CS 784: Computational Linguistics
Lecture 8: Neural Networks I
(for Text Classification)

Freda Shi

School of Computer Science, University of Waterloo
fhs@uwaterloo.ca

January 30, 2025

Check out https://pytorch.org/tutorials/intermediate/nlp_from_scratch_index.html if you aren't familiar with this topic!

Recap: A Unified View of Classification

$$\text{classify}(s) = \arg\max_{y} \mathit{score}(s, y; \boldsymbol{\Theta})$$

s: input text, y: class label, $\boldsymbol{\Theta}$: model parameters.

Recap: A Unified View of Classification

$$\text{classify}(s) = \arg\max_{y} \mathit{score}(s, y; \boldsymbol{\Theta})$$

s: input text, y: class label, $\boldsymbol{\Theta}$: model parameters.

Modeling: define $\mathit{score}(s, y; \boldsymbol{\Theta})$.

Recap: A Unified View of Classification

$$\text{classify}(s) = \arg\max_{y} \textit{score}(s, y; \boldsymbol{\Theta})$$

s: input text, y: class label, $\boldsymbol{\Theta}$: model parameters.

Modeling: define $\textit{score}(s, y; \boldsymbol{\Theta})$.

Training: learn $\boldsymbol{\Theta}$ to maximize the likelihood of the training data.

Recap: A Unified View of Classification

$$\text{classify}(s) = \arg\max_{y} \mathit{score}(s, y; \boldsymbol{\Theta})$$

s: input text, y: class label, $\boldsymbol{\Theta}$: model parameters.

Modeling: define $\mathit{score}(s, y; \boldsymbol{\Theta})$.

Training: learn $\boldsymbol{\Theta}$ to maximize the likelihood of the training data.

Inference: find the best class label y for a given input text s.

Recap: A Unified View of Classification

$$\text{classify}(s) = \arg\max_{y} \mathit{score}(s, y; \boldsymbol{\Theta})$$

s: input text, y: class label, $\boldsymbol{\Theta}$: model parameters.

Modeling: define $\mathit{score}(s, y; \boldsymbol{\Theta})$.

Training: learn $\boldsymbol{\Theta}$ to maximize the likelihood of the training data.

Inference: find the best class label y for a given input text s.

This lecture and the next: score$(\cdot)$ with artificial neural networks.

Overview of This Lecture (and the Next)

Basics: Optimization

Basics: Perceptrons and multi-layer perceptrons (MLPs)

Convolutional neural networks (CNNs)

Recurrent and recursive neural networks (RNNs/RvNNs)

Attention

Transformers

Recall: Logistic Regression with Gradient Descent

$$\arg\min_{\mathbf{w}} \text{loss}\left(\mathbf{w}; D = \{\mathbf{x}_i, y_i\}_{i=1}^{N}\right)$$

Recall: Logistic Regression with Gradient Descent

$$\arg\min_{\mathbf{w}} \text{loss}\left(\mathbf{w}; D = \{\mathbf{x}_i, y_i\}_{i=1}^{N}\right)$$

For logistic regression,

$$\text{loss}(\mathbf{w}; D) = -\sum_{i=1}^{N} y_i \log \sigma\left(\mathbf{w}^T \mathbf{x}_i\right) - (1 - y_i) \log\left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right)$$

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

Recall: Logistic Regression with Gradient Descent

$$\arg\min_{\mathbf{w}} \text{loss}\left(\mathbf{w}; D = \{\mathbf{x}_i, y_i\}_{i=1}^N\right)$$

For logistic regression,

$$\text{loss}(\mathbf{w}; D) = -\sum_{i=1}^{N} y_i \log \sigma\left(\mathbf{w}^T \mathbf{x}_i\right) - (1 - y_i) \log\left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right)$$

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

Gradient descent: update $\mathbf{w}$ in the opposite direction of the gradient of the loss function, i.e., $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D)$.

$$\nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D) = \left[\frac{\partial \text{loss}(\mathbf{w}; D)}{\partial w_1}, \ldots, \frac{\partial \text{loss}(\mathbf{w}; D)}{\partial w_n}\right]$$

Applying the Chain Rule

$$\text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} y_i \log \sigma\left(\mathbf{w}^T \mathbf{x}_i\right) + (1 - y_i) \log\left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right)$$

Applying the Chain Rule

$$\text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} y_i \log \sigma\left(\mathbf{w}^T \mathbf{x}_i\right) + (1 - y_i) \log\left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right)$$

Let $z_i(\mathbf{w}; \mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i = \sum_j w_j x_{ij}$.

$$\text{loss}(\mathbf{w}; D) = \text{loss}(\mathbf{z}; \mathbf{y}) = \sum_{i=1}^{N} y_i \log \sigma(z_i) + (1 - y_i) \log\left(1 - \sigma(z_i)\right)$$

Applying the Chain Rule

$$\text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} y_i \log \sigma\left(\mathbf{w}^T \mathbf{x}_i\right) + (1 - y_i) \log\left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right)$$

Let $z_i(\mathbf{w}; \mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i = \sum_j w_j x_{ij}$.

$$\text{loss}(\mathbf{w}; D) = \text{loss}(\mathbf{z}; \mathbf{y}) = \sum_{i=1}^{N} y_i \log \sigma(z_i) + (1 - y_i) \log\left(1 - \sigma(z_i)\right)$$

Apply the chain rule:

$$\frac{\partial \text{loss}}{\partial w_j} = \sum_{i=1}^{N} \frac{\partial \text{loss}}{\partial z_i} \frac{\partial z_i}{\partial w_j}$$

D_i: the dataset that only consists of the i-th training example.

Stochastic Gradient Descent

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D)$$

$$\nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D_i)$$

Stochastic Gradient Descent

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D)$$

$$\nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D_i)$$

Efficiency concerns: for each single update, we need to compute the gradient over the entire dataset.

Stochastic Gradient Descent

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D)$$

$$\nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D) = \sum_{i=1}^{N} \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D_i)$$

Efficiency concerns: for each single update, we need to compute the gradient over the entire dataset.

Solution (**stochastic gradient descent**): use gradients computed over a small subset (also referred to as **mini-batch**) of examples.

$$\nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D) \approx \frac{N}{B} \sum_{i=1}^{B} \nabla_{\mathbf{w}} \text{loss}(\mathbf{w}; D_i)$$

Stochastic Gradient Descent: The Idea

Consider we are estimating the gradient over the entire N examples.

The quantity we aim to estimate is:

$$\begin{aligned}\nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D) &= \sum_{i=1}^{N} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i) \\ &= N \cdot \mathbb{E}_{D_i \sim D} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i)\end{aligned}$$

Stochastic Gradient Descent: The Idea

Consider we are estimating the gradient over the entire N examples.

The quantity we aim to estimate is:

$$\begin{aligned}\nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D) &= \sum_{i=1}^{N} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i) \\ &= N \cdot \mathbb{E}_{D_i \sim D} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i)\end{aligned}$$

The expectation can be estimated by sampling $B (B << N)$ examples from D:

$$\mathbb{E}_{D_i \sim D} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i) \approx \frac{1}{B} \sum_{i=1}^{B} \nabla_{\mathbf{w}}\text{loss}(\mathbf{w}; D_i)$$

Optimizing Neural Networks

Theoretically, gradient based optimization only guarantees convergence to the global minimum for convex functions; for non-convex functions, it may converge to a local minimum.

Optimizing Neural Networks

Theoretically, gradient based optimization only guarantees convergence to the global minimum for convex functions; for non-convex functions, it may converge to a local minimum.

In (almost) every complicated real-world problems with neural network models, the loss function is non-convex.

Optimizing Neural Networks

Theoretically, gradient based optimization only guarantees convergence to the global minimum for convex functions; for non-convex functions, it may converge to a local minimum.

In (almost) every complicated real-world problems with neural network models, the loss function is non-convex.

However, empirical evidence suggests that gradient-based optimization works well in practice.

Optimizing Neural Networks

Theoretically, gradient based optimization only guarantees convergence to the global minimum for convex functions; for non-convex functions, it may converge to a local minimum.

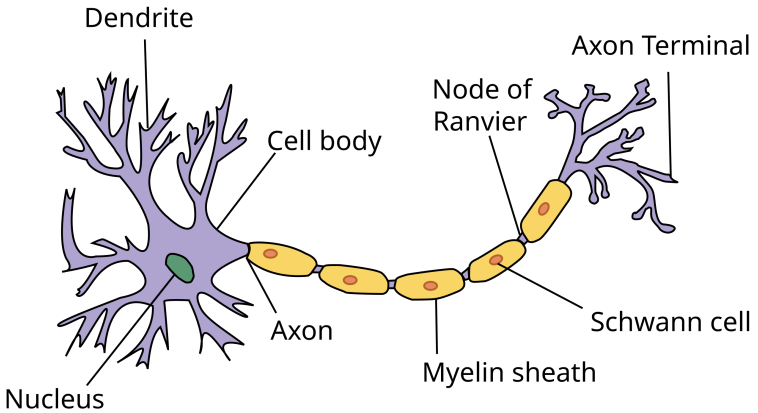
In (almost) every complicated real-world problems with neural network models, the loss function is non-convex.

However, empirical evidence suggests that gradient-based optimization works well in practice.

Adam (Kingma & Ba, 2015; momentum + adaptive learning rate) and AdamW (Loshchilov & Hutter, 2019; Adam + automatic weight decay) are popular choices now to optimize the loss function of neural networks.

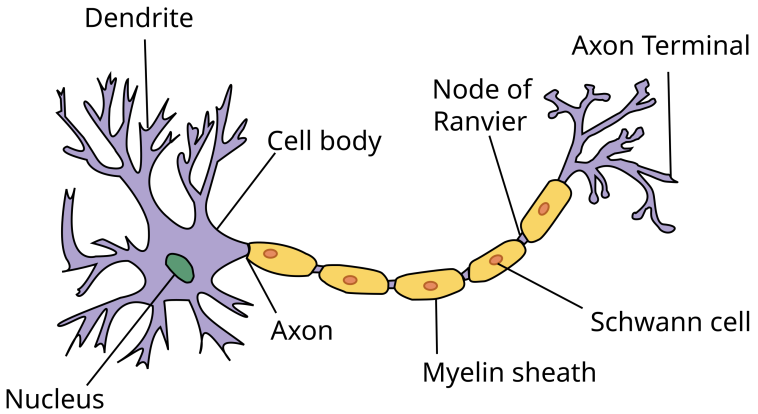
`https://pytorch.org/docs/stable/optim.html#algorithms`

From Biological Neurons to Artificial Neurons

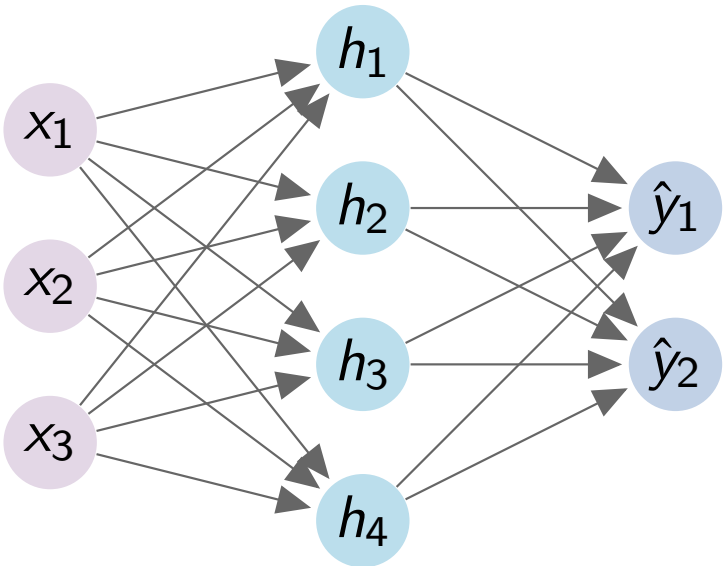


[Source: Wikipedia]

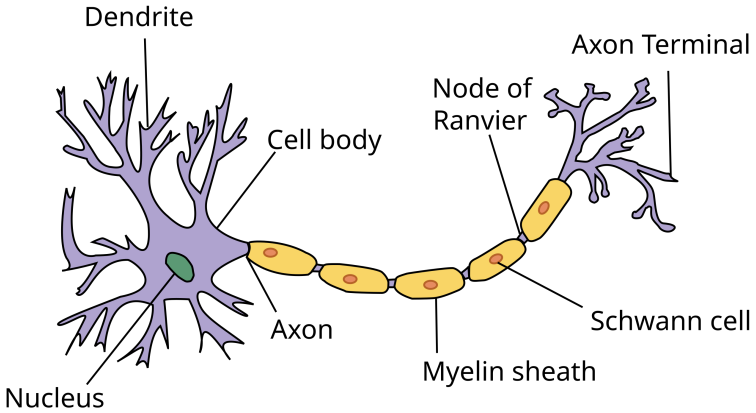
From Biological Neurons to Artificial Neurons



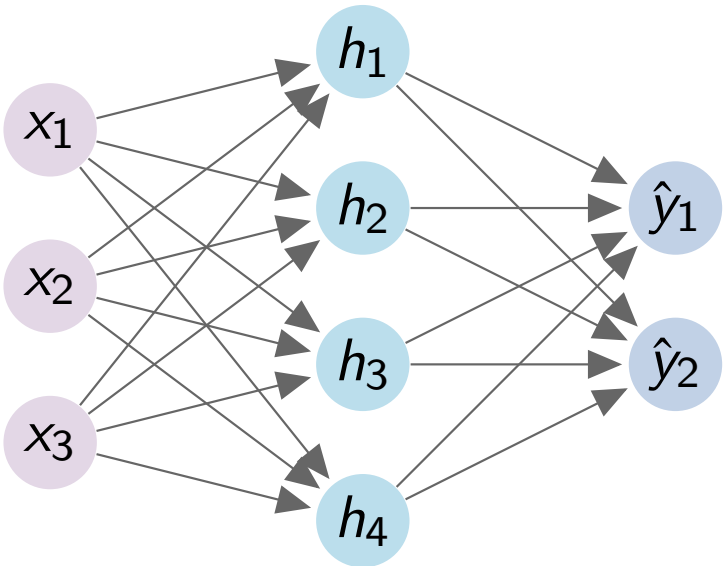
[Source: Wikipedia]



From Biological Neurons to Artificial Neurons



[Source: Wikipedia]



First computational model of a neuron (McCulloch & Pitts, 1943):

$$g(\mathbf{x}) = \sum_{i=1}^{n} x_i \qquad \widehat{y} = f_\theta(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) \geq \theta \\ 0 & \text{otherwise} \end{cases}$$

$\mathbf{x}$: input vector, θ: threshold.

What is an artificial neural network?

An artificial neural network (ANN) is a function.

What is an artificial neural network?

An artificial neural network (ANN) is a function.

In machine learning context, the term **neural network** refers to artificial neural networks.

What is an artificial neural network?

An artificial neural network (ANN) is a function.

In machine learning context, the term **neural network** refers to artificial neural networks.

Two (not necessarily exclusive) views:

- View 1 (computer scientists): The idea of neural modeling is now better thought of as **dense representation learning**, although the design of ANNs was inspired by biological neurons.

What is an artificial neural network?

An artificial neural network (ANN) is a function.

In machine learning context, the term **neural network** refers to artificial neural networks.

Two (not necessarily exclusive) views:

- View 1 (computer scientists): The idea of neural modeling is now better thought of as **dense representation learning**, although the design of ANNs was inspired by biological neurons.
- View 2 (neural scientists): The design of ANNs was inspired by biological neurons, so the study of biological neurons **may** draw insights from artificial neural network behaviors.

Notations

- $\mathbf{u}, \mathbf{v}$: vectors
- u_i, v_i: entry i in the vector

Notations

- $\mathbf{u}, \mathbf{v}$: vectors
- u_i, v_i: entry i in the vector
- $\mathbf{W}$: a matrix
- W_{ij}: entry (i, j) in the matrix

Notations

- $\mathbf{u}, \mathbf{v}$: vectors
- u_i, v_i: entry i in the vector
- $\mathbf{W}$: a matrix
- W_{ij}: entry (i, j) in the matrix
- (Future lectures) $\mathcal{Y}$: a structured object (e.g., a sequence, a tree, etc.)
- (Future lectures) y_i: entry i in the structured object

Perceptron (Minsky & Papert, 1969)

$$\text{Perceptron}(\mathbf{x}; \mathbf{w}, b) = \text{step}(\mathbf{w}^T\mathbf{x} + b), \quad \text{step}(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{o.w.} \end{cases}$$

Perceptron (Minsky & Papert, 1969)

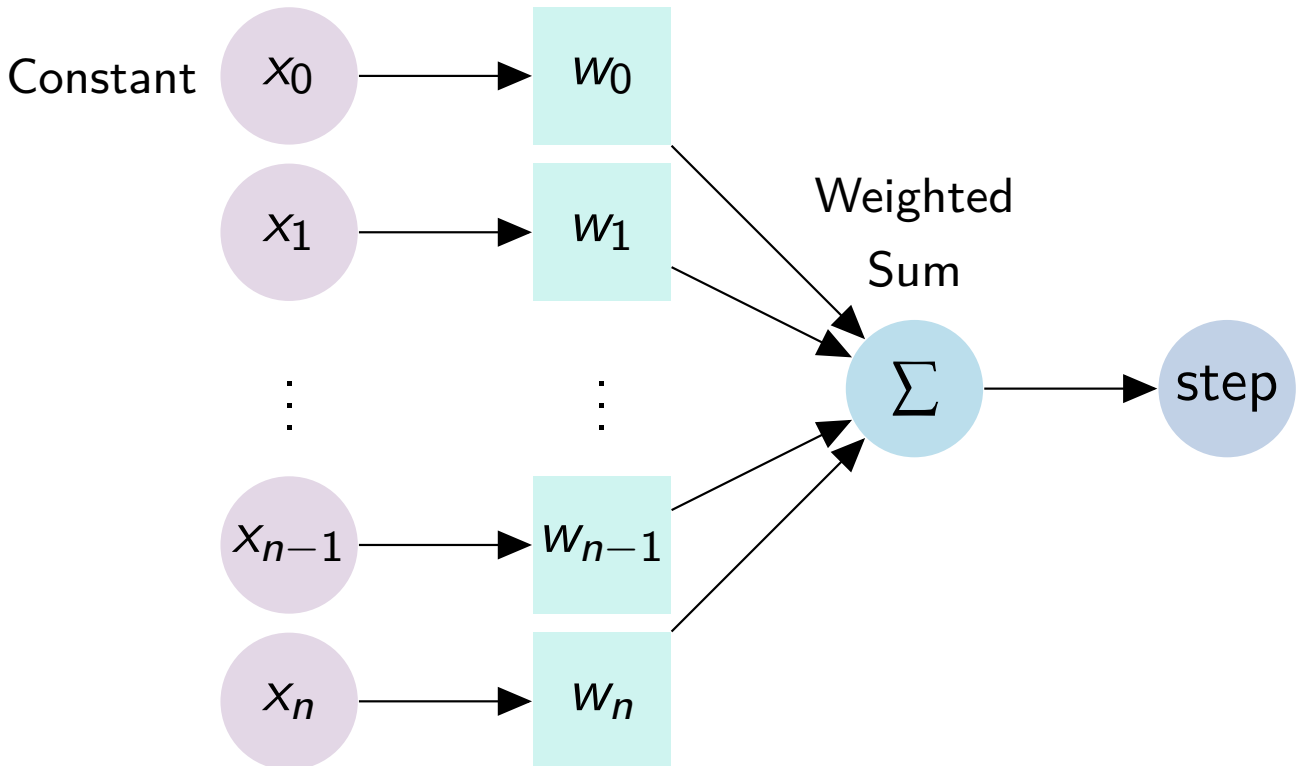
$$\text{Perceptron}(\mathbf{x}; \mathbf{w}, b) = \text{step}(\mathbf{w}^T\mathbf{x} + b), \quad \text{step}(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{o.w.} \end{cases}$$

Can be written as $\text{step}(\mathbf{w}^T\mathbf{x})$ if one entry of $\mathbf{x}$ is always constant.

Perceptron (Minsky & Papert, 1969)

$$\text{Perceptron}(\mathbf{x}; \mathbf{w}, b) = \text{step}(\mathbf{w}^T\mathbf{x} + b), \quad \text{step}(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{o.w.} \end{cases}$$

Can be written as $\text{step}(\mathbf{w}^T\mathbf{x})$ if one entry of $\mathbf{x}$ is always constant.



Learning Perceptrons

$$\text{perceptron}(\mathbf{x}) = \text{step}(\mathbf{w}^T\mathbf{x})$$

Learning Perceptrons

$$\text{perceptron}(\mathbf{x}) = \text{step}(\mathbf{w}^T\mathbf{x})$$

For each training example $(\mathbf{x}_i, y_i)$:

$$\text{Predict the label :} \quad \widehat{y}_i = \text{perceptron}(\mathbf{x}_i)$$
$$\text{Update the weights :} \quad \mathbf{w} = \mathbf{w} + \eta(y_i - \widehat{y}_i)\mathbf{x}_i$$

η: learning rate, y_i: ground-truth label, $\widehat{y}_i$: predicted label.

Learning Perceptrons

$$\text{perceptron}(\mathbf{x}) = \text{step}(\mathbf{w}^T\mathbf{x})$$

For each training example $(\mathbf{x}_i, y_i)$:

$$\begin{aligned} \text{Predict the label :} \quad & \widehat{y}_i = \text{perceptron}(\mathbf{x}_i) \\ \text{Update the weights :} \quad & \mathbf{w} = \mathbf{w} + \eta(y_i - \widehat{y}_i)\mathbf{x}_i \end{aligned}$$

η: learning rate, y_i: ground-truth label, $\widehat{y}_i$: predicted label.

- A perceptron is a binary classifier.
- $\mathbf{w}$: weights that define canonical positive class, and $-\mathbf{w}$ is the canonical negative class.
- If the prediction is incorrect, adjust $\mathbf{w}$.

Perceptron Update as Stochastic Gradient Descent

$$y_i = \text{perceptron}(\mathbf{x}_i) = \text{step}(\mathbf{w}^T \mathbf{x}_i)$$

$$\mathbf{w} = \mathbf{w} + \eta \left(y_i - \widehat{y}_i\right) \mathbf{x}_i$$

Perceptron Update as Stochastic Gradient Descent

$$y_i = \text{perceptron}(\mathbf{x}_i) = \text{step}(\mathbf{w}^T \mathbf{x}_i)$$
$$\mathbf{w} = \mathbf{w} + \eta \left(y_i - \widehat{y}_i\right) \mathbf{x}_i$$

If we set the loss function for example i as

$$\text{loss}(\mathbf{w}; \mathbf{x}_i, y_i) = \left(\widehat{y}_i - y_i\right) \mathbf{w}^T \mathbf{x}_i$$

and **view $\widehat{y}_i$ as a constant**, then the perceptron update rule is equivalent to stochastic gradient descent on the loss function.

Perceptron Update as Stochastic Gradient Descent

$$y_i = \text{perceptron}(\mathbf{x}_i) = \text{step}(\mathbf{w}^T \mathbf{x}_i)$$
$$\mathbf{w} = \mathbf{w} + \eta \left(y_i - \widehat{y}_i\right) \mathbf{x}_i$$

If we set the loss function for example i as

$$\text{loss}(\mathbf{w}; \mathbf{x}_i, y_i) = \left(\widehat{y}_i - y_i\right) \mathbf{w}^T \mathbf{x}_i$$

and **view $\widehat{y}_i$ as a constant**, then the perceptron update rule is equivalent to stochastic gradient descent on the loss function.

$\widehat{y}_i$	y_i	$\text{loss}(\mathbf{w}; \mathbf{x}_i, y_i)$
0	0	0
1	1	0
0	1	+
1	0	+

Neural Layer: Generalized Perceptron

From a machine-learning perspective,
a neural layer = affine transformation + nonlinearity.

$$\text{perceptron}(\mathbf{x}) = \text{step}(\mathbf{w}^T\mathbf{x} + b) \in \{0, 1\}$$

Neural Layer: Generalized Perceptron

From a machine-learning perspective,
a neural layer = affine transformation + nonlinearity.

$$\text{perceptron}(\mathbf{x}) = \text{step}(\mathbf{w}^T\mathbf{x} + b) \in \{0, 1\}$$

$$\text{neural-layer}(\mathbf{x}) = g(\mathbf{W}\mathbf{x} + \mathbf{b}) \in \mathbb{R}^{d_{\text{out}}}$$
$$\text{neural-layer}(\mathbf{x})_i = g(\mathbf{w}_i\mathbf{x} + b_i) \in \mathbb{R}$$

g: (nonlinear) activation function.

$\mathbf{W} \in \mathbb{R}^{d_{\text{in}} \times d_{\text{out}}}$, $\mathbf{b} \in \mathbb{R}^{d_{\text{out}}}$: parameter of the affine transformation.

$\mathbf{w}_i$: i-th row vector of $\mathbf{W}$.

d_{in}: input dimension, d_{out}: output dimension.

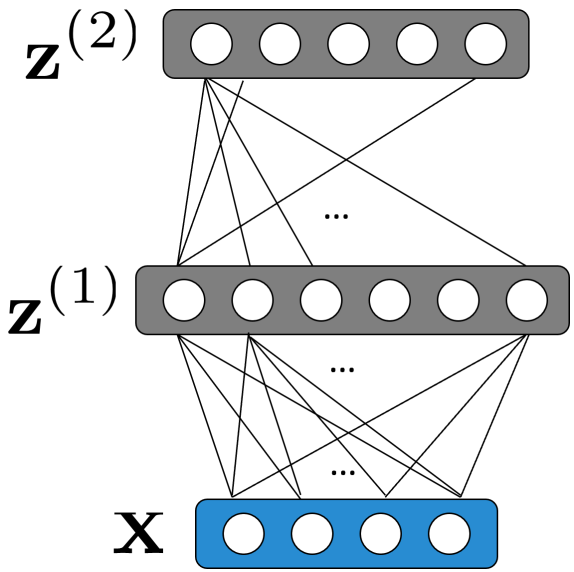
Stacking Neural Layers

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

$$\mathbf{z}^{(2)} = g\left(\mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}\right)$$

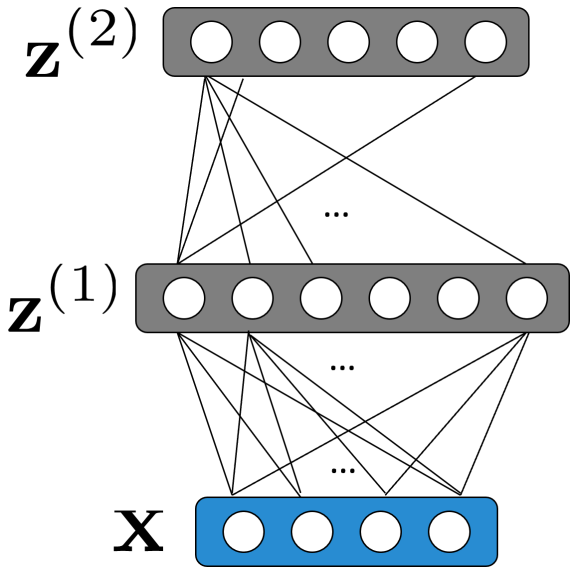
$$\dots$$

- Use the output of one layer as the input of the next layer.



Stacking Neural Layers

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{z}^{(2)} = g\left(\mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}\right)$$
$$\dots$$



- Use the output of one layer as the input of the next layer.
- Feed-Forward Neural Network
- Fully Connected Neural Network
- Multi-Layer Perceptron (MLP)

Nonlinearities: Activation Functions

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

See also the Pytorch documentation.

Nonlinearities: Activation Functions

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

- g is applied to each entry of the vector in an element-wise manner.

See also the Pytorch documentation.

Nonlinearities: Activation Functions

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

- g is applied to each entry of the vector in an element-wise manner.
- Common activation functions: sigmoid, tanh, ReLU, Leaky ReLU, etc.

See also the Pytorch documentation.

Nonlinearities: Activation Functions

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

- g is applied to each entry of the vector in an element-wise manner.
- Common activation functions: sigmoid, tanh, ReLU, Leaky ReLU, etc.

Why do we need nonlinearity?

See also the Pytorch documentation.

Nonlinearities: Activation Functions

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

- g is applied to each entry of the vector in an element-wise manner.
- Common activation functions: sigmoid, tanh, ReLU, Leaky ReLU, etc.

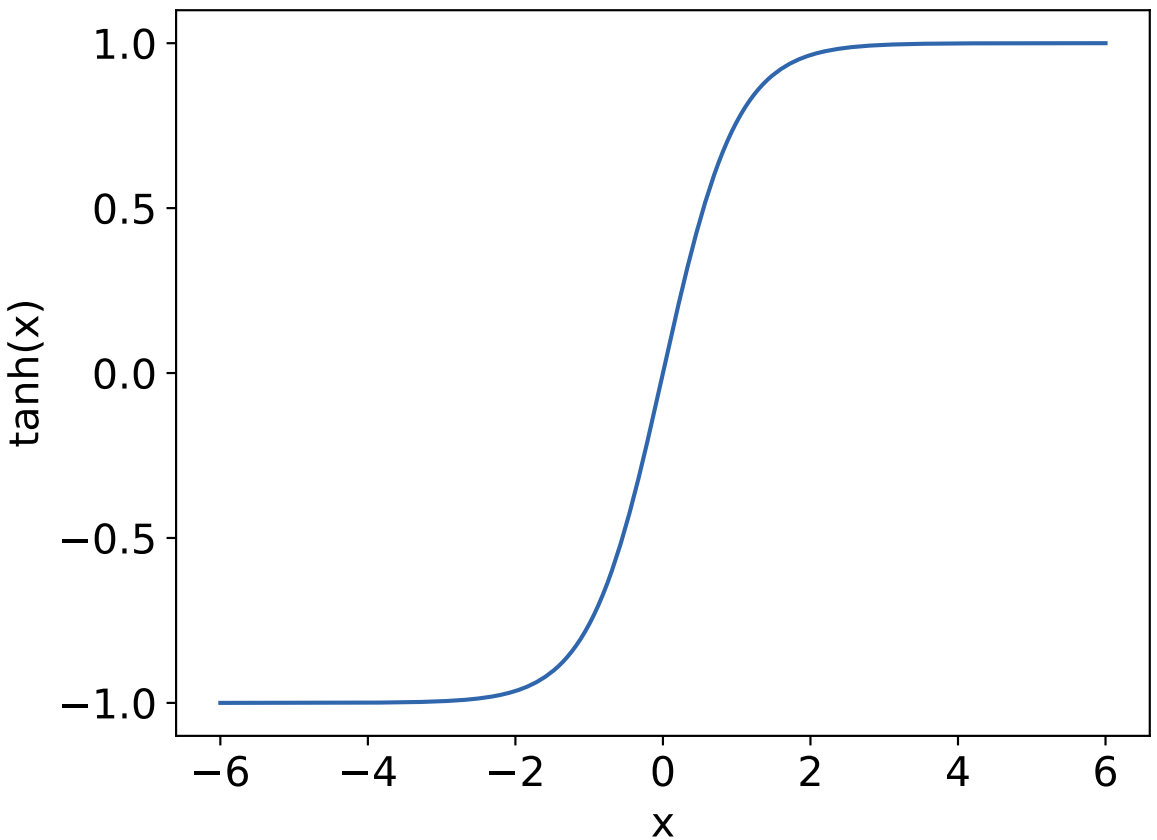
Why do we need nonlinearity?

Without nonlinearity, the composition of multiple layers of affine transformations is still an affine transformation.

See also the Pytorch documentation.

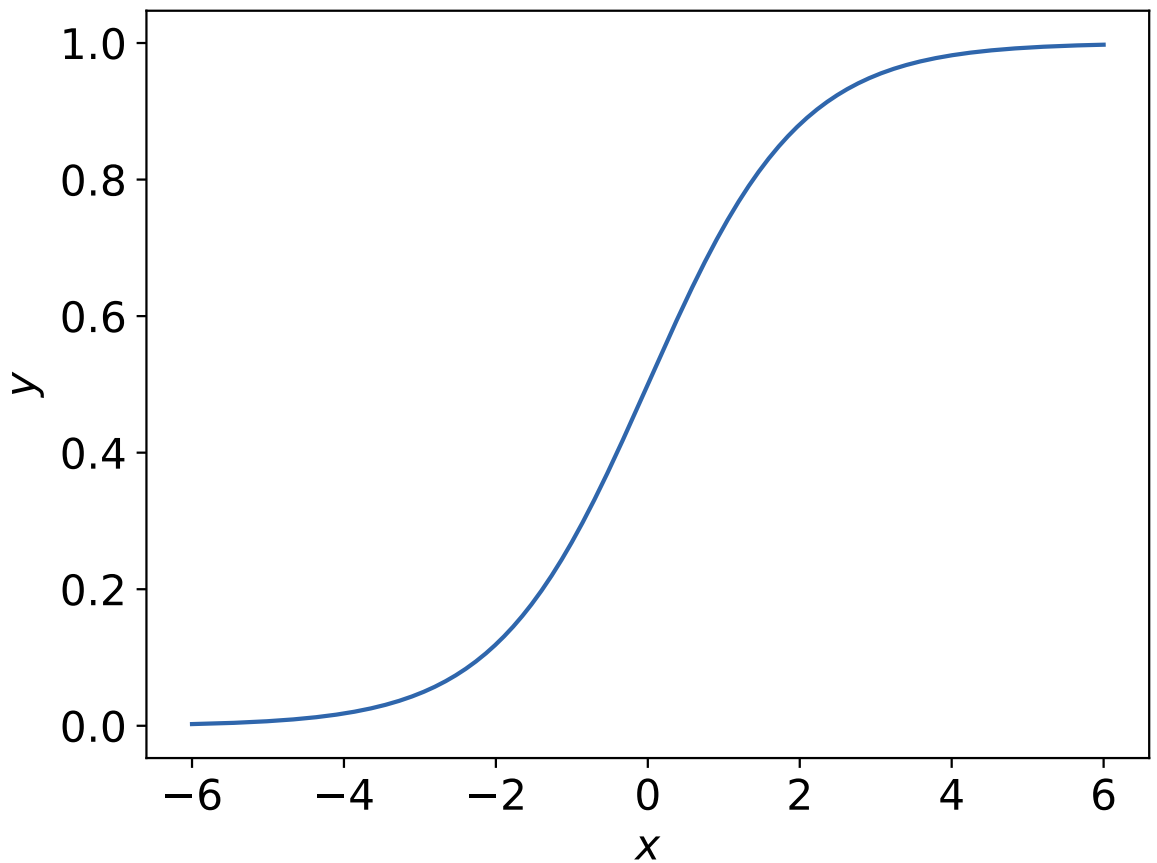
Activation Function: Tanh

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



Activation Function: Sigmoid

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$



Tanh and Sigmoid

$$
\begin{aligned}
\tanh(x) &= \frac{e^x - e^{-x}}{e^x + e^{-x}} \\
&= \frac{1 - e^{-2x}}{1 + e^{-2x}} \qquad \text{divide by } e^x \textit{ onbothsides} \\
&= \frac{1}{1 + e^{-2x}} - \frac{e^{-2x}}{1 + e^{-2x}} \\
&= \sigma(2x) - (1 - \sigma(2x)) \\
&= 2\sigma(2x) - 1
\end{aligned}
$$

Tanh and Sigmoid

$$
\begin{aligned}
\tanh(x) &= \frac{e^x - e^{-x}}{e^x + e^{-x}} \\
&= \frac{1 - e^{-2x}}{1 + e^{-2x}} && \text{divide by } e^x \textit{onbothsides} \\
&= \frac{1}{1 + e^{-2x}} - \frac{e^{-2x}}{1 + e^{-2x}} \\
&= \sigma(2x) - (1 - \sigma(2x)) \\
&= 2\sigma(2x) - 1
\end{aligned}
$$

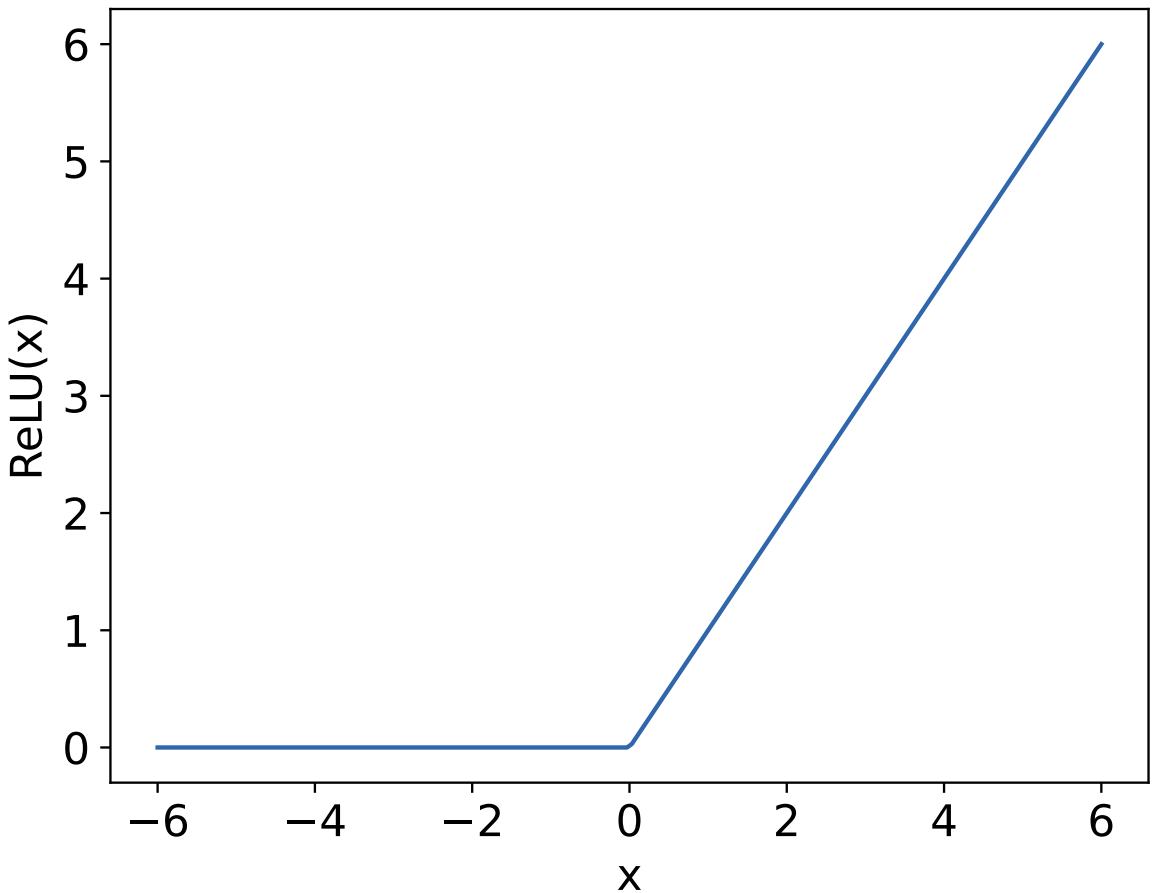
The derivatives of both tanh and sigmoid can be expressed in terms of the function itself.

$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x)$$

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x))$$

Activation Function: Rectified Linear Unit (ReLU)

$$\text{ReLU}(x) = \max(0, x)$$



The Dying ReLU Problem

ReLU was once the most popular activation function in deep learning.

However, it can be fragile during training.

The Dying ReLU Problem

ReLU was once the most popular activation function in deep learning.

However, it can be fragile during training.

Due to problematic **weight initialization**, or **imbalanced data**, the input of a ReLU unit can become negative for all training examples.

These neurons will never activate again.

The Dying ReLU Problem

ReLU was once the most popular activation function in deep learning.

However, it can be fragile during training.

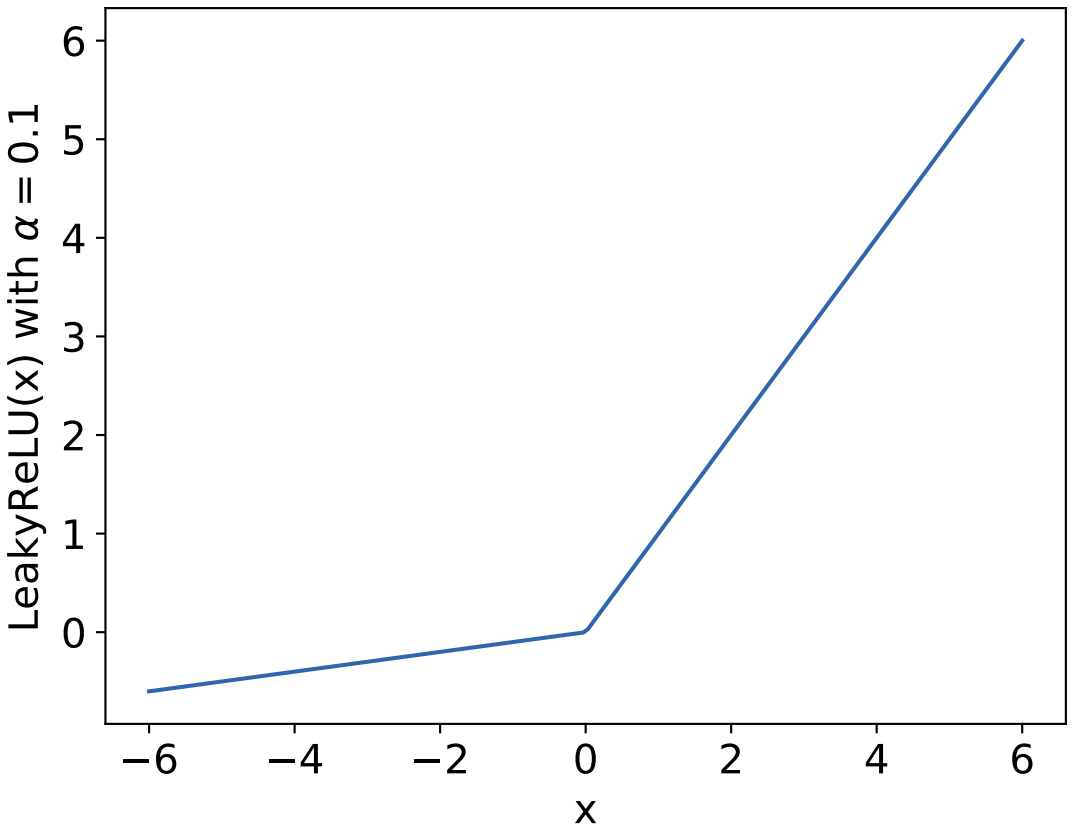
Due to problematic **weight initialization**, or **imbalanced data**, the input of a ReLU unit can become negative for all training examples.

These neurons will never activate again.

Solution: Leaky ReLU, Parametric ReLU, GELU, SELU, etc.

Leaky ReLU

$$\text{LeakyReLU}(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x (\alpha < 1) & \text{otherwise} \end{cases}$$



Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Remaining Questions:

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Remaining Questions:

- How can we obtain the text representation $\mathbf{x}$?

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Remaining Questions:

- How can we obtain the text representation $\mathbf{x}$?
  Anyhow we can convert text into a fixed-dimensional vector.

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Remaining Questions:

- How can we obtain the text representation $\mathbf{x}$?
  Anyhow we can convert text into a fixed-dimensional vector.
- How do we train the model (update model parameters)?

Text Classification with MLP

A 2-layer MLP is a simple and general text classification model:

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$\mathbf{x}$: text features, $\mathbf{s} \in \mathbb{R}^{|\mathcal{Y}|}$: score$(\mathbf{x}, \cdot)$.

We empirically do not add nonlinear activation to the output layer—we'll see the reason soon!

Remaining Questions:

- How can we obtain the text representation $\mathbf{x}$?
  Anyhow we can convert text into a fixed-dimensional vector.
- How do we train the model (update model parameters)?
  By minimizing the objective function (e.g., cross-entropy loss) over the training data, using gradient-based optimization methods.

The `softmax` Operator

The `softmax` operator converts **a list of scores** into probabilities:

$$\texttt{softmax}: \mathbb{R}^d \rightarrow \mathbb{R}^d$$

$$\widehat{P}(Y = y_i) = \texttt{softmax}(\mathbf{s})_i = \frac{e^{s_i}}{\sum_{j=1}^{|Y|} e^{s_j}}$$

The `softmax` Operator

The `softmax` operator converts **a list of scores** into probabilities:

$$\texttt{softmax}: \mathbb{R}^d \rightarrow \mathbb{R}^d$$

$$\widehat{P}(Y = y_i) = \texttt{softmax}(\mathbf{s})_i = \frac{e^{s_i}}{\sum_{j=1}^{|Y|} e^{s_j}}$$

`softmax` is a differentiable operator so that we can compute the gradient of its output with respect to input.

The `softmax` Operator

The `softmax` operator converts **a list of scores** into probabilities:

$$\texttt{softmax}: \mathbb{R}^d \rightarrow \mathbb{R}^d$$

$$\widehat{P}(Y = y_i) = \texttt{softmax}(\mathbf{s})_i = \frac{e^{s_i}}{\sum_{j=1}^{|Y|} e^{s_j}}$$

`softmax` is a differentiable operator so that we can compute the gradient of its output with respect to input.

In some tasks, particularly language model inference, `softmax` is usually coupled with a **temperature** τ.

$$\texttt{softmax}_\tau(\mathbf{s})_i = \frac{e^{s_i/\tau}}{\sum_j e^{s_j/\tau}}$$

The `softmax` Operator

The `softmax` operator converts **a list of scores** into probabilities:

$$\texttt{softmax}: \mathbb{R}^d \to \mathbb{R}^d$$

$$\widehat{P}(Y = y_i) = \texttt{softmax}(\mathbf{s})_i = \frac{e^{s_i}}{\sum_{j=1}^{|Y|} e^{s_j}}$$

`softmax` is a differentiable operator so that we can compute the gradient of its output with respect to input.

In some tasks, particularly language model inference, `softmax` is usually coupled with a **temperature** τ.

$$\texttt{softmax}_\tau(\mathbf{s})_i = \frac{e^{s_i/\tau}}{\sum_j e^{s_j/\tau}}$$

When $\tau \to 0$ (temperature annealing), `softmax` becomes **argmax**.

The `softmax` Operator

Many activation functions restrict the range of the output to some narrow interval.

Some probability distributions can not be represented by `softmax`, if passing the output of these functions to `softmax`.

The `softmax` Operator

Many activation functions restrict the range of the output to some narrow interval.

Some probability distributions can not be represented by `softmax`, if passing the output of these functions to `softmax`.

Example:

$$\mathbf{s} = \tanh(\mathbf{a}) \in \mathbb{R}^2$$

$\texttt{softmax}(\mathbf{s})$ cannot represent a distribution sharper than

$$\left[\frac{e^{-1}}{e + e^{-1}}, \frac{e}{e + e^{-1}}\right] = [0.12, 0.88].$$

The `softmax` Operator

Many activation functions restrict the range of the output to some narrow interval.

Some probability distributions can not be represented by `softmax`, if passing the output of these functions to `softmax`.

Example:

$$\mathbf{s} = \tanh(\mathbf{a}) \in \mathbb{R}^2$$

$\texttt{softmax}(\mathbf{s})$ cannot represent a distribution sharper than

$$\left[\frac{e^{-1}}{e + e^{-1}}, \frac{e}{e + e^{-1}}\right] = [0.12, 0.88].$$

This explains why we drop nonlinear activation for the output layer.

Softmax vs. Sigmoid

Softmax is a generalization of sigmoid to multiple classes.

Softmax vs. Sigmoid

Softmax is a generalization of sigmoid to multiple classes.

$\sigma(x)$ gives the distribution

$$\left[\frac{1}{1+e^{-x}}, \frac{e^{-x}}{1+e^{-x}}\right] = \left[\frac{e^{0}}{e^{0}+e^{-x}}, \frac{e^{-x}}{e^{0}+e^{-x}}\right]$$

$$= \texttt{softmax}([0, -x])$$

Softmax vs. Sigmoid

Softmax is a generalization of sigmoid to multiple classes.

$\sigma(x)$ gives the distribution

$$\left[\frac{1}{1+e^{-x}}, \frac{e^{-x}}{1+e^{-x}}\right] = \left[\frac{e^{0}}{e^{0}+e^{-x}}, \frac{e^{-x}}{e^{0}+e^{-x}}\right]$$

$$= \texttt{softmax}([0, -x])$$

Logistic regression can be considered as a single-layer neural network with sigmoid activation for 2-way classification.

Training Objective: The Cross-Entropy Loss

Recall the cross-entropy loss between the population distribution $Pop(\cdot \mid \mathbf{x})$ and the predicted distribution $\widehat{P}(\cdot \mid \mathbf{x})$:

$$H(Pop, \widehat{P}) = \mathbb{E}_{\mathbf{x}, y \sim Pop} \left[-\log \widehat{P}(y \mid \mathbf{x}) \right]$$

Training Objective: The Cross-Entropy Loss

Recall the cross-entropy loss between the population distribution $Pop(\cdot \mid \mathbf{x})$ and the predicted distribution $\widehat{P}(\cdot \mid \mathbf{x})$:

$$H(Pop, \widehat{P}) = \mathbb{E}_{\mathbf{x}, y \sim Pop} \left[-\log \widehat{P}(y \mid \mathbf{x}) \right]$$

In practice, we **estimate** $H(Pop, \widehat{P})$ using the training data, with the assumption that they are i.i.d. samples from the population distribution.

Training Objective: The Cross-Entropy Loss

Recall the cross-entropy loss between the population distribution $Pop(\cdot \mid \mathbf{x})$ and the predicted distribution $\widehat{P}(\cdot \mid \mathbf{x})$:

$$H(Pop, \widehat{P}) = \mathbb{E}_{\mathbf{x}, y \sim Pop} \left[-\log \widehat{P}(y \mid \mathbf{x}) \right]$$

In practice, we **estimate** $H(Pop, \widehat{P})$ using the training data, with the assumption that they are i.i.d. samples from the population distribution.

For single-label classification, the cross-entropy loss then becomes the negative log-likelihood loss:

$$\text{loss}(\mathbf{x}_i, y_i) = -\log \widehat{P}(y_i \mid \mathbf{x}_i) = -\log \texttt{softmax}(\mathbf{s}(\mathbf{x}))_{y_i}$$

Training Neural Classifiers

Assume $\mathbf{x}_i$ is a text feature vector (obtained by bag-of-words over pretrained word embeddings).

For a mini-batch of examples $\{(\mathbf{x}_i, y_i)\}_{i=1}^{B}$:

- Compute the scores $\mathbf{s} = NN_{\mathbf{\Theta}}(\mathbf{x}_i)$ and $\text{loss}(\mathbf{x}_i, y_i)$ for each example.
- Compute the average loss over the mini-batch.
- Compute the gradient of the average loss with respect to the model parameters $\mathbf{\Theta}$ – using back propagation.
- Update the model parameters using the gradients.

Back Propagation

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$$\text{loss}(\mathbf{x}, y) = -\log \texttt{softmax}(\mathbf{s})_y$$

Back Propagation

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$
$$\text{loss}(\mathbf{x}, y) = -\log \texttt{softmax}(\mathbf{s})_y$$

The gradient for the parameters $\mathbf{W}^{(0)}, \mathbf{b}^{(0)}, \mathbf{W}^{(1)}, \mathbf{b}^{(1)}$ can be computed using the chain rule.

$$\frac{\partial \text{loss}}{\partial \mathbf{W}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{W}^{(1)}} \quad \frac{\partial \text{loss}}{\partial \mathbf{b}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{b}^{(1)}} \quad \frac{\partial \text{loss}}{\partial \mathbf{z}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}}$$

$$\frac{\partial \text{loss}}{\partial \mathbf{W}^{(0)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \qquad \frac{\partial \text{loss}}{\partial \mathbf{b}^{(0)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{b}^{(0)}}$$

Back Propagation

$$\mathbf{z}^{(1)} = g\left(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$
$$\mathbf{s} = \mathbf{z}^{(2)} = \mathbf{W}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$
$$\text{loss}(\mathbf{x}, y) = -\log \texttt{softmax}(\mathbf{s})_y$$

The gradient for the parameters $\mathbf{W}^{(0)}, \mathbf{b}^{(0)}, \mathbf{W}^{(1)}, \mathbf{b}^{(1)}$ can be computed using the chain rule.

$$\frac{\partial \text{loss}}{\partial \mathbf{W}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{W}^{(1)}} \quad \frac{\partial \text{loss}}{\partial \mathbf{b}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{b}^{(1)}} \quad \frac{\partial \text{loss}}{\partial \mathbf{z}^{(1)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}}$$

$$\frac{\partial \text{loss}}{\partial \mathbf{W}^{(0)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \qquad \frac{\partial \text{loss}}{\partial \mathbf{b}^{(0)}} = \frac{\partial \text{loss}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{b}^{(0)}}$$

SGD and advanced optimizers can be applied as long as the gradients are computable!

Some Philosophy: KL Divergence in Classification

[Source: David McAllester]

Recall: The Kullback–Leibler (KL) divergence serves as a natural measurement of the difference between two distributions.

$$KL(P \parallel Q) = \mathbb{E}_{y \sim P} \log \frac{P(y)}{Q(y)}$$

How many more bits are needed to encode samples from P using the optimal code of Q, compared to the optimal code of P.

Some Philosophy: KL Divergence in Classification

[Source: David McAllester]

Recall: The Kullback–Leibler (KL) divergence serves as a natural measurement of the difference between two distributions.

$$KL(P \parallel Q) = \mathbb{E}_{y \sim P} \log \frac{P(y)}{Q(y)}$$

How many more bits are needed to encode samples from P using the optimal code of Q, compared to the optimal code of P.

What we really aim to optimize is $KL(Pop \parallel \widehat{P})$.

Some Philosophy: KL Divergence in Classification

[Source: David McAllester]

Recall: The Kullback–Leibler (KL) divergence serves as a natural measurement of the difference between two distributions.

$$KL(P \parallel Q) = \mathbb{E}_{y \sim P} \log \frac{P(y)}{Q(y)}$$

How many more bits are needed to encode samples from P using the optimal code of Q, compared to the optimal code of P.

What we really aim to optimize is $KL(Pop \parallel \widehat{P})$.

$$KL(Pop \parallel \widehat{P}) = \mathbb{E}_{\mathbf{x}, y \sim Pop} \log \frac{Pop(y \mid \mathbf{x})}{\widehat{P}(y \mid \mathbf{x})}$$

However, we don't have a good estimation of $Pop(y \mid \mathbf{x})$ due to lack of data.

Some Philosophy: KL Divergence vs. Cross Entropy

$$
\begin{aligned}
KL(Pop \,\|\, \widehat{P}) &= \mathbb{E}_{\mathbf{x},y\sim Pop} \log \frac{Pop(y \mid \mathbf{x})}{\widehat{P}(y \mid \mathbf{x})} \\
&= H(Pop, \widehat{P}) - H(Pop) \\
H(Pop, \widehat{P}) &= \mathbb{E}_{\mathbf{x},y\sim Pop} - \log \widehat{P}(y \mid \mathbf{x})
\end{aligned}
$$

Some Philosophy: KL Divergence vs. Cross Entropy

$$
\begin{aligned}
KL(Pop \,\|\, \widehat{P}) &= \mathbb{E}_{\mathbf{x},y\sim Pop} \log \frac{Pop(y \mid \mathbf{x})}{\widehat{P}(y \mid \mathbf{x})} \\
&= H(Pop, \widehat{P}) - H(Pop) \\
H(Pop, \widehat{P}) &= \mathbb{E}_{\mathbf{x},y\sim Pop} - \log \widehat{P}(y \mid \mathbf{x})
\end{aligned}
$$

Although the optimal $\widehat{P}$ are the same, we can use the training data to estimate $H(Pop, \widehat{P})$, but not $KL(Pop \,\|\, \widehat{P})$.

Some Philosophy: KL Divergence vs. Cross Entropy

$$KL(Pop \,\|\, \widehat{P}) = \mathbb{E}_{\mathbf{x},y\sim Pop} \log \frac{Pop(y \mid \mathbf{x})}{\widehat{P}(y \mid \mathbf{x})}$$
$$= H(Pop, \widehat{P}) - H(Pop)$$
$$H(Pop, \widehat{P}) = \mathbb{E}_{\mathbf{x},y\sim Pop} - \log \widehat{P}(y \mid \mathbf{x})$$

Although the optimal $\widehat{P}$ are the same, we can use the training data to estimate $H(Pop, \widehat{P})$, but not $KL(Pop \,\|\, \widehat{P})$.

We are never simply interested in minimizing the cross-entropy loss between the training data distribution and the model predictions.

We are interested in doing so because training data is the only information we have about the **population distribution**.

Next

Advanced neural network architectures.