Deep Feedforward Networks

Paolo Favaro

Workshop on Machine Learning - Observatoire de Geneve

Contents

- Introduction to Feedforward Neural Networks: definition, design, training

- Based on **Chapter 6** (and 4) of Deep Learning by Goodfellow, Bengio, Courville

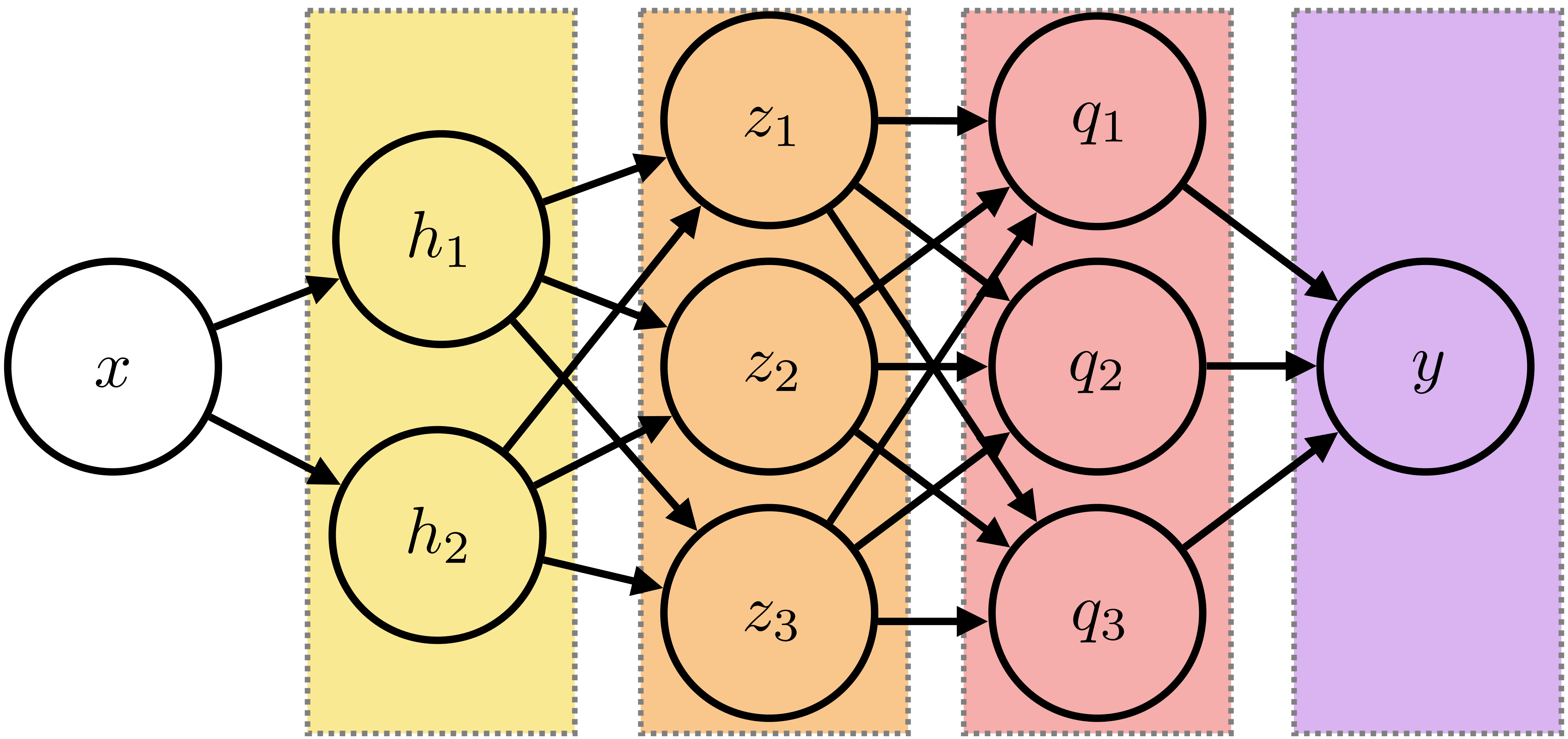
- References to Machine Learning and Pattern Recognition by Bishop

Resources

- Books and online material for further studies
  - CS231 @ Stanford (Fei-Fei Li)
  - **Pattern Recognition and Machine Learning**
    by Christopher M. Bishop
  - **Machine Learning: a Probabilistic Perspective**
    by Kevin P. Murphy

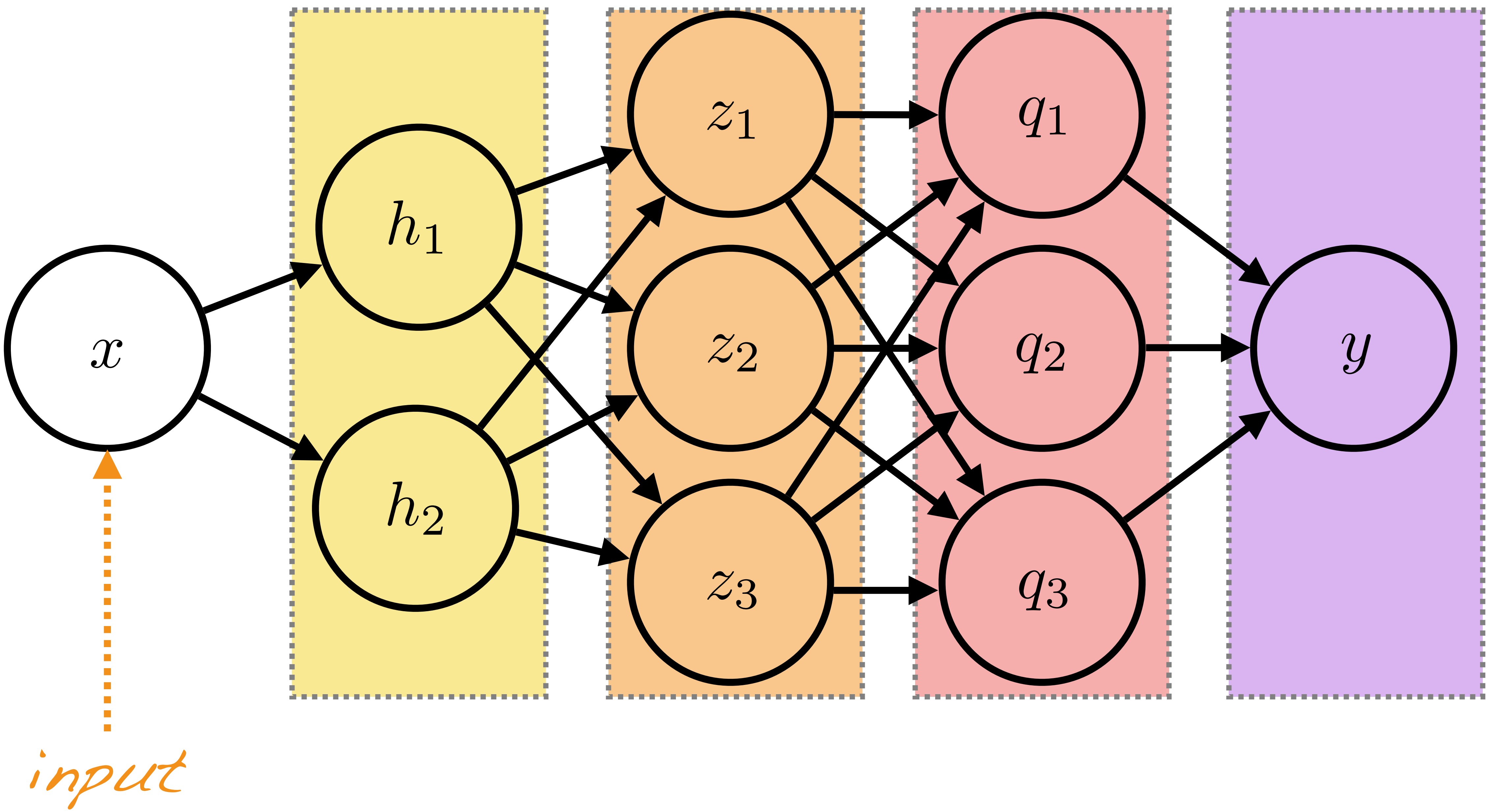
Feedforward Neural Networks

- Feedforward networks are a sequence of layers, each processing the output of the previous layer(s)



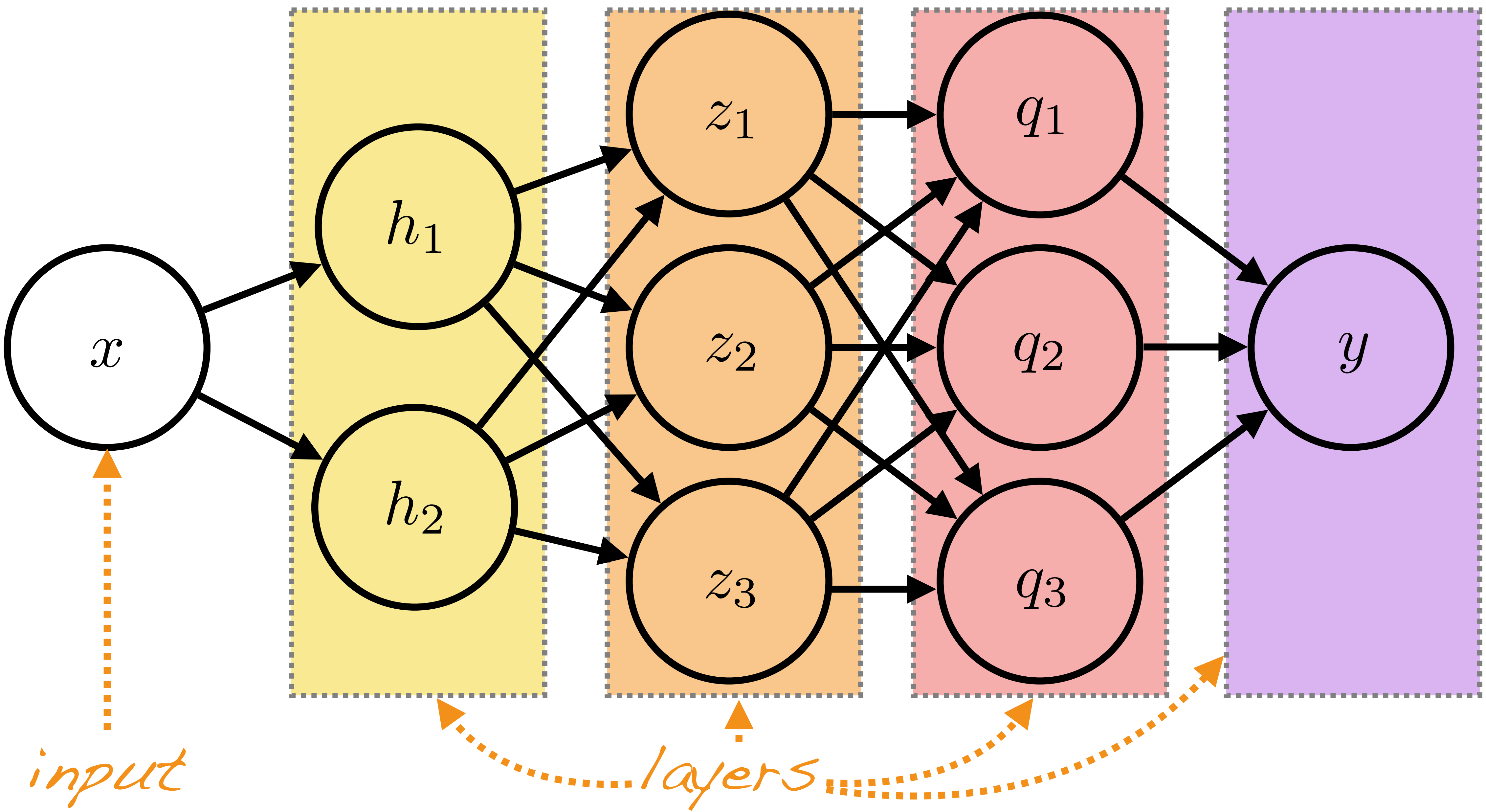
Feedforward Neural Networks

- Feedforward networks are a sequence of layers, each processing the output of the previous layer(s)



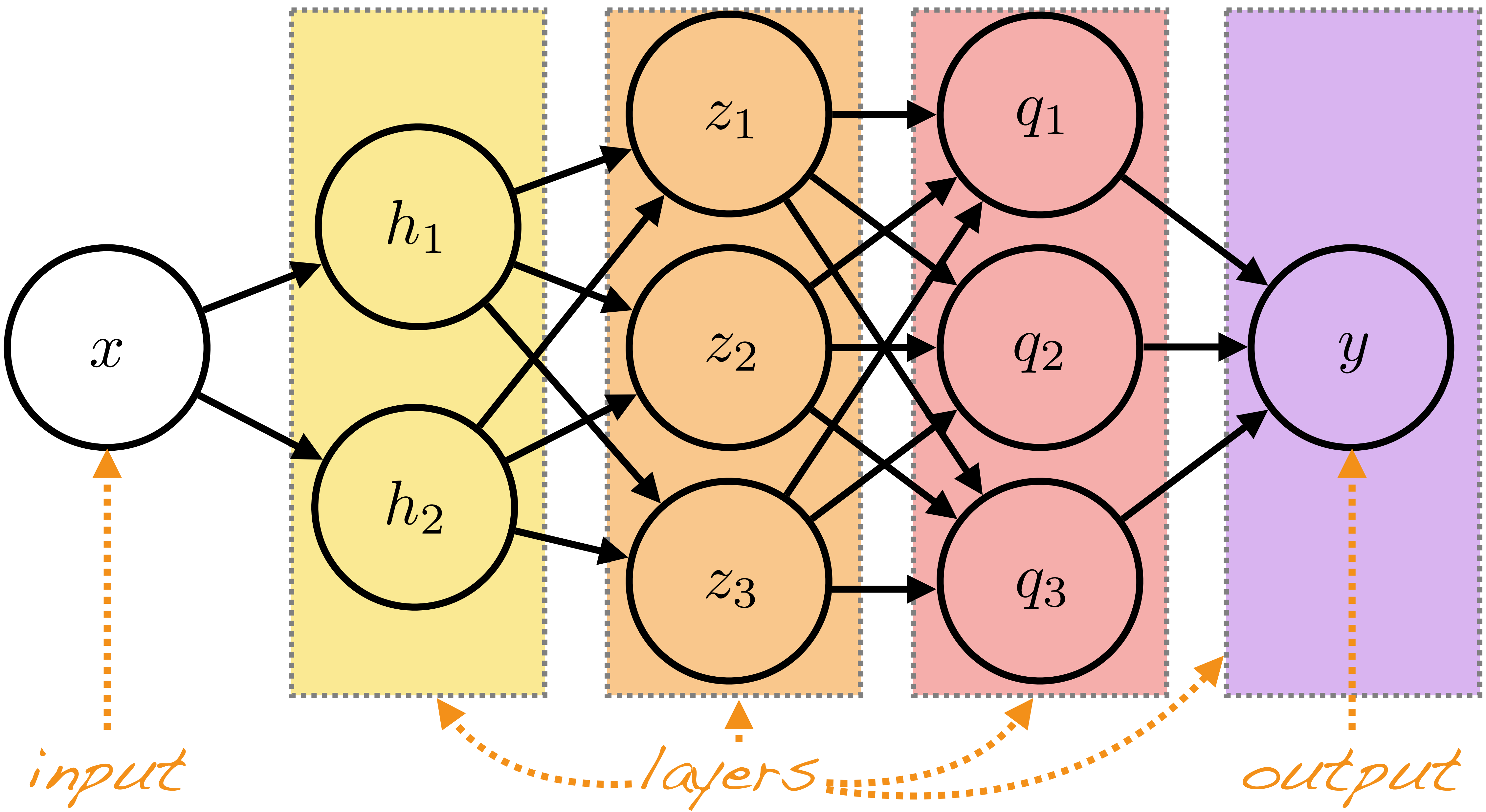
Feedforward Neural Networks

- Feedforward networks are a sequence of layers, each processing the output of the previous layer(s)

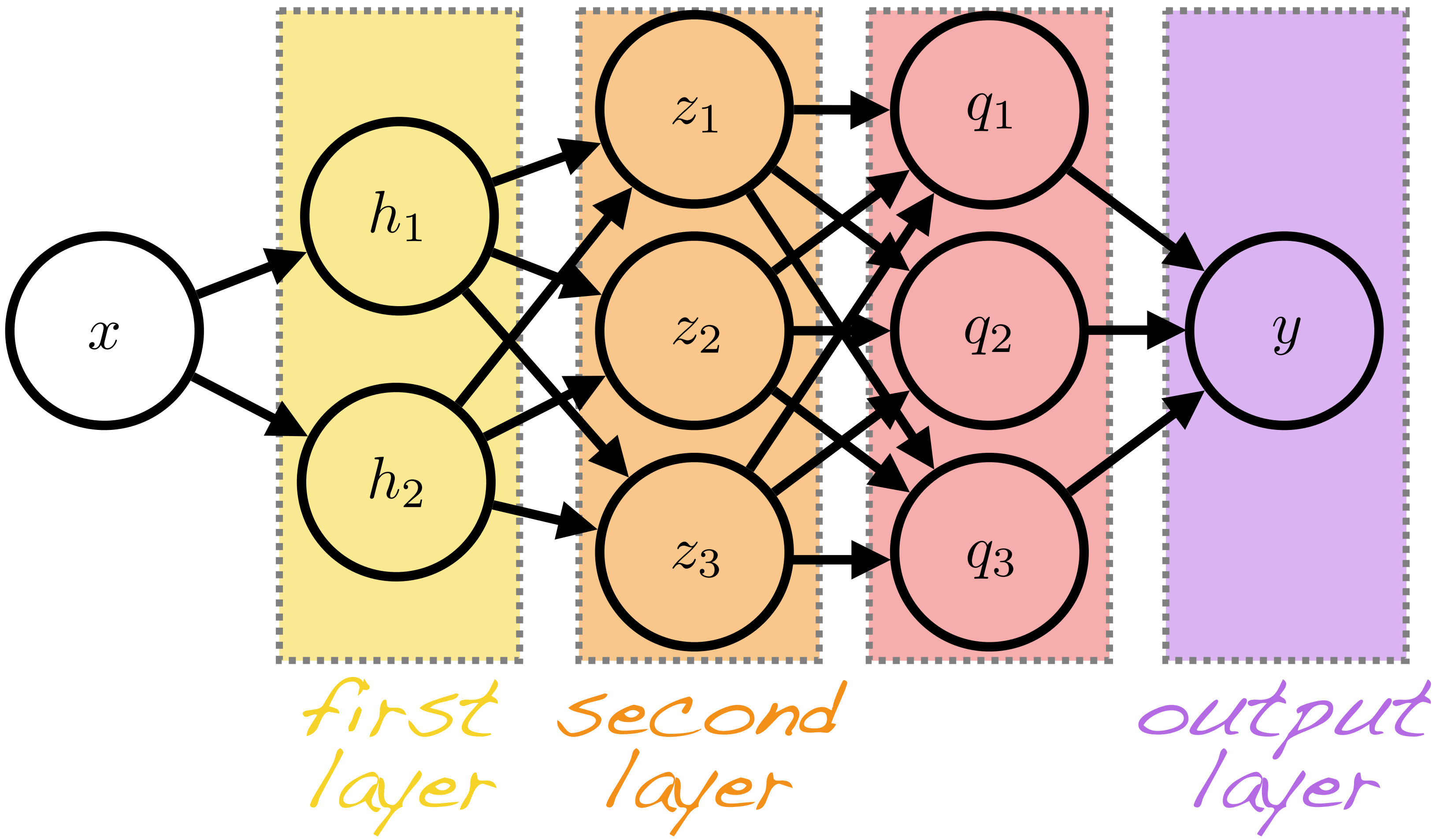


Feedforward Neural Networks

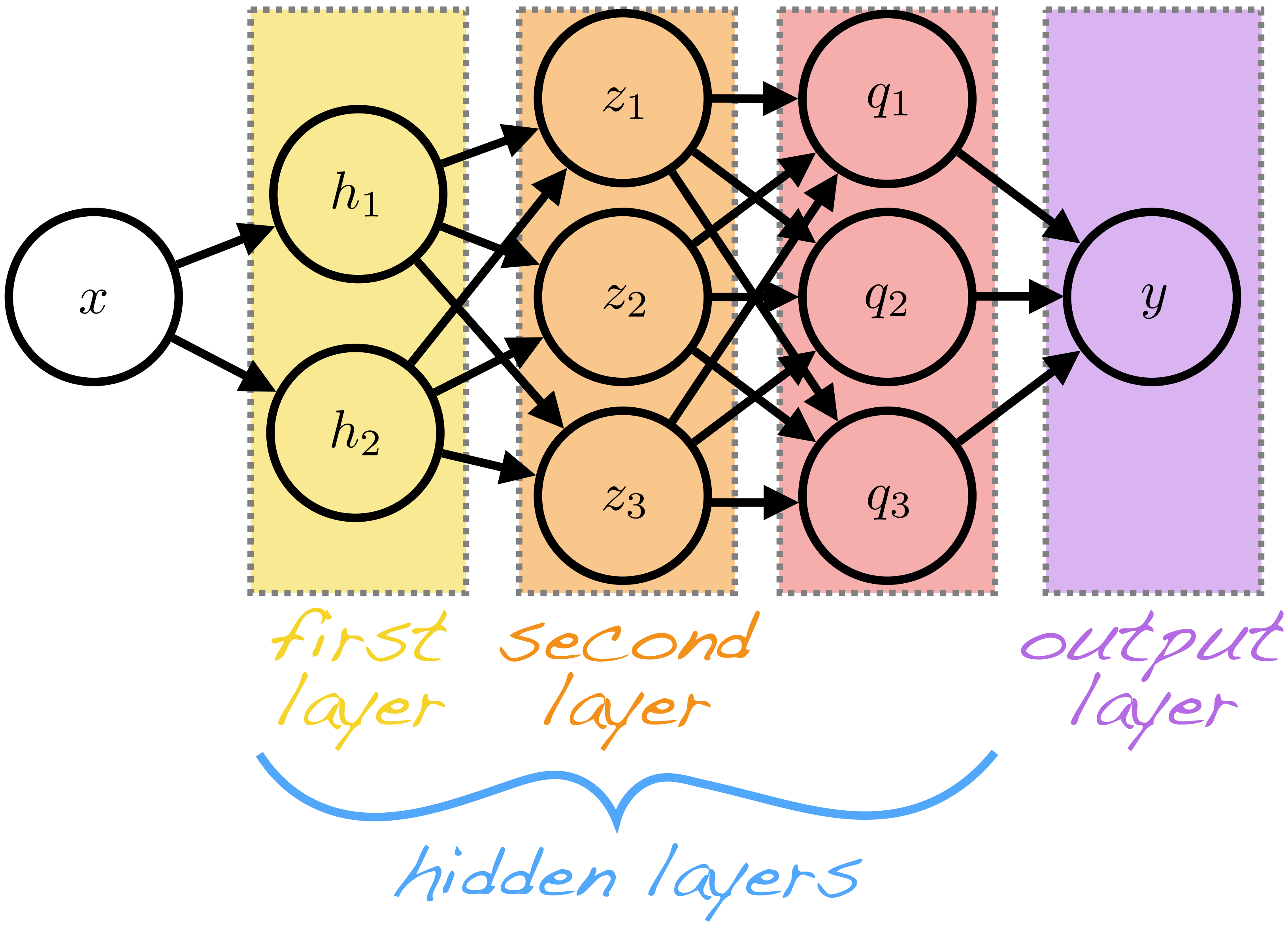
- Feedforward networks are a sequence of layers, each processing the output of the previous layer(s)



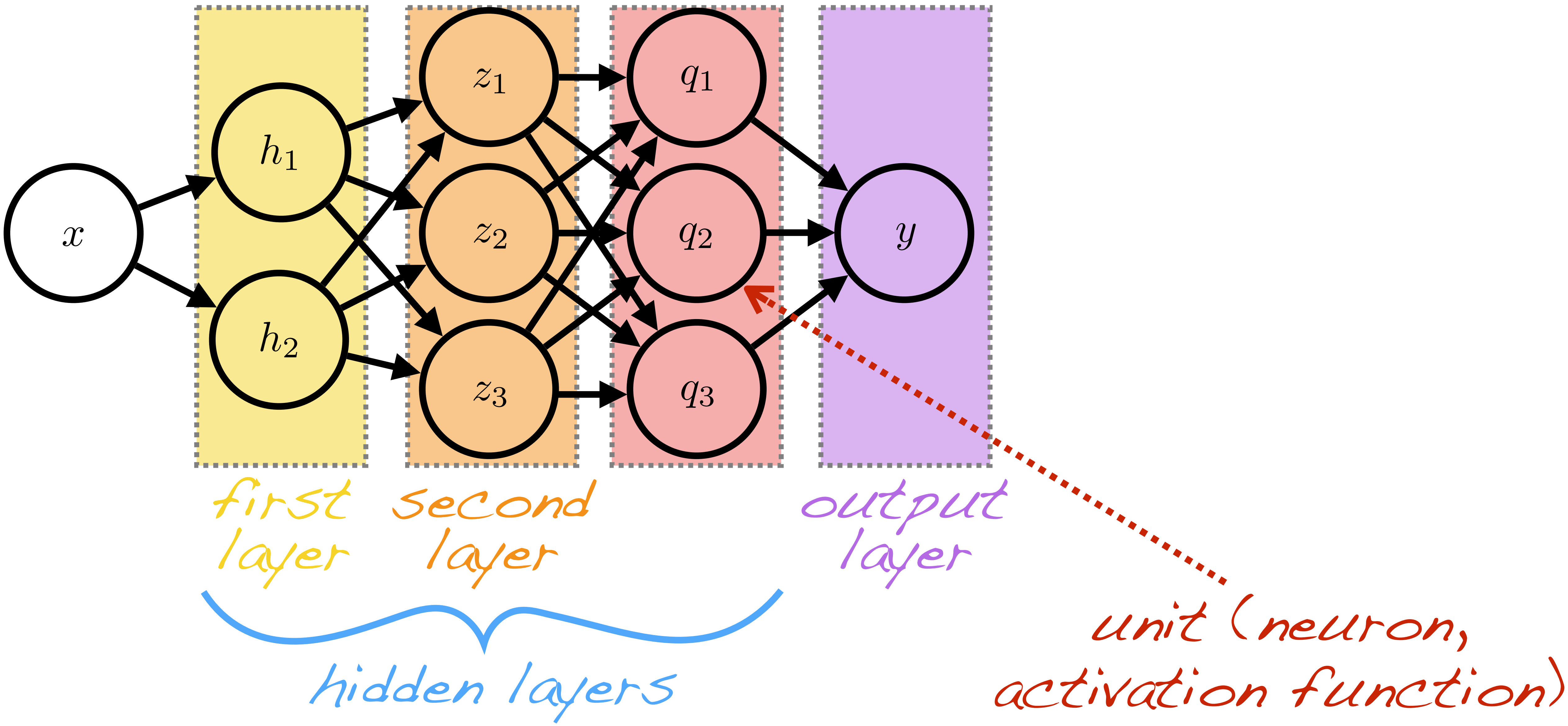
Feedforward Neural Networks



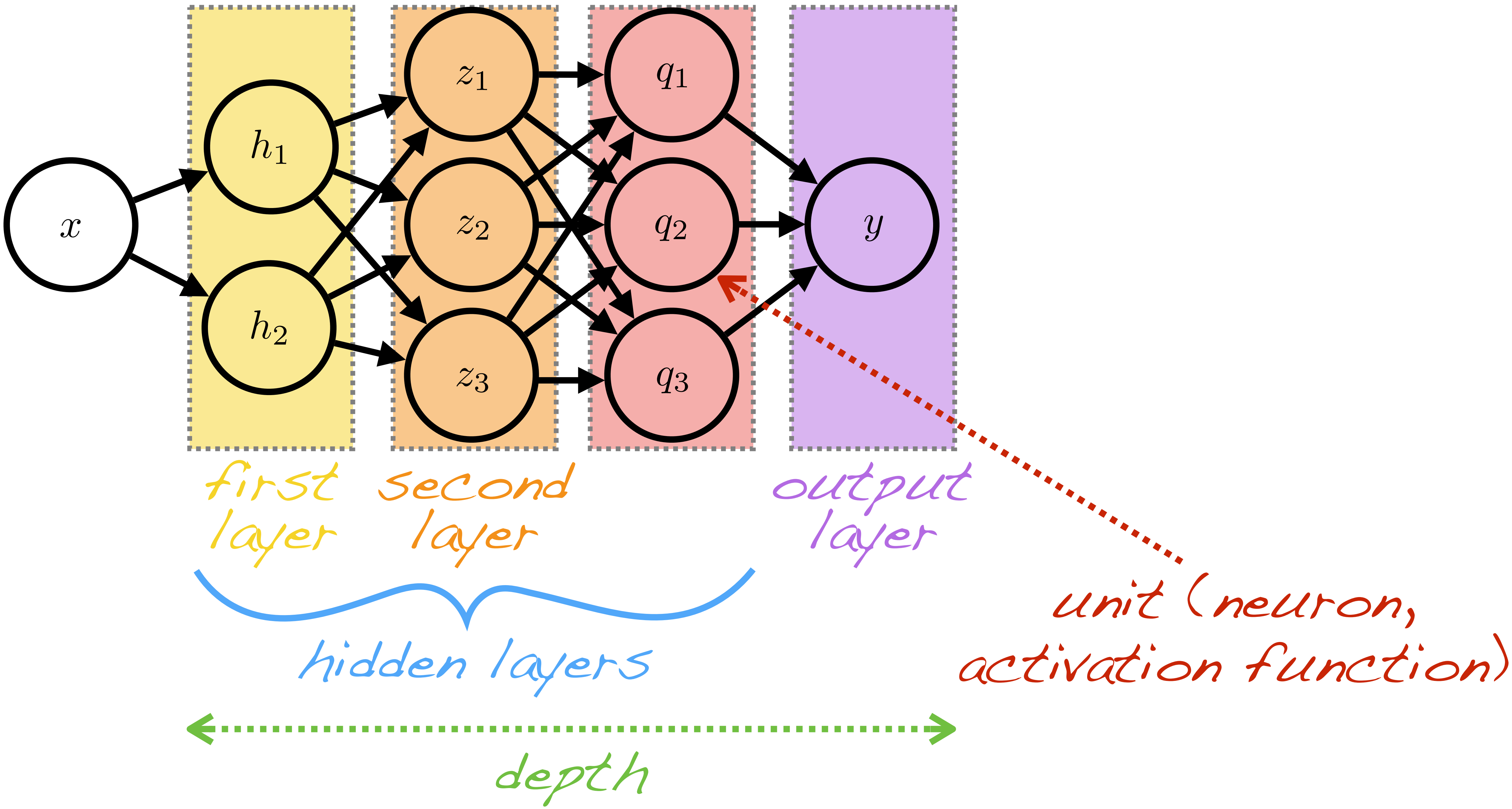
Feedforward Neural Networks



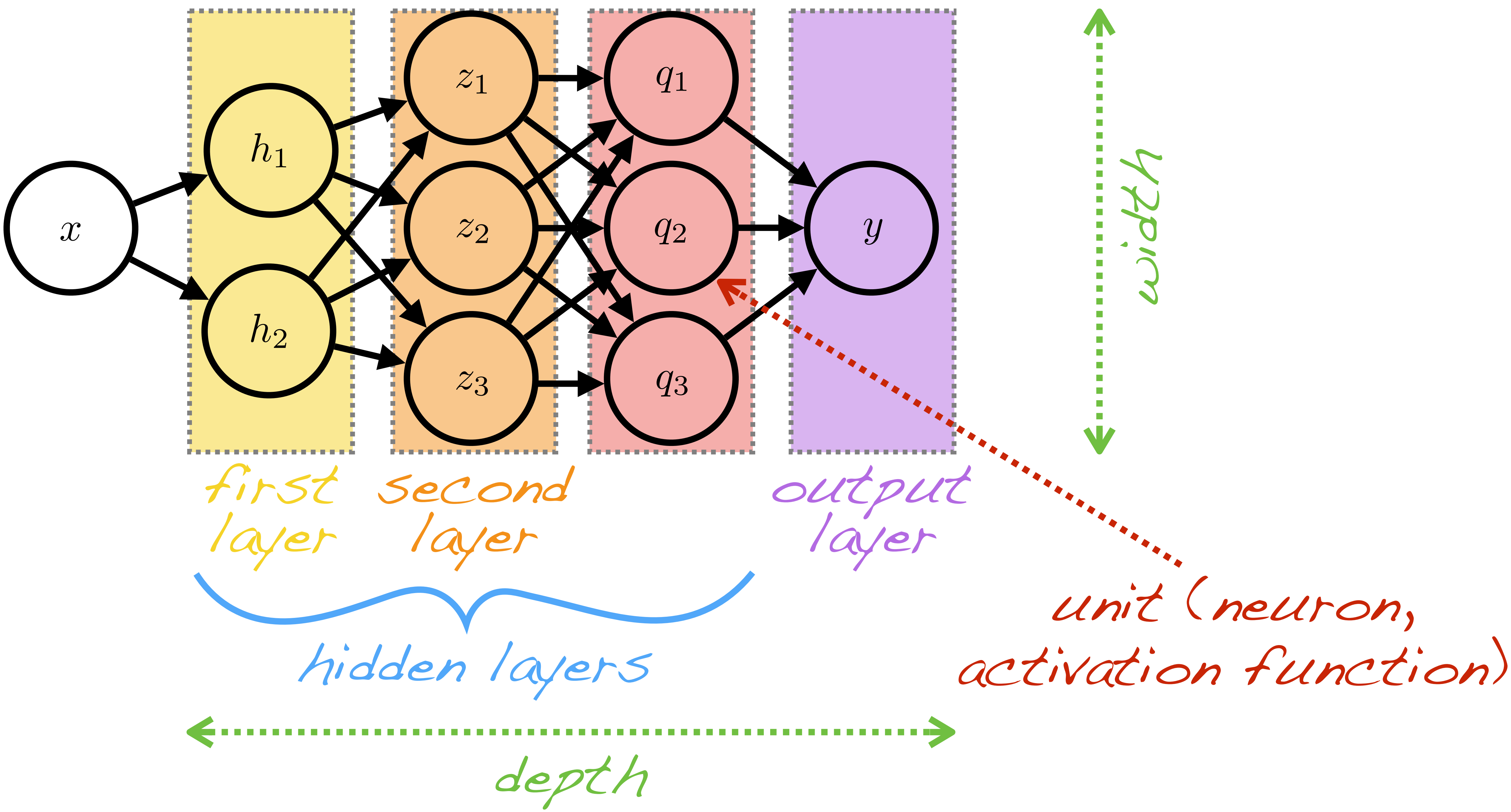
Feedforward Neural Networks



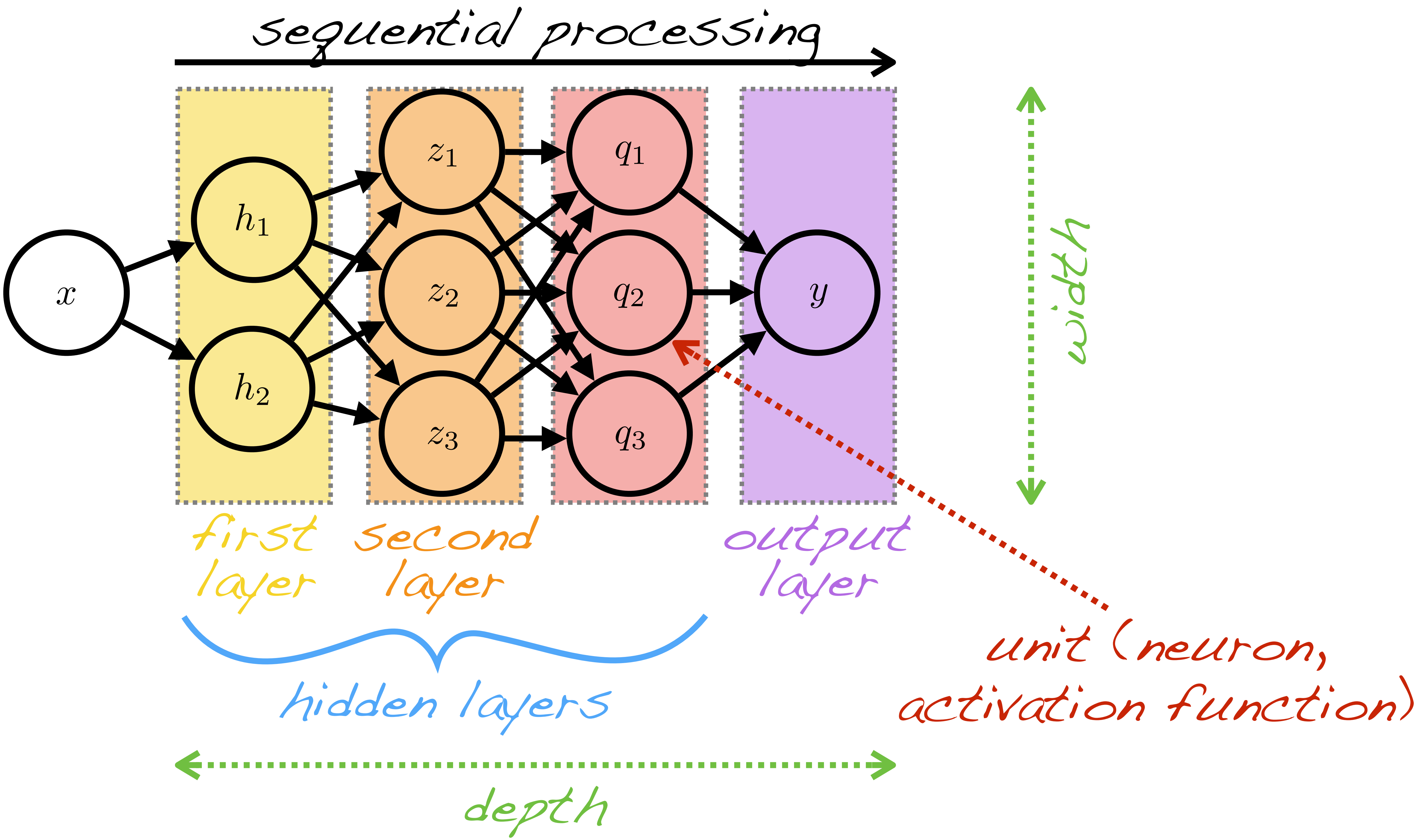
Feedforward Neural Networks



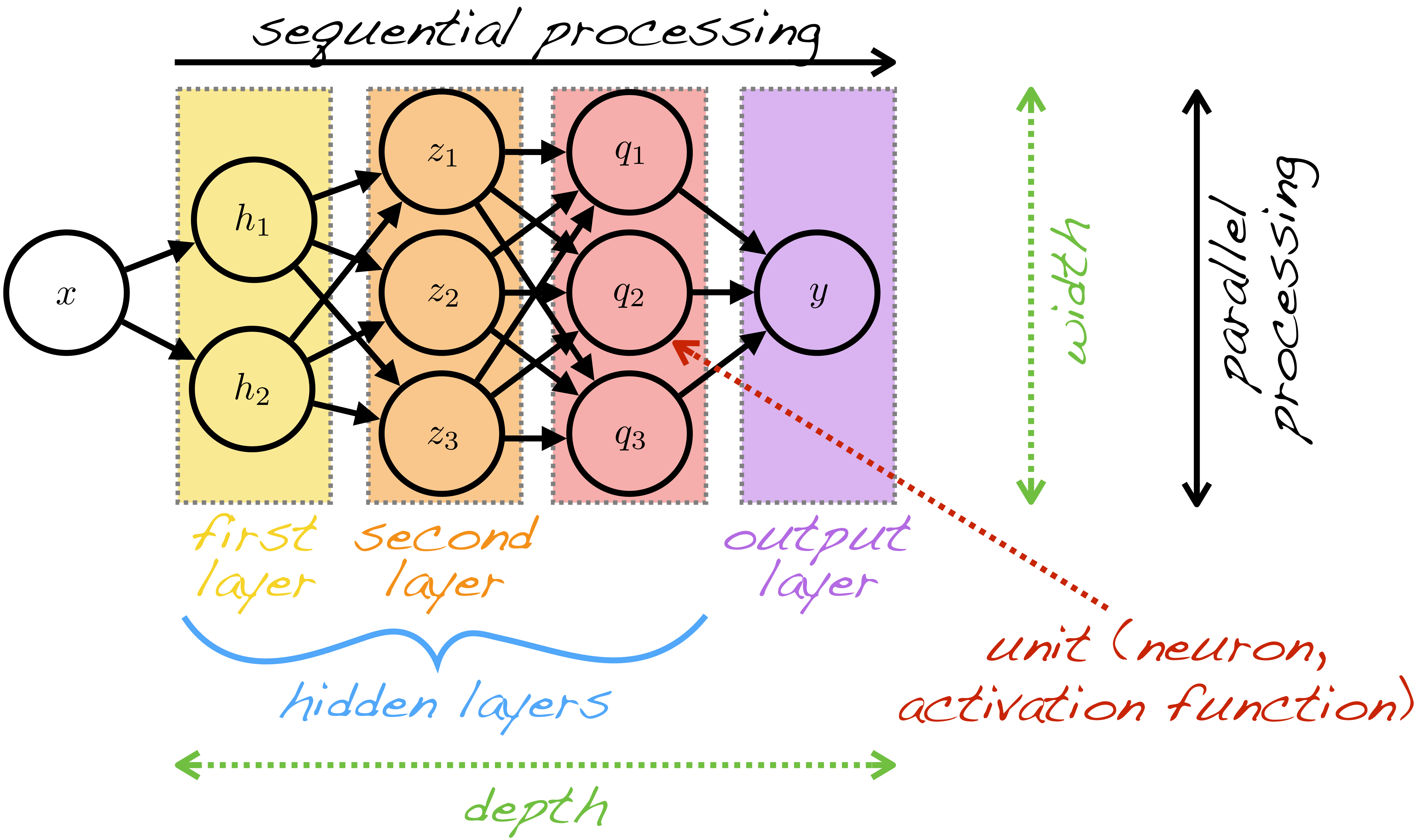
Feedforward Neural Networks



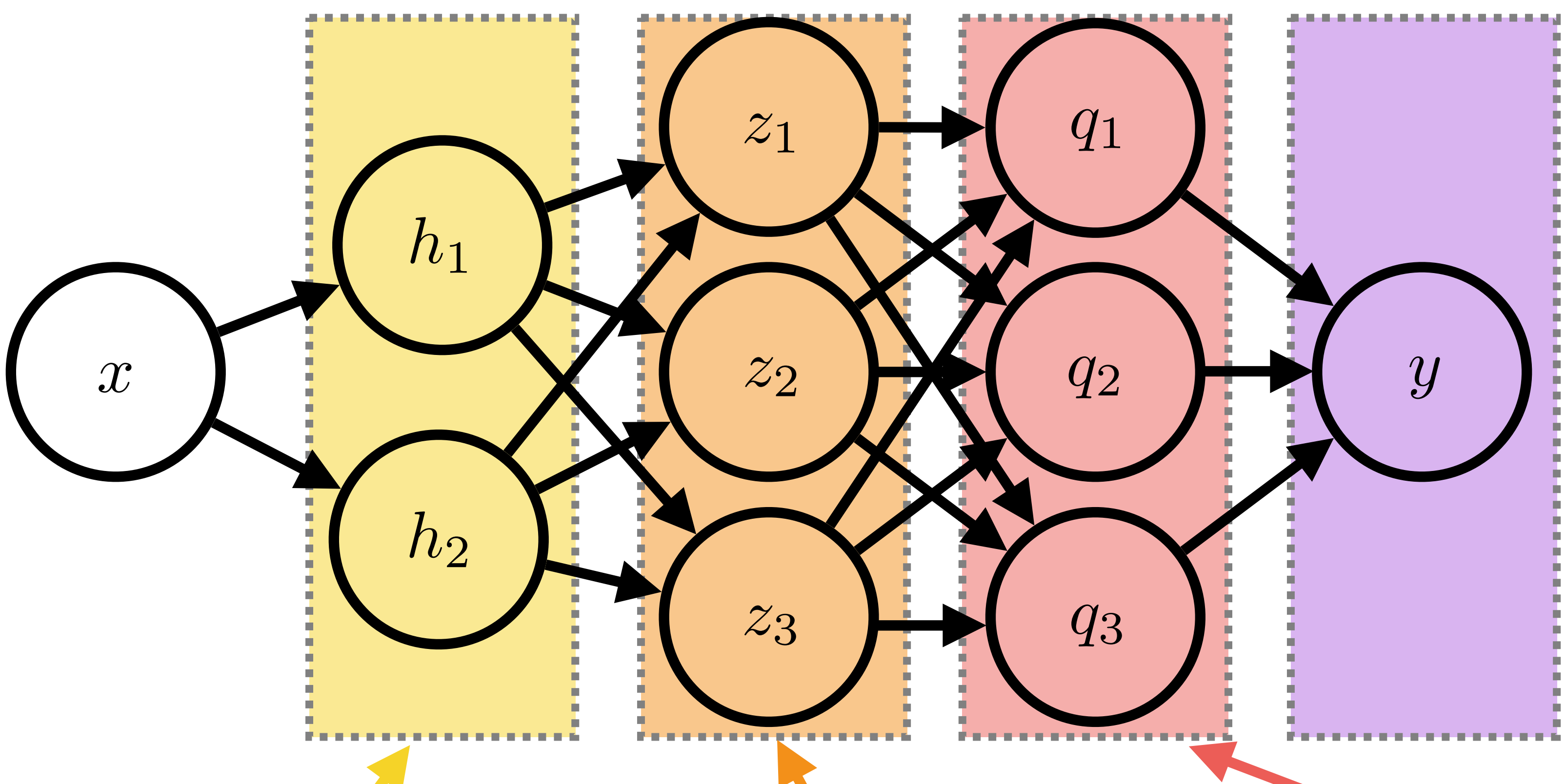
Feedforward Neural Networks



Feedforward Neural Networks



Feedforward Neural Networks



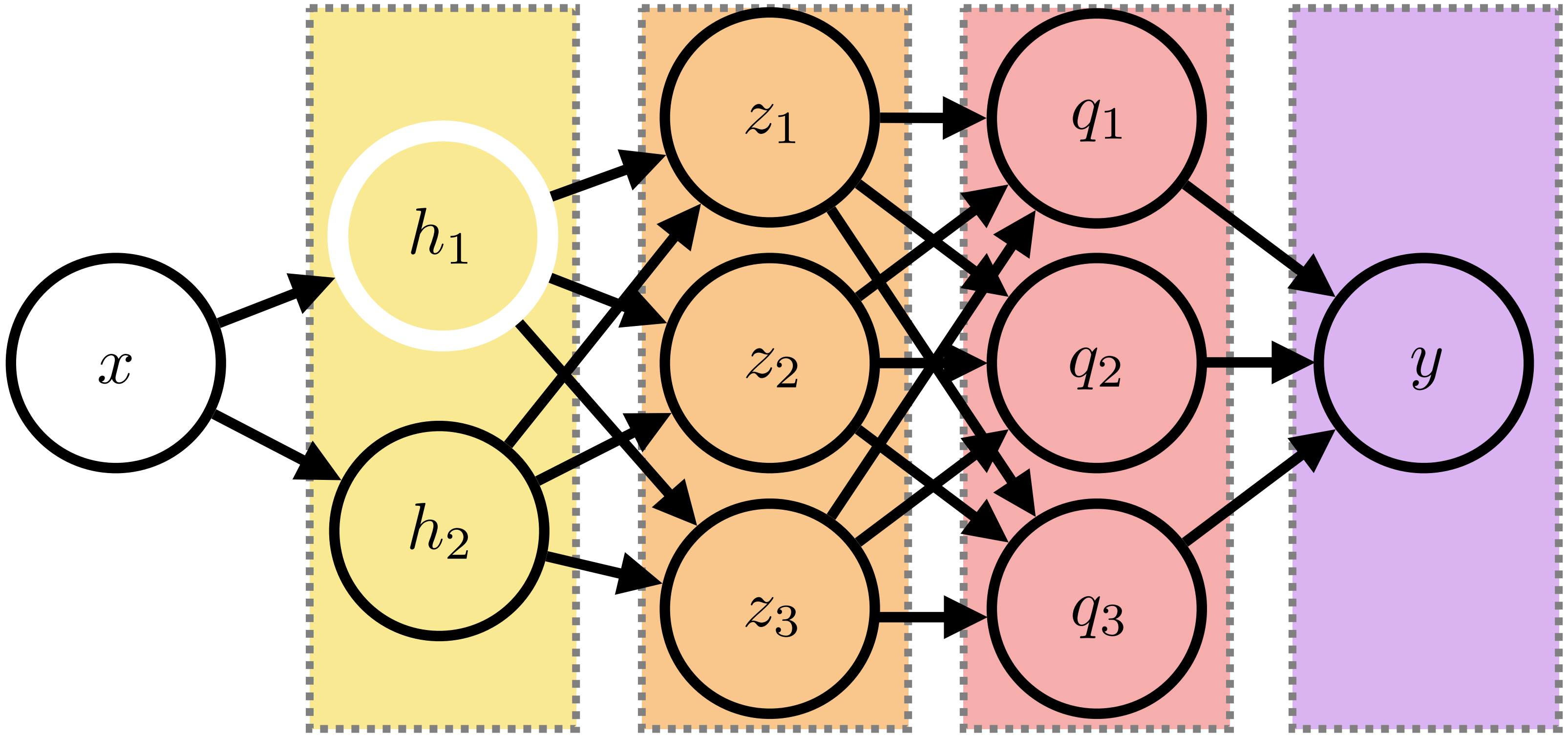
$$y = f_4(q_1, q_2, q_3)$$

$$h_1 = f_{1,1}(x)$$
$$h_2 = f_{1,2}(x)$$

$$z_1 = f_{2,1}(h_1, h_2)$$
$$z_2 = f_{2,2}(h_1, h_2)$$
$$z_3 = f_{2,3}(h_1, h_2)$$

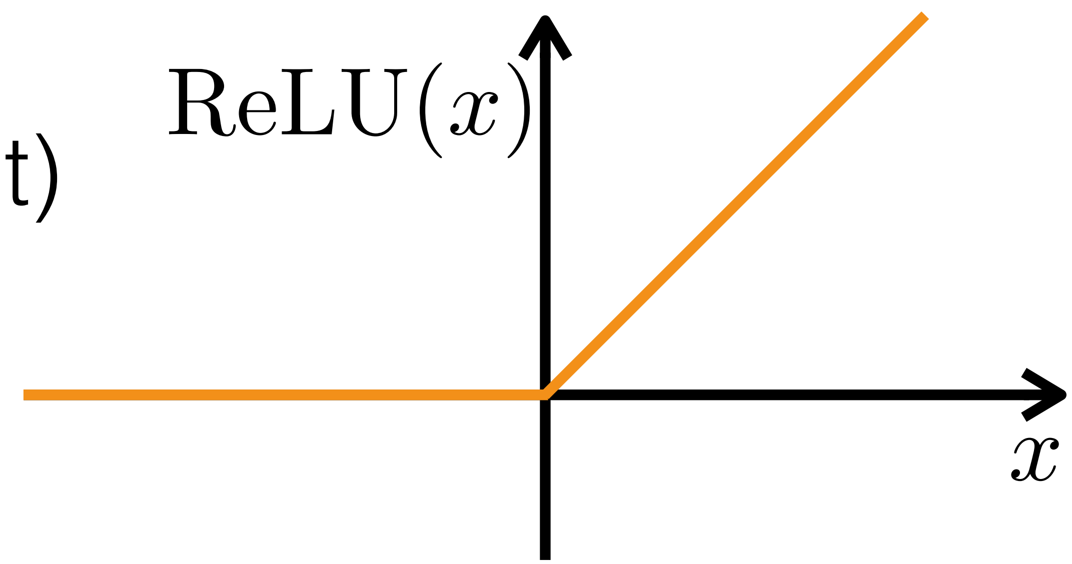
$$q_1 = f_{3,1}(z_1, z_2, z_3)$$
$$q_2 = f_{3,2}(z_1, z_2, z_3)$$
$$q_3 = f_{3,3}(z_1, z_2, z_3)$$

Feedforward Neural Networks

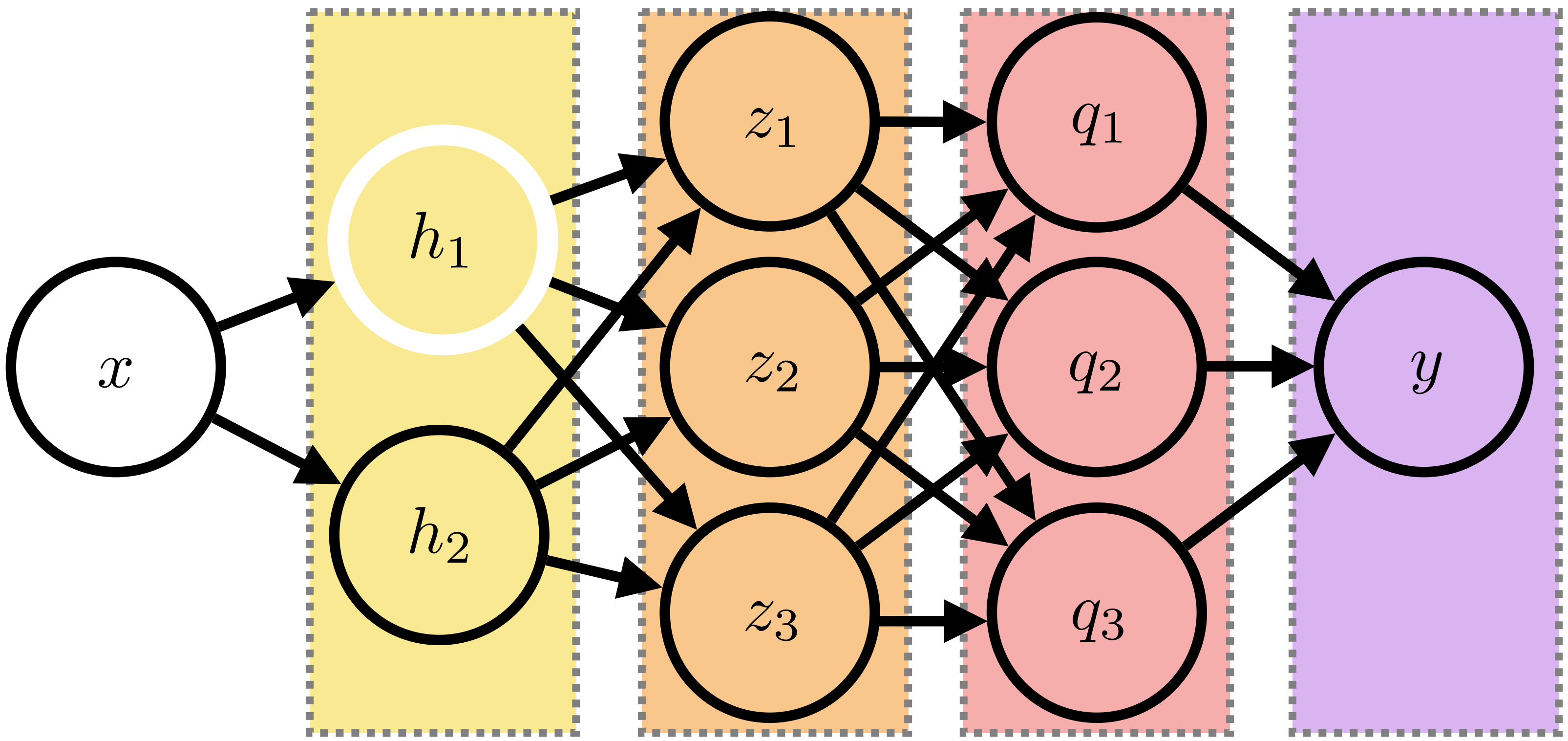


Example (rectified linear unit)

$$f_{1,1}(x) = \mathrm{ReLU}(x)$$

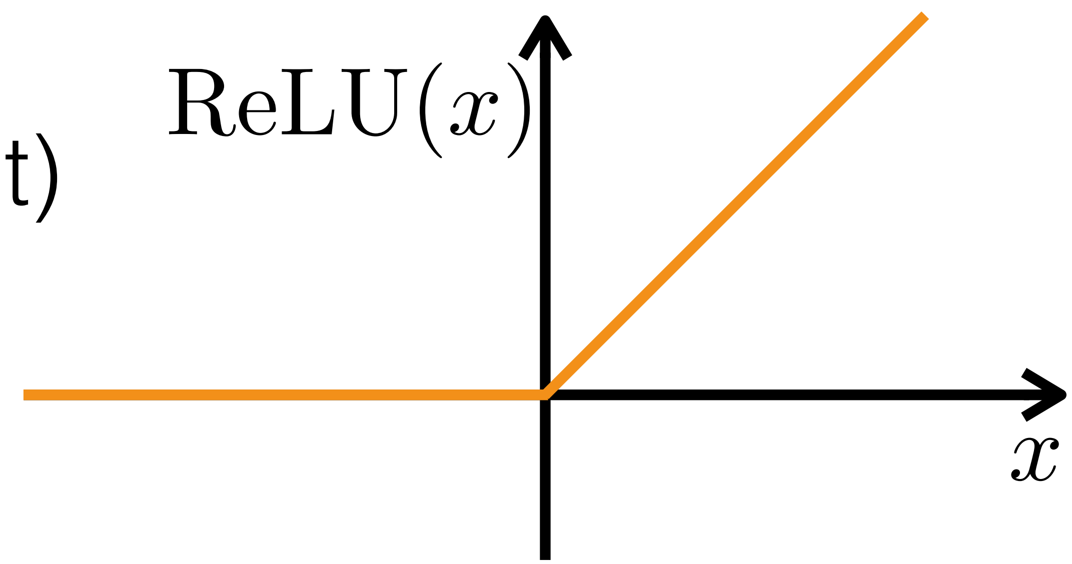


Feedforward Neural Networks

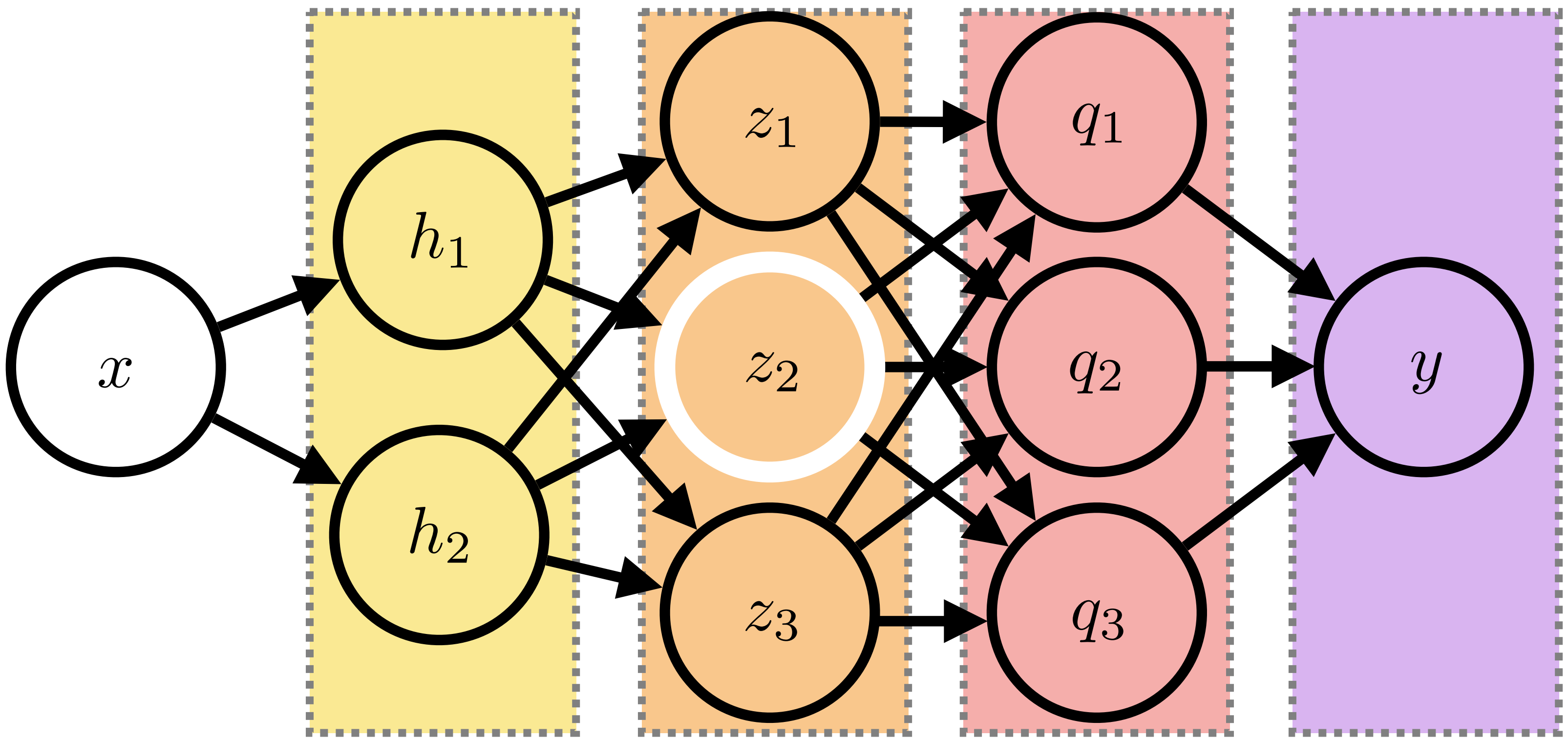


Example (rectified linear unit)

$$f_{1,1}(x) = \mathrm{ReLU}(x)$$



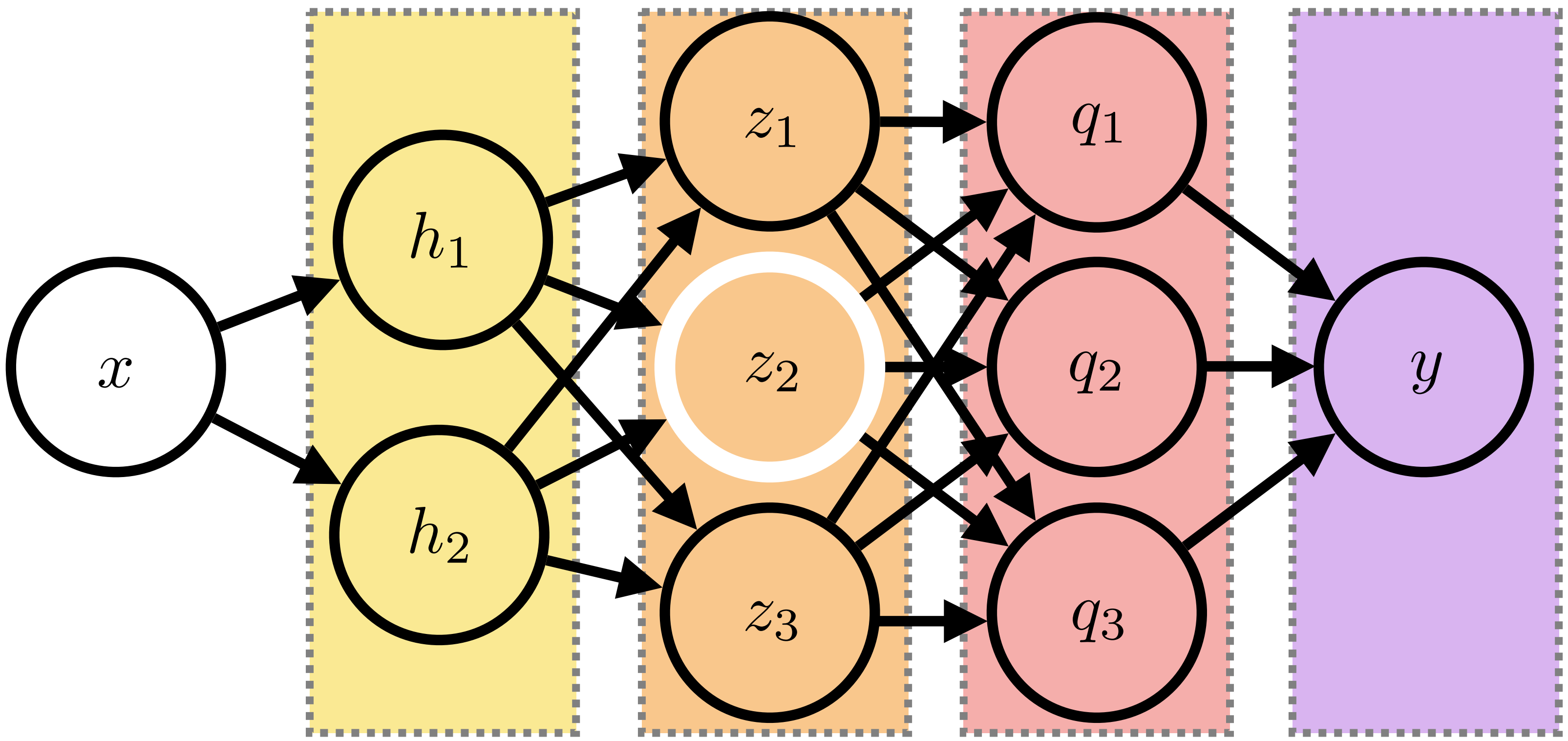
Feedforward Neural Networks



Example (fully connected unit)

$$f_{2,2}(h_1, h_2) = w_1 h_1 + w_2 h_2$$

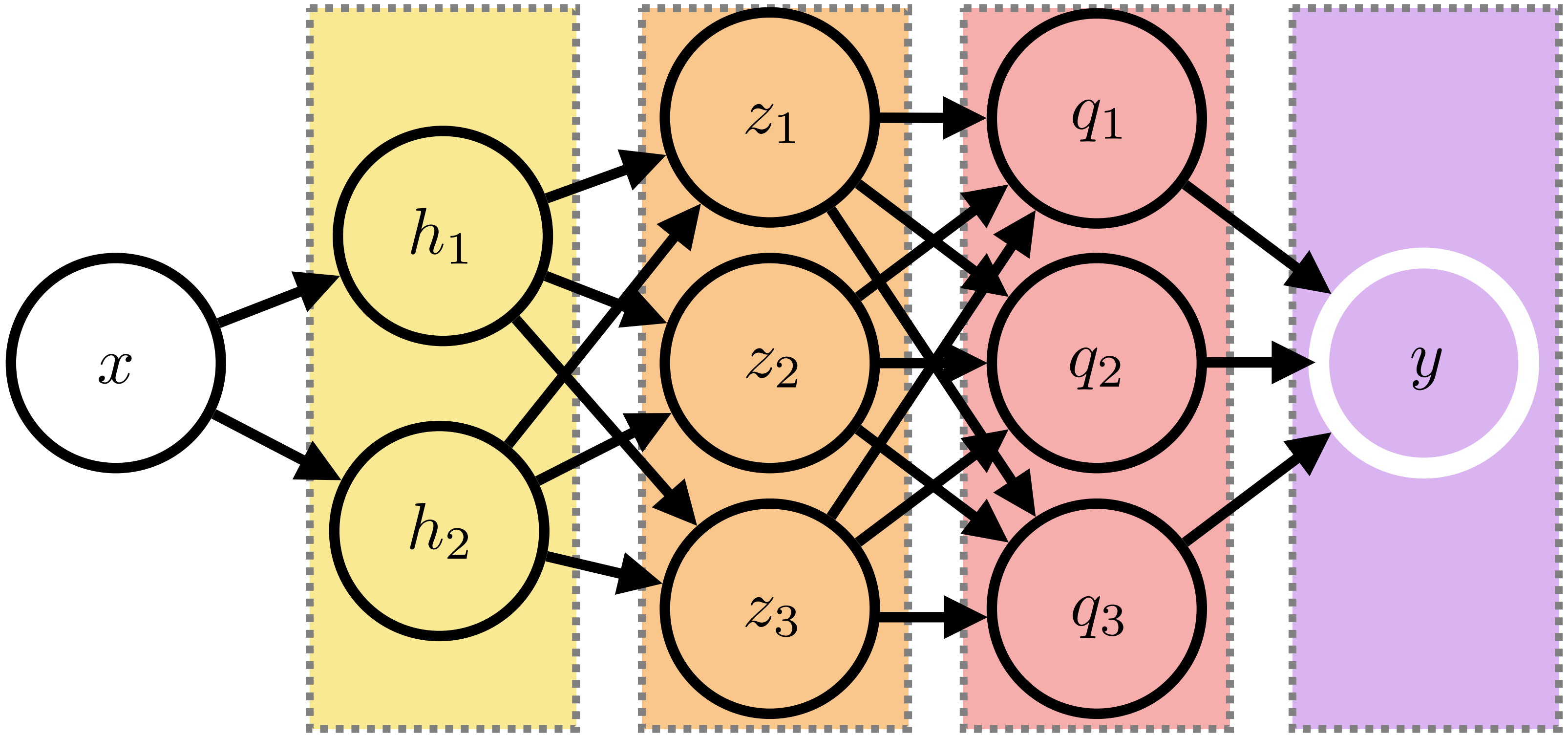
Feedforward Neural Networks



Example (fully connected unit)

$$f_{2,2}(h_1, h_2) = w_1 h_1 + w_2 h_2$$

Feedforward Neural Networks

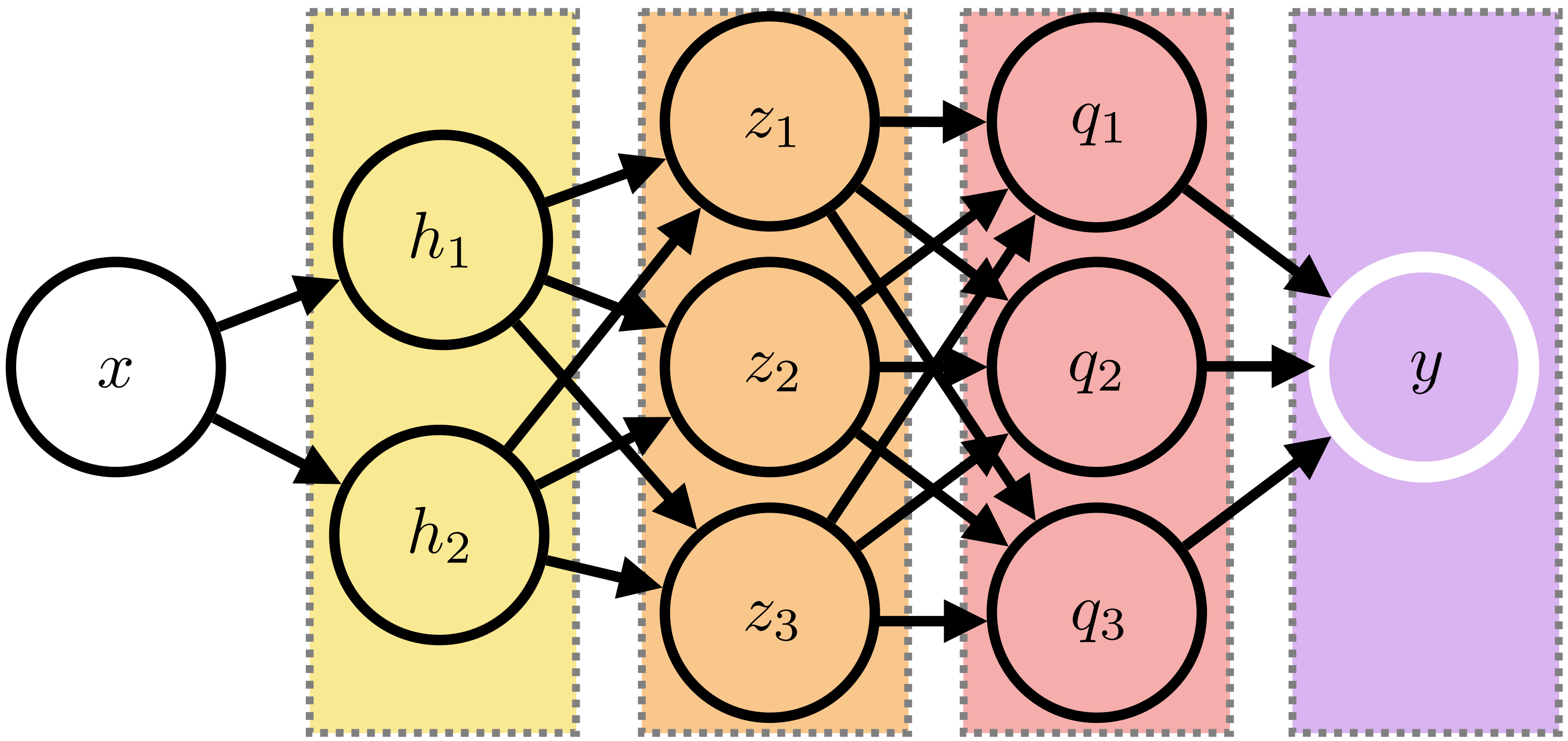


$$y = f_4(q_1, q_2, q_3)$$

Hierarchical composition of functions

$$y = f_4(f_{3,1}(f_{2,1}(f_{1,1}(x), f_{1,2}(x)), \ldots), \ldots)$$

Feedforward Neural Networks



$$y = f_4(q_1, q_2, q_3)$$

Hierarchical composition of functions

$$y = f_4(f_{3,1}(f_{2,1}(f_{1,1}(x), f_{1,2}(x)), \ldots), \ldots)$$

Feedforward Neural Networks

- Feedforward neural networks define a family of functions $f(x;\theta)$

- The goal is to find parameters θ that define the best mapping

$$y = f(x;\theta)$$

  between input x and output y

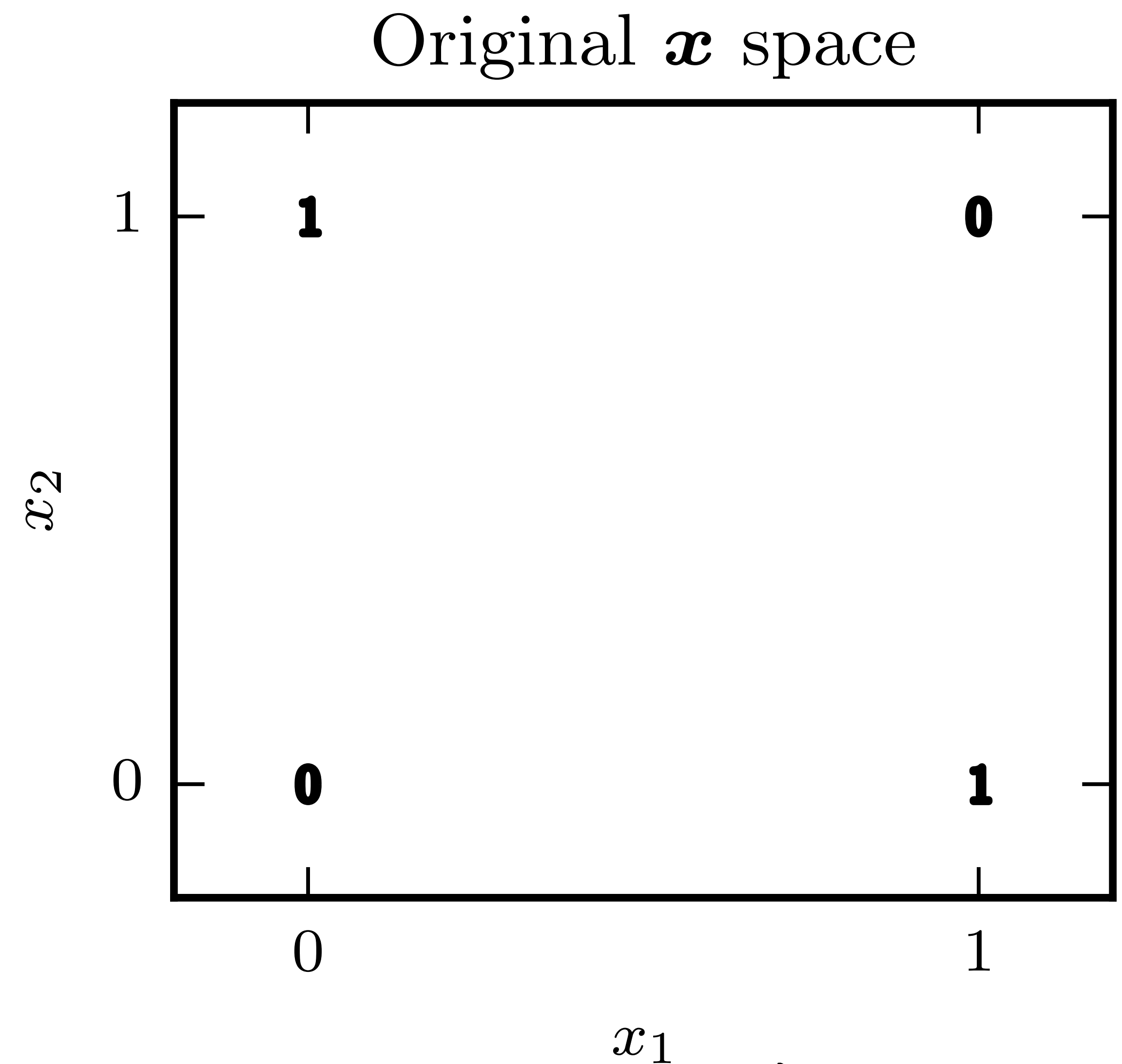
- The key constraints are the I/O dependencies

Deploying a Neural Network

- Given a **task** (in terms of I/O mappings)
- We need
  - **Cost function**
  - **Neural network model** (e.g., choice of units, their number, their connectivity)
  - **Optimization method** (back-propagation)

Example: Learning XOR

- Objective function is the XOR operation between two binary inputs x_1 and x_2



- Training set of (x,y) pairs

$$\left\{ \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, 0 \right), \left(\begin{bmatrix} 0 \\ 1 \end{bmatrix}, 1 \right), \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix}, 1 \right), \left(\begin{bmatrix} 1 \\ 1 \end{bmatrix}, 0 \right) \right\}$$

Cost Function

- Let us use the Mean Squared Error (MSE) as a first attempt

$$J(\theta) = \frac{1}{4} \sum_{i=1}^{4} \left(y^i - f(x^i; \theta)\right)^2$$

Linear Model

- Let us try a linear model of the form

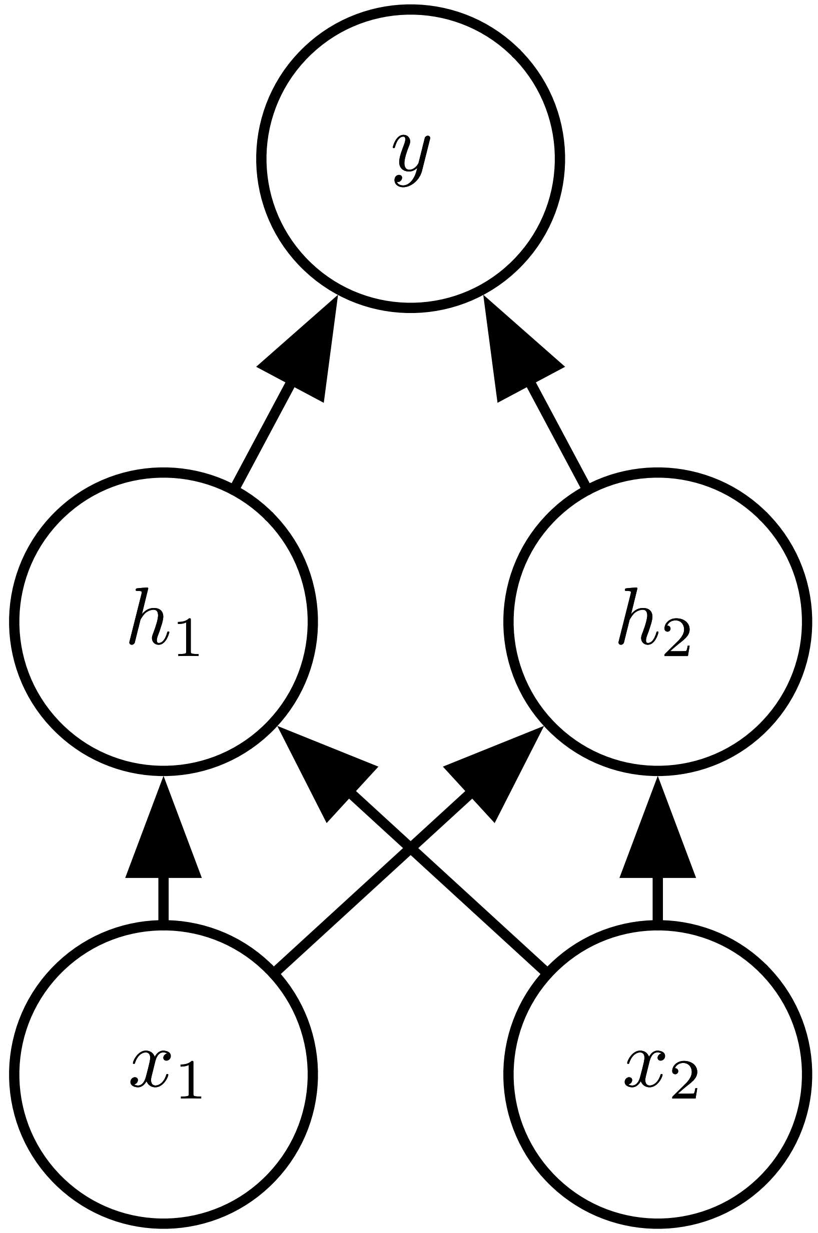
$$f(x; w, b) = w^\top x + b$$

- This choice leads to the normal equations (see slides on Machine Learning Review) and the following values for the parameters

$$w = 0, \qquad b = \frac{1}{2}$$

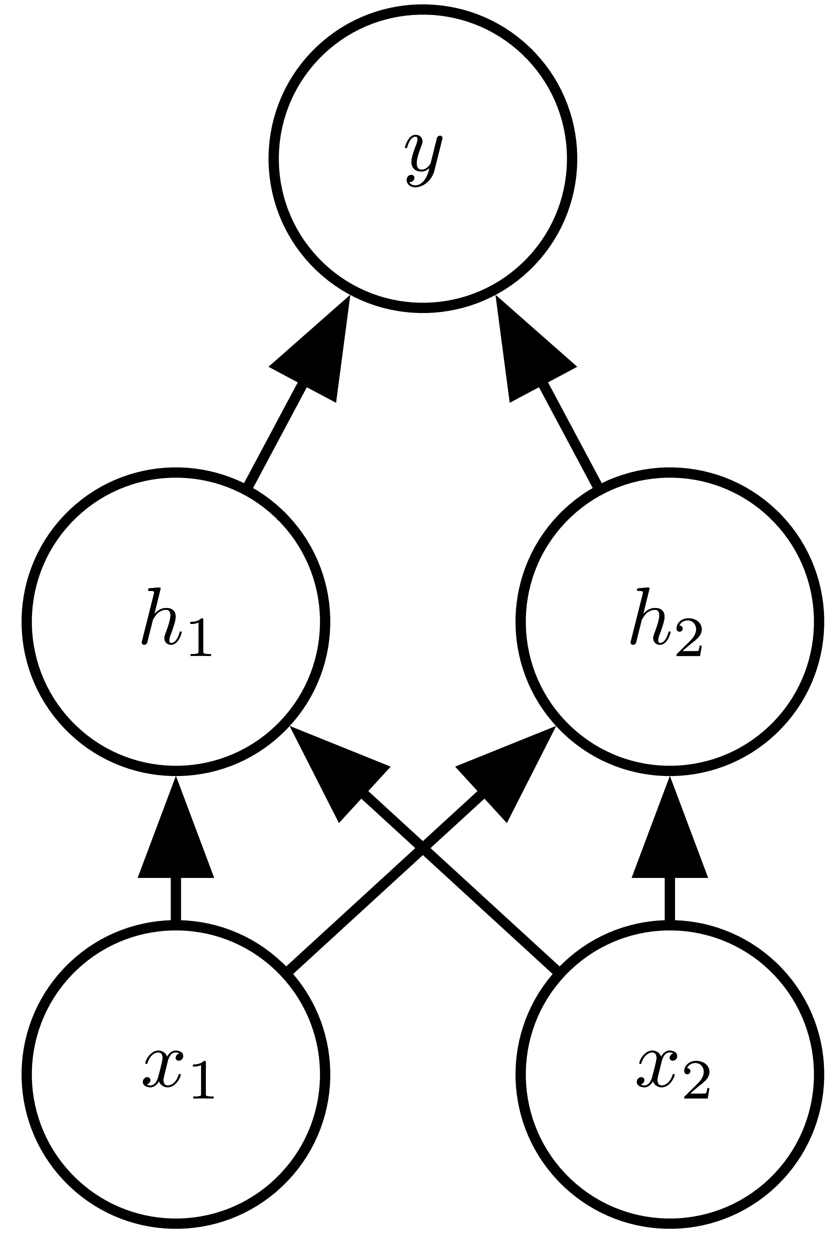
Nonlinear Model

- Let us try a simple feedforward network with one hidden layer and two hidden units



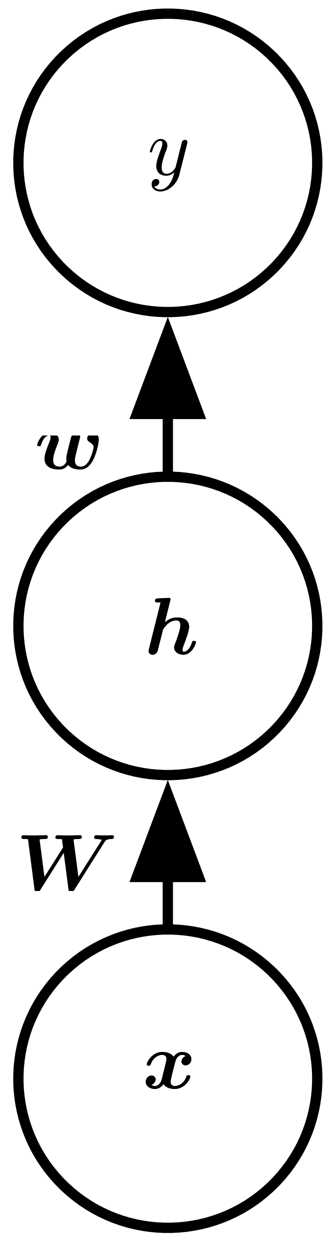
Nonlinear Model

- If each activation function is linear then the composite function would also be linear
- We would have the same poor result as before
- We must consider nonlinear activation functions



Nonlinear Model

$$f(x;W,c,w,b) = w^\top \max\{0, W^\top x + c\} + b$$



$$y(h) = w^\top h + b$$

$$h(x) = \mathrm{ReLU}(W^\top x + c)$$

Optimization

$$f(x; W, c, w, b) = w^\top \max\{0, W^\top x + c\} + b$$

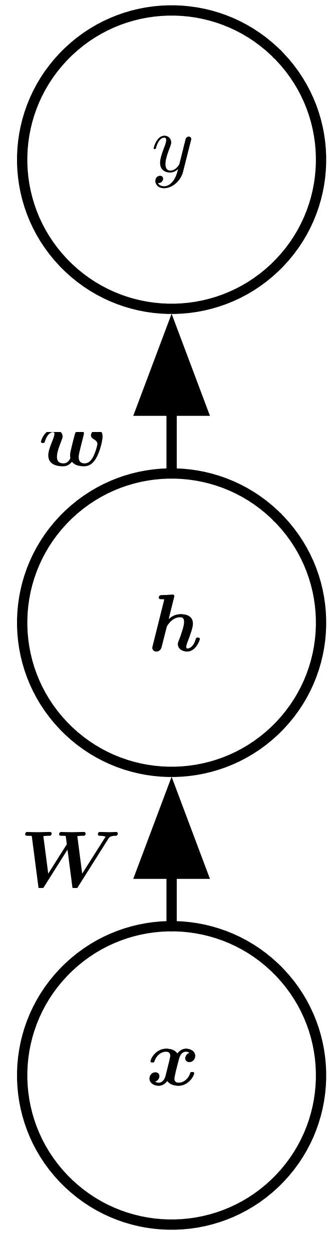
At this stage we would use optimization to fit f to the y in the training set. In this example, we skip this step and assume that some oracle gives us the parameters

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \qquad c = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$$

$$w = \begin{bmatrix} 1 \\ -2 \end{bmatrix} \qquad b = 0$$

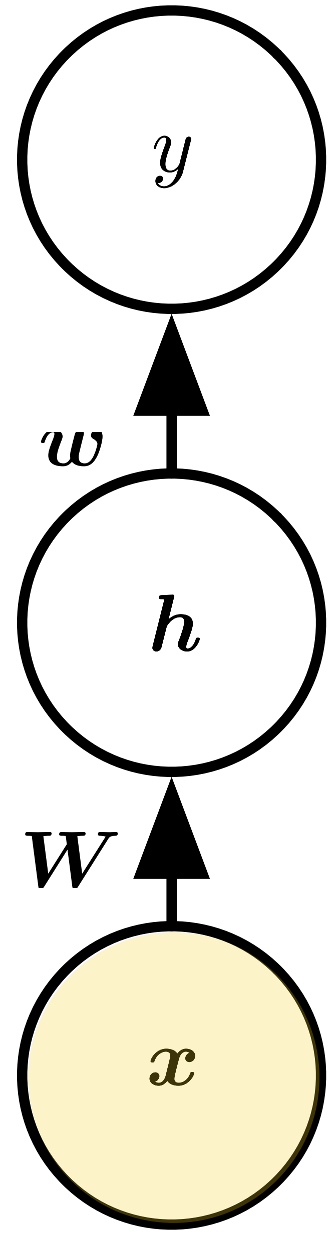
Simulation

$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$



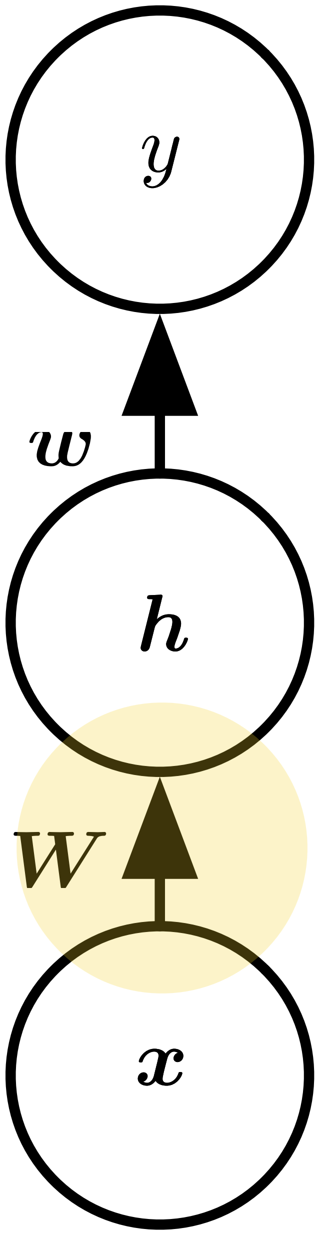
Simulation

$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$



Simulation

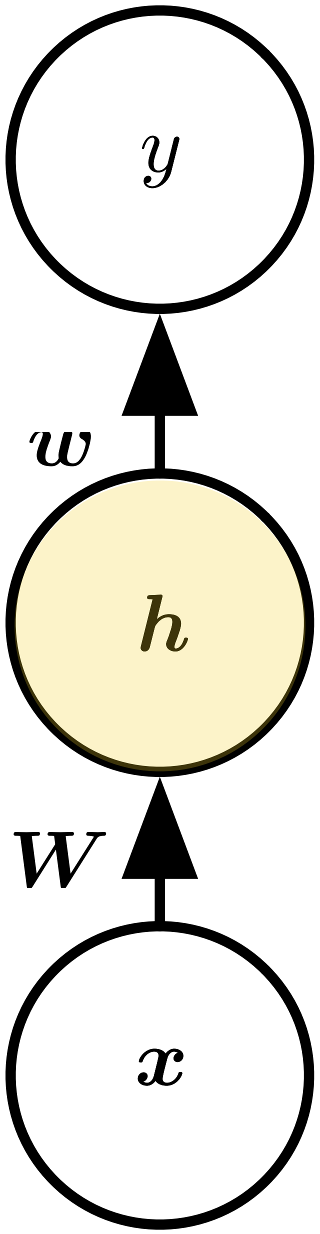
$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \Rightarrow XW + \mathbf{1}c = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$



Simulation

$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \Rightarrow XW + \mathbf{1}c = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

$$\Rightarrow \max\{0, XW + \mathbf{1}c\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$



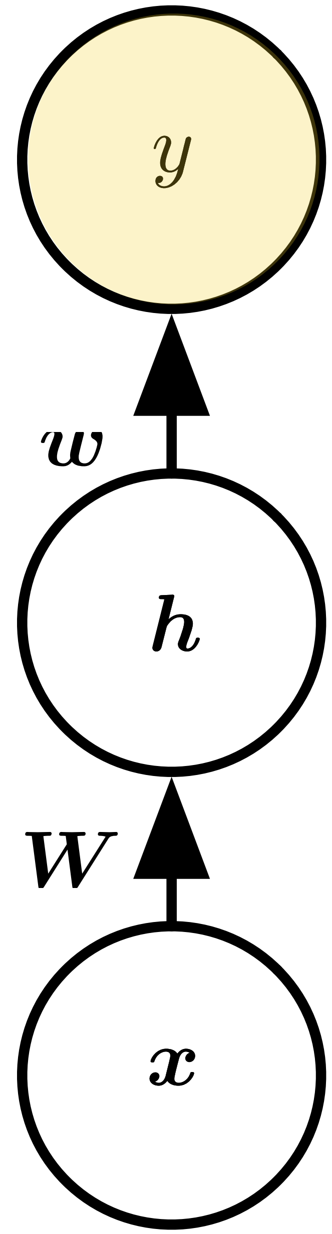
Simulation

$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$

$$XW + \mathbf{1}c = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

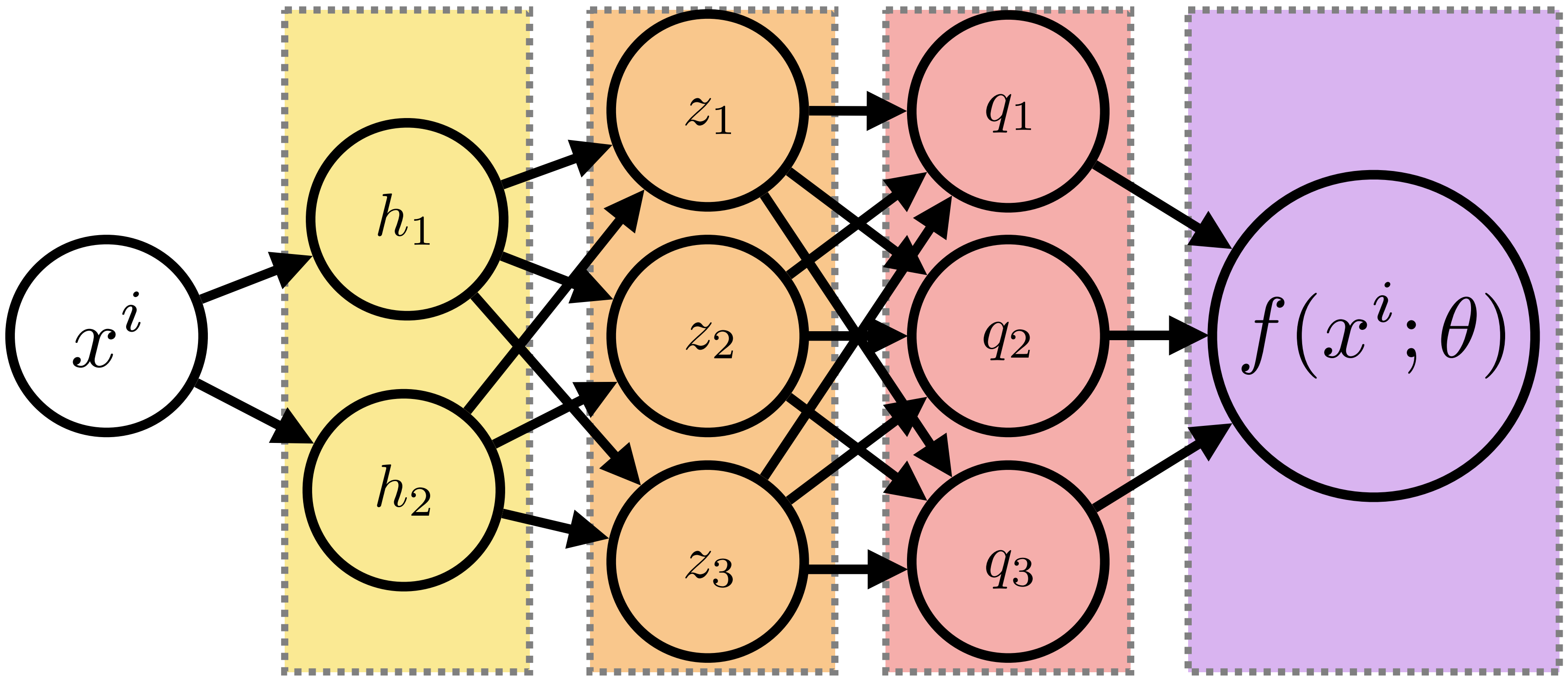
$$\max\{0, XW + \mathbf{1}c\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

$$\max\{0, XW + \mathbf{1}c\}w + \mathbf{1}b = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$



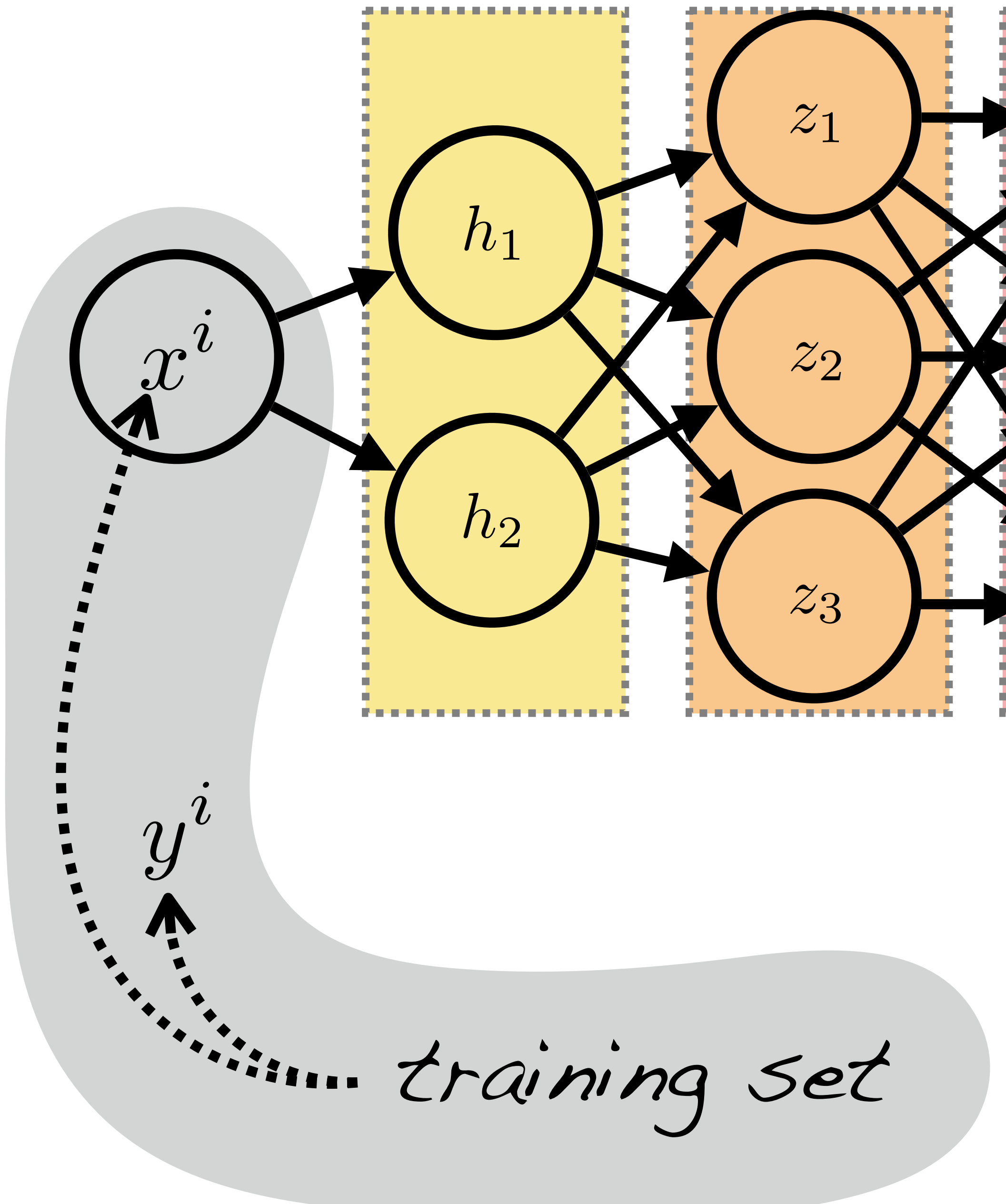
the XOR function
(matches Y)

Step-by-Step Analysis

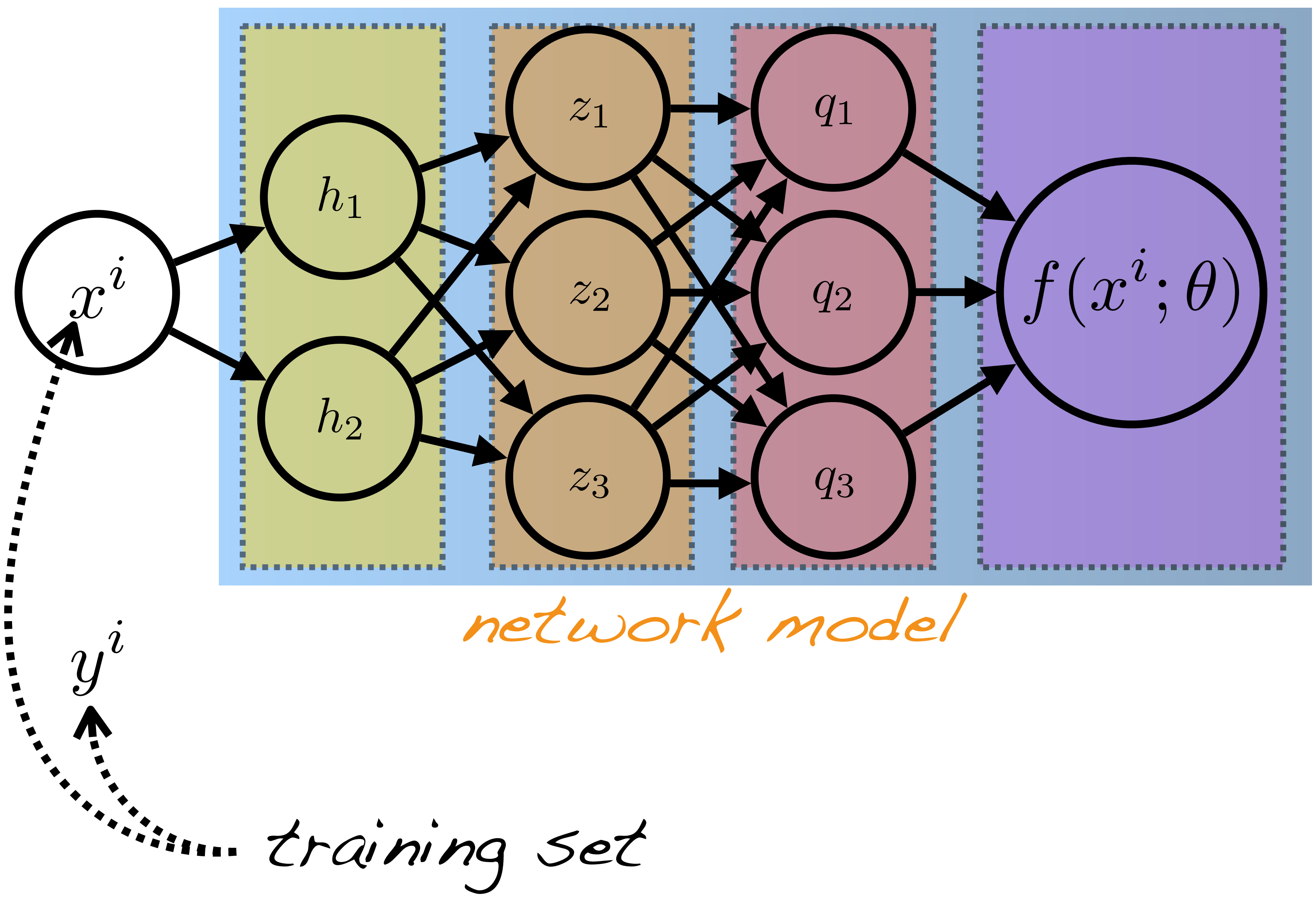


y^i

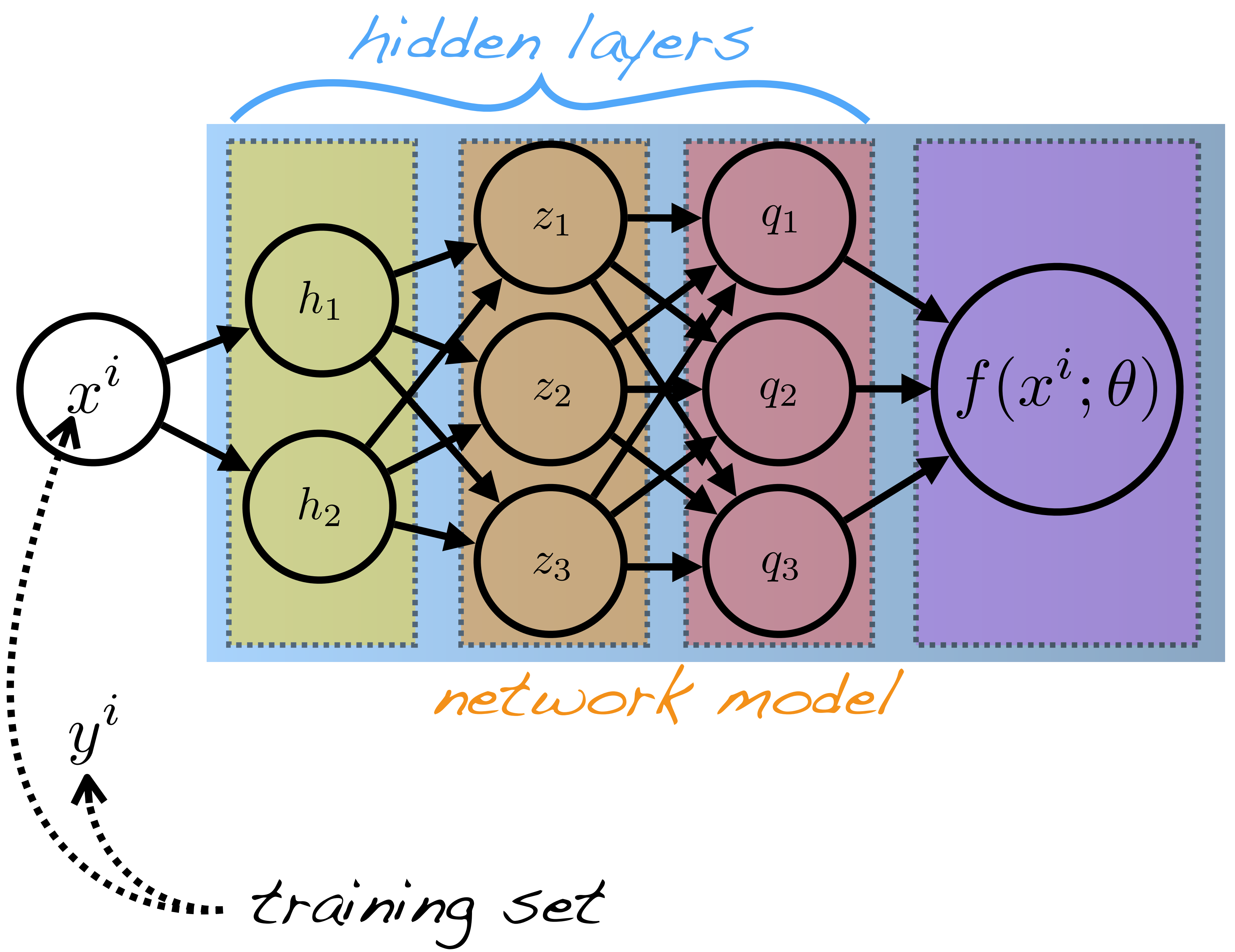
Step-by-Step Analysis



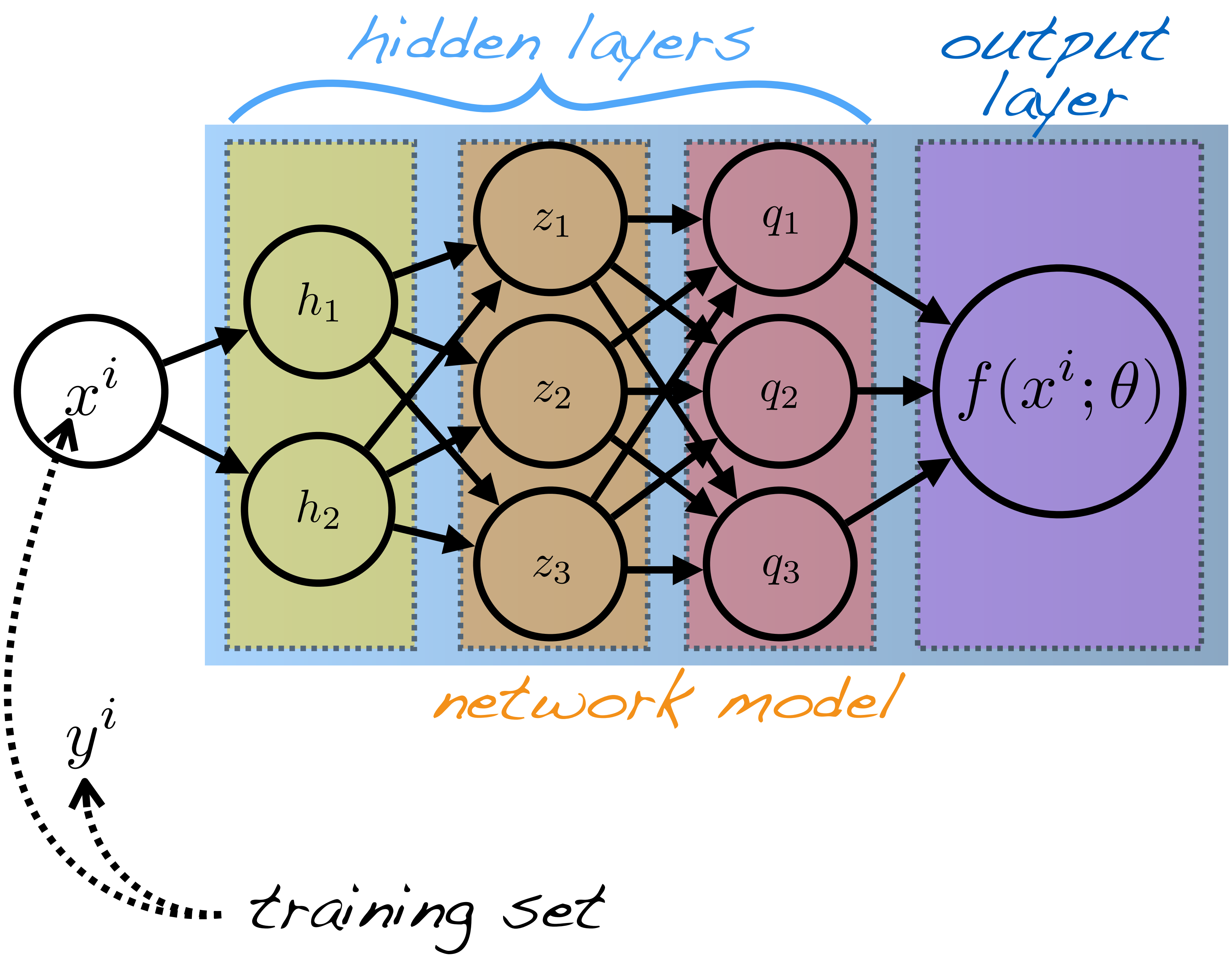
Step-by-Step Analysis



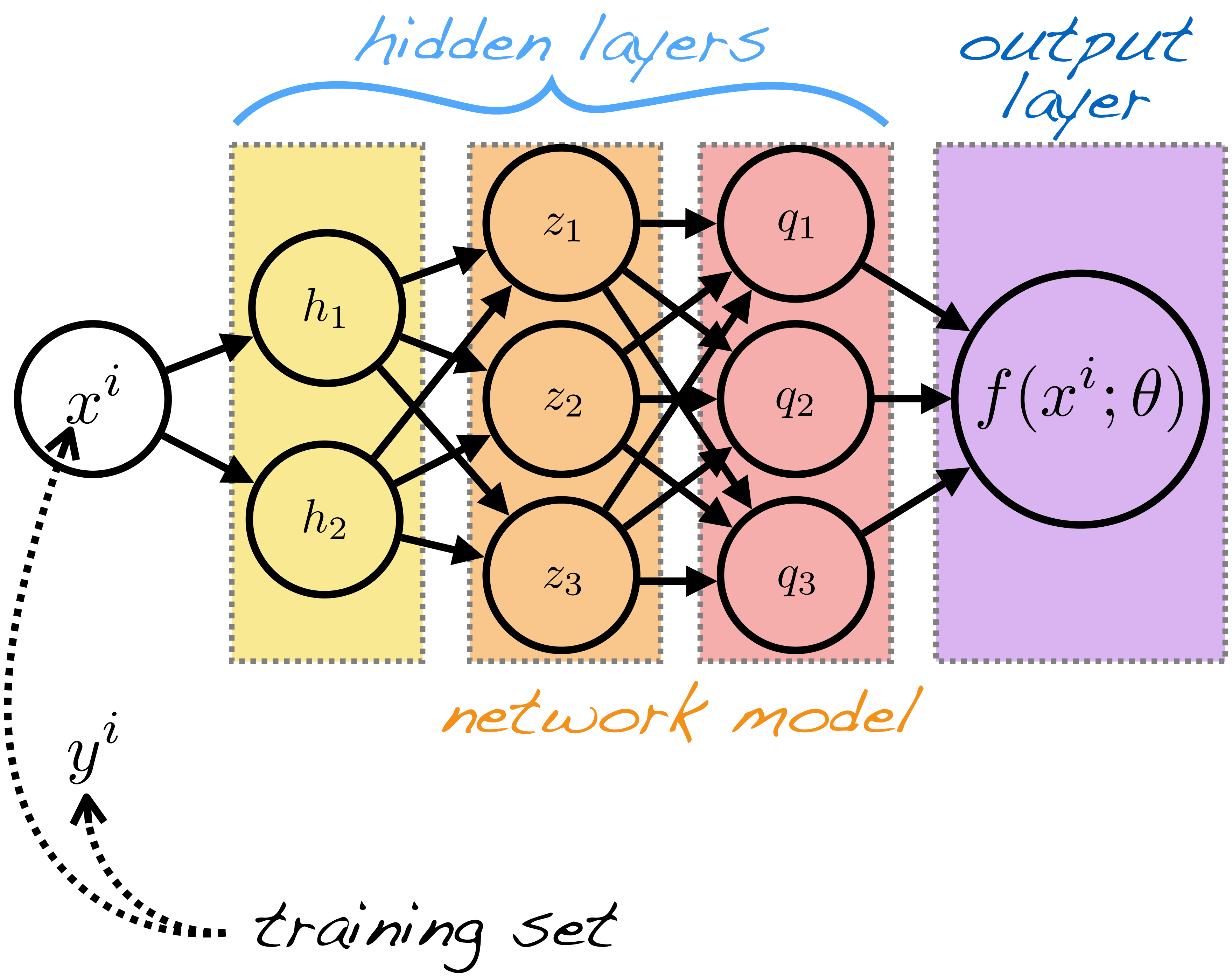
Step-by-Step Analysis



Step-by-Step Analysis



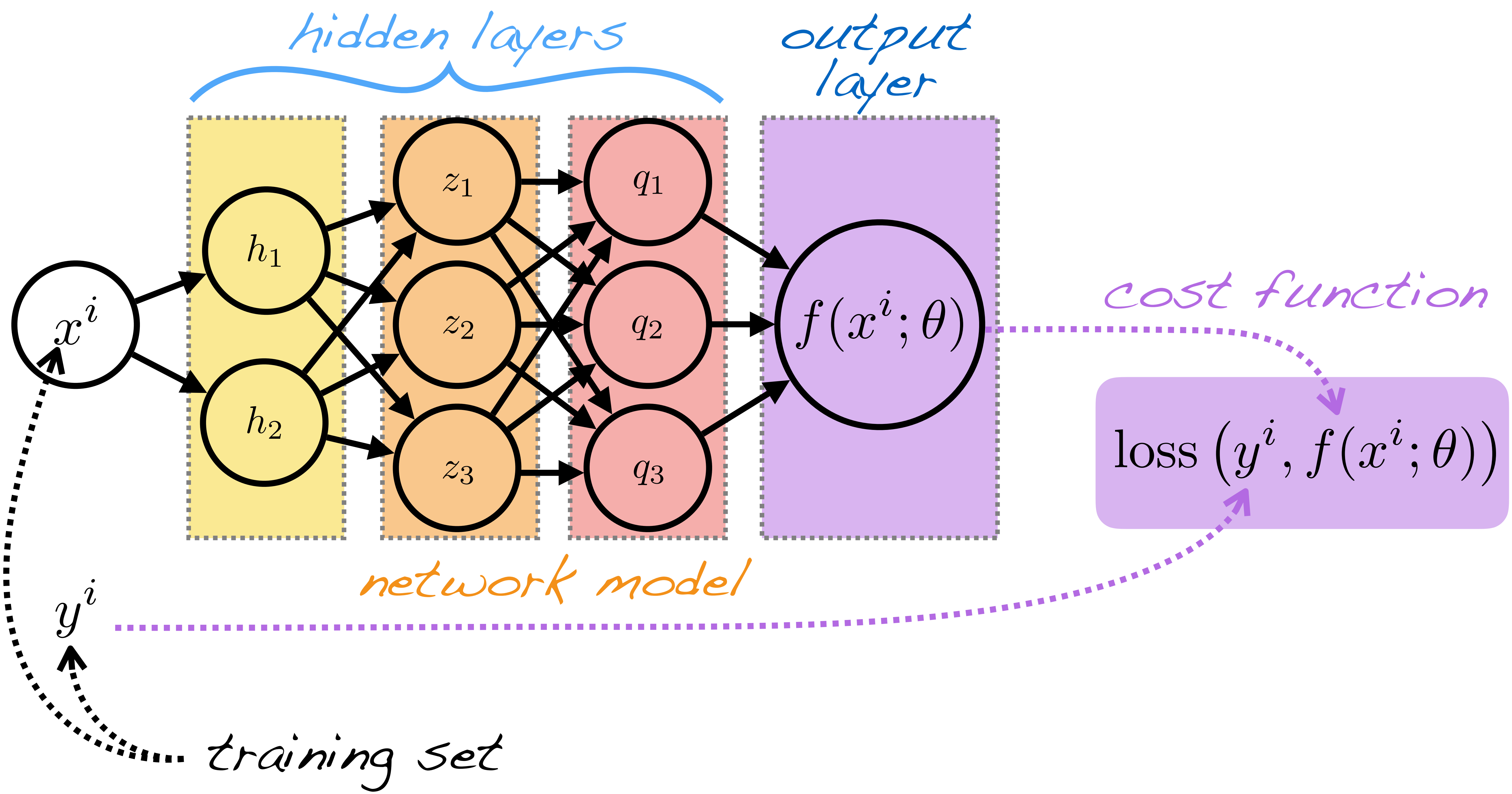
Step-by-Step Analysis



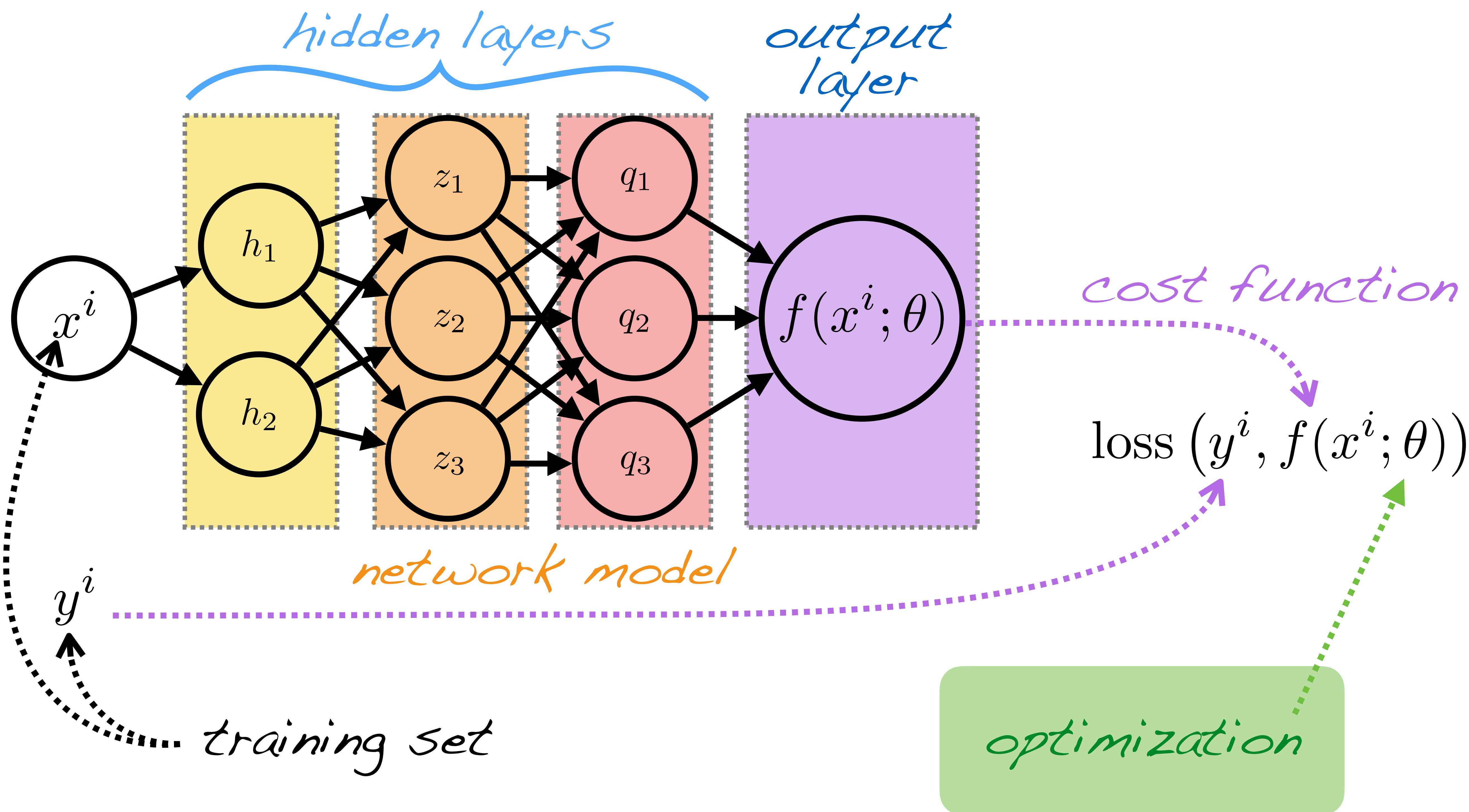
cost function

$$\text{loss}\left(y^i, f(x^i;\theta)\right)$$

Step-by-Step Analysis



Step-by-Step Analysis



Cost Function

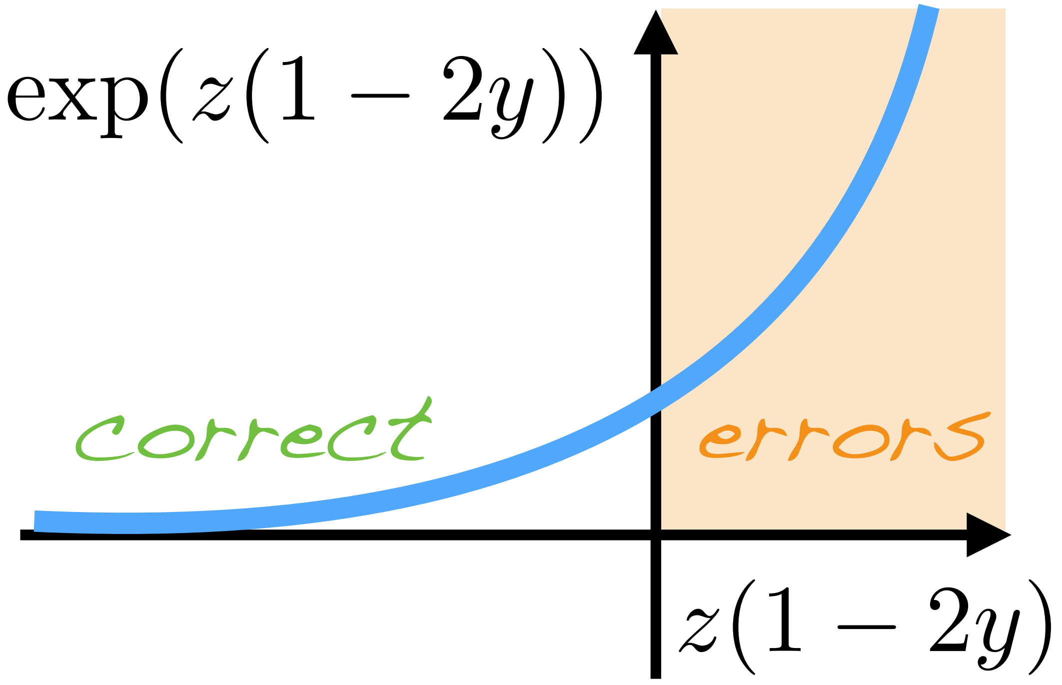
- Based on the **conditional distribution** $p_{\text{model}}(y|x;\theta)$

  - Maximum Likelihood (i.e., **cross-entropy** between model pdf and data pdf)

$$\min_{\theta} -E_{x,y\sim\hat{p}_{\text{data}}}[\log p_{\text{model}}(y|x;\theta)]$$

Saturation

- Functions that saturate (have flat regions) have a very small gradient and slow down gradient descent
- We choose loss functions that have a non flat region when the answer is incorrect (it might be flat otherwise)
- E.g., exponential functions saturate in the negative domain; with a binary variable $y \in \{0, 1\}$ map errors to the nonflat region and then minimize



- The logarithm also helps with saturation (see next slides)

Output Units

- The choice of the output representation (e.g., a probability vector or the mean estimate) determines the cost function
- Let us denote with

$$h = f(x; \theta)$$

the output of the layer before the output unit

Linear Units

- With a little abuse of terminology, linear units include **affine transformations**

$$\hat{y} = W^\top h + b$$

can be seen as the mean of the conditional Gaussian distribution (in the Maximum Likelihood loss)

$$p(y|x) = \mathcal{N}(y; \hat{y}, I)$$

- The Maximum Likelihood loss becomes

$$-\log p(y|\hat{y}) = |y - \hat{y}|^2 + \text{const}$$

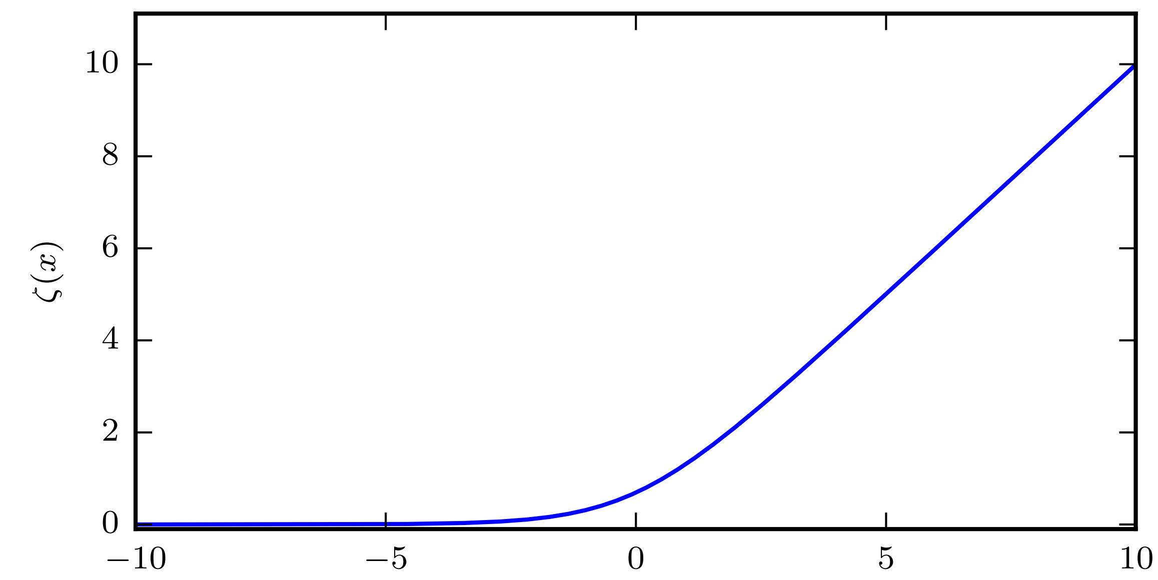
Softplus

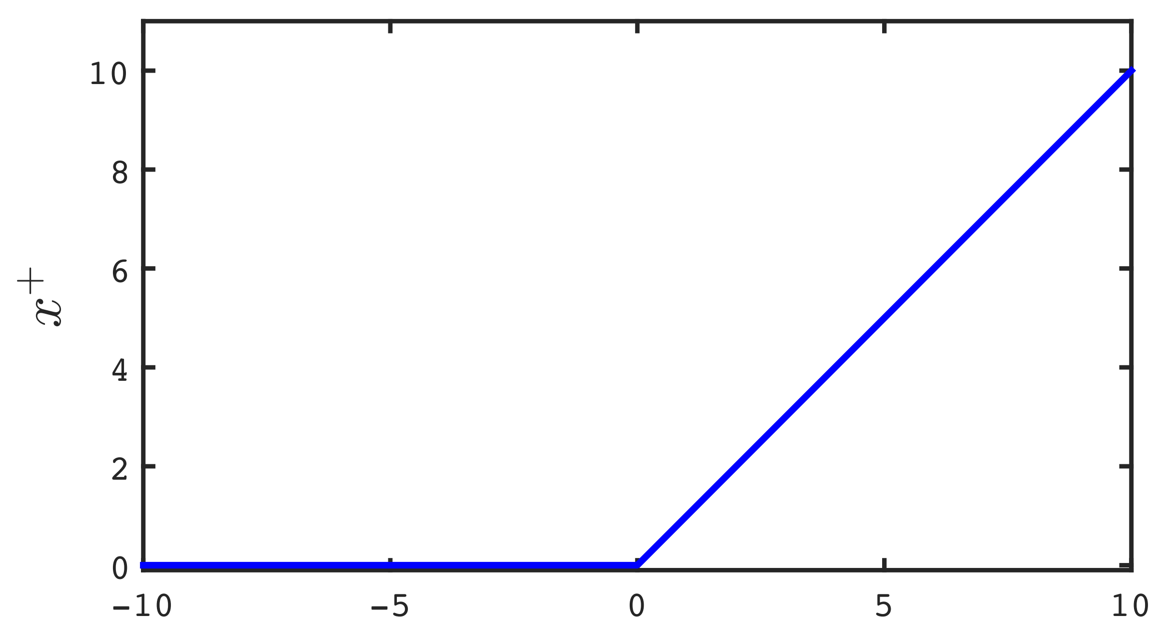
- The **softplus** function is defined as

$$\zeta(x) = \log(1 + \exp(x))$$

and it is a smooth approximation of the Rectified Linear Unit (ReLU)

$$x^+ = \max(0, x)$$





Sigmoid Units

- Use to predict binary variables or to predict the probability of binary variables

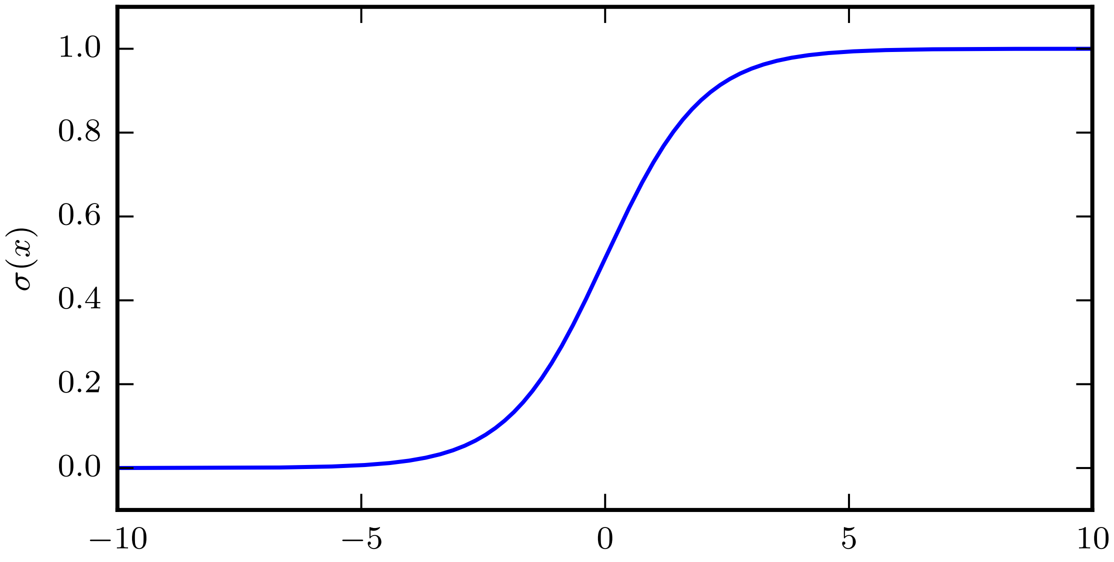
$$p(y = 0|x) \in [0, 1]$$

- The sigmoid unit defines a suitable mapping and has no flat regions (useful in gradient descent)

$$\hat{y} = \sigma(w^\top h + b)$$

where we have used the **logistic sigmoid** function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



Bernoulli Parametrization

- Let $z = w^\top h + b$. Then, we can define the Bernoulli distribution

$$p(y|z) = \sigma((2y-1)z)$$

- The loss function with Maximum Likelihood is then

$$-\log p(y|z) = \zeta((1-2y)z) \simeq \max(0, (1-2y)z)$$

and saturation occurs only when the output is correct (y=0 and z<0 or y=1 and z>0)

Smoothed Max

- An extension to the softplus function is the smoothed max

$$\log \sum_j \exp(z_j)$$

which gives a smooth approximation to $\max_j z_j$

- If we rewrite the softplus function as

$$\log(1 + \exp(z)) = \log(\exp(0) + \exp(z))$$

we can see that it is the case with $z_1 = 0, z_2 = z$

Softmax Units

- An extension of the logistic sigmoid to multiple variables
- Used as the output of a multi-class classifier
- The **Softmax** function is defined as

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- Shift-invariance: $\text{softmax}(z + \mathbf{1}c) = \text{softmax}(z)$

  gives numerically stable implementation

$$\text{softmax}(z - \max_j z_j) = \text{softmax}(z)$$

Softmax Units

- In Maximum Likelihood we have

$$\log \operatorname{softmax}(z)_i = z_i - \log \sum_j \exp(z_j)$$

- Recall the smoothed max, then we can write

$$\log \operatorname{softmax}(z)_i \simeq z_i - \max_j z_j$$

- Maximization, with $i = \arg\max_j z_j$, yields

$$\operatorname{softmax}(z)_i = 1 \quad \text{and} \quad \operatorname{softmax}(z)_{j \neq i} = 0$$

Softmax Units

- Softmax is an extension to the logistic sigmoid where we have 2 variables and $z_1 = 0, z_2 = z$

$$p(y = 1|x) = \mathrm{softmax}(z)_1 = \sigma(z_2)$$

- Softmax is a winner-take-all formulation

- Softmax is more related to the arg max function than the max function

Hidden Units

- The design of a neural network is so far still an art

- The basic principle is the **trial and error** process:
  1. Start from a known model
  2. Modify
  3. Implement and test (go back to 2. if needed)

- A good choice is to always use ReLUs

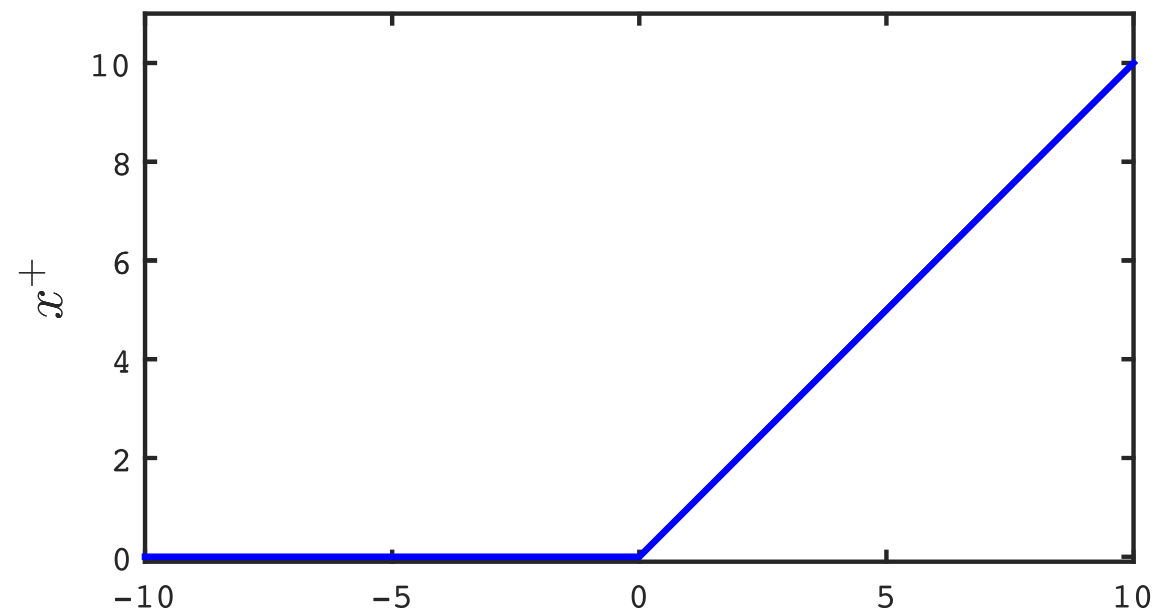
- In general the hidden unit picks a g for

$$h(x) = g(W^\top x + b)$$

Rectified Linear Units

- ReLUs typically use also an affine transformation

$$g(z) = \max\{0, z\}$$



- Good initialization is b = 0.1 (initially, a linear layer)
- Negative axis cannot learn due to null gradient
- Generalizations help avoid the null gradient

Leaky ReLUs and More

- A generalisation of ReLU is

$$g(z, \alpha) = \max\{0, z\} + \alpha \min\{0, z\}$$

- To avoid a null gradient the following are in use

1. Absolute value rectification $\alpha = -1$
2. Leaky ReLU $\alpha = 0.01$
3. Parametric ReLU α learnable
4. Maxout Units

$$g(z)_i = \max_{j \in S_i} z_j$$

$$\cup_i S_i = [1, \ldots, m]$$

$$S_i \cap S_j = \varnothing \quad i \neq j$$

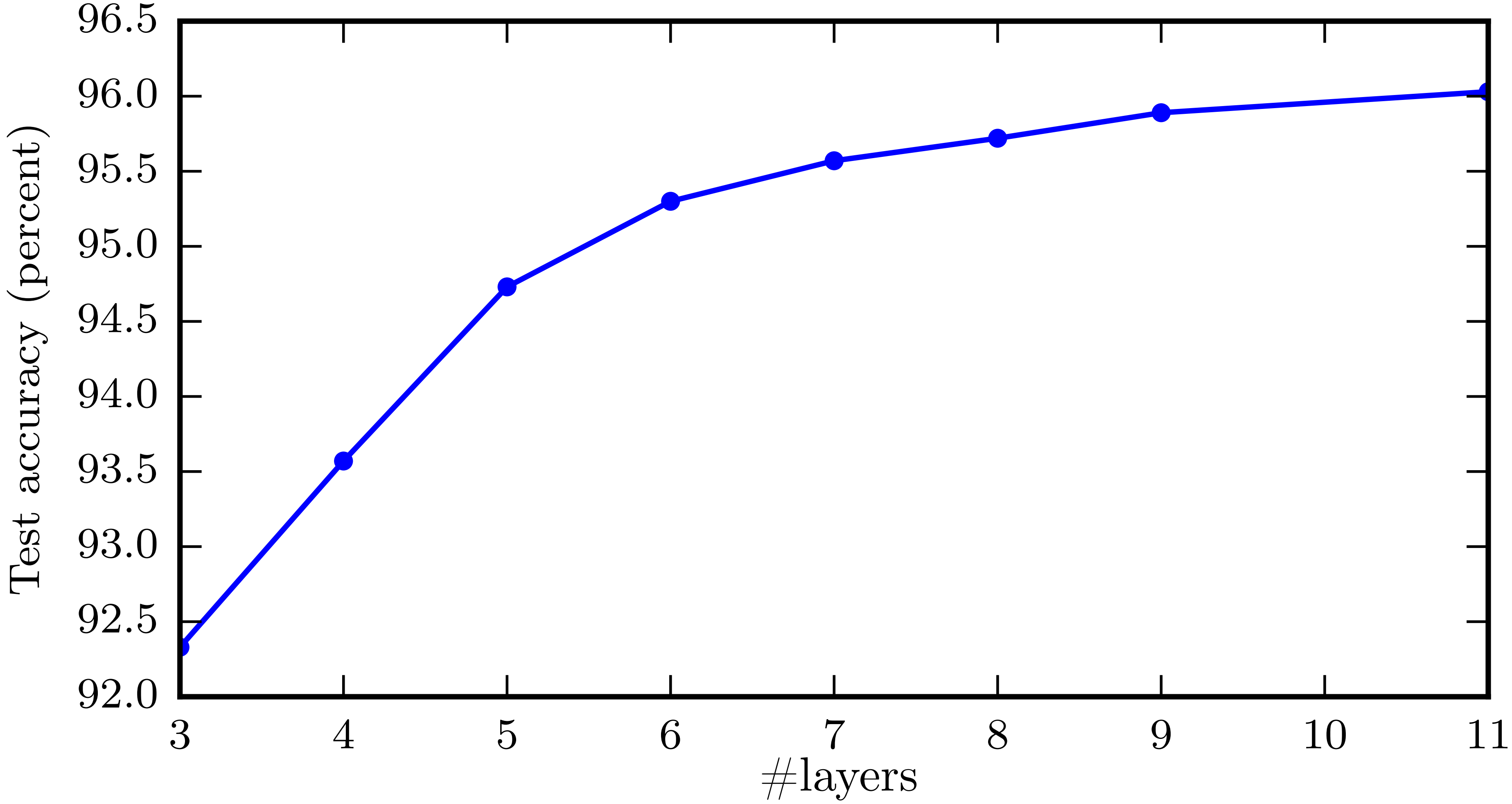
Network Design

- The **network architecture** is the overall structure of the network: number of units and their connectivity

- Today, the design for a task must be found experimentally via a careful analysis of the training and validation error

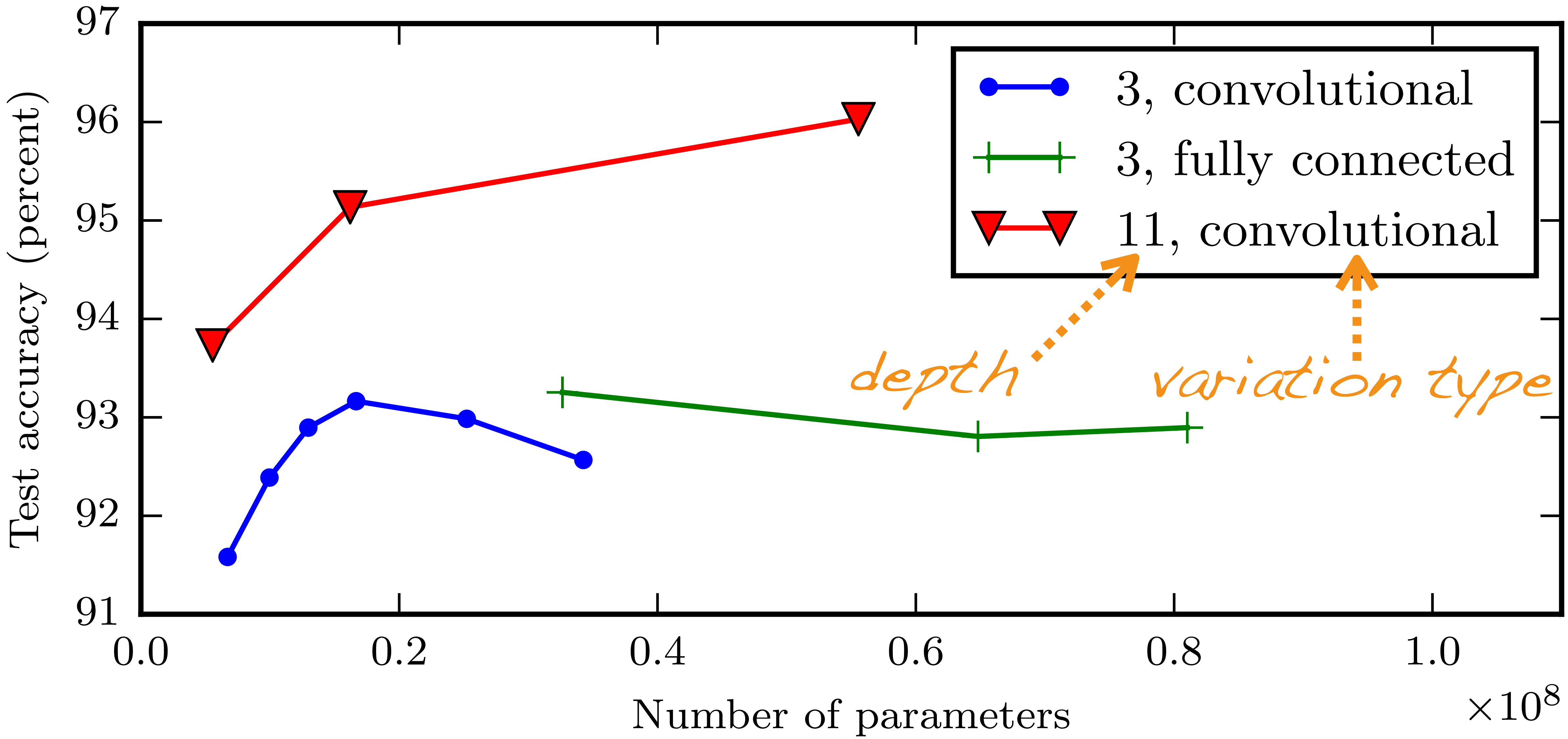
Depth

- A general rule is that depth helps generalization
- It is better to have many simple layers than few highly complex ones



Depth

- Other network modifications do not have the same effect

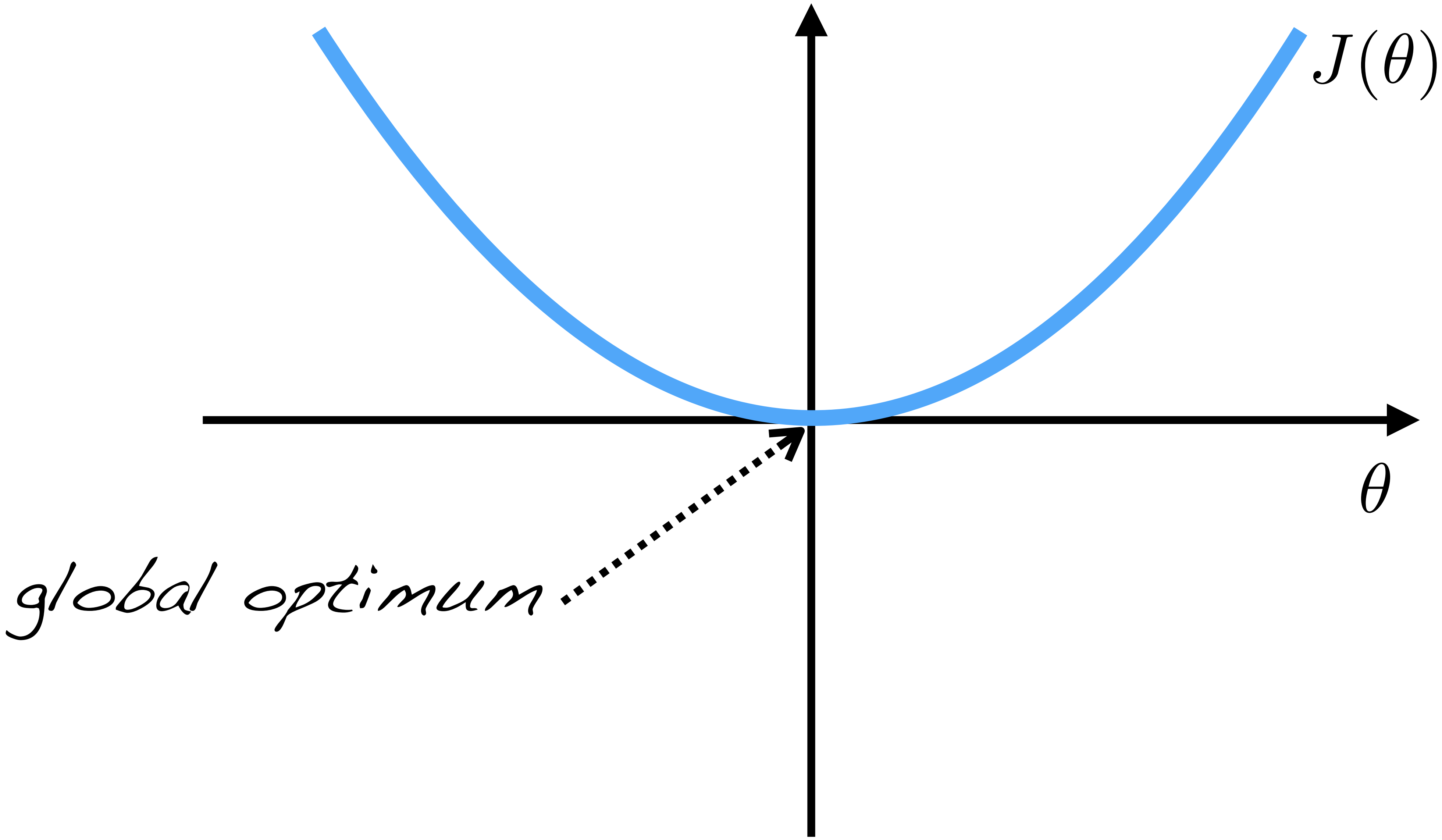


Optimization

- Given a task we define
  - The training data $\{x^i, y^i\}_{i=1,\ldots,m}$
  - A network design $f(x;\theta)$
  - The loss function $J(\theta) = \sum_{i=1}^{m} \text{loss}\left(y^i, f(x^i;\theta)\right)$
- Next, we **optimize** the network parameters θ
- This operation is called **training**

Optimization

- The MSE cost function $J(\theta)$ is **convex** with a linear model



Optimization

- However, since the cost function $J(\theta)$ is typically **non convex** in the parameters, we use an iterative solution

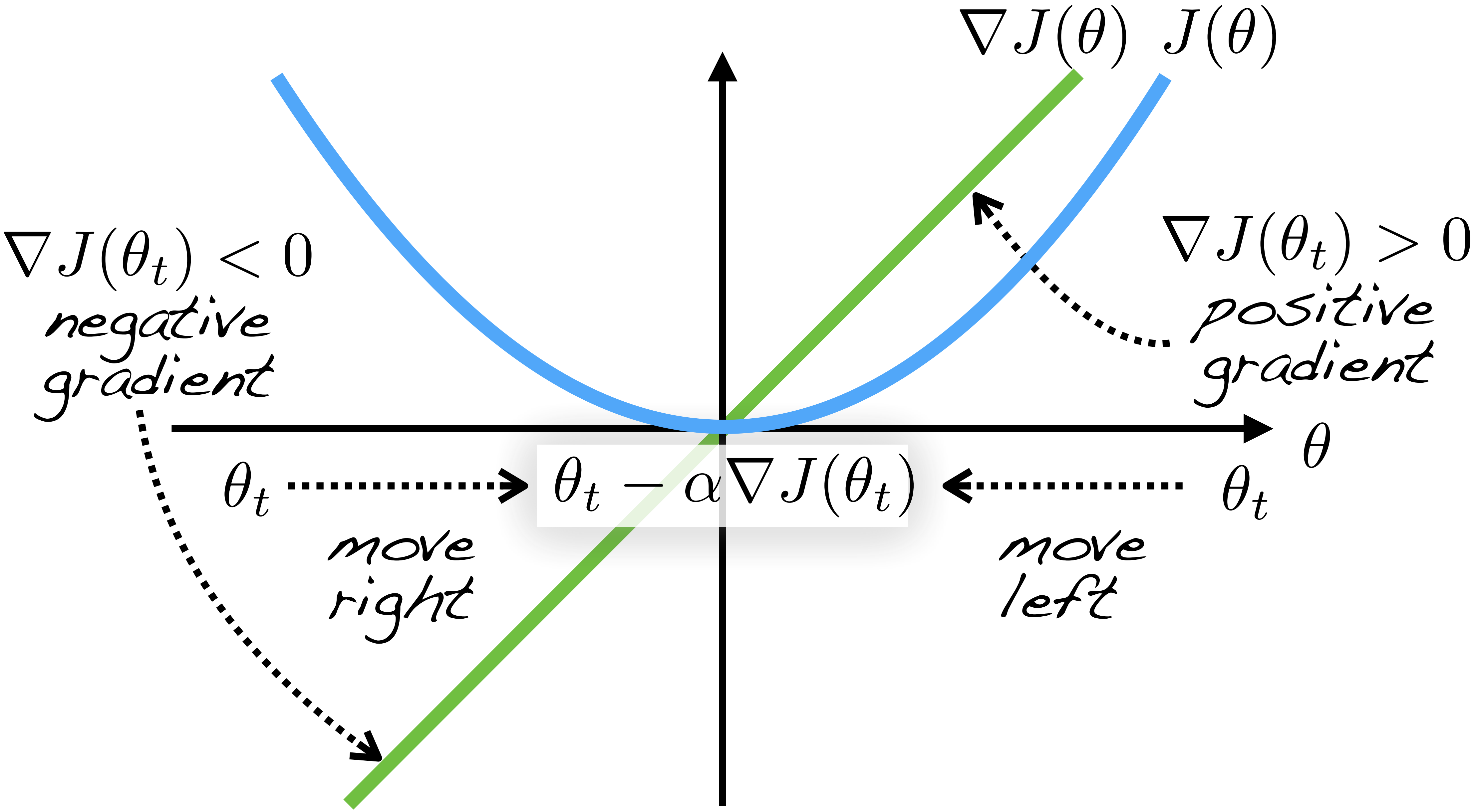
- We consider the **gradient descent** method

$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

where $\alpha > 0$ is the learning rate

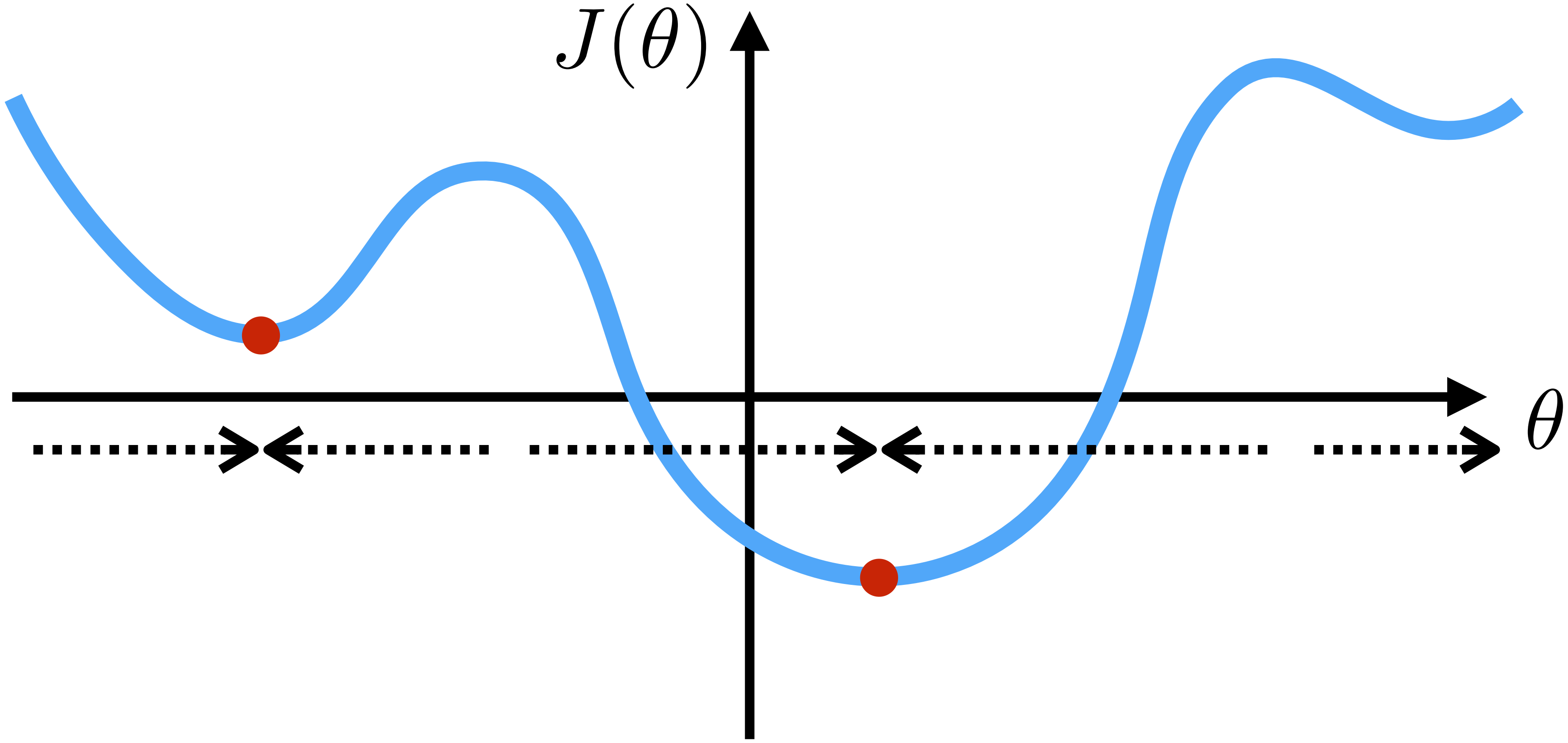
Optimization

gradient descent $\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$



Local Minima

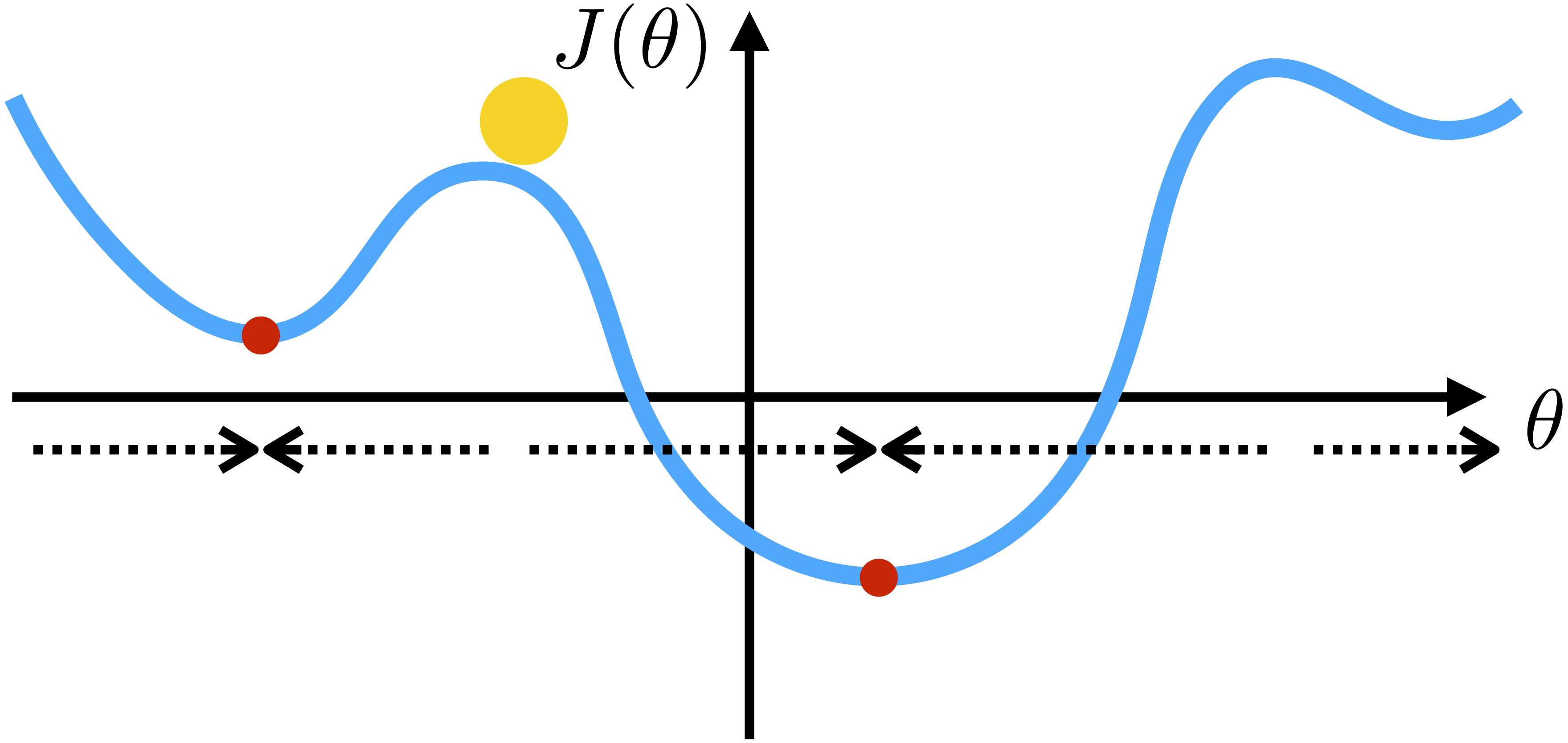
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

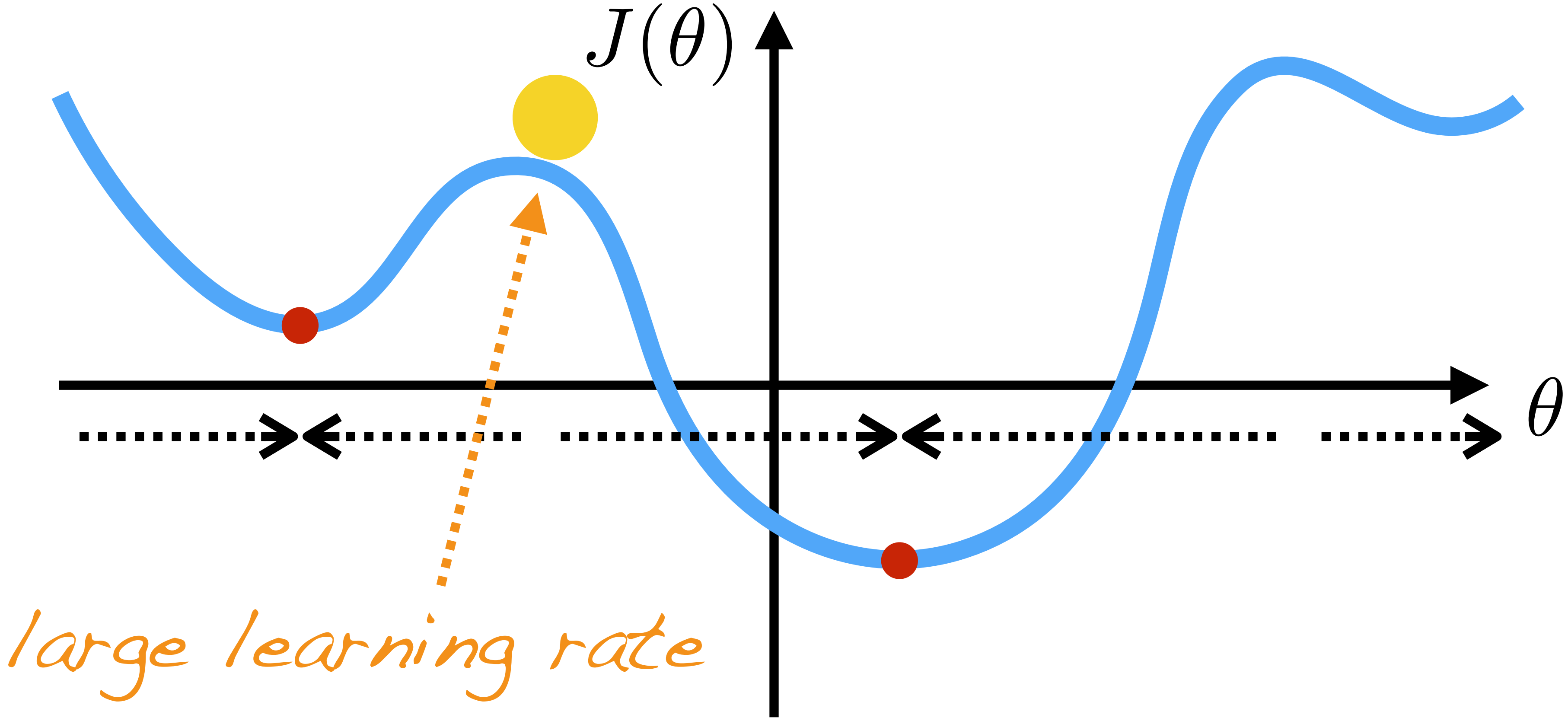
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

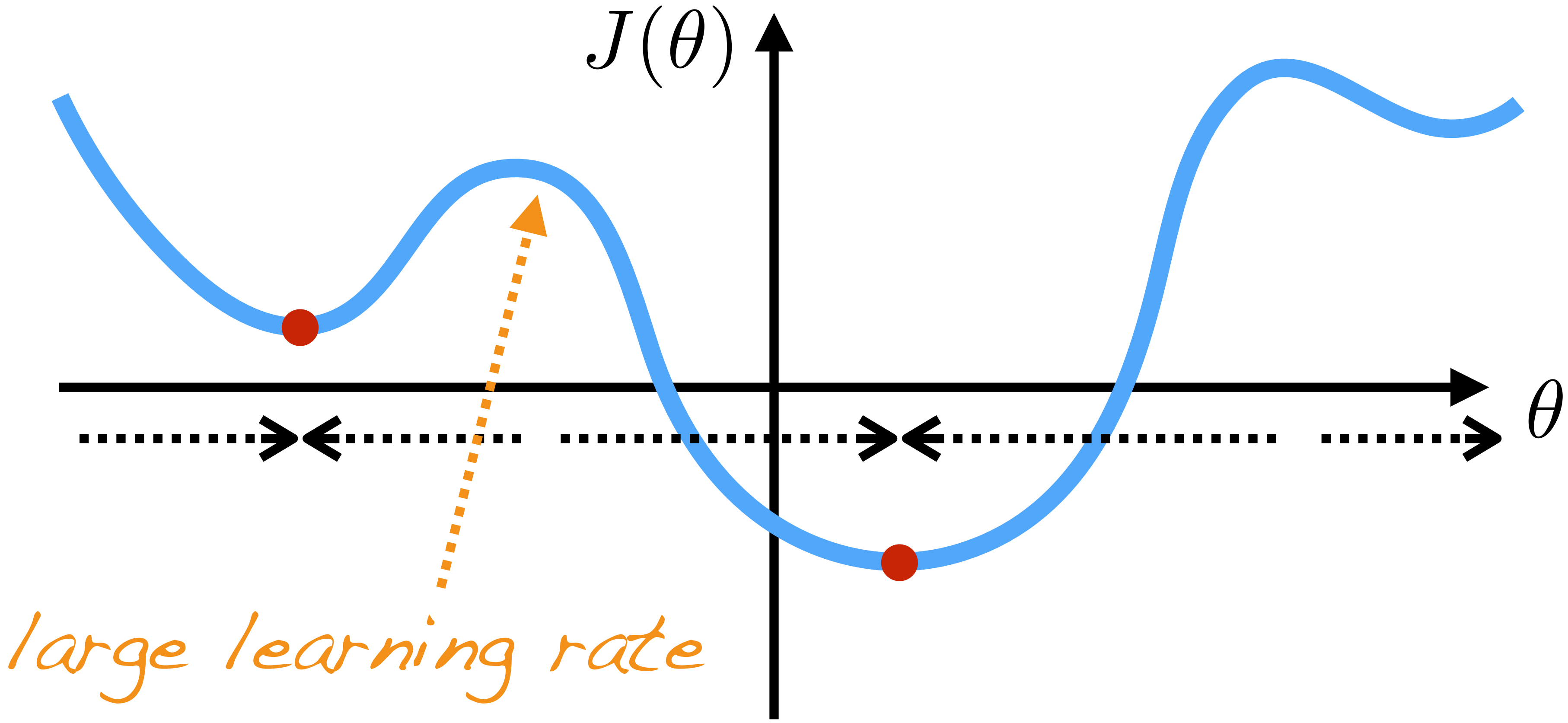
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

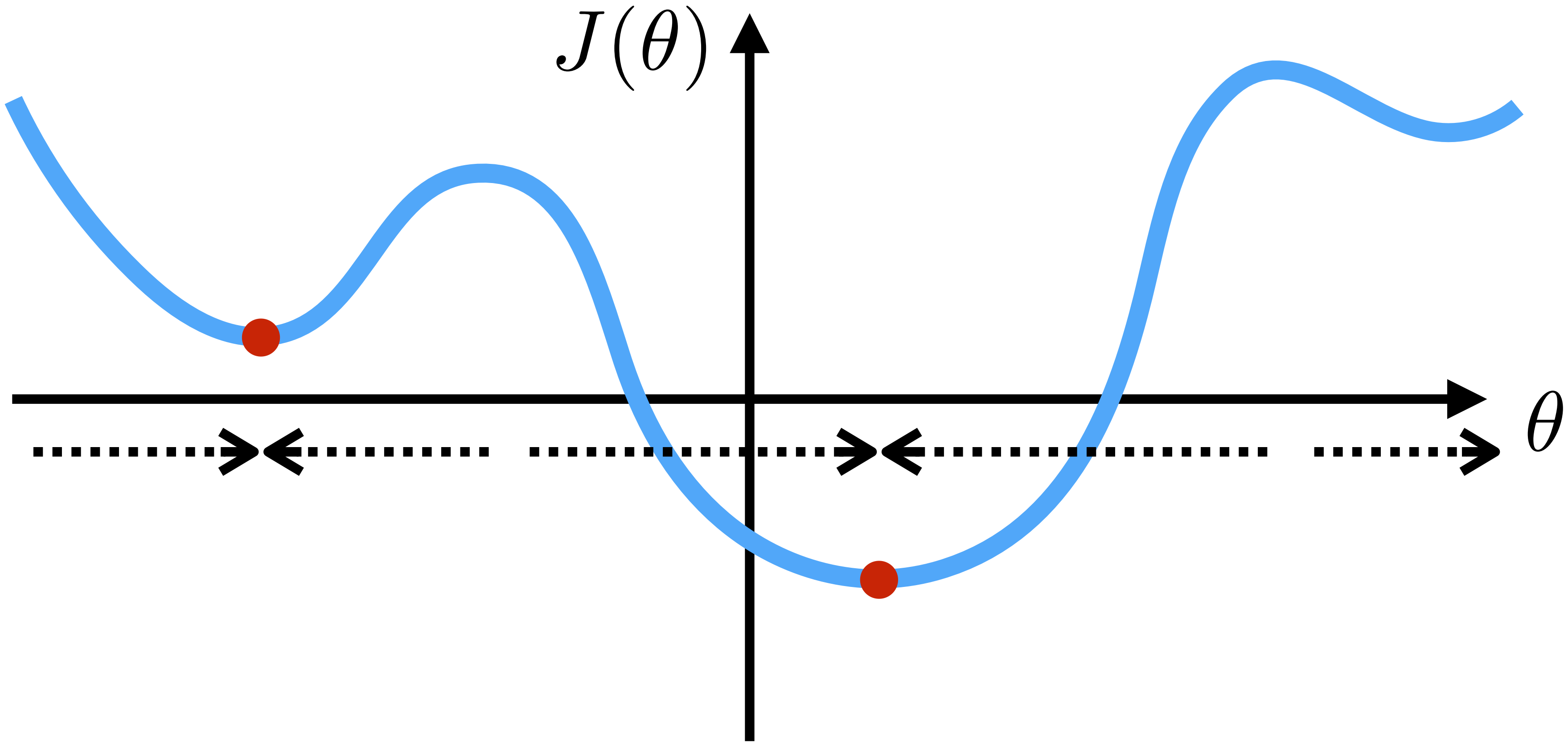
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

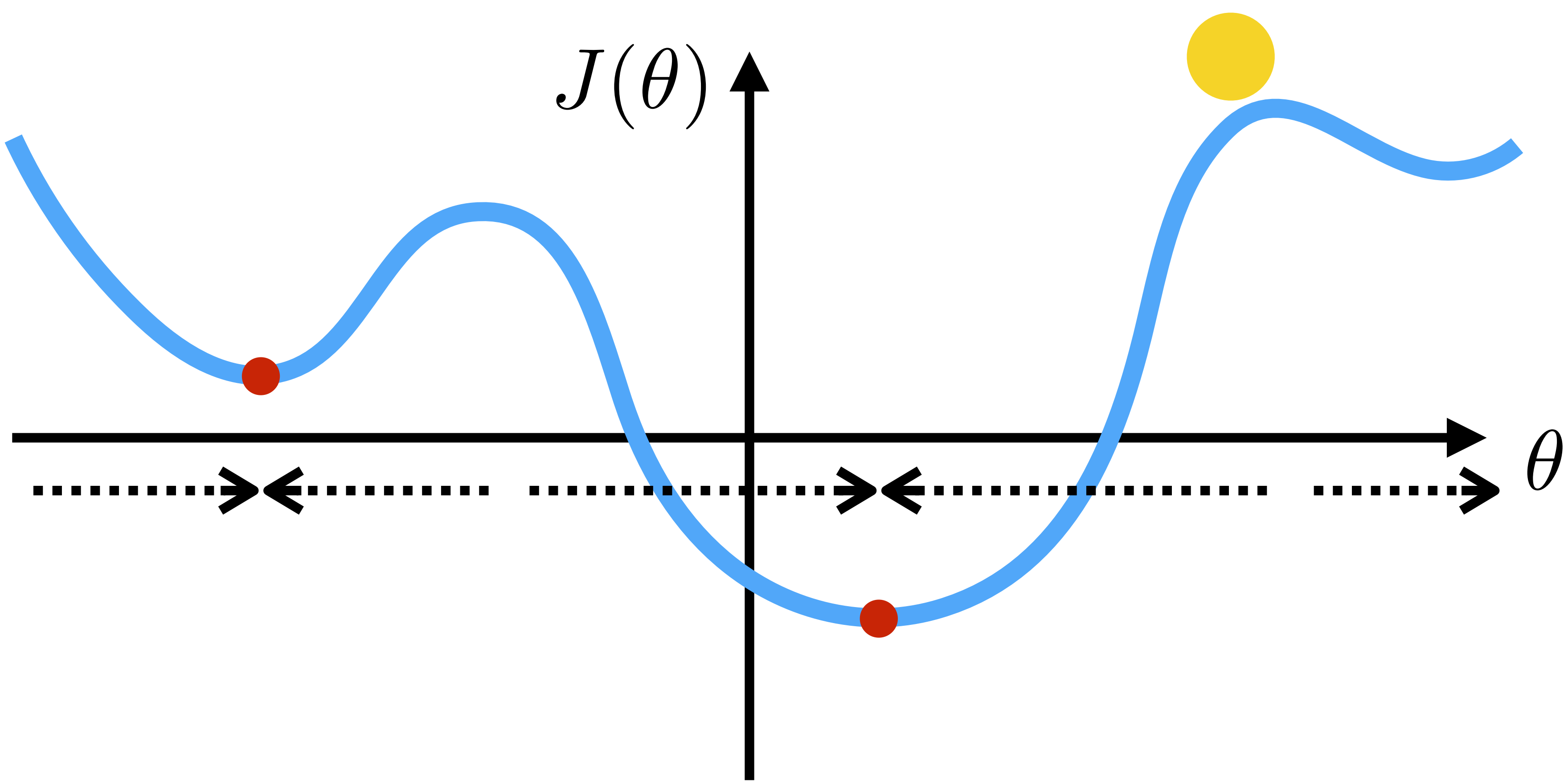
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

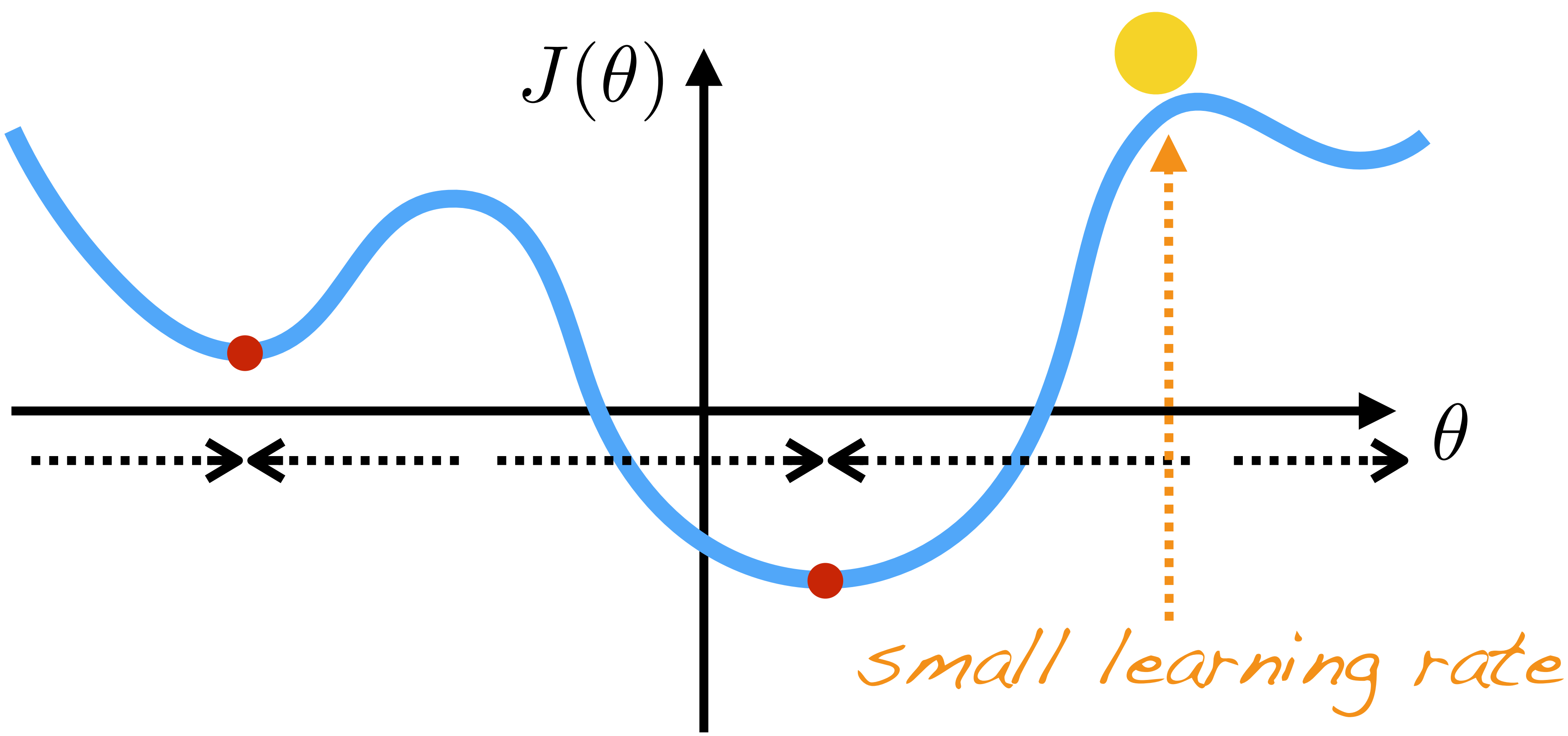
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

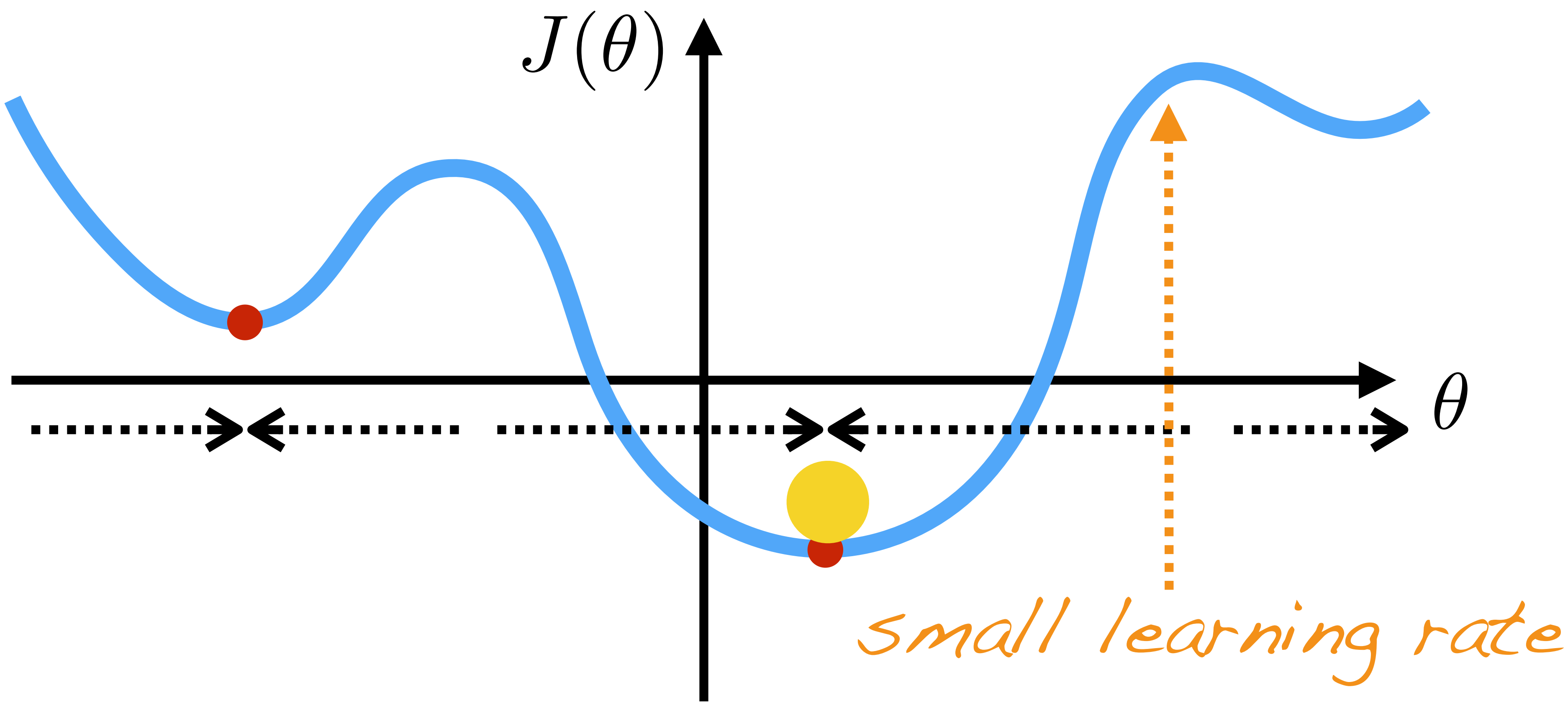
- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Local Minima

- Does gradient descent reach a (local) minimum even with a non convex function?



$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Optimization

- For more efficiency, we use the **stochastic gradient descent** method

- The gradient of the loss function is computed on a small set of samples from the training set

$$\tilde{J}(\theta) = \sum_{i\sim[1,\ldots,m]} \text{loss}\left(y^i, f\left(x^i;\theta\right)\right)$$

and the iteration is as before

$$\theta_{t+1} = \theta_t - \alpha \nabla \tilde{J}(\theta_t)$$