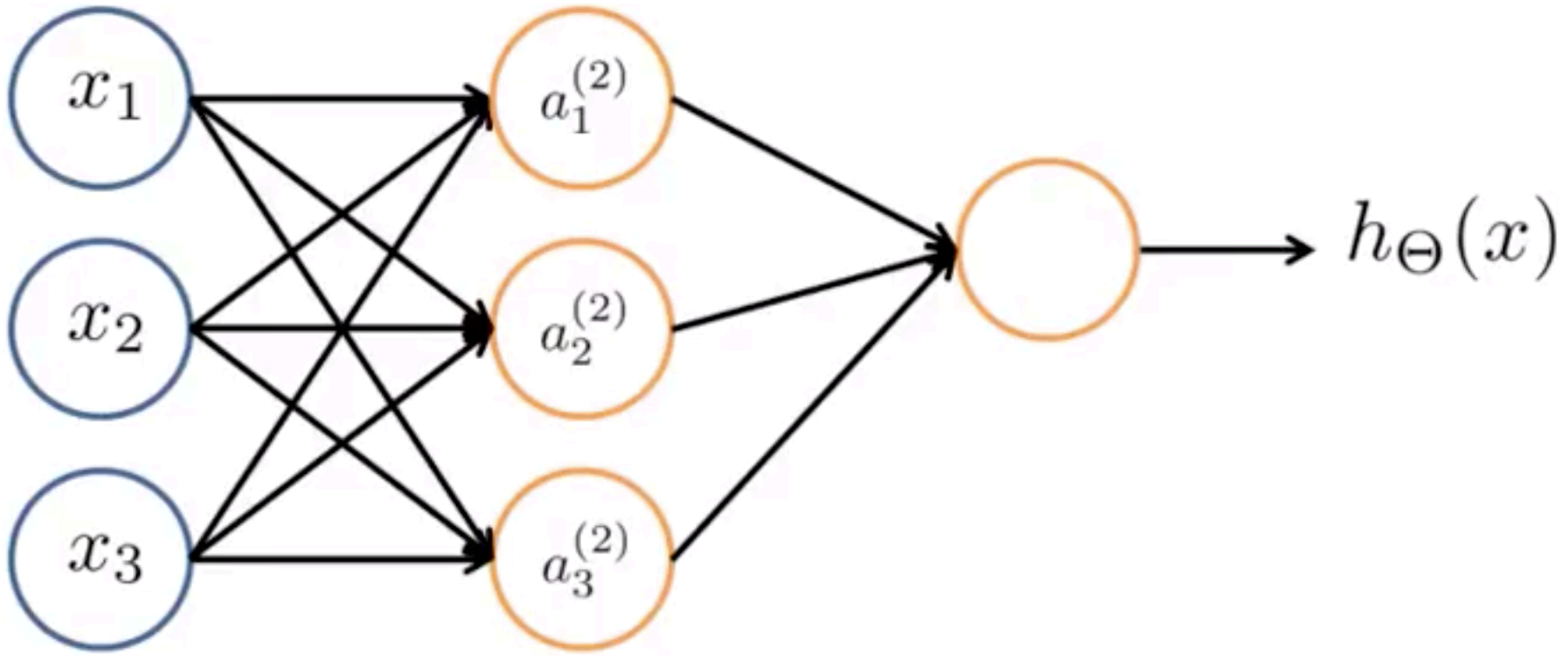
Suppose we have an input layer composed of features $x_1, x_2, \ldots$

Let's use the notation $a_i^{(j)}$ to indicate the activation of the ith unit in the jth layer *e.g.*

- $a_1^{(2)}$ is the output of the first hidden unit in the first hidden layer;
- $a_1^{(3)}$ is the output of the first unit in the second hidden layer (or the output layer in a network with only one hidden layer).

To unify the notation, we let $a_i^{(1)} = x_i$ *i.e.* we treat the input as layer 1.

Neural Network's Notation



Layer 1 **Layer 2** **Layer 3**

"input layer" **"hidden layer"** **"output layer"**

Activation Functions

We saw a simple ReLU network already.

Logistic regression can also be treated as a simple neural network with one output unit and no hidden units *i.e.*

$$g(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^T \boldsymbol{x}}}$$

can be written in neural networks as two steps:

1. Calculate the linear response $z = \theta_0 + \Sigma_{i=1}^{n} \theta_i x_i$
2. Calculate the activation function $a = \sigma(z)$ where $\sigma(z) = \dfrac{1}{1 + e^{-z}}$

Activation Functions

Usually, $g(z)$ is non-linear.

The most common activation functions are:

1. Sigmoid: $g(z) = \dfrac{1}{1 + e^{-z}}$
2. ReLU (the default activation function in modern neural networks): $g(z) = \max(z,0)$
3. Hyperbolic tangent: $g(z) = \dfrac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$

Forward Propagation

- The full calculation proceeds as follows:
- For the first hidden unit in the first hidden layer, we calculate:

$$z_1^{(2)} = \Theta^{(1)^T} \boldsymbol{x} + \theta_0^{(1)}$$

Play a role of bias, which always output 1

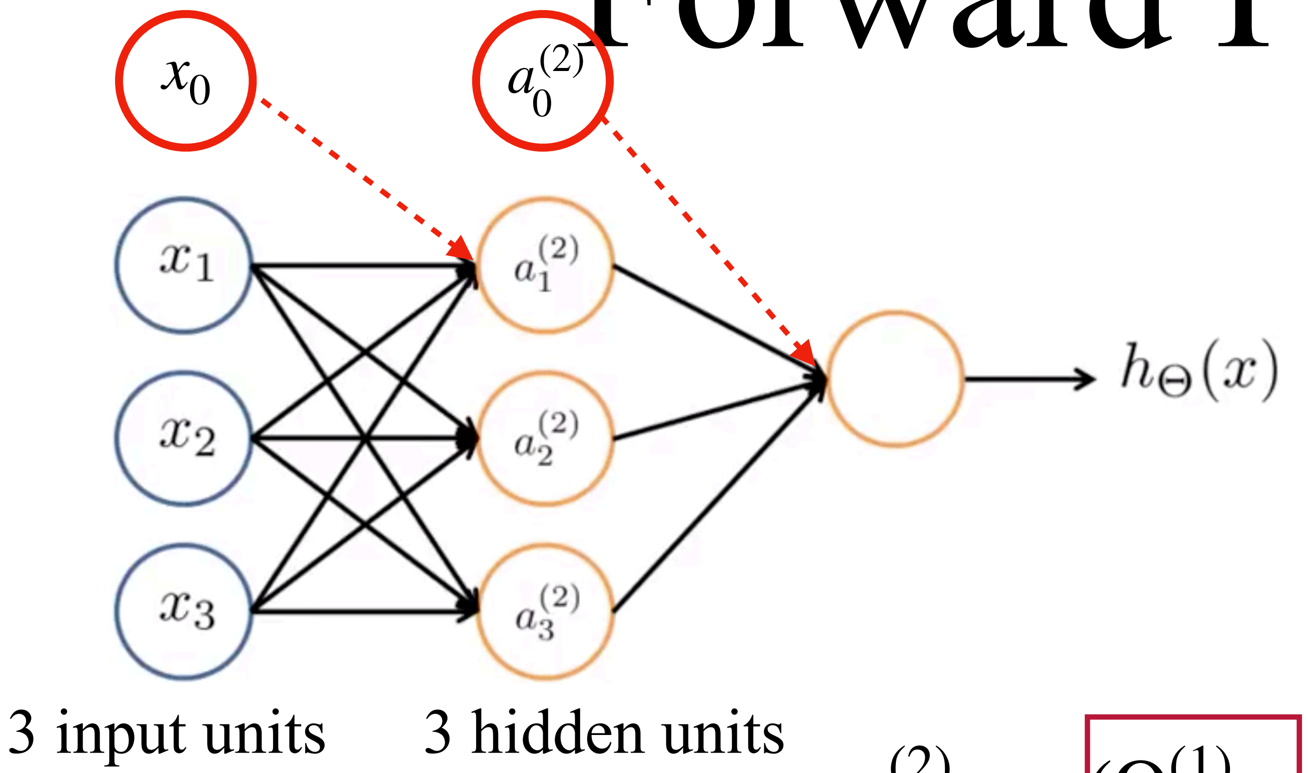
and

$$a_1^{(2)} = g(z_1^{(2)})$$

where $\Theta^{(j)}$ is a matrix of parameters or weights controlling function mapping from layer j to layer $j+1$.

- We repeat for each unit in each layer to get the final output layer.

Forward Propagation



$a_i^{(j)}$ = 'activation' of unit i in layer j

$\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$

$\Theta^{(i)} \in \mathbb{R}^{3\times4}$

$$a_1^{(2)} = g(\boxed{\Theta_{10}^{(1)}x_0} + \boxed{\Theta_{11}^{(1)}x_1} + \boxed{\Theta_{12}^{(1)}x_2} + \boxed{\Theta_{13}^{(1)}x_3})$$
$$a_2^{(2)} = g(\boxed{\Theta_{20}^{(1)}x_0} + \boxed{\Theta_{21}^{(1)}x_1} + \boxed{\Theta_{22}^{(1)}x_2} + \boxed{\Theta_{23}^{(1)}x_3})$$
$$a_3^{(2)} = g(\boxed{\Theta_{30}^{(1)}x_0} + \boxed{\Theta_{31}^{(1)}x_1} + \boxed{\Theta_{32}^{(1)}x_2} + \boxed{\Theta_{33}^{(1)}x_3})$$

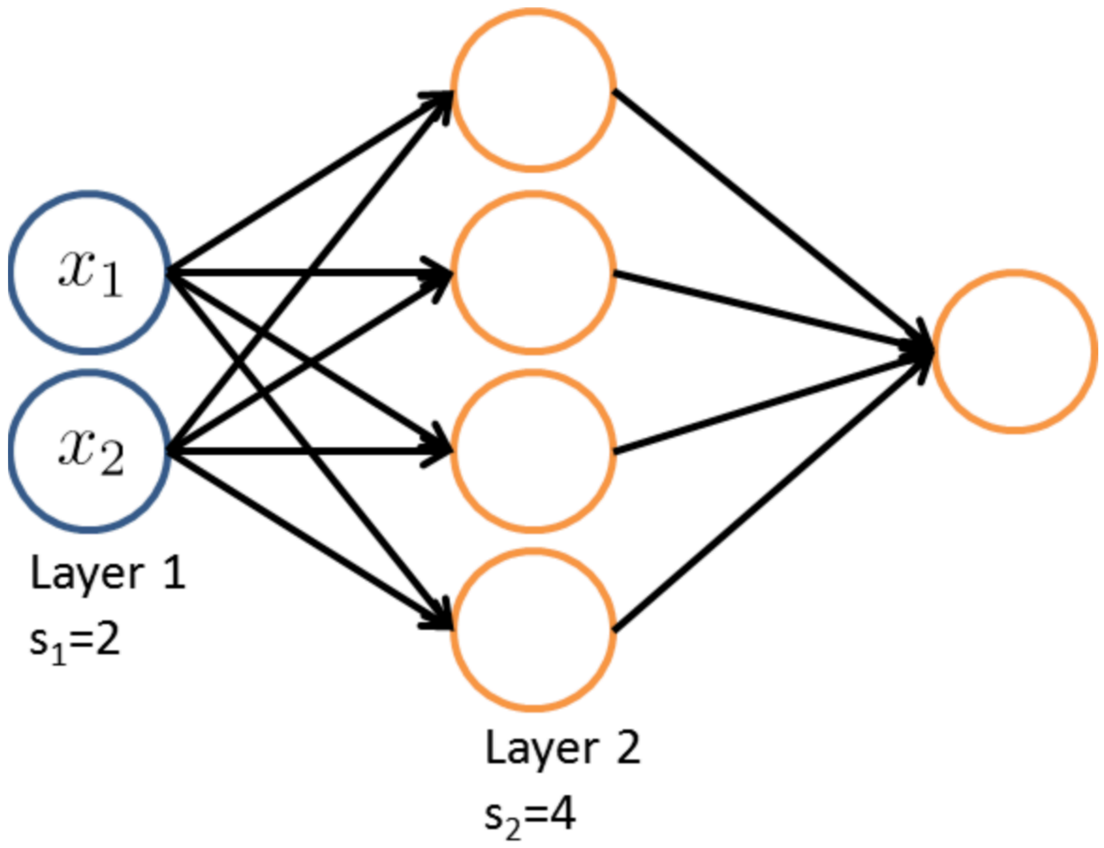
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

Formally, If network has s_j units in layer j, s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

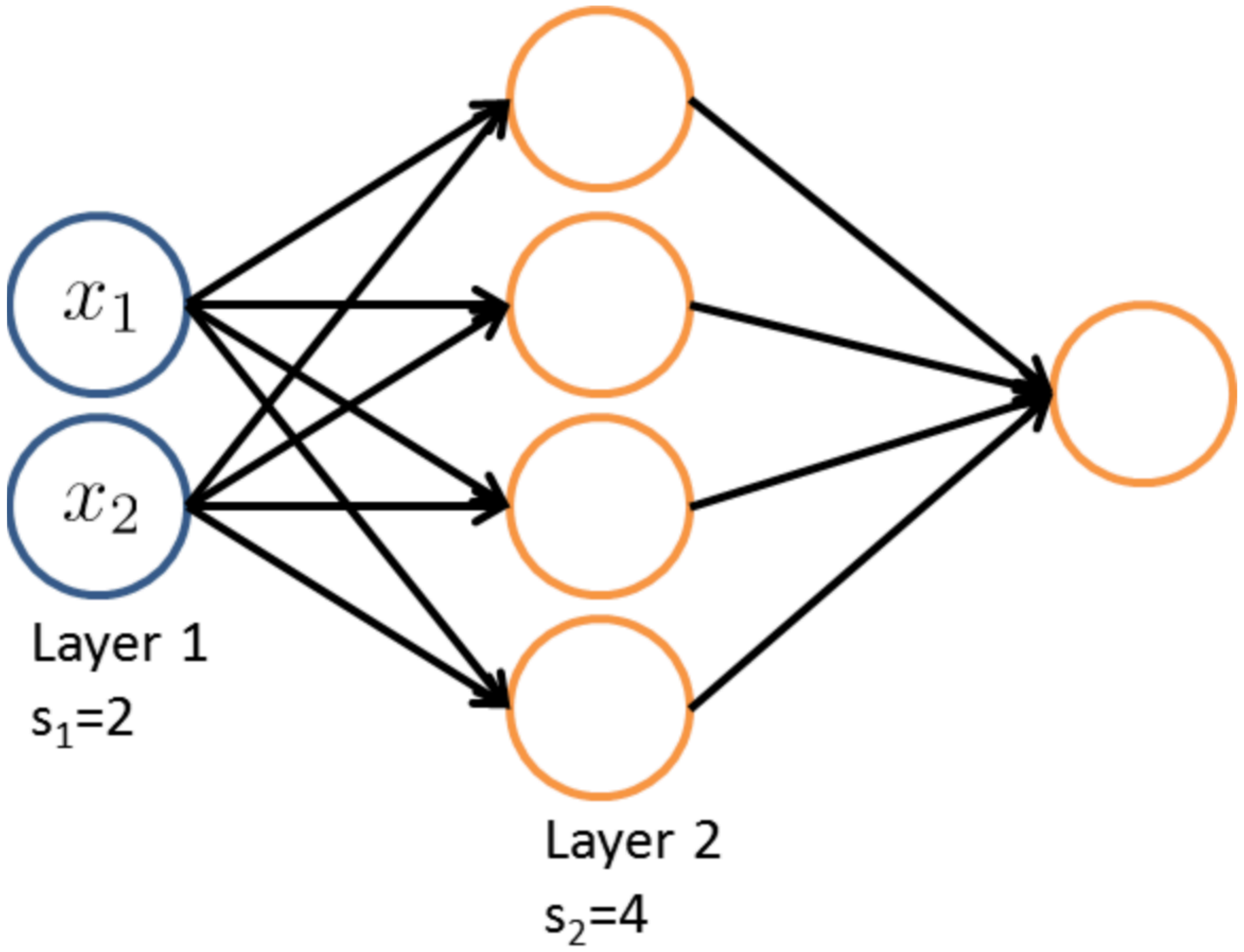
Question

Consider the neural network.
What is the dimension of $\Theta^{(1)}$?

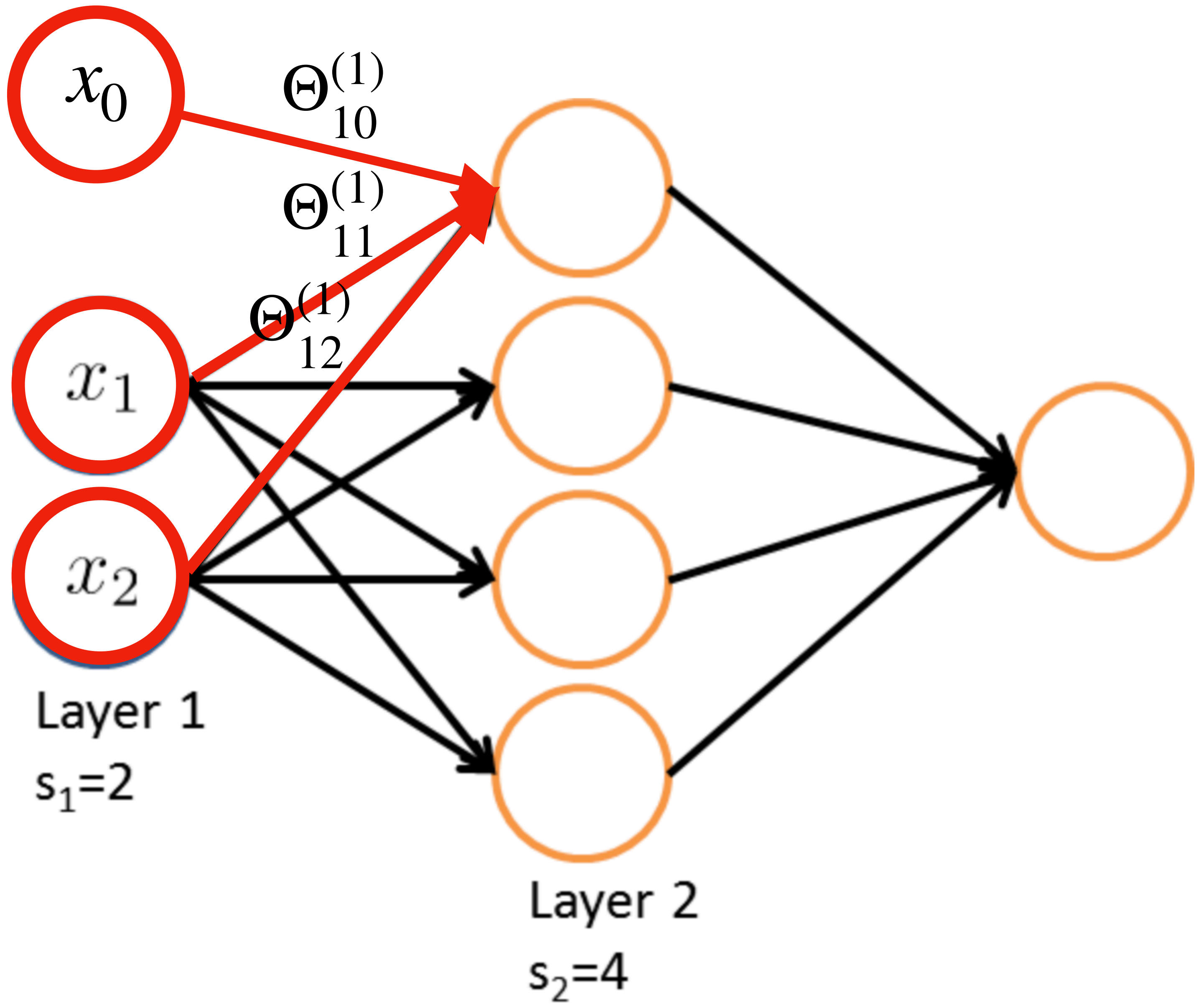
(i) 2 x 4
(ii) 4 x 2
(iii) 3 x 4
(iv) 4 x 3



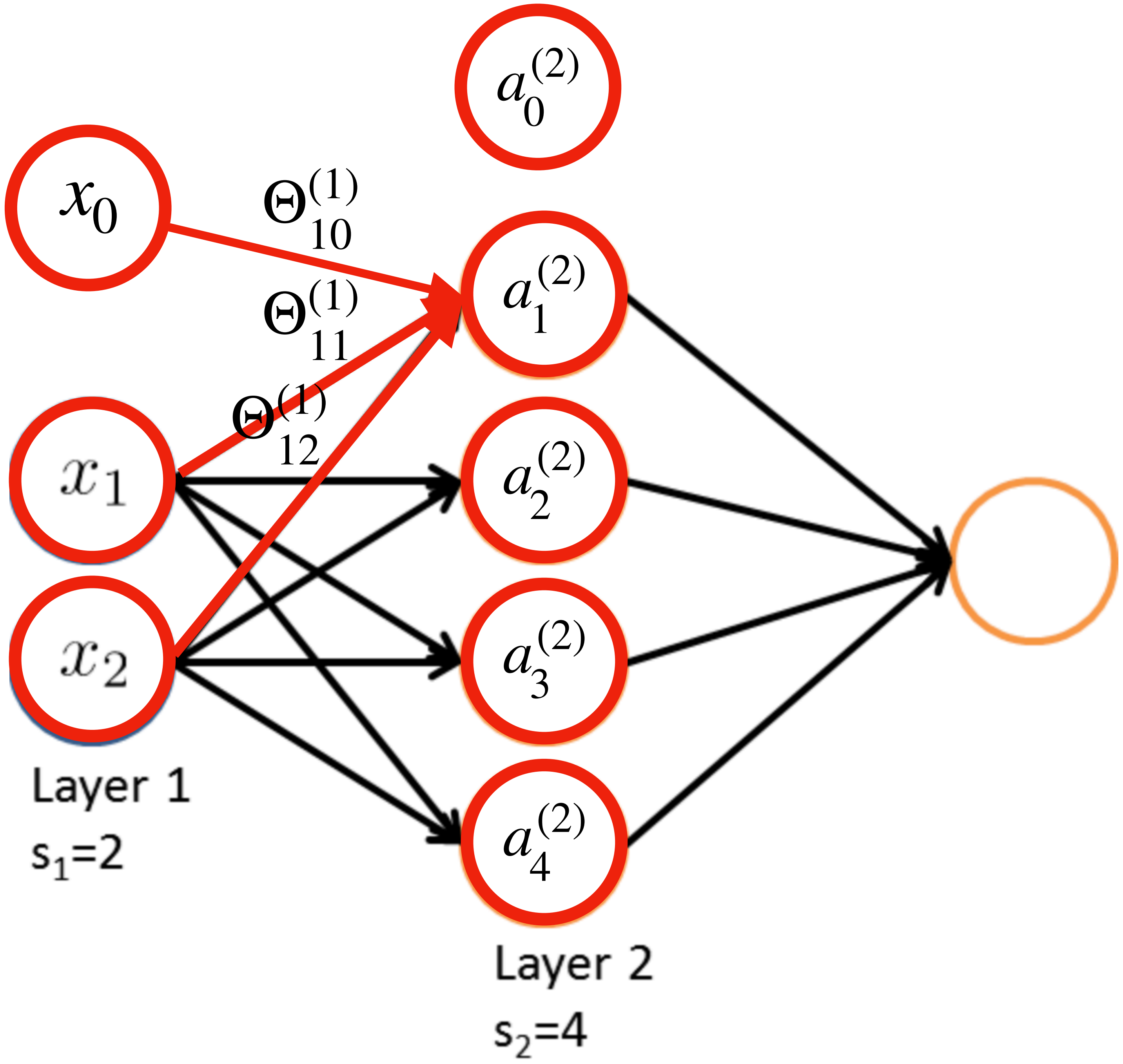
Feedforward Propagation



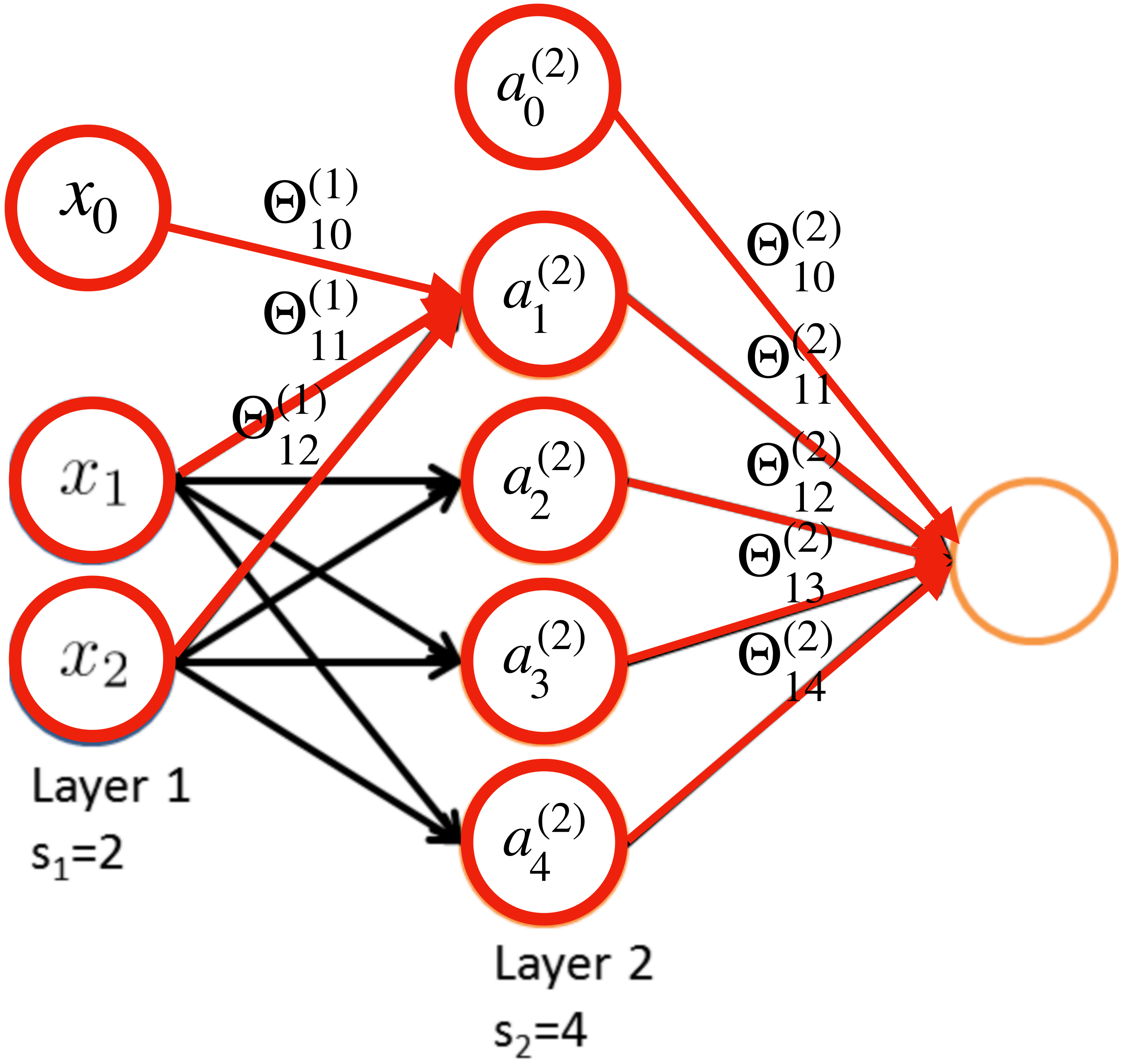
Feedforward Propagation



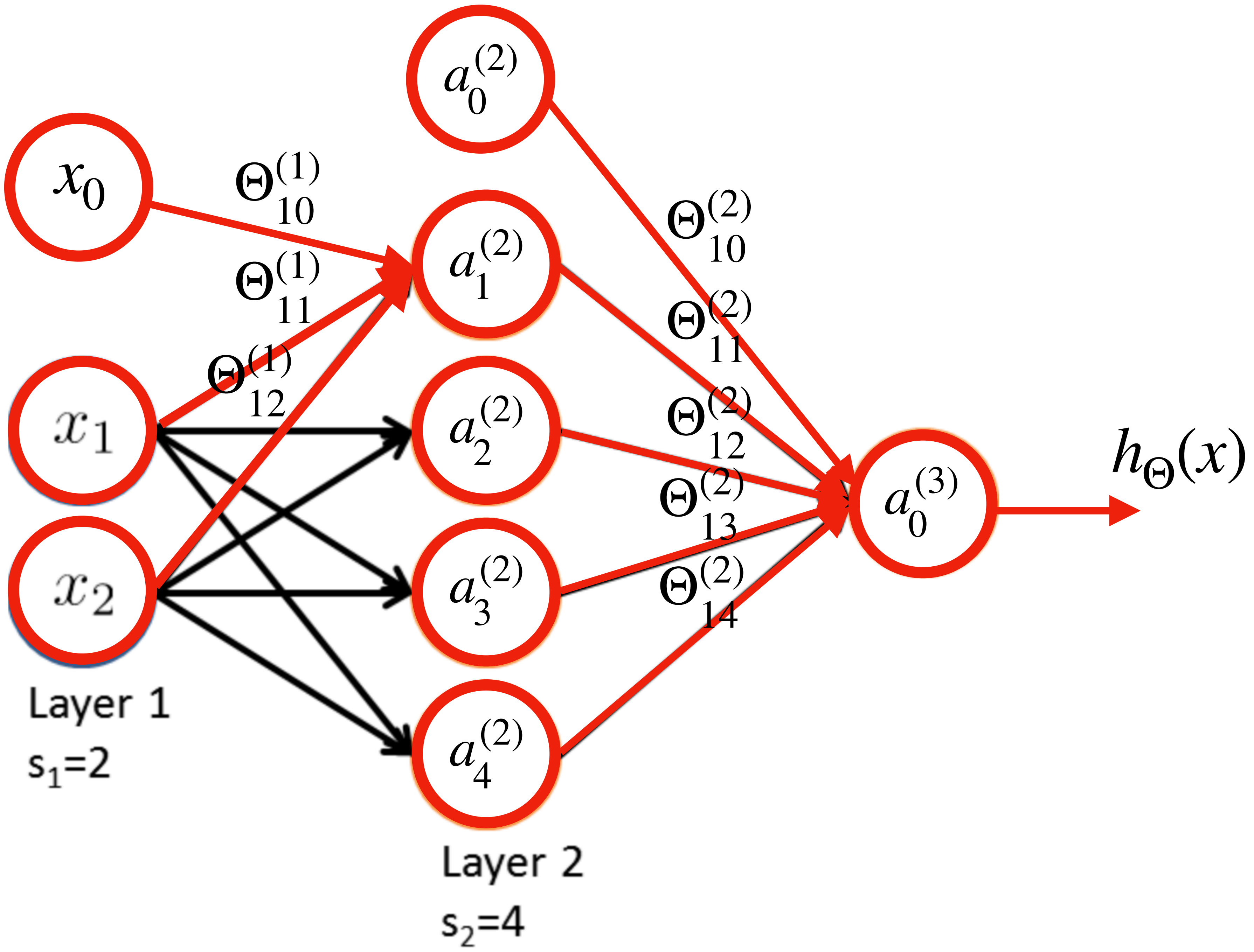
Feedforward Propagation



Feedforward Propagation



Feedforward Propagation



Forward Propagation

What remains?

Now that we understand the feed-forward computation of a neural network. Then, let's talk about:

- Efficient execution of the feed-forward computation,
- The gradient descent process used to learn the weights Θ

Remark: Ng uses the notation Θ for weights but some of other materials use **W**. So, our lecture slides will use them interchangeably.

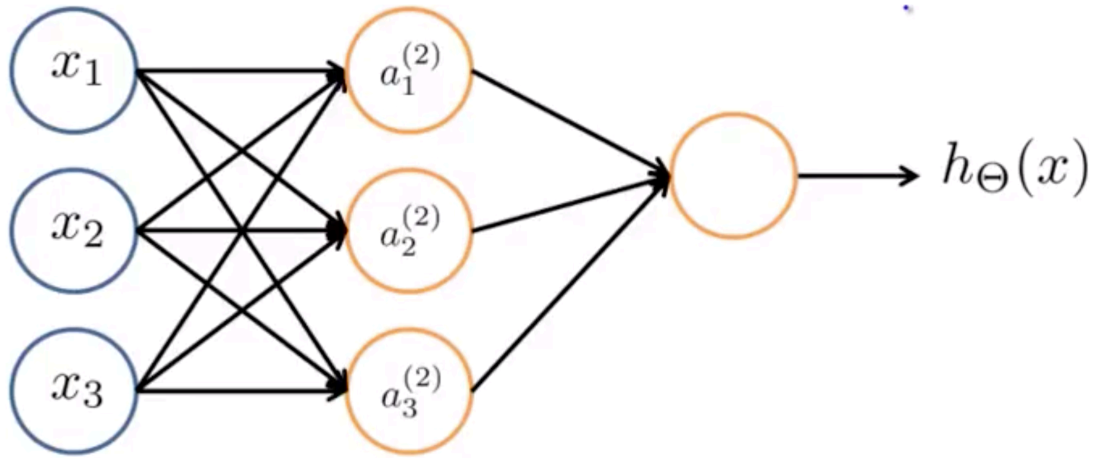
Efficient Computation

Consider calculating hidden unit activations. We have:

$$\mathbf{z}_1^{(2)} = \mathbf{W}_1^{(1)^T} x + \mathbf{b}_1^{(1)} \quad \text{and} \quad \mathbf{a}_1^{(2)} = g(\mathbf{z}_1^{(2)})$$

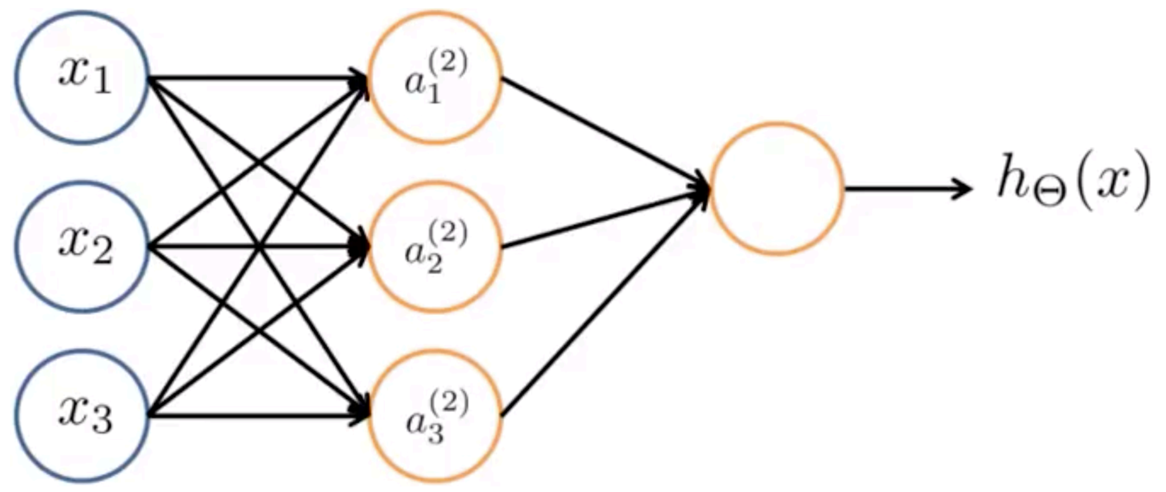
$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$\mathbf{z}_4^{(2)} = \mathbf{W}_4^{(1)^T} x + \mathbf{b}_4^{(1)} \quad \text{and} \quad \mathbf{a}_4^{(2)} = g(\mathbf{z}_4^{(2)})$$



Efficient Computation

Consider calculating hidden unit activations of the following network:



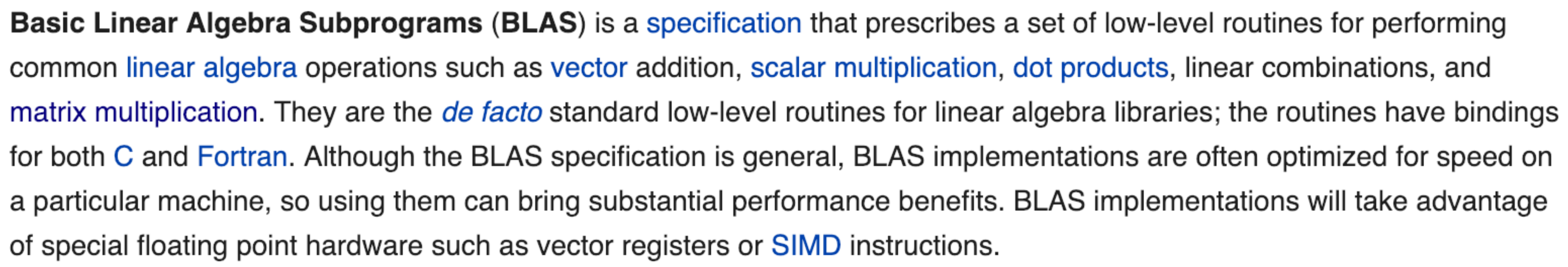
Depending on the 'deepness' of an architecture, for a single input, we may be doing a calculation of activations for 100 or 1,000 of units.

Code to implement this procedure using 'for' loops and the like will run very slowly, especially if implemented in a bytecode based on language like Python or Java.

Efficient Computation

What is needed is the ability to perform matrix algebra with a single library call or instruction that is highly optimized, using CPU instructions provided for vector operations.

BLAS is a well-known library that does this and is used by numpy:



Basic Linear Algebra Subprograms (**BLAS**) is a specification that prescribes a set of low-level routines for performing common linear algebra operations such as vector addition, scalar multiplication, dot products, linear combinations, and matrix multiplication. They are the *de facto* standard low-level routines for linear algebra libraries; the routines have bindings for both C and Fortran. Although the BLAS specification is general, BLAS implementations are often optimized for speed on a particular machine, so using them can bring substantial performance benefits. BLAS implementations will take advantage of special floating point hardware such as vector registers or SIMD instructions.

(from Wikipedia)

Alternatively, we may parallelize computation by recruiting GPU resources.

Efficient Computation

For an entire layer, to use vectorized computation, we need to perform the operation in one operation:

$$\begin{aligned}
a_1^{(2)} &= g(\boxed{\Theta_{10}^{(1)}x_0} + \boxed{\Theta_{11}^{(1)}x_1} + \boxed{\Theta_{12}^{(1)}x_2} + \boxed{\Theta_{13}^{(1)}x_3}) \\
a_2^{(2)} &= g(\boxed{\Theta_{20}^{(1)}x_0} + \boxed{\Theta_{21}^{(1)}x_1} + \boxed{\Theta_{22}^{(1)}x_2} + \boxed{\Theta_{23}^{(1)}x_3}) \\
a_3^{(2)} &= g(\boxed{\Theta_{30}^{(1)}x_0} + \boxed{\Theta_{31}^{(1)}x_1} + \boxed{\Theta_{32}^{(1)}x_2} + \boxed{\Theta_{33}^{(1)}x_3})
\end{aligned}$$

This can be implemented in a single Python statement:

```
W1 = np.matrix(np.random.normal(0, 1, (3, 4)))
 x = np.matrix(np.random.normal(0, 1, (4, 1)))
z2 = np.dot(W1, x)
```

} This would run much faster than the equivalent doubly-nested for loop !

Efficient Computation

For an entire layer, to use vectorized computation, we need to perform the operation in one operation:

$$\mathbf{z}_1^{(2)} = {\mathbf{W}_1^{(1)}}^T \boldsymbol{x} + \mathbf{b}_1^{(1)}$$

This can be implemented in a single Python statement:

```
W1 = np.matrix(np.random.normal(0, 1, (3, 4)))
b1 = np.matrix(np.random.normal(0, 1, (4, 1)))
 x = np.matrix(np.random.normal(0, 1, (3, 1)))

z2 = W1.T*x + b1
```

This would run much faster than the equivalent doubly-nested for loop !

Efficient Computation

Then, to calculate $a^{(2)}$ as a vector operation, we can hopefully use vectorized functions in our implementation language.

If we have the sigmoid function, for example, we implement:

$$g(z^{(2)}) = \frac{1}{1 + e^{-z^{(2)}}}$$

as

```
def g(z):
    return 1 / (1 + exp(-z))

z2 = np.matrix([[1, 2, 3]]).T
a2 = g(z2)
```

$\Big\}$ This will run much faster than executing the exp( ) function within a Python loop !

Efficient Computation

Next, consider performing a computation over many training examples.

Performing the operation:

$$\mathbf{z}_1^{(2)} = {\mathbf{W}_1^{(1)}}^T \boldsymbol{x}^{(i)} + \mathbf{b}_1^{(1)}$$

inside a loop for every training example *i* would be slower than the vectorized operation.

$$\mathbf{z}_1^{(2)} = {\mathbf{W}_1^{(1)}}^T X^T + \mathbf{b}_1^{(1)}$$

Efficient Computation

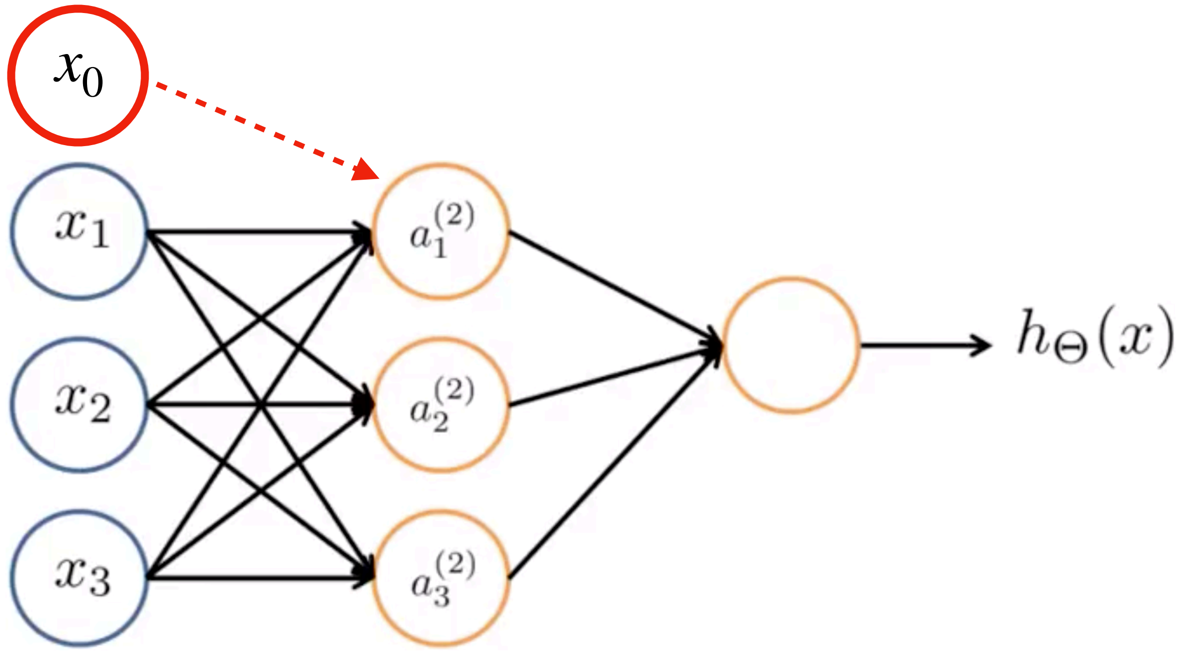
Noted that some languages *e.g.* Python also allow broadcasting of the addition operation horizontally:

```
A = np.matrix([[1, 2, 3], [2, 3, 4]])
b = np.matrix([[2, 3]]).T
>> A + b
```

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \end{bmatrix} + \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix}$$

With broadcasting, the computation will be much more efficient than for loop!

Efficient Computation



$z_i^{(j)}$: a weighted linear combination of the inputs that go into a neuron *e.g.* $a_1^{(2)} = g(z_1^{(2)})$

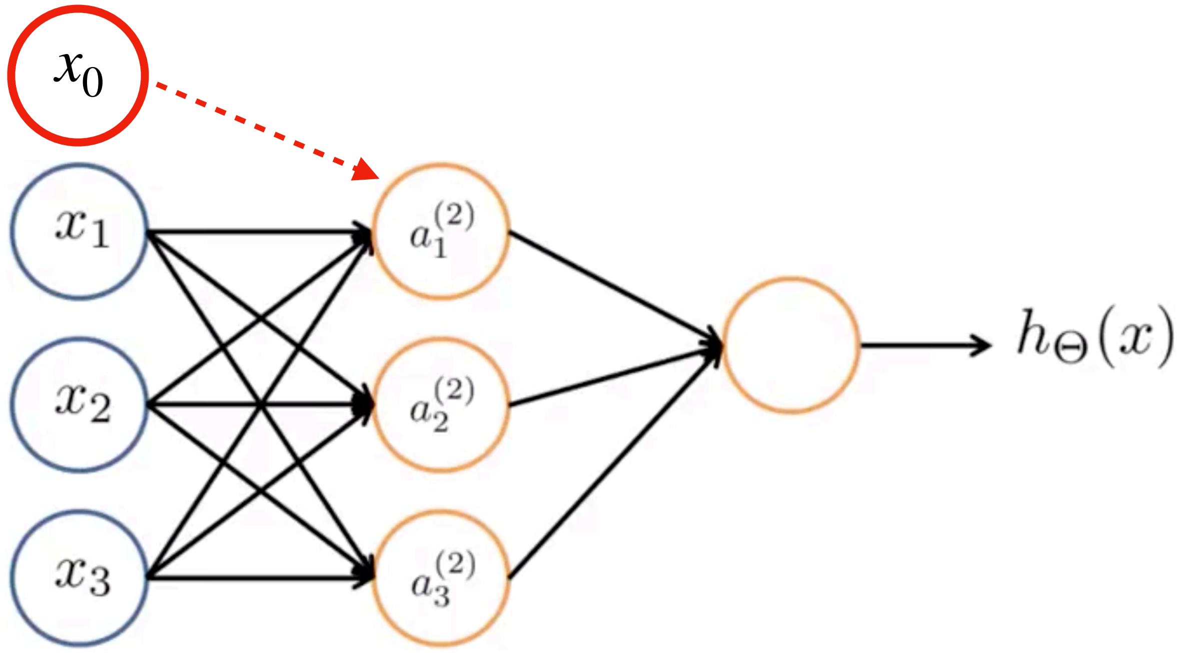
$$a_1^{(2)} = g(\boxed{\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3}) \dashrightarrow z_1^{(2)}$$

$$a_2^{(2)} = g(\boxed{\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3}) \dashrightarrow z_2^{(2)}$$

$$a_3^{(2)} = g(\boxed{\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3}) \dashrightarrow z_3^{(2)}$$

$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

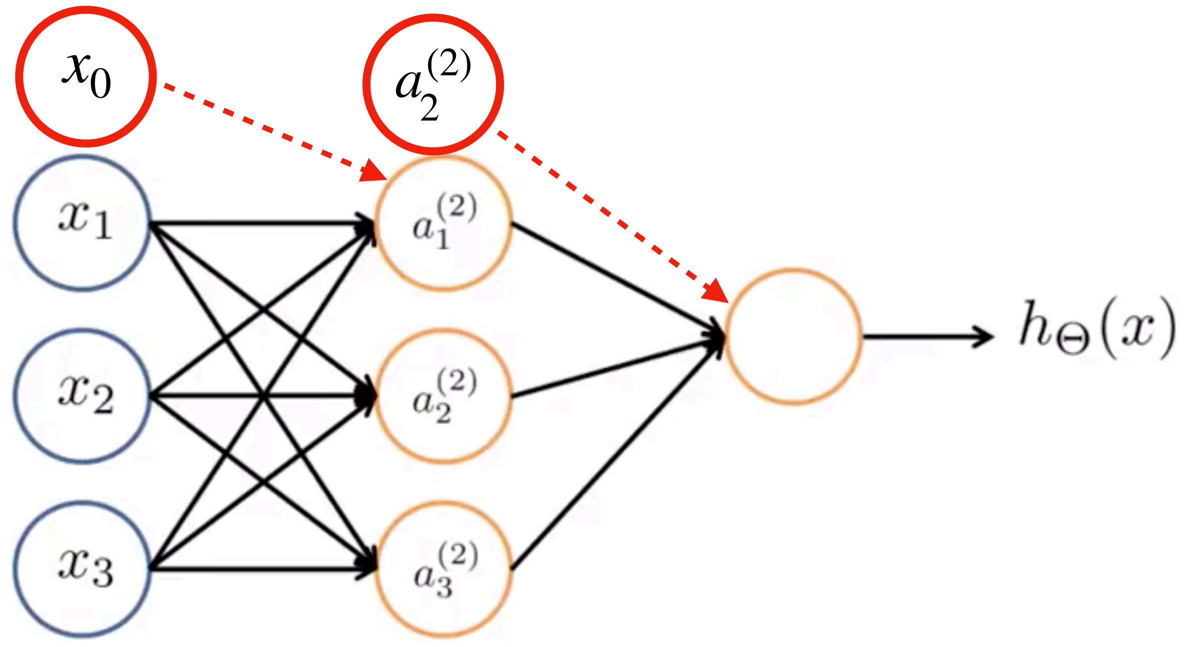
Efficient Computation



$z_i^{(j)}$: a weighted linear combination of the inputs that go into a neuron *e.g.* $a_1^{(2)} = g(z_1^{(2)})$

$$\left.\begin{aligned} z_1^{(2)} &= \Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3 \\ z_2^{(2)} &= \Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3 \\ z_3^{(2)} &= \Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3 \end{aligned}\right\} \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix} = \begin{bmatrix} \Theta_{10}^{(1)} & \Theta_{11}^{(1)} & \Theta_{12}^{(1)} & \Theta_{13}^{(1)} \\ \Theta_{20}^{(1)} & \Theta_{21}^{(1)} & \Theta_{22}^{(1)} & \Theta_{23}^{(1)} \\ \Theta_{30}^{(1)} & \Theta_{31}^{(1)} & \Theta_{32}^{(1)} & \Theta_{33}^{(1)} \end{bmatrix} \times \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Efficient Computation



$$a_0^{(2)} = 1 \Longrightarrow a^2 \in \mathbb{R}^4$$

$$\therefore z^{(3)} = \Theta^{(2)} a^{(2)}$$

$$h_\Theta(x) = a^{(3)} = g(z^{(3)})$$

$z_i^{(j)}$: a weighted linear combination of the inputs that go into a neuron *e.g.* $a_1^{(2)} = g(z_1^{(2)})$

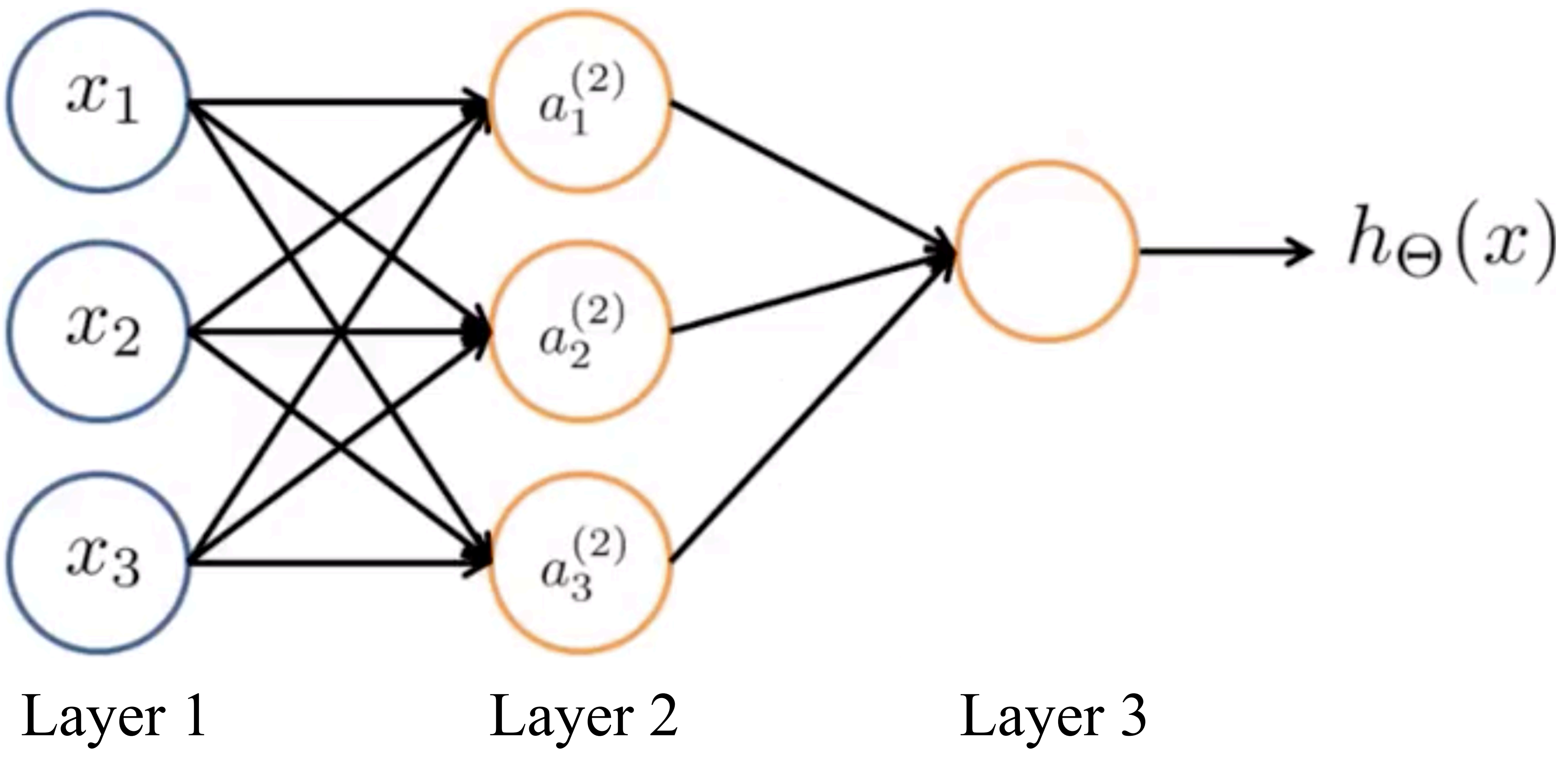
$$\left.\begin{aligned} z_1^{(2)} &= \Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3 \\ z_2^{(2)} &= \Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3 \\ z_3^{(2)} &= \Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3 \end{aligned}\right\} \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix} = \begin{bmatrix} \Theta_{10}^{(1)} & \Theta_{11}^{(1)} & \Theta_{12}^{(1)} & \Theta_{13}^{(1)} \\ \Theta_{20}^{(1)} & \Theta_{21}^{(1)} & \Theta_{22}^{(1)} & \Theta_{23}^{(1)} \\ \Theta_{30}^{(1)} & \Theta_{31}^{(1)} & \Theta_{32}^{(1)} & \Theta_{33}^{(1)} \end{bmatrix} \times \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

i.e. $z^{(2)} = \Theta^{(1)} a^{(1)}$

$a^{(2)} = g(z^{(2)})$

Forward Propagation

As aforementioned, if there are no hidden units, depending on a type of an activation function, a network may become a regression setting.



Forward Propagation

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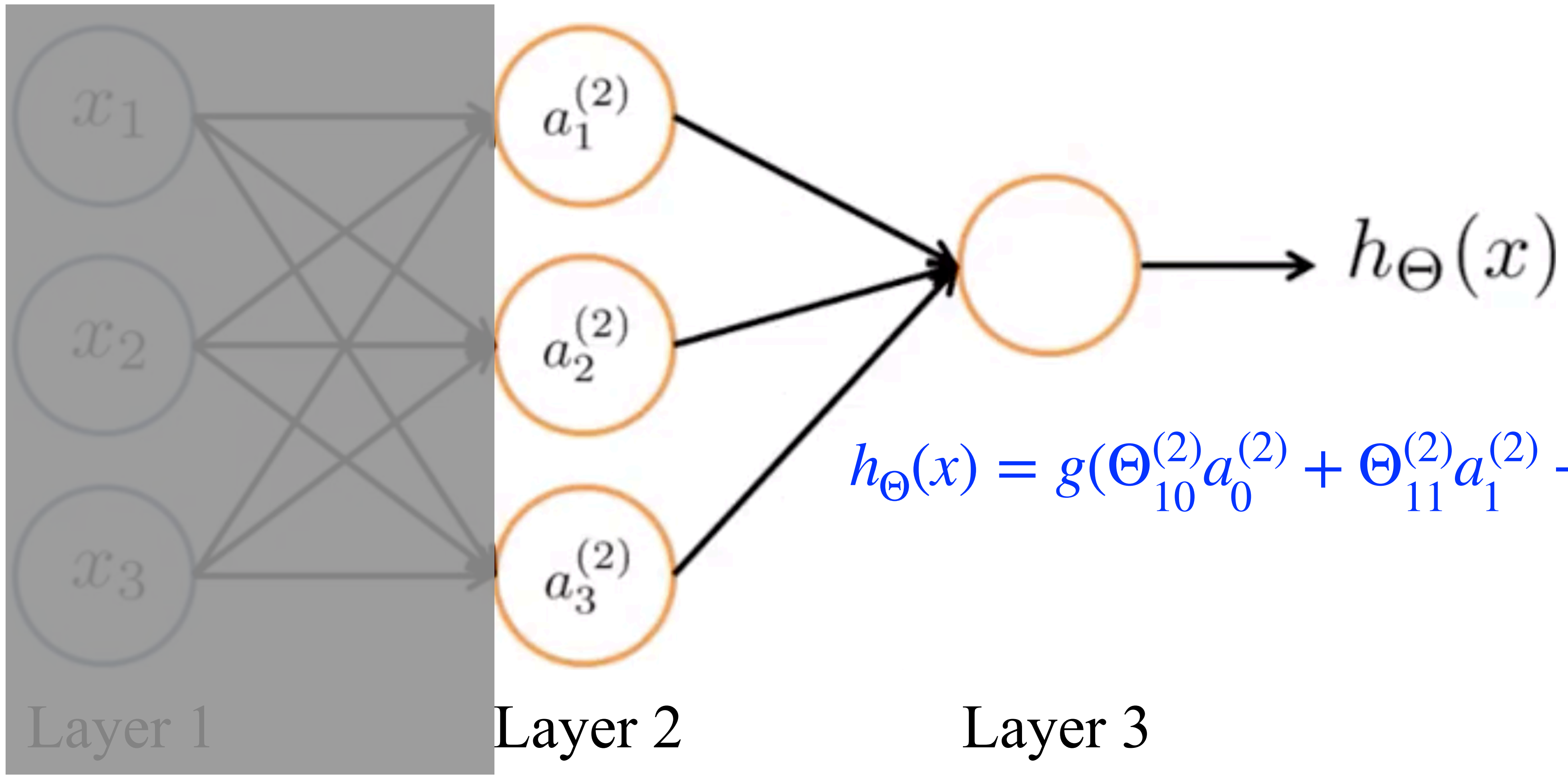
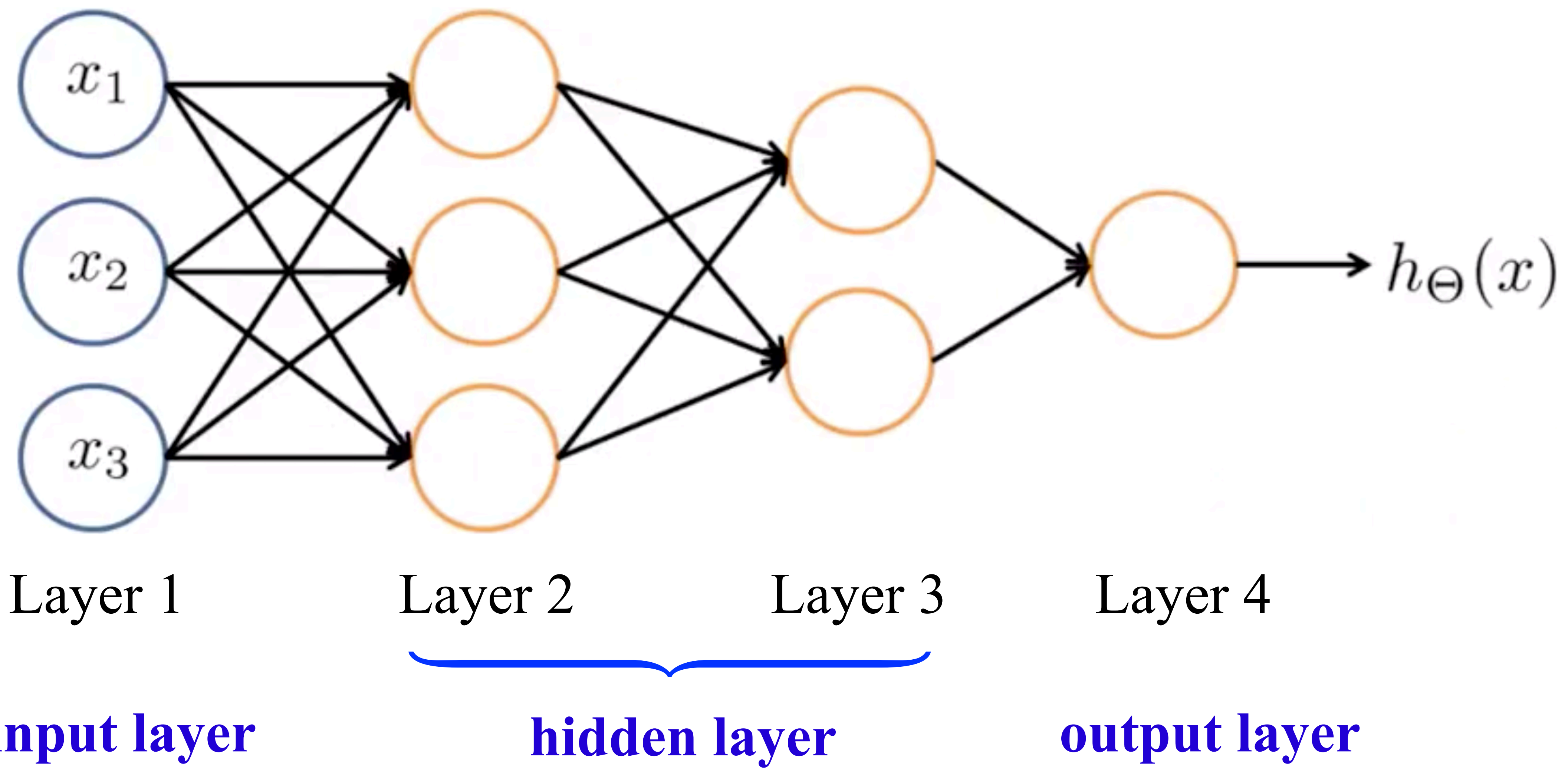


$$h_\Theta(x) = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

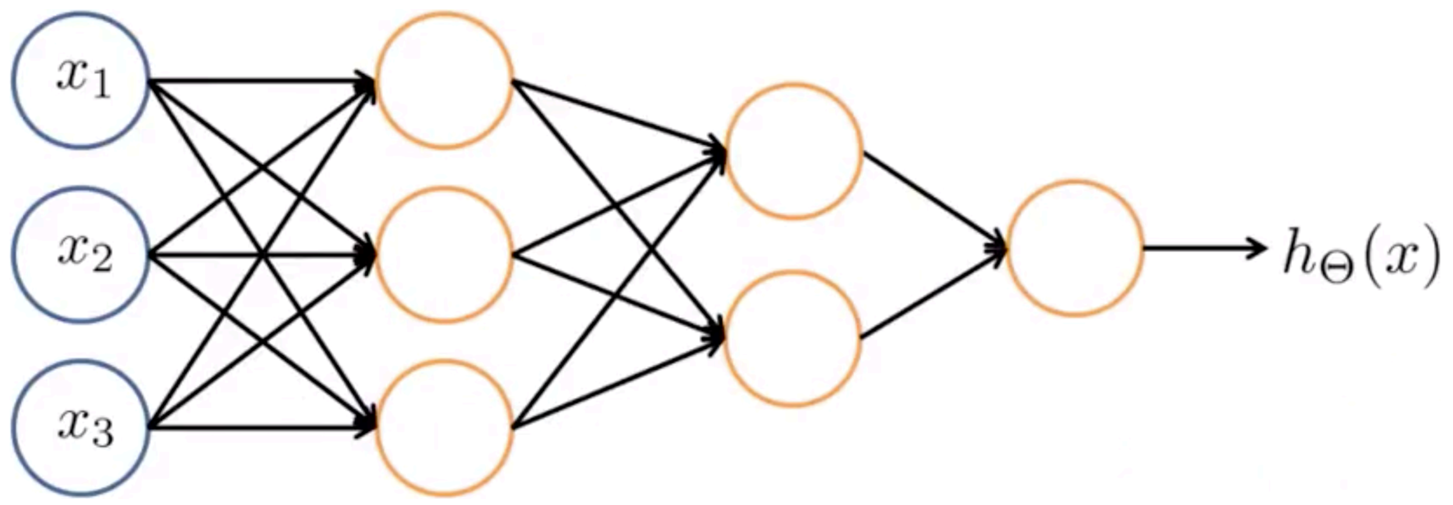
Other Network Architectures

The term ‘architecture’ refers to how different neurons are connected to each other (*e.g.* number of layers, units, type of units, connectivity between units).



Question

Consider the network.
Let $a^{(1)} = x \in \mathbb{R}^{n+1}$
denote the input
(with $a_0^{(1)} = 1$).
How would you
compute $a^{(2)}$?



(i) $a^{(2)} = \Theta^1 a^{(1)}$

(ii) $z^{(2)} = \Theta^2 a^{(1)}$; $a^{(2)} = g(z^{(2)})$

(iii) $z^{(2)} = \Theta^1 a^{(1)}$; $a^{(2)} = g(z^{(2)})$

(iv) $z^{(2)} = \Theta^2 g(a^{(1)})$; $a^{(2)} = g(z^{(2)})$