

Neural Networks Training, SGD and Backpropagation

Machine Learning Course - CS-433
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Recap

Neural Networks: Key Facts

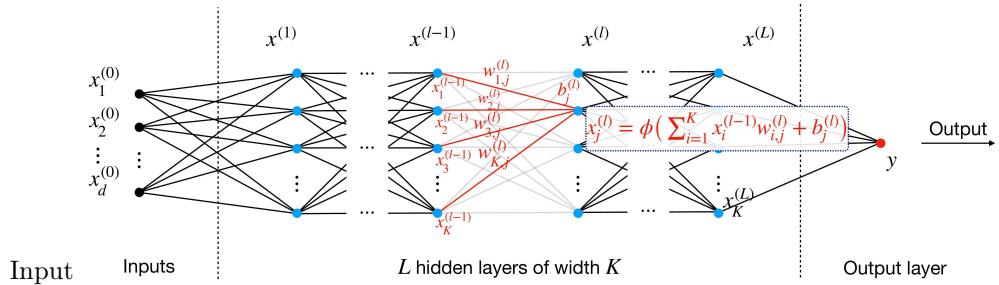
Supervised learning : we observe some data $S_{\text{train}} = \{x_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y} \Rightarrow$ given a new x , we want to predict its label y

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

Prediction with a NN:

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

Fully Connected Neural Networks



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

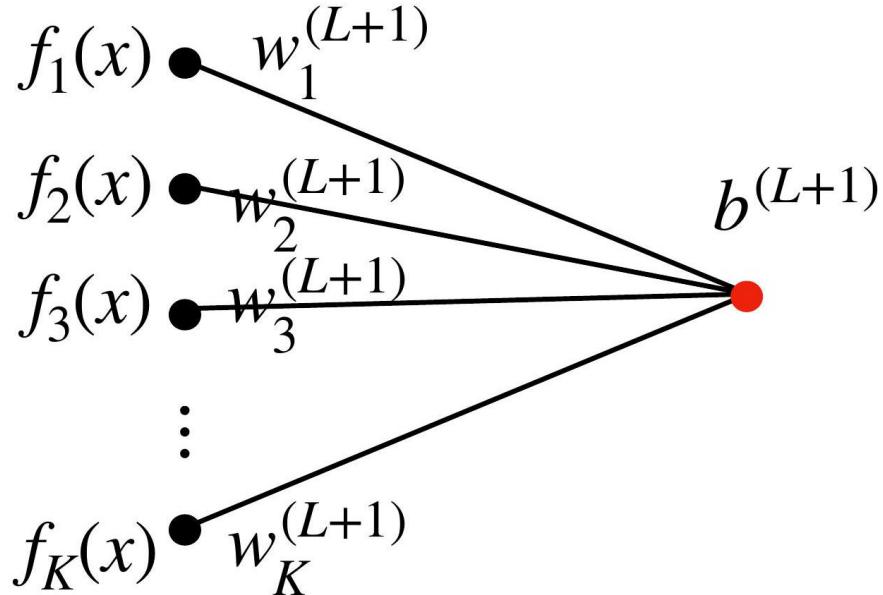
Important: ϕ is non-linear otherwise we can only represent linear functions

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

$h(x)$

$\text{sign}(h(x))$

Binary Classification

with $y \in \{-1, 1\}$

Multi-Class Classification

with $y \in \{1, \dots, K\}$

with $y \in \mathbb{R}$ Training

$\ell(y, h(x)) = (h(x) - y)^2$

$\text{argmax}_{c \in \{1, \dots, K\}} h(x)_c$ $\ell(y, h(x)) = \log(1 + \exp(-yh(x)))$

$\ell(y, h(x)) = -\log \frac{e^{h(x)y}}{\sum_{i=1}^K e^{h(x)_i}}$

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 $S_{\text{train}} = \{(x_n, y_n)\}_{n=1}^N$:

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

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

Task:

Remarks:

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

- Regularization can be added to avoid overfitting and is easy to implement
- Non-convex optimization problem
 \Rightarrow not guaranteed to converge to a global minimum

Training of NNs with SGD

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

$$\begin{pmatrix} w_{i,j}^{(l)} \end{pmatrix}_{t+1} = \begin{pmatrix} w_{i,j}^{(l)} \end{pmatrix}_t - \gamma \frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} \quad \begin{pmatrix} b_i^{(l)} \end{pmatrix}_{t+1} = \begin{pmatrix} b_i^{(l)} \end{pmatrix}_t - \gamma \frac{\partial \mathcal{L}_n}{\partial b_i^{(l)}}$$

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

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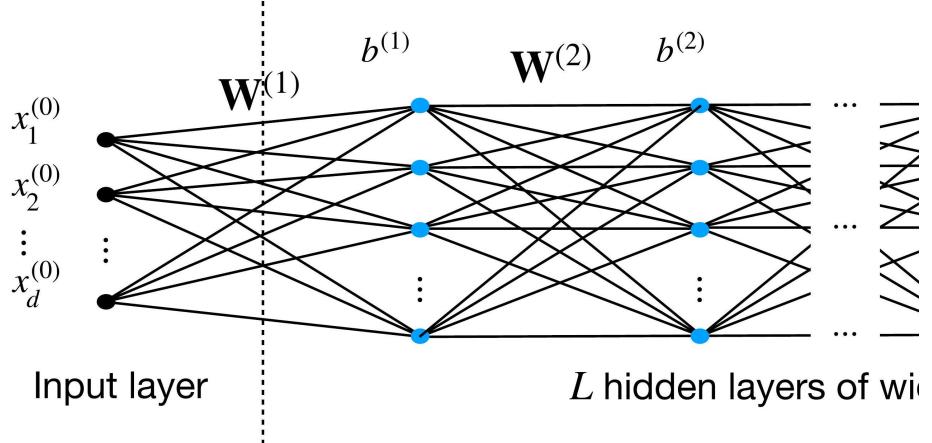
In Practice: Step size schedule, mini-batch, momentum, Adam

Problem: With $O(K^2 L)$ 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

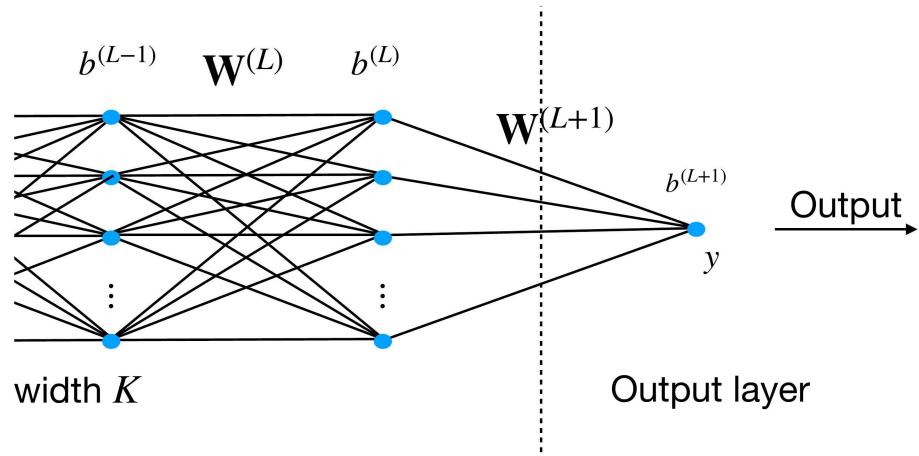
Description of NN parameters

Input



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

- $\mathbf{W}^{(1)} \in \mathbb{R}^{d \times K}$



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

- $\mathbf{W}^{(l)} \in \mathbb{R}^{K \times K}$ 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:

- $x^{(1)} = f^{(1)}(x^{(0)}) := \phi\left(\left(\mathbf{W}^{(1)}\right)^\top x^{(0)} + b^{(1)}\right)$
- $x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi\left(\left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}\right)$
- $y = f^{(L+1)}(x^{(L)}) := \left(\mathbf{W}^{(L+1)}\right)^\top x^{(L)} + b^{(L+1)}$

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

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

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:

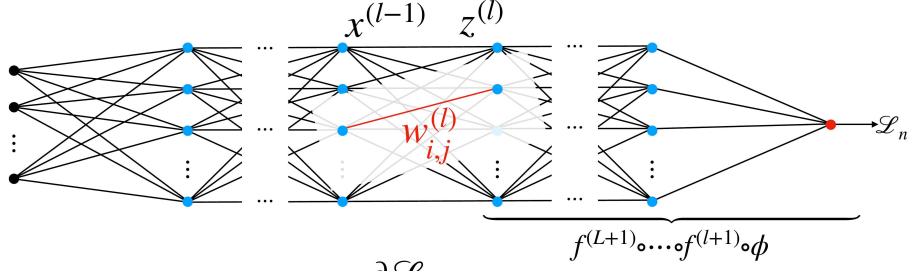
$$\mathcal{L}_n = \frac{1}{2} \left(y_n - f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(x_n) \right)^2$$

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

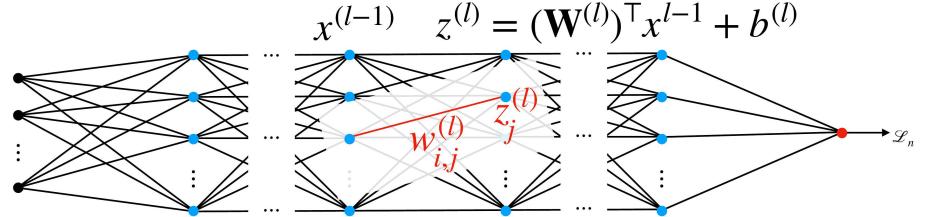
$$\mathcal{L}_n = \frac{1}{2} \left(y_n - f^{(L+1)} \circ \dots \circ f^{(l+1)} \circ \phi(\underbrace{\left(\mathbf{W}^{(l)} \right)^\top x^{(l-1)} + b^{(l)} \right)) \right)^2$$



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

Chain rule

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



Apply the chain rule:

$$\begin{aligned} \frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} &= \sum_{k=1}^K \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} \\ &= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} \quad \text{since } \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = 0 \text{ for } k \neq j \\ &= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \cdot x_i^{(l-1)} \quad \text{since } z_j^{(l)} = \sum_{k=1}^K w_{k,j}^{(l)} x_k^{(l-1)} + b_j^{(l)} \end{aligned}$$

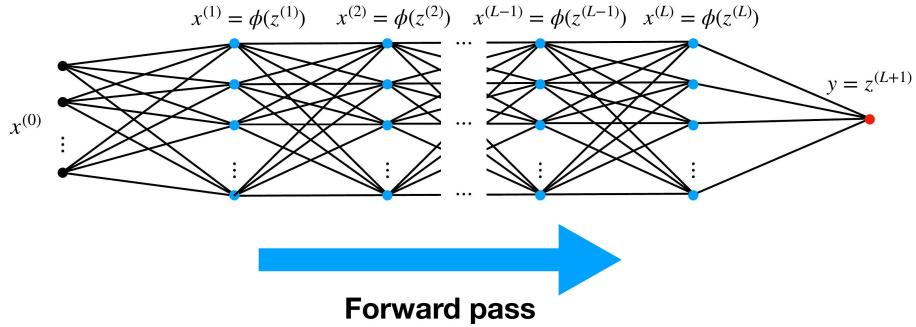
We need to compute $\frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}}, z^{(l)}, x_i^{(l-1)}$ and reuse them for different $\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}}$

Forward Pass

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

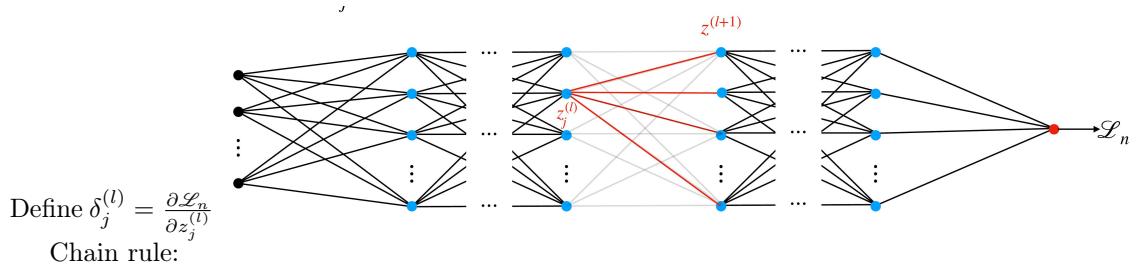
$$\begin{aligned} x^{(0)} &= x_n \in \mathbb{R}^d \\ z^{(l)} &= (\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)} \\ x^{(l)} &= \phi(z^{(l)}) \end{aligned}$$

Computational complexity:



\Rightarrow one pass over the network $O(K^2L)$

Backward pass (I)



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

Backward pass (II)

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

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

Thus

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

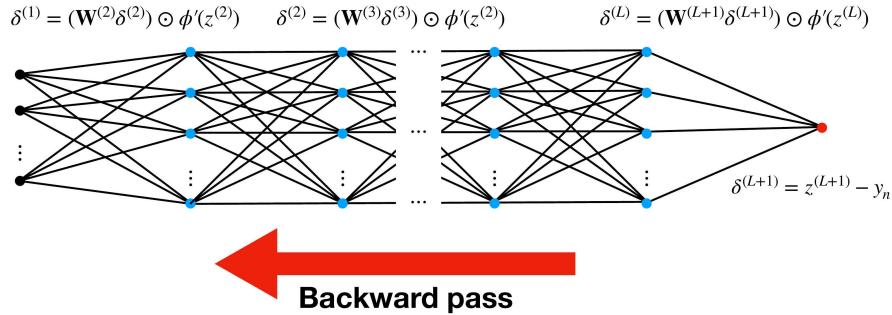
It can be written in vector form:

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

Backward pass (III)

Initialization:

$$\begin{aligned} \delta^{(L+1)} &= \frac{\partial}{\partial z^{(L+1)}} \frac{1}{2} (y_n - z^{(L+1)})^2 \\ &= z^{(L+1)} - y_n \end{aligned}$$

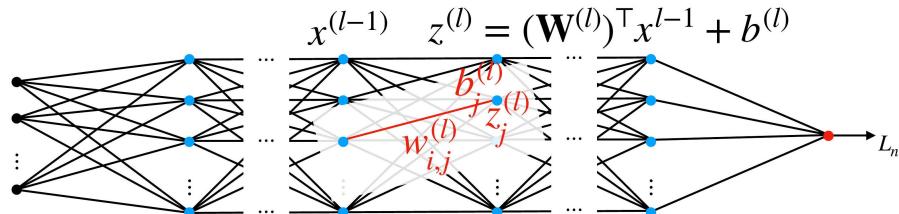


Compute all the $\delta^{(l)}$ by a backward pass in the network:

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

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

Derivatives computation



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

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

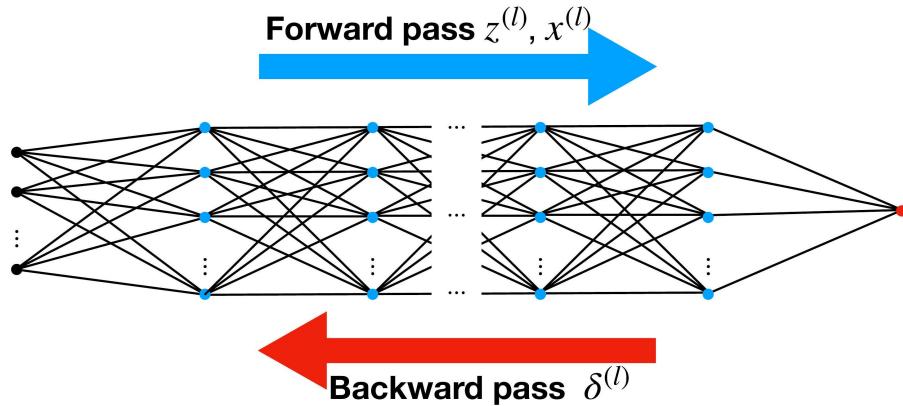
Backpropagation algorithm

Forward pass:

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

Backward pass:

$$\begin{aligned} \delta^{(L+1)} &= z^{(L+1)} - y_n \\ \delta^{(l)} &= (\mathbf{W}^{(l+1)} \delta^{(l+1)}) \odot \phi'(z^{(l)}) \end{aligned}$$



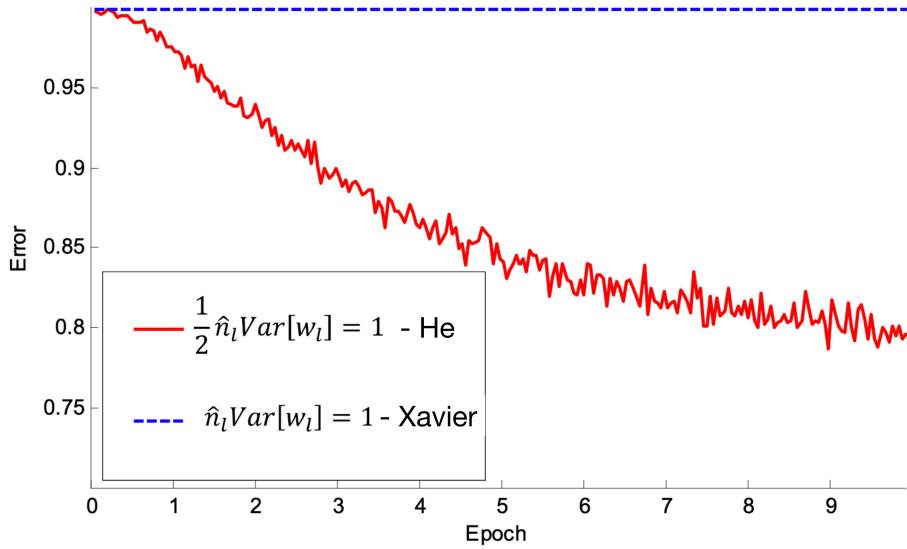
Compute the derivatives:

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

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



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

Variance-Preserving Initialization

Variance-preserving initialization for ReLU networks:

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

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

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

Derivation: Refer to the exercise for the derivation

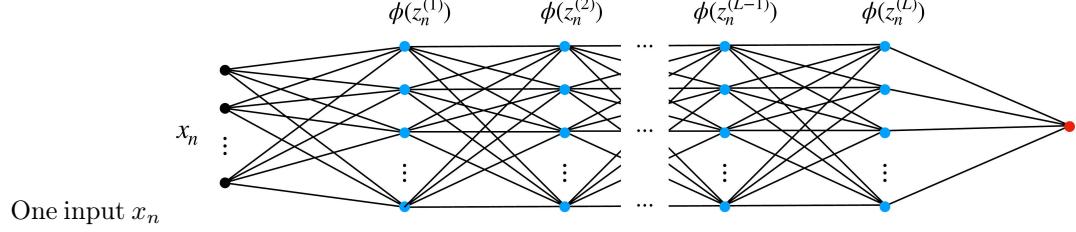
Normalization Layers

Batch Normalization

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

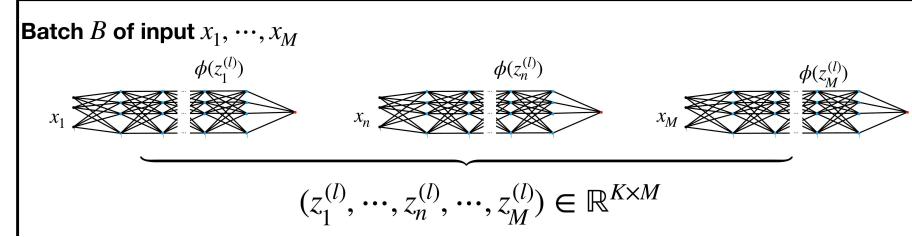
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Consider a batch $B = (x_1, \dots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

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

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

Component-wise

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

Step 2: Introduce learnable parameters $\gamma^{(l)}, \beta^{(l)} \in \mathbb{R}^K$ to be able to reverse the normalization if needed:

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

Batch Normalization

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

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

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

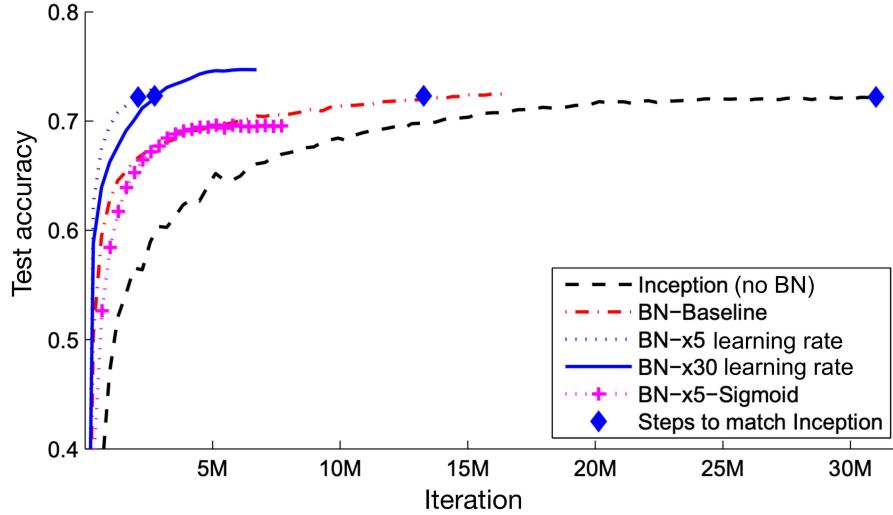
Inference: The prediction for one sample should not depend on other samples

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

Implementation:

- Requires sufficiently large batches to get good estimates of $\mu_B^{(l)}, \sigma_B^{(l)}$
- BatchNorm is applied a bit differently for non-fully-connected nets (see the pytorch docs 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

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

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

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

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

Remarks:

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

- 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
- Additional regularization effect from noisy $\mu_B^{(l)}, \sigma_B^{(l)}$ in batch norm
- Stabilizes and speeds up training, allows larger learning rates

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