Natural Language Processing

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Part 1: Feedforward neural networks

Log-linear models versus Neural networks

Feedforward neural networks

Stochastic Gradient Descent

Motivating example: XOR

Computation Graphs

Log linear model

- Let there be m features, $f_k(\mathbf{x}, y)$ for $k = 1, \ldots, m$
- Define a parameter vector $\mathbf{v} \in \mathbb{R}^m$
- A log-linear model for classification into labels $y \in \mathcal{Y}$:

$$\Pr(y \mid \mathbf{x}; \mathbf{v}) = \frac{exp\left(\mathbf{v} \cdot \mathbf{f}(\mathbf{x}, y)\right))}{\sum_{y' \in \mathcal{Y}} exp\left(\mathbf{v} \cdot \mathbf{f}(\mathbf{x}, y')\right))}$$

Advantages

The feature representation $\mathbf{f}(\mathbf{x}, y)$ can represent any aspect of the input that is useful for classification.

Disadvantages

The feature representation $\mathbf{f}(\mathbf{x}, y)$ has to be designed by hand which is time-consuming and error-prone.

Log linear model

Figure from [1]

Disadvantages: number of combined features can explode

farmers eat	steak → **high** hay → **low**	cows eat	steak → **low** hay → **high**
farmers grow	steak → **low** hay → **high**	cows grow	steak → **low** hay → **low**

Neural Networks

Advantages

- Neural networks replace hand-engineered features with **representation learning**
- Empirical results across many different domains show that learned representations give significant improvements in accuracy
- Neural networks allow end to end training for complex NLP tasks and do not have the limitations of multiple chained pipeline models

Disadvantages

For many tasks linear models are much faster to train compared to neural network models

Alternative Form of Log linear model

Log-linear model:

$$\Pr(y \mid \mathbf{x}; \mathbf{v}) = \frac{exp\left(\mathbf{v} \cdot \mathbf{f}(\mathbf{x}, y)\right))}{\sum_{y' \in \mathcal{Y}} exp\left(\mathbf{v} \cdot \mathbf{f}(\mathbf{x}, y')\right))}$$

Alternative form using functions:

$$\Pr(y \mid x; v) = \frac{exp\left(v(y) \cdot f(x) + \gamma_y\right)}{\sum_{y' \in \mathcal{Y}} exp\left(v(y') \cdot f(x) + \gamma_{y'}\right)}$$

- Feature vector $f(x)$ maps input x to $\mathbb{R}^d$
- Parameters $v(y) \in \mathbb{R}^d$ and $\gamma_y \in \mathbb{R}$ for each $y \in \mathcal{Y}$
- We assume $v(y) \cdot f(x)$ is a dot product. Using matrix multiplication it would be $v(y) \cdot f(x)^T$
- Let $v = \{(v(y), \gamma_y) : y \in \mathcal{Y}\}$

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Representation Learning: Feedforward Neural Network

Replace hand-engineered features f with learned features ϕ:

$$\Pr(y \mid x; \theta, v) = \frac{exp\left(v(y) \cdot \phi(x; \theta) + \gamma_y\right)}{\sum_{y' \in \mathcal{Y}} exp\left(v(y') \cdot \phi(x; \theta) + \gamma_{y'}\right)}$$

- Replace $f(x)$ with $\phi(x; \theta) \in \mathbb{R}^d$ where θ are new parameters
- Parameters θ are learned from training data
- Using θ the model ϕ maps input x to $\mathbb{R}^d$: a learned representation from x
- $x \in \mathbb{R}^d$ is a pre-trained vector of size d
- We will use feedforward neural networks to define $\phi(x; \theta)$
- $\phi(x; \theta)$ will be a **non-linear** mapping to $\mathbb{R}^d$
- ϕ replaces f which was a **linear** model

A Single Neuron aka Perceptron

A single neuron maps input $x \in \mathbb{R}^d$ to output h:

$$h = g(w \cdot x + b)$$

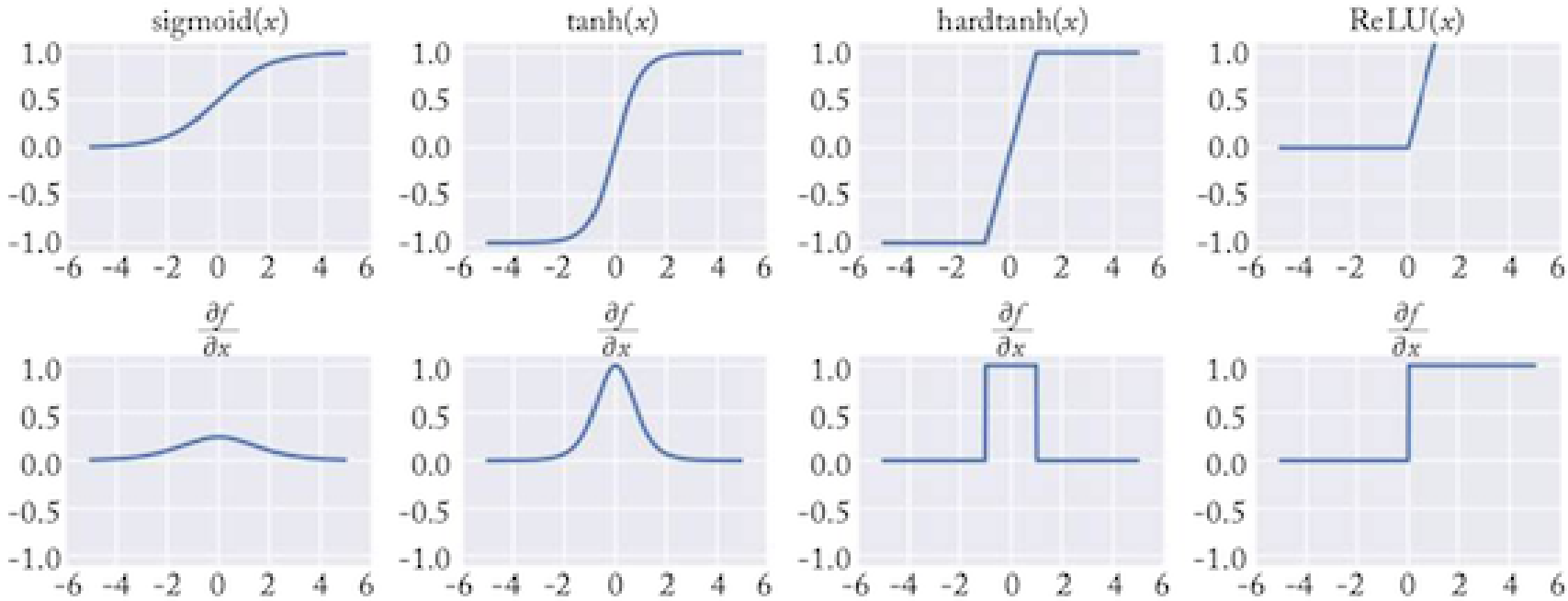
- Weight vector $w \in \mathbb{R}^d$, a bias $b \in \mathbb{R}$ are the parameters of the model learned from training data
- *Transfer function* (also called *activation function*)

$$g : \mathbb{R} \to \mathbb{R}$$

- It is important that g is a **non-linear** transfer function
- Linear $g(z) = \alpha \cdot z + \beta$ for constants α, β (linear perceptron)

Activation Functions and their Gradients

from [2], Fig. 4.3



The sigmoid Transfer Function: σ

sigmoid transfer function:

$$g(z) = \frac{1}{1 - \exp(z)}$$

Derivative of sigmoid:

$$\frac{dg(z)}{dz} = g(z)(1 - g(z))$$

The tanh Transfer Function

tanh transfer function:

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

Derivative of tanh:

$$\frac{dg(z)}{dz} = 1 - g(z)^2$$

Alternatives to tanh

hardtanh:

$$g(z) = \begin{cases} 1 & \text{if } z > 1 \\ -1 & \text{if } z < -1 \\ z & \text{otherwise} \end{cases}$$

$$\frac{dg(z)}{dz} = \begin{cases} 1 & \text{if } -1 \leq z \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

softsign:

$$g(z) = \frac{z}{1 + |z|}$$

$$\frac{dg(z)}{dz} = \begin{cases} \frac{1}{(1+z)^2} & \text{if } z \geq 0 \\ \frac{-1}{(1+z)^2} & \text{if } z < 0 \end{cases}$$

The ReLU Transfer Function

Rectified Linear Unit (ReLU):

$$g(z) = \{z \text{ if } z \geq 0 \text{ or } 0 \text{ if } z < 0\}$$

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

Derivative of ReLU:

$$\frac{dg(z)}{dz} = \{1 \text{ if } z > 0 \text{ or } 0 \text{ if } z < 0\}$$

non-differentiable or undefined if $z = 0$
(in practice: choose a value for $z = 0$)

The GeLU Transfer Function

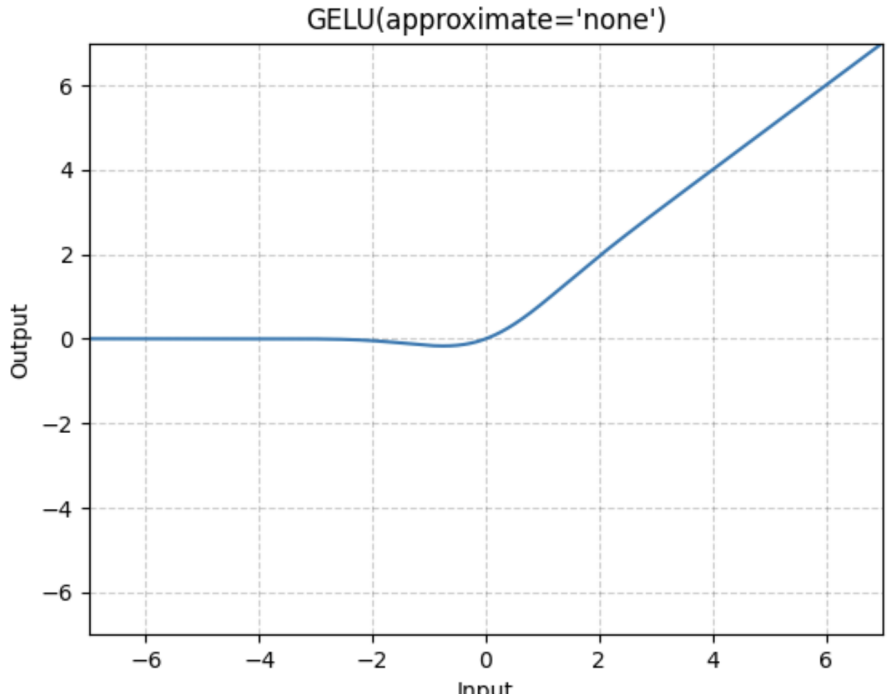
Gaussian Error Linear Unit (GELU):

$$g(z) = \{\frac{z}{2}(1 + (\sqrt{\frac{2}{\pi}} \times (z + 0.044715 \times z^3)))\}$$

or

$$g(z) = \{\frac{z}{2}(1 + \tanh(\sqrt{\frac{2}{\pi}} \times (z + 0.044715 \times z^3)))\}$$

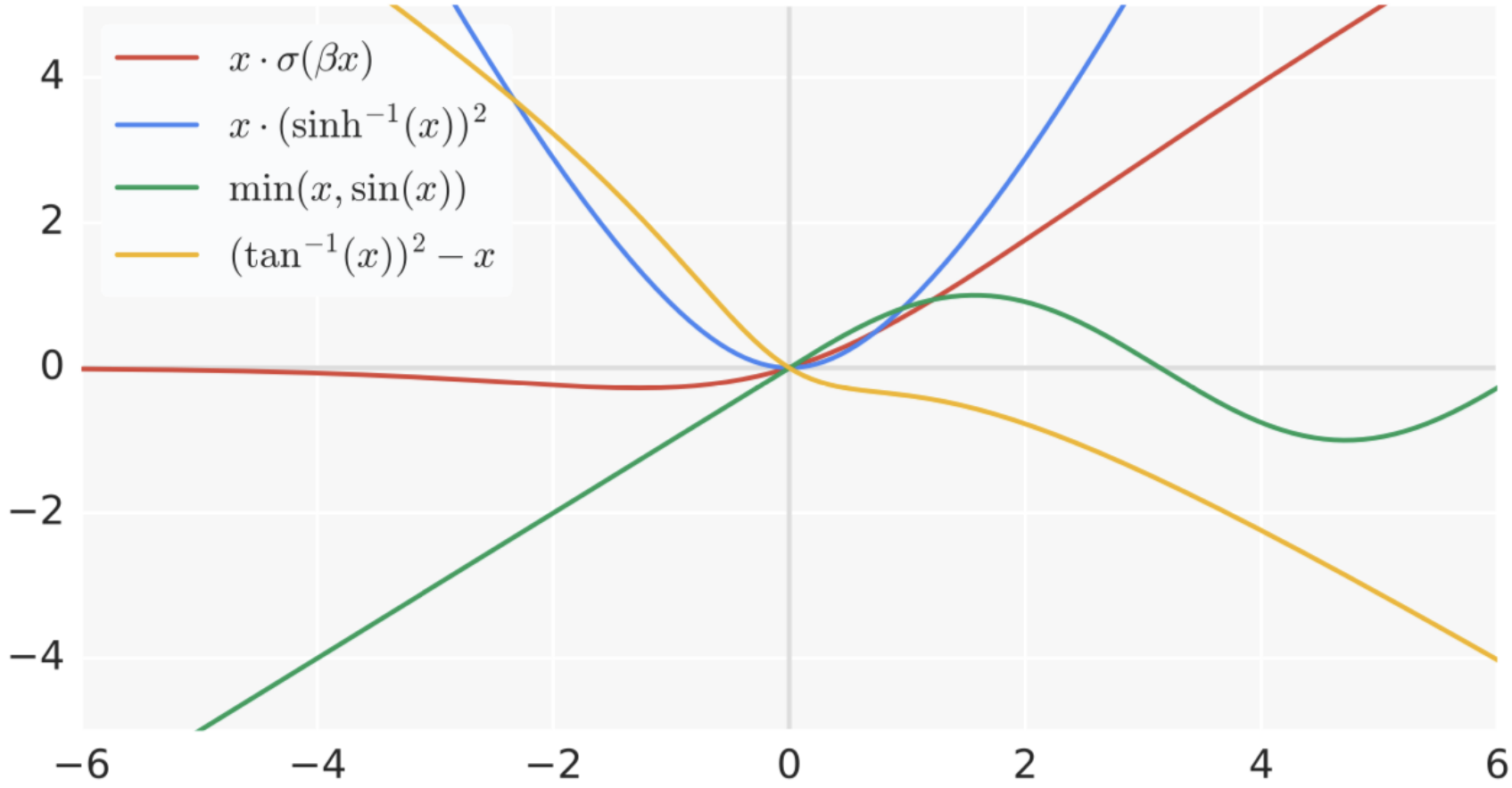
Transfer function of choice for Transformer language models.



Desperately Seeking Transfer Functions

from [3]

Enumeration of non-linear functions



Desperately Seeking Transfer Functions

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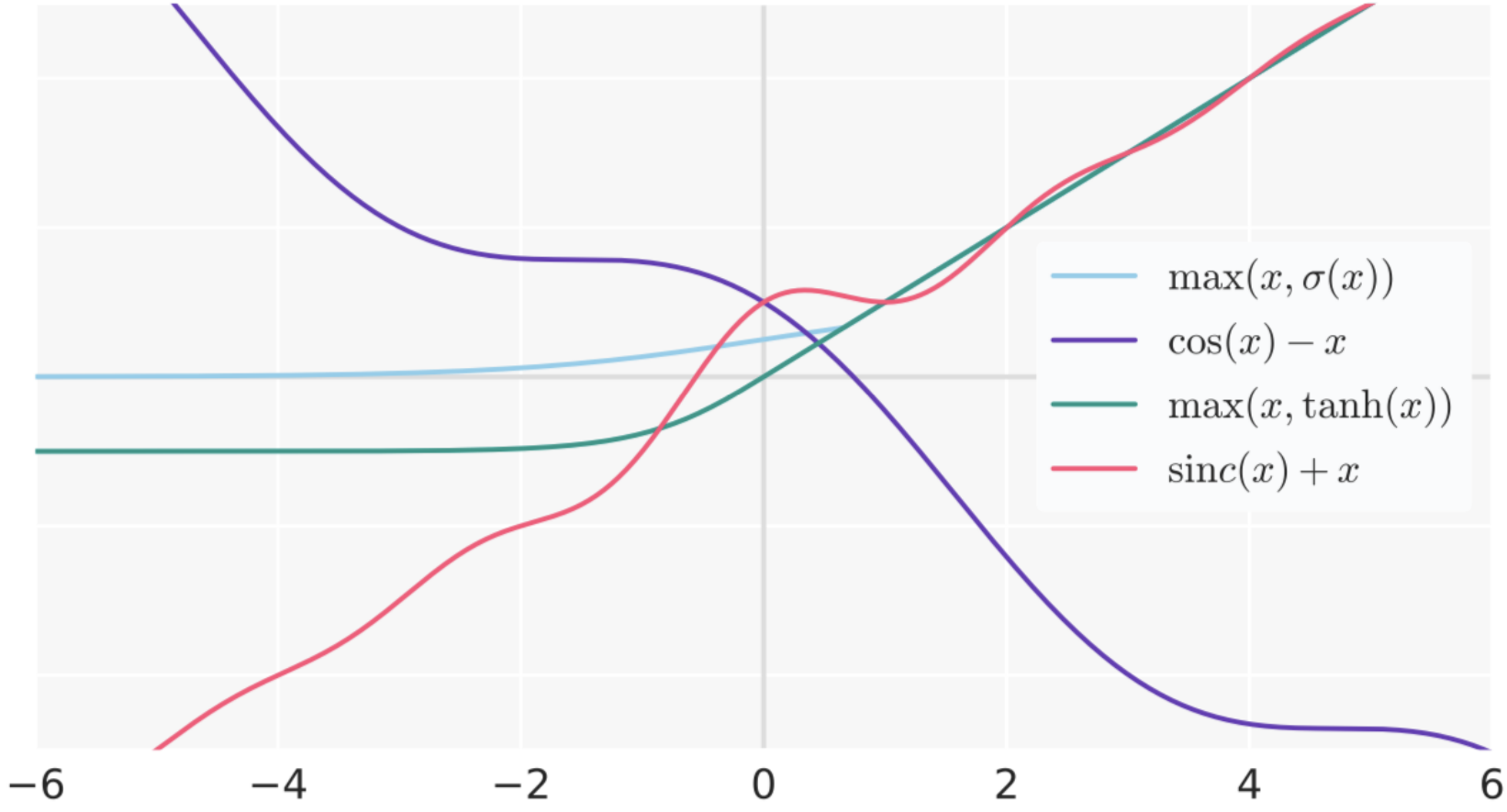


The Swish Transfer Function [3]

Enumeration of activation functions:

Swish was the end result of comparing all the auto-generated activation functions for accuracy on standard datasets.

Swish uses the sigmoid σ:

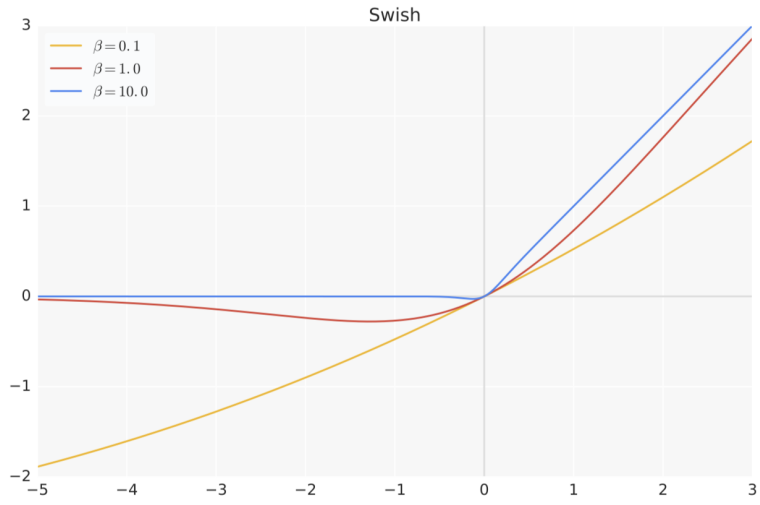
$$g(z) = z \cdot \sigma(\beta z)$$

- If $\beta = 0$ then $g(z) = \frac{z}{2}$ (a linear function; so avoid this)
- If $\beta \to \infty$ then $g(z) = \mathrm{ReLu}$

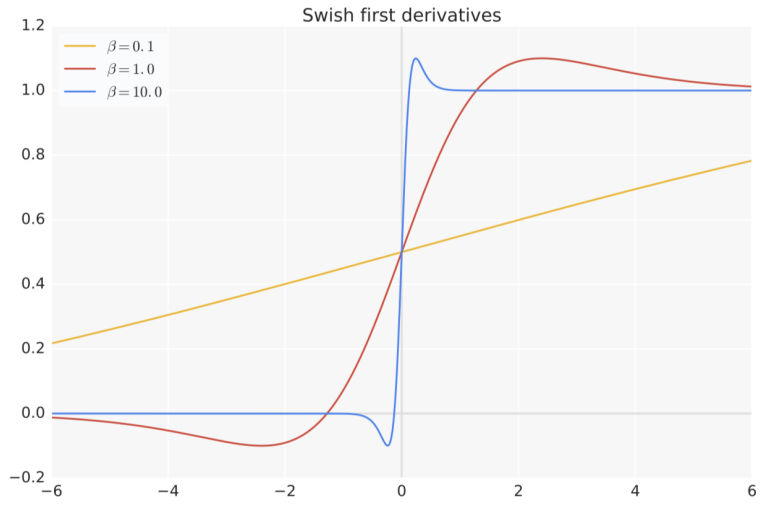
Derivative of Swish:

$$\frac{dg(z)}{dz} = \beta g(z) + \sigma(\beta z)(1 - \beta g(z))$$

The Swish Transfer Function [3]



Swish transfer function with different values of β



First derivative of the Swish transfer function

Derivatives w.r.t. parameters

Derivatives w.r.t. w:

Given

$$h = g(w \cdot x + b)$$

derivatives w.r.t. $w_1, \ldots, w_j, \ldots w_d$:

$$\frac{dh}{dw_j}$$

Derivatives w.r.t. b:

derivatives w.r.t. b:

$$\frac{dh}{db}$$

Chain Rule of Differentiation

Introduce an intermediate variable $z \in \mathbb{R}$

$$z = w \cdot x + b$$

$$h = g(z)$$

Then by the chain rule to differentiate w.r.t. w:

$$\frac{dh}{dw_j} = \frac{dh}{dz}\frac{dz}{dw_j} = \frac{dg(z)}{dz} \times x_j$$

And similarly for b:

$$\frac{dh}{db} = \frac{dh}{dz}\frac{dz}{db} = \frac{dg(z)}{dz} \times 1$$

Single Layer Feedforward model

A single layer feedforward model consists of:

- An integer d specifying the input dimension. Each input to the network is $x \in \mathbb{R}^d$
  - Think of it as a d dimensional word embedding
- An integer m specifying the number of hidden units
- A parameter matrix $W \in \mathbb{R}^{m \times d}$. The vector $W_k \in \mathbb{R}^d$ for $1 \leq k \leq m$ is the kth row of W
- A vector $b \in \mathbb{R}^d$ of bias parameters
- A transfer function $g : \mathbb{R} \to \mathbb{R}$
  $g(z) = \mathrm{ReLU}(z)$ or $g(z) = \tanh(z)$

Single Layer Feedforward model (continued)

For $k = 1, \ldots, m$:

- The input to the kth neuron is: $z_k = W_k \cdot x + b_k$
- The output from the kth neuron is: $h_k = g(z_k)$
- Define vector $\phi(x; \theta) \in \mathbb{R}^m$ as: $\phi(x; \theta) = h_k$
- $\theta = (W, b)$ where $W \in \mathbb{R}^{m \times d}$ and $b \in \mathbb{R}^d$
- Size of θ is $m \times (d + 1)$ parameters

Some intuition

The neural network employs m hidden units, each with their own parameters W_k and b_k, and these neurons are used to construct a *hidden* representation $h \in \mathbb{R}^m$

Matrix Form

We can replace the operation:

$$z_k = W_k \cdot x + b \text{ for } k = 1, \ldots, m$$

with

$$z = Wx + b$$

where the dimensions are as follows (vector of size m equals a matrix of size $m \times 1$):

$$\underbrace{z}_{m\times 1} = \underbrace{\underbrace{W}_{m\times d}\ \underbrace{x}_{d\times 1}}_{m\times 1} + \underbrace{b}_{m\times 1}$$

Single Layer Feedforward model (matrix form)

A single layer feedforward model consists of:

- An integer d specifying the input dimension. Each input to the network is $x \in \mathbb{R}^d$
- An integer m specifying the number of hidden units
- A parameter matrix $W \in \mathbb{R}^{m \times d}$
- A vector $b \in \mathbb{R}^d$ of bias parameters
- A transfer function $g : \mathbb{R}^m \to \mathbb{R}^m$
  $g(z) = [\ldots, \mathrm{ReLU}(z_i), \ldots]$ or
  $g(z) = [\ldots, \tanh(z_i), \ldots]$ or
  $g(z) = [\ldots, \sigma(z_i), \ldots]$ or
  for $i = 1, \ldots, m$

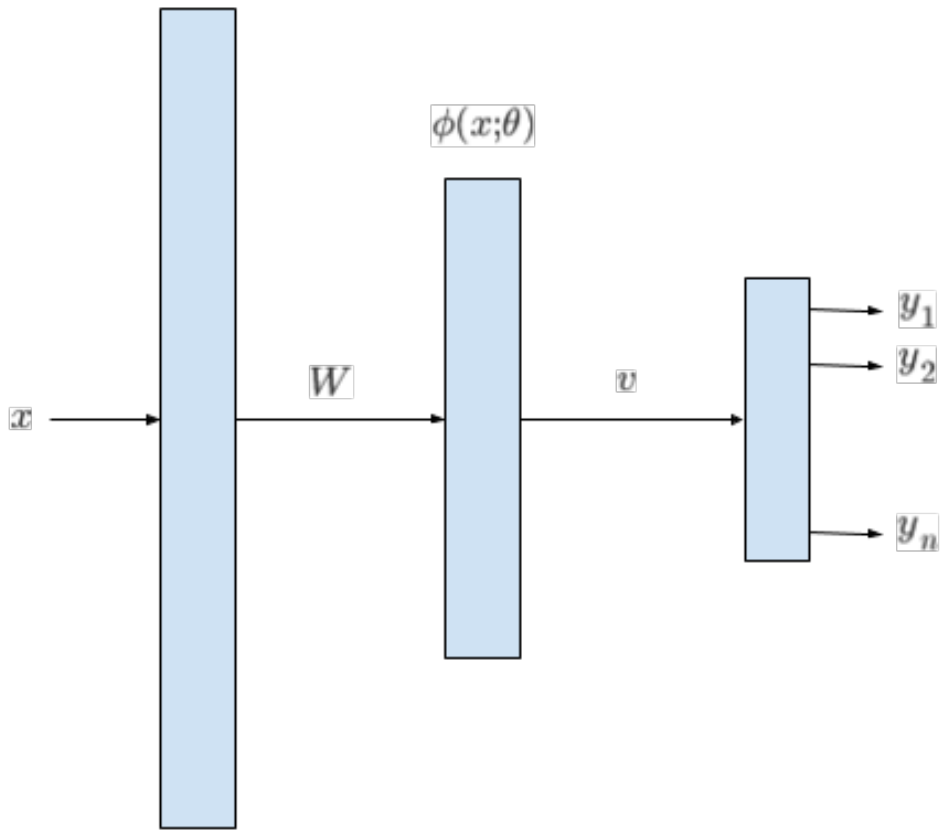
Single Layer Feedforward model (matrix form, continued)

- Vector of inputs to the hidden layer $z \in \mathbb{R}^m$: $z = Wx + b$
- Vector of outputs from hidden layer $h \in \mathbb{R}^m$: $h = g(z)$
- Define $\phi(x; \theta) = h$ where $\theta = (W, b)$
- Define $\text{softmax}_y = \frac{exp(r_y)}{\sum_{y'} exp(r_{y'})}$ for $r_y = v(y) \cdot h + \gamma_y$
- Let $V = [\ldots, v_y, \ldots]$ for $y \in \mathcal{Y}$. $v_y \in \mathbb{R}^m$ so $V \in \mathbb{R}^{|\mathcal{Y}| \times m}$.
- Let $\Gamma = [\ldots, \gamma_y, \ldots]$ for $y \in \mathcal{Y}$. $\Gamma \in \mathbb{R}^{|\mathcal{Y}|}$.

Putting it all together:

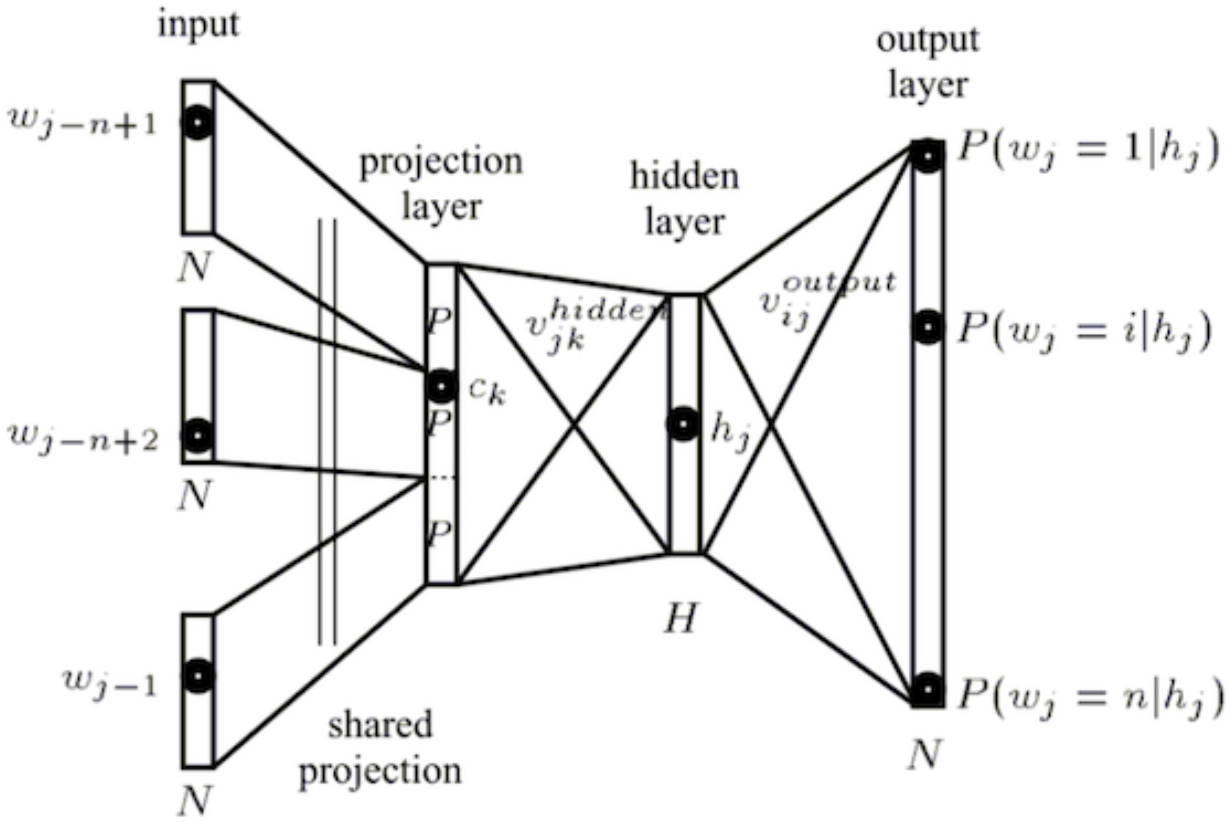
$$\underbrace{r}_{\text{vector of size } |\mathcal{Y}|} = \underbrace{\text{softmax}(\underbrace{V \cdot \phi(x; \theta) + \Gamma}_{\text{for each } y \in \mathcal{Y} \text{ an } \mathbb{R} \text{ value}})}_{\text{A vector of size } \mathbb{R}^{\mathcal{Y}} \text{ that sums to 1}}$$

Feedforward neural network



n-gram Feedforward neural network

from [5]



Log-linear models versus Neural networks

Feedforward neural networks

Stochastic Gradient Descent

Motivating example: XOR

Computation Graphs

Simple stochastic gradient descent

Inputs:

- Training examples (x^i, y^i) for $i = 1, \ldots, n$
- A feedforward representation $\phi(x; \theta)$
- Integer T specifying the number of updates
- A sequence of learning rates: $\eta^1, \ldots, \eta^T$ where $\eta^t \in [0, 1]$
  - One should experiment with learning rates: 0.001, 0.01, 0.1, 1
  - Bottou (2012) suggests a learning rate $\eta^t = \frac{\eta^1}{1+\eta^1 \times \lambda \times t}$ where λ is a hyperparameter that can be tuned experimentally

Initialization:

Set $v = (v(y), \gamma_y)$ for all y, and θ to random values

Gradient descent

Algorithm:

- For $t = 1, \ldots, T$
  - Select an integer i uniformly at random from $\{1, \ldots, n\}$
  - Define $L(\theta, v) = -\log P(y_i \mid x_i; \theta, v)$
  - For each parameter θ_j and $v_k(y)$ and γ_y (for each label y):

$$\begin{aligned}
\theta_j &= \theta_j - \eta^t \times \frac{dL(\theta, v)}{d\theta_j} \\
v_k(y) &= v_k(y) - \eta^t \times \frac{dL(\theta, v)}{dv_k(y)} \\
\gamma(y) &= \gamma(y) - \eta^t \times \frac{dL(\theta, v)}{d\gamma(y)}
\end{aligned}$$

- **Output**: parameters θ, $v = (v(y), \gamma_y)$ for all y

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Computation Graphs

Motivating example: the XOR problem

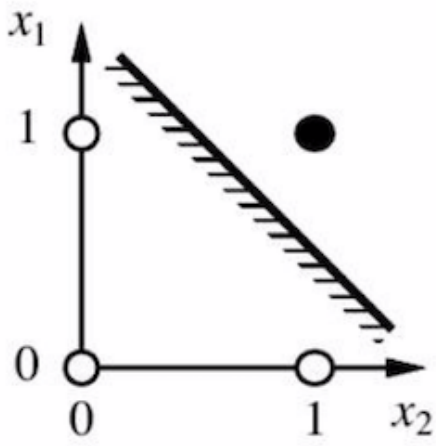
From *Deep Learning* by Goodfellow, Bengio, Courville

We will assume a training set where each label is in the set $\mathcal{Y} = \{-1, +1\}$

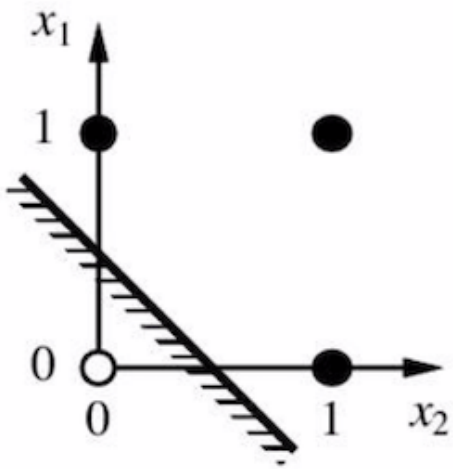
There are four training examples:

$$\begin{aligned} x^1 &= [0,0], y^1 = -1 \\ x^2 &= [0,1], y^2 = +1 \\ x^3 &= [1,0], y^3 = +1 \\ x^4 &= [1,1], y^4 = -1 \end{aligned}$$

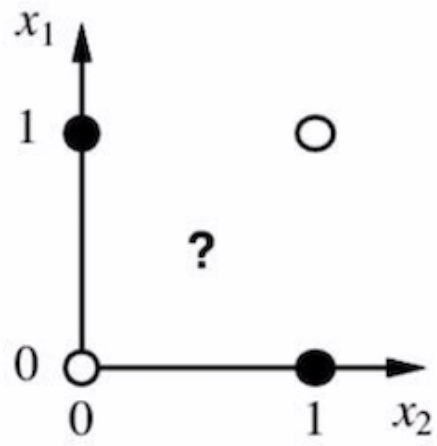
Motivating example: the XOR problem



x_1 **and** x_2



x_1 **or** x_2



x_1 **xor** x_2

Motivating example: the XOR problem

Theorem

For examples (x^i, y^i) for $i = 1, \ldots, 4$ as defined previously for the feedforward neural network:

$$\Pr(y \mid x; W, b, v) = \frac{exp\left(v(y) \cdot g(Wx + b) + \gamma_y\right)}{\sum_{y' \in \mathcal{Y}} exp\left(v(y') \cdot g(Wx + b) + \gamma_{y'}\right)}$$

where $x \in \mathbb{R}^2$ ($d = 2$) and let $m = 2$ so $W \in \mathbb{R}^{2 \times 2}$ and $b \in \mathbb{R}^2$ and g is a ReLU transfer function.

Then there are parameter settings $v(-1)$, $v(+1)$, γ_{-1}, γ_{+1}, W, b such that

$$p(y^i \mid x^i; v) > 0.5 \text{ for } i = 1, \ldots, 4$$

Motivating example: the XOR problem

Proof Sketch

Define $W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ and $b = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$ Then for each input x calculate values of $z = Wx + b$ and $h = g(z)$:

$$
\begin{aligned}
x = [0, 0] &\Rightarrow z = [0, -1] \Rightarrow h = [0, 0] \\
x = [1, 0] &\Rightarrow z = [1, 0] \Rightarrow h = [1, 0] \\
x = [0, 1] &\Rightarrow z = [1, 0] \Rightarrow h = [1, 0] \\
x = [1, 1] &\Rightarrow z = [2, 1] \Rightarrow h = [2, 1]
\end{aligned}
$$

Motivating example: the XOR problem

Proof Sketch (continued)

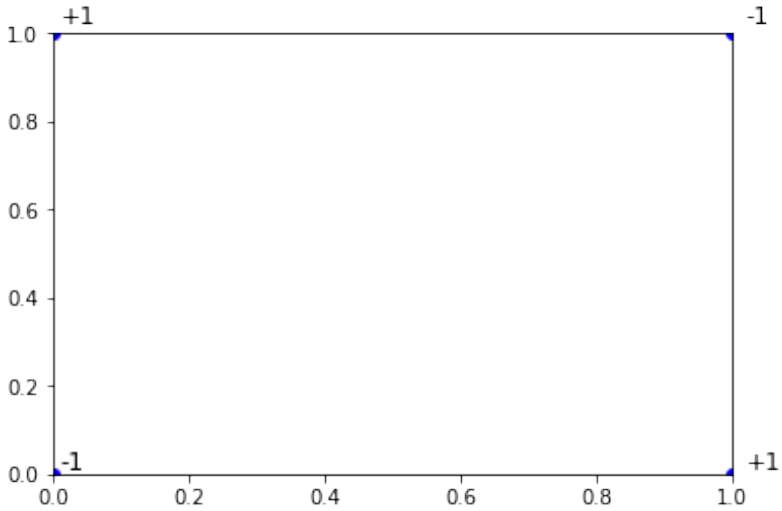
$$
\begin{aligned}
p(+1 \mid x; v) &= \frac{exp(v(+1) \cdot h + \gamma_{+1})}{exp(v(+1) \cdot h + \gamma_{+1}) + exp(v(-1) \cdot h + \gamma_{-1})} \\
&= \frac{1}{1 + exp(-(u \cdot h + \gamma))}
\end{aligned}
$$

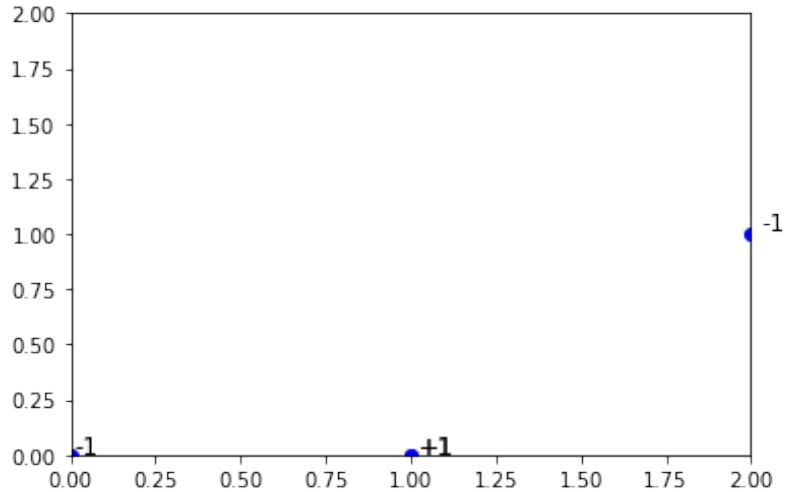
To satisfy $P(y^i \mid x^i; v) > 0.5$ for $i = 1, \ldots, 4$ we have to find parameters $u = v(+1) - v(-1)$ and $\gamma = \gamma_{+1} - \gamma_{-1}$ such that:

$$
\begin{aligned}
u \cdot [0, 0] + \gamma &< 0 \\
u \cdot [1, 0] + \gamma &> 0 \\
u \cdot [1, 0] + \gamma &> 0 \\
u \cdot [2, 1] + \gamma &< 0
\end{aligned}
$$

$u = [1, -2]$ and $\gamma = -0.5$ satisfies these constraints.

Solving the XOR problem





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Complex neural networks

Neural network with a loss function

Consider a neural network trained using a **squared-error loss**. For the correct answer y^* the output value y is compared using the function $(y^* - y)^2$.

$$\begin{aligned} h' &= W_{xh}x + b_h \\ h &= \tanh(h') \\ y &= w_{hy}h + b_y \\ \ell &= (y^* - y)^2 \end{aligned}$$

Derivative wrt loss

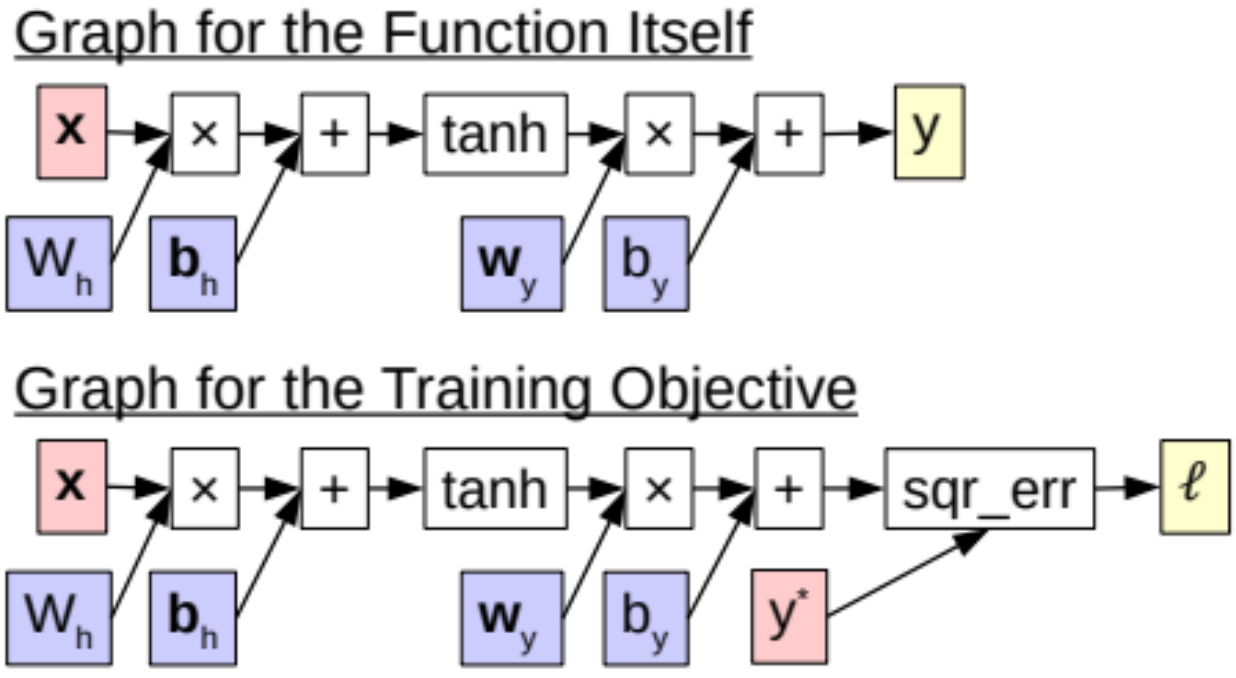
$$
\begin{aligned}
h' &= W_{xh}x + b_h \\
h &= \tanh(h') \\
y &= w_{hy}h + b_y \\
\ell &= (y^* - y)^2
\end{aligned}
$$

We want to compute $\frac{d\ell}{db_y}$, $\frac{d\ell}{dw_{hy}}$, $\frac{d\ell}{db_h}$, $\frac{d\ell}{dW_{xh}}$

$$
\begin{aligned}
\frac{d\ell}{db_y} &= \frac{d\ell}{dy}\frac{dy}{db_y} \\
\frac{d\ell}{dw_{hy}} &= \frac{d\ell}{dy}\frac{dy}{dw_{hy}} \\
\frac{d\ell}{db_h} &= \frac{d\ell}{dy}\frac{dy}{dh}\frac{dh}{dh'}\frac{dh'}{db_h} \\
\frac{d\ell}{dW_{xh}} &= \frac{d\ell}{dy}\frac{dy}{dh}\frac{dh}{dh'}\frac{dh'}{dW_{xh}}
\end{aligned}
$$

Computation graphs and automatic differentiation

Figure from [1]



Computation graphs and automatic differentiation

- Automatic differentiation is a two-step dynamic programming algorithm that operates over the second graph and performs:

  Forward calculation which traverses the nodes in the graph in topological order, calculating the actual result of the computation.

  Back propagation which traverses the nodes in reverse topological order, calculating the gradients.

- Many neural network toolkits can perform auto differentiation for very large computation graphs.

[1] Graham Neubig
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2003.

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