Neural Networks Training, SGD and Backpropagation

Machine Learning Course - CS-433

Nov 5, 2024

Nicolas Flammarion

EPFL

Recap

Neural Networks: Key Facts

Supervised learning : we observe some data $S_{\text{train}} = \{x_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y}$

➡ given a new x, we want to predict its label y

Linear prediction (with augmented features): $y = f_{\text{Lin}}(x) = \phi(x)^\top w$

Features are given

Prediction with a NN:

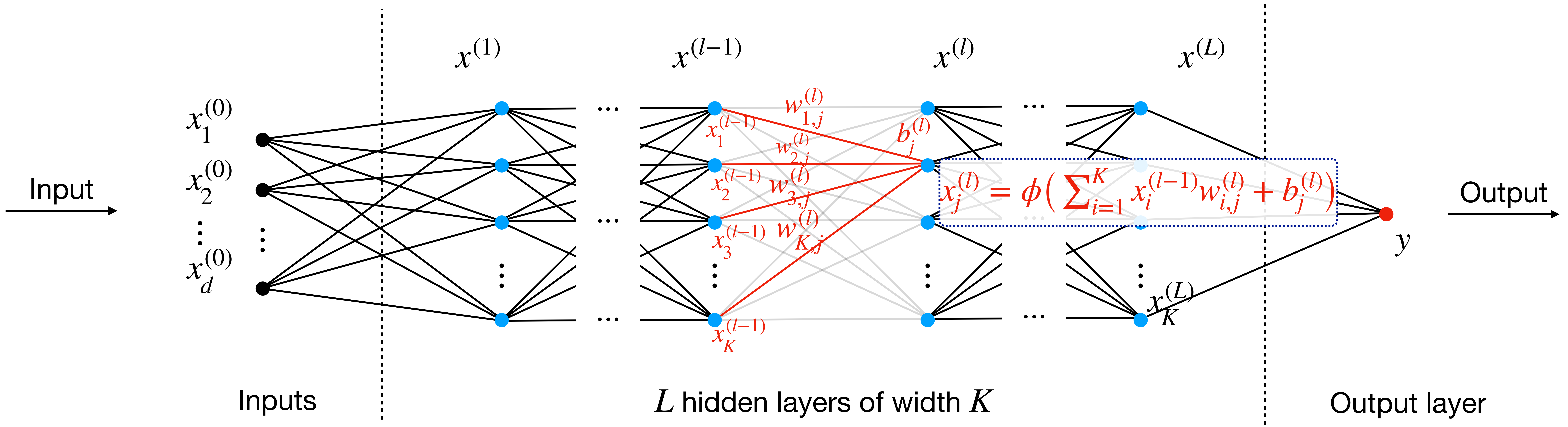
$$y = f_{\text{NN}}(x) = f(x)^\top w$$

Function implemented by the NN parameters: weights and biases

First layers transform the input into a good representation

Last layer is performing a linear prediction

Fully Connected Neural Networks



$$x_j^{(l)} = \phi\left(\sum_{i=1}^{K} x_i^{(l-1)} w_{i,j}^{(l)} + b_j^{(l)} \right)$$

Important: ϕ is non-linear otherwise we can only represent linear functions

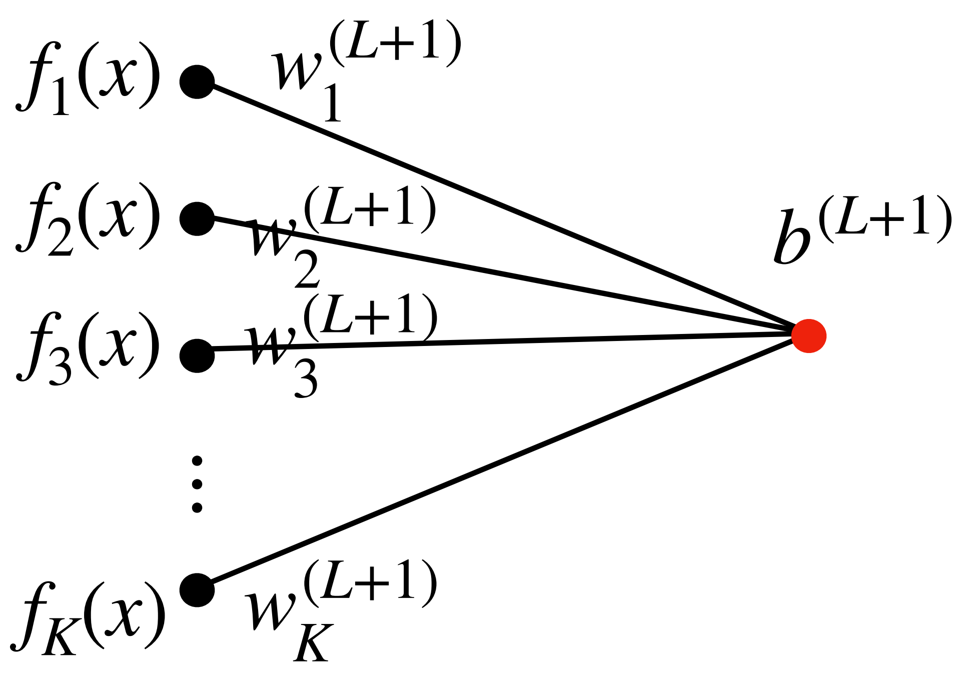
weight of the edge going from node i in layer $l-1$ to node j in layer l

bias term associated with node j in layer l

NNs: Inference vs. Training

Linear prediction on features $f(x)$

$$h(x) = f(x)^\top w^{(L+1)} + b^{(L+1)}$$



	Inference	**Training**
Regression with $y \in \mathbb{R}$	$h(x)$	$\ell(y, h(x)) = (h(x) - y)^2$
Binary Classification with $y \in \{-1,1\}$	$sign\big(h(x)\big)$	$\ell(y, h(x)) = log(1 + exp(-yh(x)))$
Multi-Class Classification with $y \in \{1,\dots,K\}$	$argmax_{c\in\{1,\dots,K\}}\ h(x)_c$	$\ell(y, h(x)) = -\ log \frac{e^{h(x)_y}}{\sum_{i=1}^{K} e^{h(x)_i}}$

With a suitable representation of the data $f(x)$ learned by the network, the last layer only performs a linear regression or classification step

Today: How do we train a NN?

Training of NNs

Training loss for a regression problem with $S_{\text{train}} = \{(x_n, y_n)\}_{n=1}^N$:

$$\mathscr{L}(f) = \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - f(x_n)\right)^2$$

where f is the function represented by a NN with weights $\left(w_{i,j}^{(l)}\right)$ and biases $\left(b_i^{(l)}\right)$

<u>Task</u>:

$$\min_{w_{i,j}^{(l)}, b_i^{(l)}} \mathscr{L}(f)$$

<u>Remarks</u>:

- Regularization can be added to avoid overfitting and is easy to implement
- Non-convex optimization problem

  ➡ not guaranteed to converge to a global minimum

Training of NNs with SGD

SGD algorithm: Uniformly sample n, compute the gradient of $\mathscr{L}_n = \frac{1}{2}(y_n - f(x_n))^2$ to update:

$$(w_{i,j}^{(l)})_{t+1} = (w_{i,j}^{(l)})_t - \gamma \frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} \qquad (b_i^{(l)})_{t+1} = (b_i^{(l)})_t - \gamma \frac{\partial \mathscr{L}_n}{\partial b_i^{(l)}}$$

In Practice: Step size schedule, mini-batch, momentum, Adam

Training of NNs with SGD

SGD algorithm: Uniformly sample n, compute the gradient of $\mathscr{L}_n = \frac{1}{2}(y_n - f(x_n))^2$ to update:

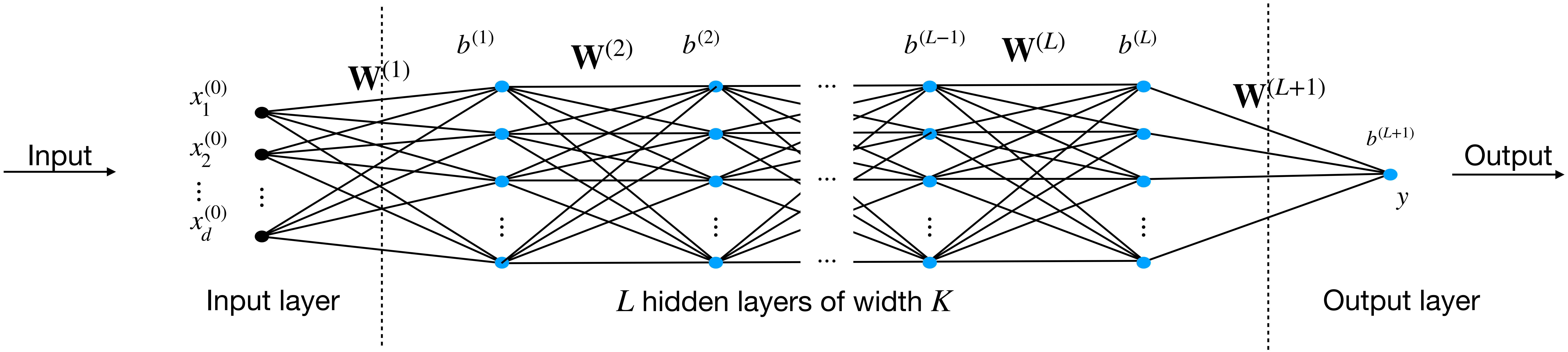
$$(w_{i,j}^{(l)})_{t+1} = (w_{i,j}^{(l)})_t - \gamma \frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} \qquad (b_i^{(l)})_{t+1} = (b_i^{(l)})_t - \gamma \frac{\partial \mathscr{L}_n}{\partial b_i^{(l)}}$$

In Practice: Step size schedule, mini-batch, momentum, Adam

Problem: With $O(K^2L)$ parameters, applying chain-rules **independently** is inefficient due to the compositional structure of f

Solution: the **Backpropagation algorithm** computes gradients via the chain rule but reuses intermediate computations

Description of NN parameters



Weight matrices: $\mathbf{W}^{(l)}$ such that $\mathbf{W}^{(l)}_{i,j} = w^{(l)}_{i,j}$, of size

- $\mathbf{W}^{(1)} \in \mathbb{R}^{d \times K}$
- $\mathbf{W}^{(l)} \in \mathbb{R}^{K \times K}$ for $2 \leq l \leq L$
- $\mathbf{W}^{(L+1)} \in \mathbb{R}^{K}$

Bias vectors: $b^{(l)}$ such that the i-th component is $b_i^{(l)}$

- $b^{(l)} \in \mathbb{R}^{K}$ for $1 \leq l \leq L$
- $b^{(L+1)} \in \mathbb{R}$

Compact description of output

The functions implemented by each layer can be written as:

- $x^{(1)} = f^{(1)}(x^{(0)}) := \phi\Big((\mathbf{W}^{(1)})^\top x^{(0)} + b^{(1)}\Big)$

  ...

- $x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi\Big((\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)}\Big)$

  ...

- $y = f^{(L+1)}(x^{(L)}) := (\mathbf{W}^{(L+1)})^\top x^{(L)} + b^{(L+1)}$

The overall function $y = f(x^{(0)})$ is just the composition of the layer functions:

$$\boxed{f = f^{(L+1)} \circ f^{(L)} \circ \cdots \circ f^{(l)} \circ \cdots \circ f^{(2)} \circ f^{(1)}}$$

Cost function

Cost function:

$$\mathcal{L} = \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(x_n)\right)^2$$

Remarks:

- The specific form of the loss is not crucial
- $\mathcal{L}$ is a function of all weight matrices and bias vectors
- Each function $f^{(l)}$ is parameterized by weights $\mathbf{W}^{(l)}$ and biases $b^{(l)}$

Individual loss for SGD:

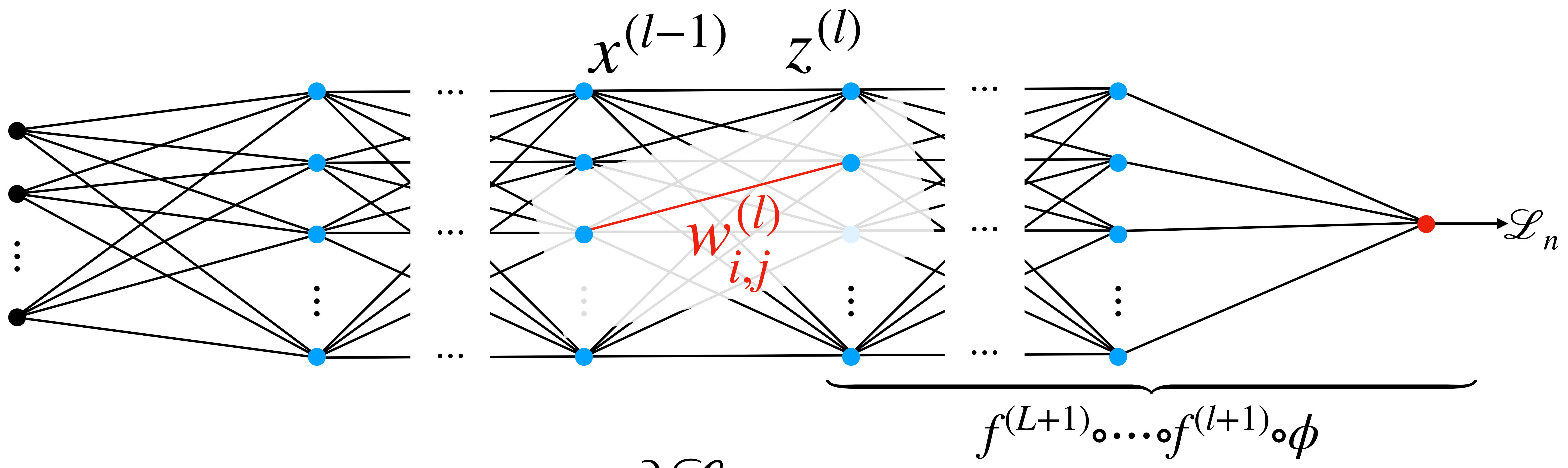
$$\mathcal{L}_n = \frac{1}{2}\left(y_n - f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(x_n)\right)^2$$

Goal: Compute for all (i, j, l)

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} \quad \text{and} \quad \frac{\partial \mathcal{L}_n}{\partial b_i^{(l)}}$$

Chain rule

$$\mathcal{L}_n = \frac{1}{2}\Big(y_n - f^{(L+1)} \circ \cdots \circ f^{(l+1)} \circ \phi\big(\underbrace{(\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)}}_{z^{(l)}}\big)\Big)^2$$

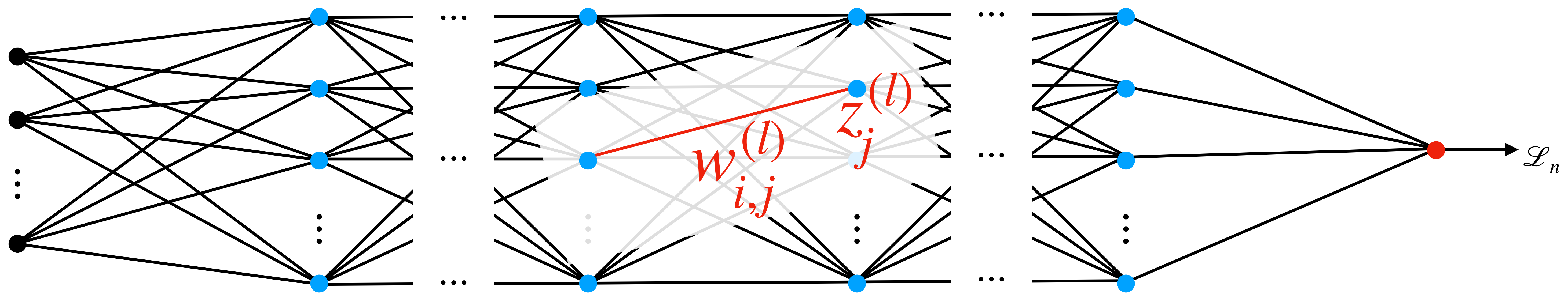


$$\frac{\partial \mathcal{L}_n}{\partial w^{(l)}_{i,j}} \quad ?$$

Chain rule

$$\mathcal{L}_n = \frac{1}{2}\left(y_n - f^{(L+1)} \circ \cdots \circ f^{(l+1)} \circ \phi\left(z^{(l)}\right)\right)^2$$

$$x^{(l-1)} \quad z^{(l)} = (\mathbf{W}^{(l)})^\top x^{l-1} + b^{(l)}$$



<u>Apply the chain rule</u>:

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} = \sum_{k=1}^{K} \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}}$$

$$= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} \qquad \text{since } \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = 0 \text{ for } k \neq j$$

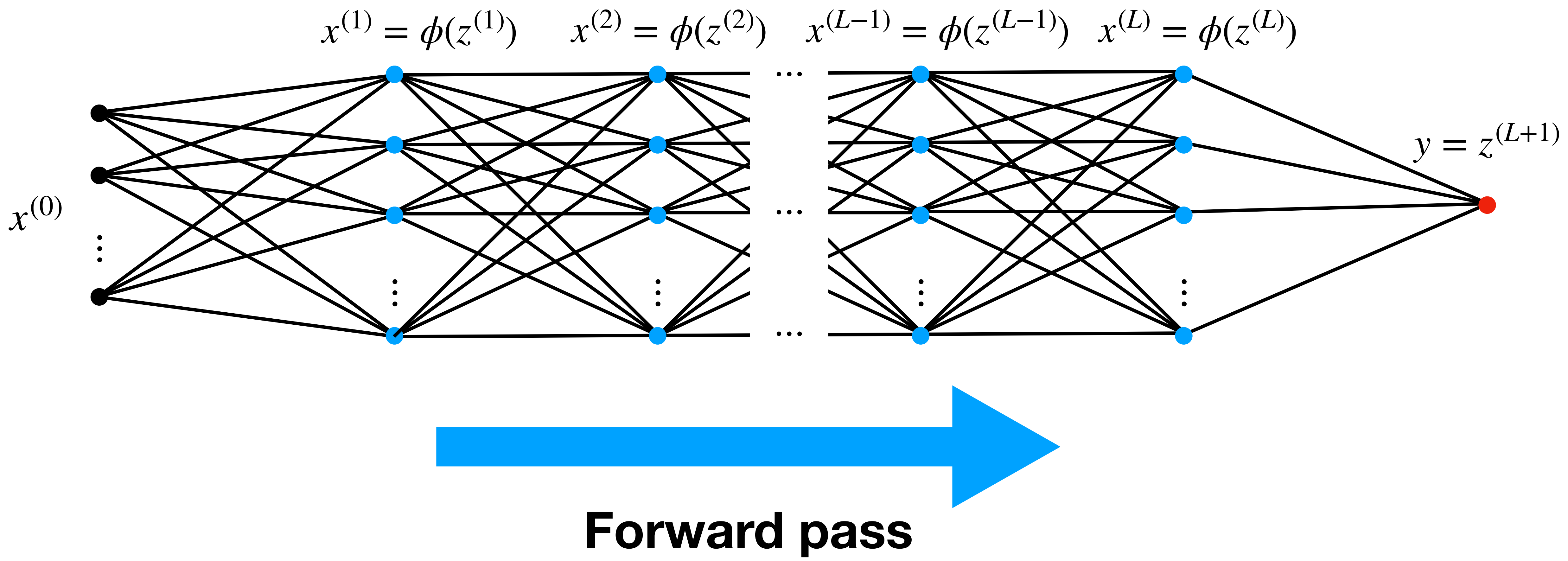
$$= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \cdot x_i^{(l-1)} \qquad \text{since } z_j^{(l)} = \sum_{k=1}^{K} w_{k,j}^{(l)} x_k^{(l-1)} + b_j^{(l)}$$

We need to compute $\frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}}$, $z^{(l)}$, $x_i^{(l-1)}$ and reuse them for different $\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}}$

Forward Pass

We can compute $z^{(l)}$ and $x^{(l)}$ by a forward pass in the network:

$$x^{(0)} = x_n \in \mathbb{R}^d$$
$$z^{(l)} = (\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)}$$
$$x^{(l)} = \phi(z^{(l)})$$

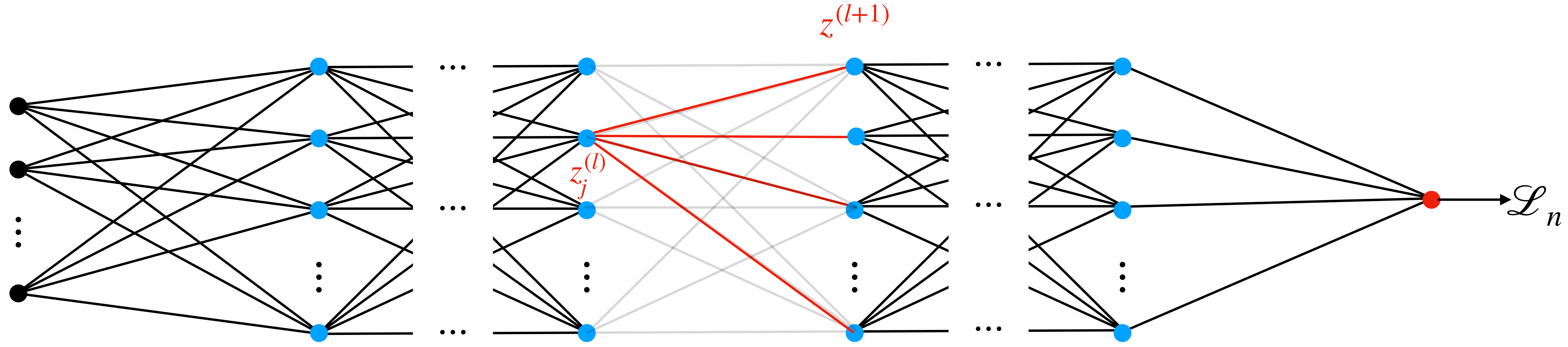


Computational complexity:

➡ one pass over the network $O(K^2L)$

Backward pass (I)

Define $\delta_j^{(l)} = \dfrac{\partial \mathscr{L}_n}{\partial z_j^{(l)}}$



Chain rule:

$$\delta_j^{(l)} = \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} = \sum_k \frac{\partial \mathscr{L}_n}{\partial z_k^{(l+1)}} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \sum_k \delta_k^{(l+1)} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}}$$

Backward pass (II)

Using $z_k^{(l+1)} = \sum_{i=1}^{K} w_{i,k}^{(l+1)} x_i^{(l)} + b_k^{(l+1)} = \sum_{i=1}^{K} w_{i,k}^{(l+1)} \phi(z_i^{(l)}) + b_k^{(l+1)}$

We obtain $\frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \phi'(z_j^{(l)}) w_{j,k}^{(l+1)}$

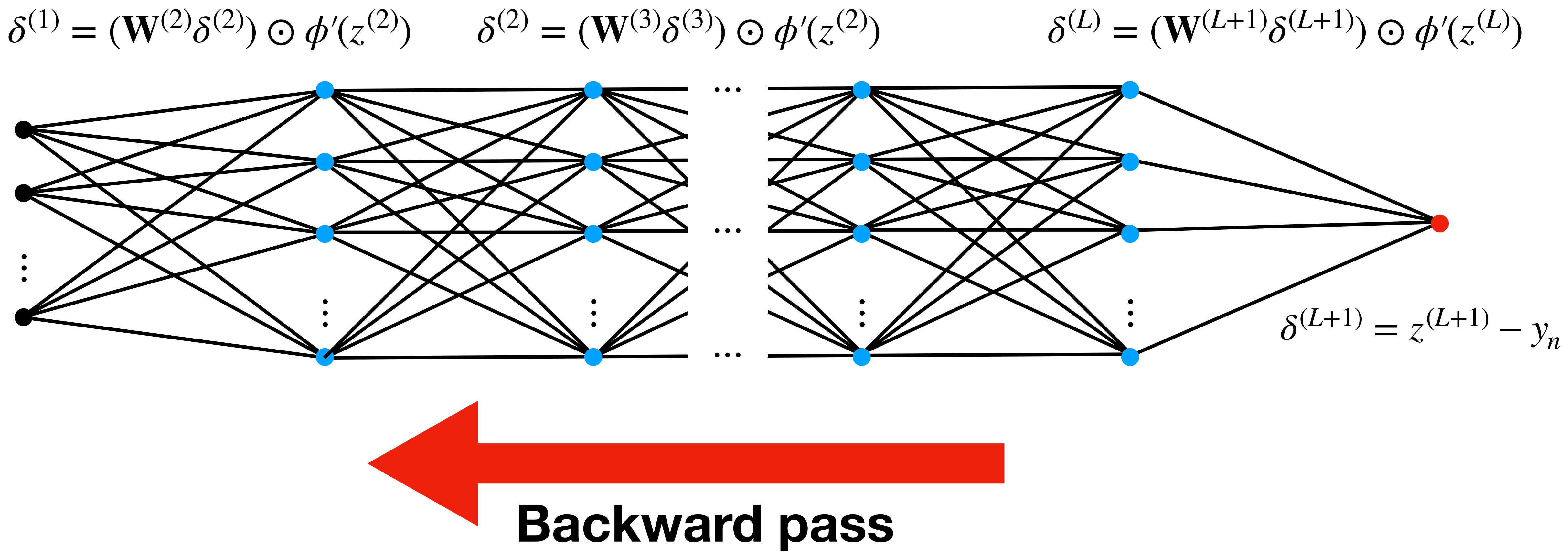
Thus $$\delta_j^{(l)} = \sum_k \delta_k^{(l+1)} \phi'(z_j^{(l)}) w_{j,k}^{(l+1)}$$

It can be written in vector form:

$$\delta^{(l)} = (\mathbf{W}^{(l+1)} \delta^{(l+1)}) \odot \phi'(z^{(l)})$$

$\odot$: Hadamard product, i.e.,
pointwise multiplication of vector

Backward pass (III)



<u>Initialization</u>:

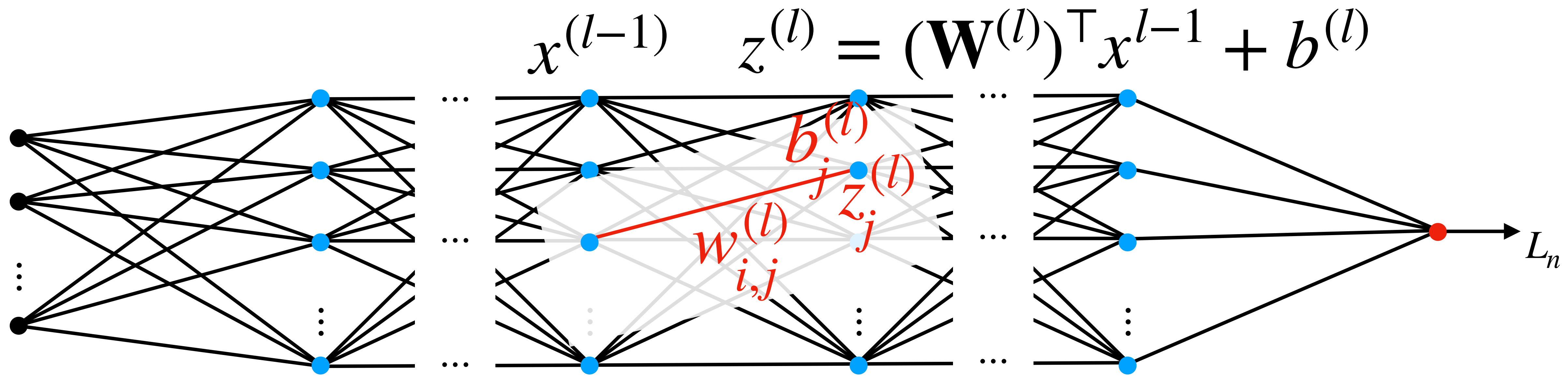
$$\delta^{(L+1)} = \frac{\partial}{\partial z^{(L+1)}} \frac{1}{2}\left(y_n - z^{(L+1)}\right)^2$$
$$= z^{(L+1)} - y_n$$

Compute all the $\delta^{(l)}$ by a backward pass in the network:

$$\delta^{(l)} = (\mathbf{W}^{(l+1)}\delta^{(l+1)}) \odot \phi'(z^{(l)})$$

Computational complexity: one pass over the network $O(K^2L)$

Derivatives computation



Using that $z_m^{(l)} = \sum_{k=1}^{K} w_{k,m}^{(l)} x_k^{(l-1)} + b_m^{(l)}$:

- $\dfrac{\partial \mathscr{L}_n}{\partial b_j^{(l)}} = \sum_{k=1}^{K} \dfrac{\partial \mathscr{L}_n}{\partial z_k^{(l)}} \dfrac{\partial z_k^{(l)}}{\partial b_j^{(l)}} = \dfrac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \dfrac{\partial z_j^{(l)}}{\partial b_j^{(l)}} = \delta_j^{(l)}$
- $\dfrac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} = \sum_{k=1}^{K} \dfrac{\partial \mathscr{L}_n}{\partial z_k^{(l)}} \dfrac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = \dfrac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \dfrac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} = \delta_j^{(l)} \cdot x_i^{(l-1)}$

Backpropagation algorithm

Forward pass:

$$x^{(0)} = x_n \in \mathbb{R}^d$$
$$z^{(l)} = (\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)}$$
$$x^{(l)} = \phi(z^{(l)})$$

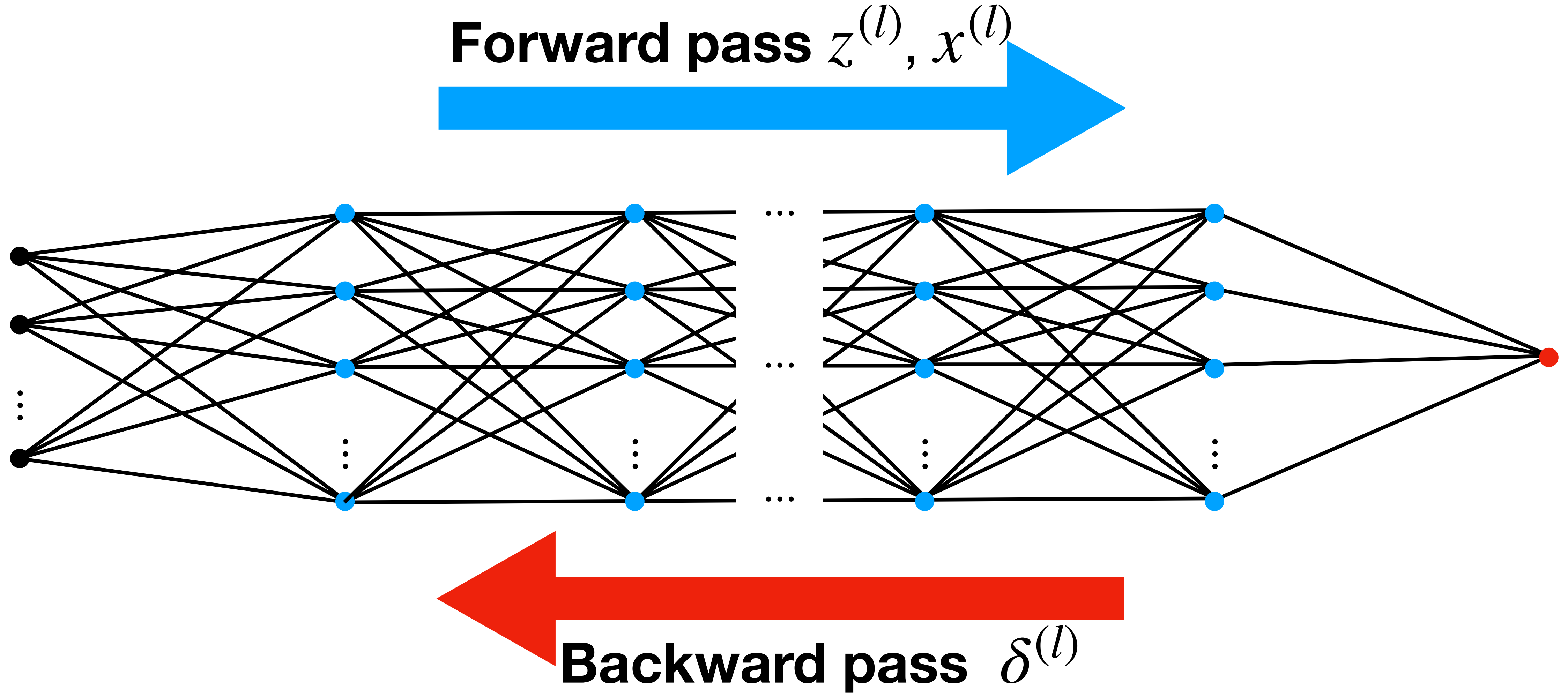
Backward pass:

$$\delta^{(L+1)} = z^{(L+1)} - y_n$$

$$\delta^{(l)} = (\mathbf{W}^{(l+1)}\delta^{(l+1)}) \odot \phi'(z^{(l)})$$

Compute the derivatives:

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} = \delta_j^{(l)} x_i^{(l-1)}$$
$$\frac{\partial \mathcal{L}_n}{\partial b_j^{(l)}} = \delta_j^{(l)}$$



Overall Complexity: $O(K^2L)$

Common issues with gradient descent

- Gradient exploding / vanishing: As the network depth L increases, the gradient magnitude can decrease or grow uncontrollably, slowing the training process.

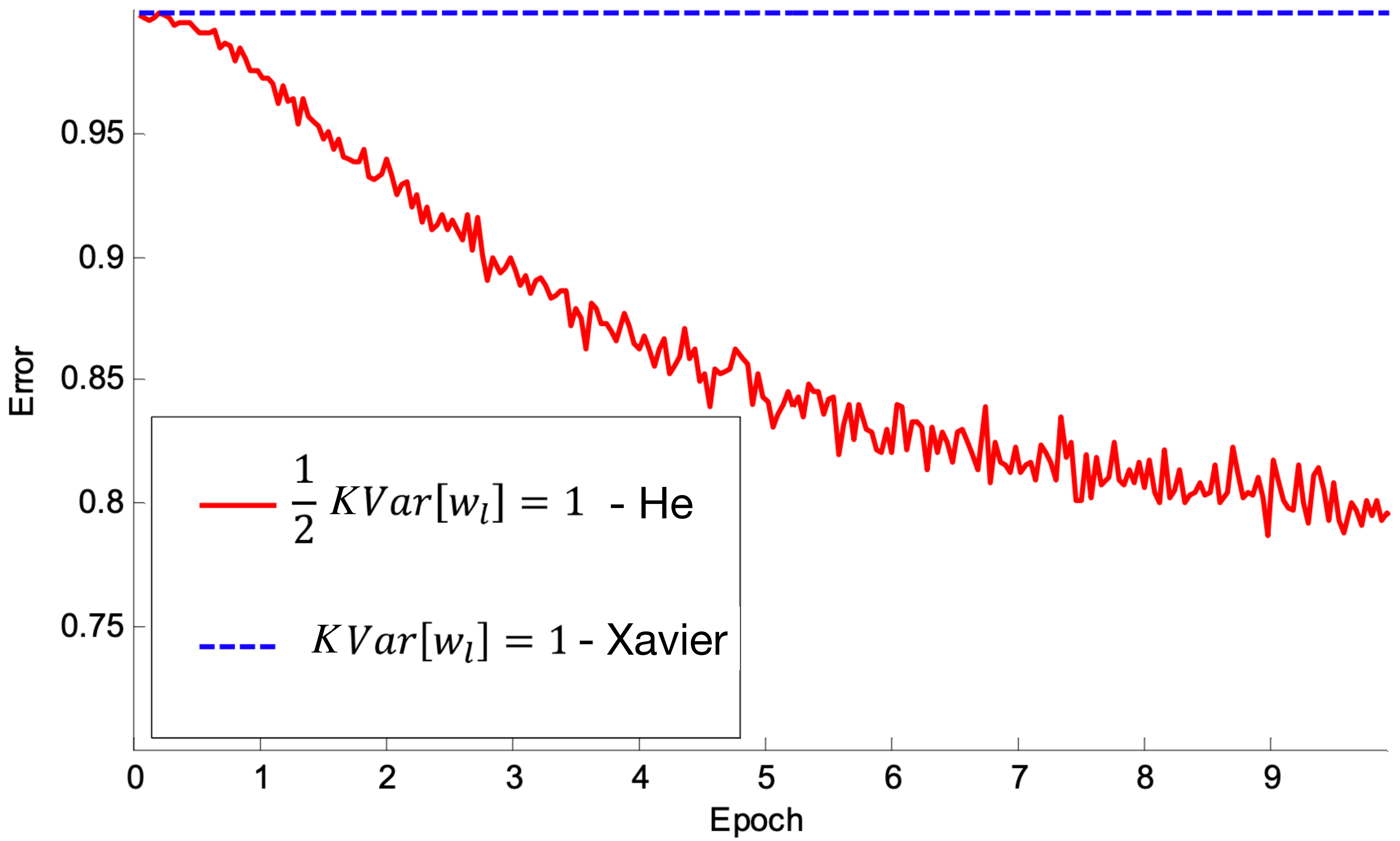
- Cause: Back propagation uses chain rule. Where there are L times multiplication of small or big values, gradients decrease or grow exponentially.

- Remedy: Effective strategies include choosing suitable activation functions, using weight normalization, initializing weights properly, and implementing skip connections.

Parameter Initialization

Importance of Parameter Initialization

- In deep networks, improper parameter initialization can lead to the **vanishing** or **exploding gradients problem**
- **Problem**: Extremely slow or unstable optimization
- **Solution**: Control the layerwise variance of neurons (aka **He initialization**)
- **Note**: As illustrated, even a two-fold difference in the scale of initialization can be crucial



Source: Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification (CVPR 2015)

Variance-Preserving Initialization

Variance-preserving initialization for ReLU networks:

- $z^{(l)} \sim \mathcal{N}(0, \mathbf{I}_K)$: pre-activations at layer l (note: $Var[z_i^{(l)}] = 1$)
- $w_i^{(l+1)} \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_K)$: the i-th weight vector at layer $l+1$
- $z_i^{(l+1)} = ReLU(z^{(l)})^\top w_i^{(l+1)}$: the i-th pre-activation at layer $l+1$

Question: How should we set σ so that $Var[z_i^{(l+1)}] = 1$?

Answer: $\sigma = \sqrt{2/K}$

Derivation: Refer to the exercise for the derivation

Normalization Layers

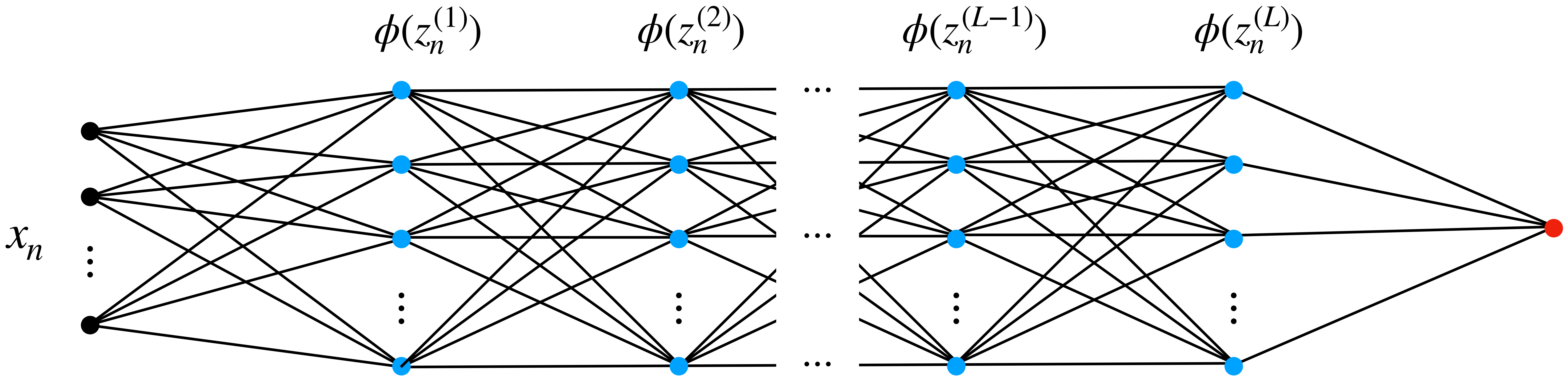
Batch Normalization

Consider a batch $B = (x_1, \cdots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

Batch Normalization

Consider a batch $B = (x_1, \cdots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

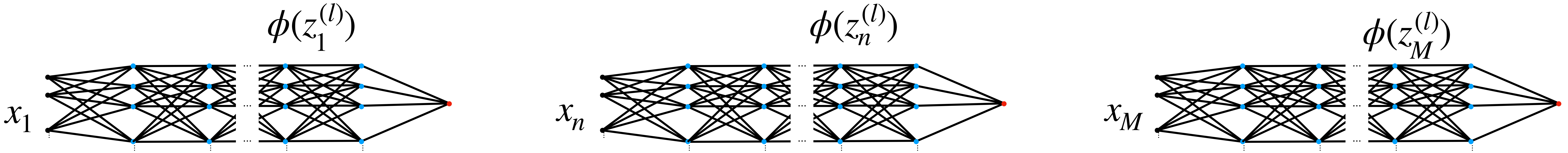
One input x_n



Batch Normalization

Consider a batch $B = (x_1, \cdots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

Batch B of input $x_1, \cdots, x_M$



$$\underbrace{\hphantom{xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx}}_{(z_1^{(l)}, \cdots, z_n^{(l)}, \cdots, z_M^{(l)}) \in \mathbb{R}^{K \times M}}$$

Batch Normalization

Consider a batch $B = (x_1, \cdots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

<u>Step 1</u>: Normalize each layer's input using its mean and its variance over the batch:

$$\bar{z}_n^{(l)} = \frac{z_n^{(l)} - \mu_B^{(l)}}{\sqrt{(\sigma_B^{(l)})^2 + \varepsilon}}$$

Component-wise

where $\mu_B^{(l)} = \frac{1}{M} \sum_{n=1}^{M} z_n^{(l)}$ and $(\sigma_B^{(l)})^2 = \frac{1}{M} \sum_{n=1}^{M} (z_n^{(l)} - \mu_B^{(l)})^2$, and $\varepsilon \in \mathbb{R}_{\geq 0}$ is a small value added for numerical stability

<u>Step 2</u>: Introduce learnable parameters $\gamma^{(l)} \in \mathbb{R}^K$ (scale) and $\beta^{(l)} \in \mathbb{R}^K$ (shift) to be able to recover the original activations if needed:

$$\hat{z}_n^{(l)} = \gamma^{(l)} \odot \bar{z}_n^{(l)} + \beta^{(l)}$$

Batch Normalization

<u>Scale-invariance:</u> For $\varepsilon \approx 0$, the output is invariant to activation-wise affine scaling of $z_n^{(l)}$

$$\text{BN}(a \odot z_n^{(l)} + b) = \text{BN}(z_n^{(l)}) \text{ for } a \in \mathbb{R}_{>0}^K \text{ and } b \in \mathbb{R}^K$$

Thus, for example, there is no need to include a bias *before* BatchNorm.

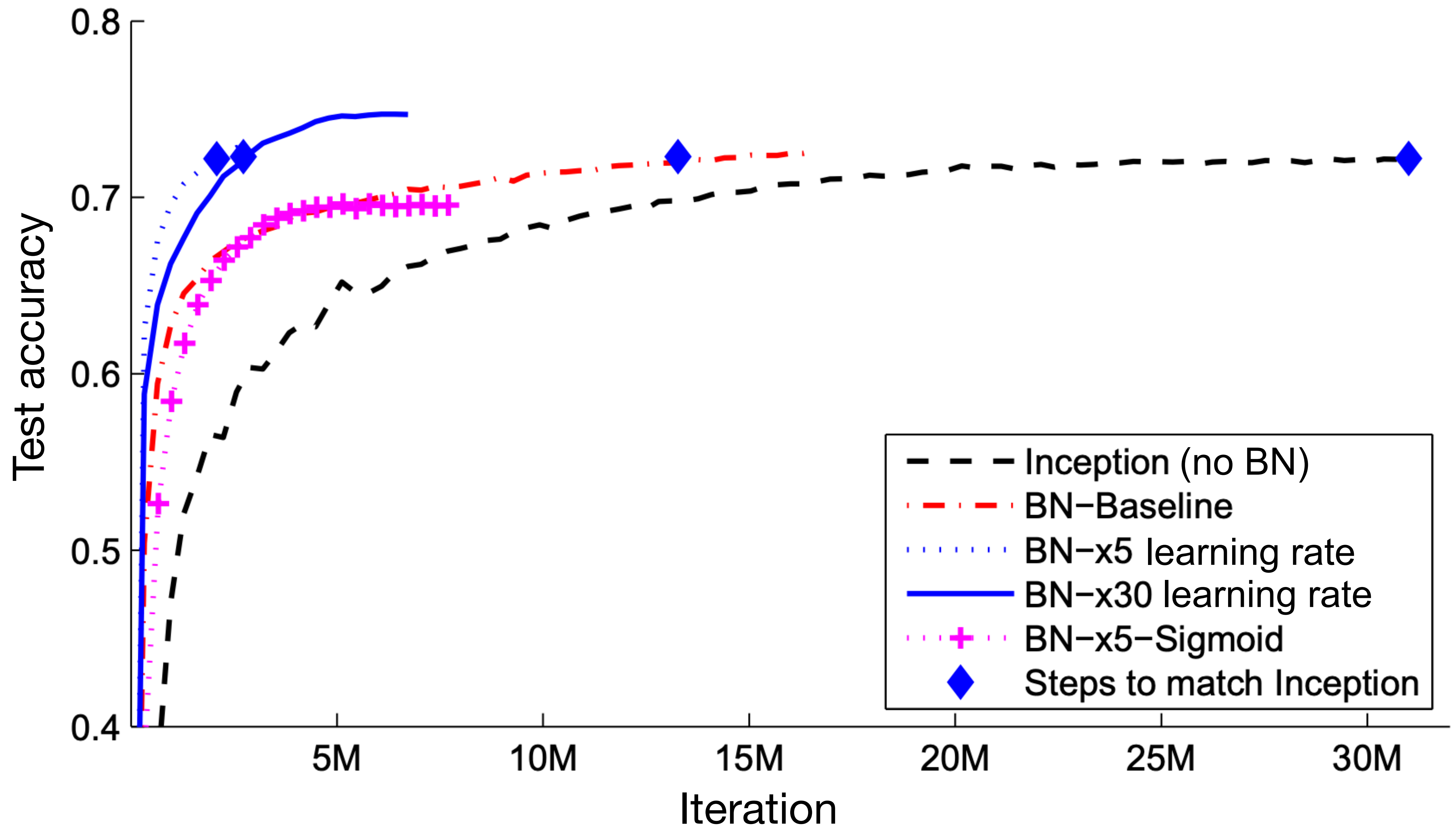
<u>Inference</u>: Use *fixed* mean and variance for normalization, as samples may arrive one at a time

- Estimate $\hat{\mu}^{(l)} = \mathbf{E}_{B \sim \mathcal{D}^{Train}}[\mu_B^{(l)}]$ and $\hat{\sigma}^{(l)} = \mathbf{E}_{B \sim \mathcal{D}^{Train}}[\sigma_B^{(l)}]$ during training, use these for inference
- Exponential moving averages are commonly used in practice

<u>Implementation:</u>

- Requires <u>sufficiently large batches</u> to get good estimates of $\mu_B^{(l)}, \sigma_B^{(l)}$
- BatchNorm is applied a bit differently for non-fully-connected nets (see the <u>pytorch docs</u> for CNNs)
- In PyTorch, switch modes by using model.train() for training and model.eval() for inference

Batch Normalization - Results



Source: Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift (ICML 2015)

- BatchNorm leads to **much faster convergence**
- BatchNorm allows to use **much larger learning rates** (up to $30\times$)

Layer Normalization

<u>Step 1</u>: Normalize each layer's input using its mean and its variance over *the features* (instead of over *the inputs*):

$$\bar{z}_n^{(l)} = \frac{z_n^{(l)} - \mu_n^{(l)} \cdot 1_K}{\sqrt{(\sigma_n^{(l)})^2 + \varepsilon}}$$

where $\mu_n^{(l)} = \frac{1}{K} \sum_{k=1}^{K} z_n^{(l)}(k)$ and $(\sigma_n^{(l)})^2 = \frac{1}{K} \sum_{k=1}^{K} (z_n^{(l)}(k) - \mu_n^{(l)})^2$, and $\varepsilon \in \mathbb{R}_{\geq 0}$

<u>Step 2</u>: Introduce learnable parameters $\gamma^{(l)}, \beta^{(l)} \in \mathbb{R}^K$:

$$\hat{z}_n^{(l)} = \gamma^{(l)} \odot \bar{z}_n^{(l)} + \beta^{(l)}$$

<u>Remarks:</u>

- Normalize across features, independently for each observation
- Very common alternative, widely used for transformers and text data
- No batch dependency, use the same for training and inference

Normalization - conclusion

Benefits of normalization layers:

- Stabilizes activation magnitudes / reduces initialization impact
- Stabilizes and speeds up training, allows larger learning rates
- Additional regularization effect from noisy batch statistics $\mu_B^{(l)}, \sigma_B^{(l)}$

Used in almost all modern deep learning architectures

- Often inserted after every convolutional layer, before non-linearity

Recap

- Neural networks are trained with gradient-based methods such as **SGD**

- To compute the gradients, we use **backpropagation**, which involves the chain rule to efficiently calculate the gradients based on the network's intermediate outputs $z^{(l)}$ and $\delta^{(l)}$

- Proper **parameter initialization** should avoid exploding and vanishing gradients by carefully controlling the layerwise variance

- **Batch and Layer normalization** dynamically stabilize the training process, allowing for faster convergence and the use of larger learning rates