Neural Networks I

Wei Li

Syracuse University

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OVERVIEW

Projection Pursuit Regression

Single Hidden Layer Neural Networks

Deep Neural Networks

Stochastic Gradient Descent

Backpropagation

Projection Pursuit Regression

Projection Pursuit Regression

Let X be a p-dimensional predictors. Y be some target response. The PPR function takes the form

$$f(X) = \sum_{m=1}^{M} g_m\left(\omega_m^\top X\right)$$

- $\omega_m : 1, \ldots, M$ unit p-vector (directions) unknown, $\|\omega\| = 1$
- g_m unknown, $g_m\left(\omega_m^\top X\right)$ is called a ridge function in $\mathbb{R}^p$
- The scalar variable $V_m = \omega_m^\top X$ is the projection of X onto the unit vector ω_m

The parameters are $\{g_m, \omega_m\}_{m=1}^{M}$.

The model takes the form

$$Y_i = \sum_{m=1}^{M} g_m\left(\omega_m^\top X_i\right) + \epsilon_i$$

Given data $\{Y_i, X_i\}_{i=1}^n$, the estimates are defined by

$$\min_{g_m, \omega_m} \sum_{i=1}^{n} \left(Y_i - \sum_{m=1}^{M} g_m\left(\omega_m^\top X_i\right) \right)^2$$

Note: the PPR model is a generalization of the so-called *one-hidden layer neural network* when g_m's are assumed to be known

$$g_m\left(\omega_m^\top X\right) = \beta_m \sigma\left(\alpha_{m0} + \alpha_m^\top X\right) = \beta_m \sigma\left(\alpha_{m0} + \|\alpha_m\| \left(\omega_m^\top X\right)\right)$$

where $\omega_m = \alpha_m / \|\alpha_m\|$ is the m-th unit-vector.

Single-index model

When $m = 1$ (single-index model), the parameters can be estimated via a recursive algorithm:

1. Given ω, forms $\nu_i = \omega^\top x_i$, solve for g (one-dimensional smoothing).
2. Given g, minimize the lass over ω through iteration (quasi-Newton): note that

$$g\left(\omega^\top x_i\right) \approx g\left(\omega_{\text{old}}^\top x_i\right) + g'\left(\omega_{\text{old}}^\top x_i\right)\left(\omega - \omega_{\text{old}}\right)^\top x_i$$

Thus $\sum_{i=1}^n \left(y_i - g\left(\omega^\top x_i\right)\right)^2 \approx$

$$\sum_{i=1}^n g'\left(\omega_{\text{old}}^\top x_i\right)^2 \left(\left(\omega_{\text{old}}^\top x_i + \frac{y_i - g\left(\omega_{\text{old}}^\top x_i\right)}{g'\left(\omega_{\text{old}}^\top x_i\right)}\right) - \omega^\top x_i\right)^2$$

m>1

Forward stage-wise manner: adding a pair (ω_m, g_m) at each stage (Forward Stagewise Algorithm 10.2). It is hinted that the backfitting algorithm (Algorithm 9.1) may be also applied for each step m to readjust previous g terms.

- Backfitting algorithm: for each m in turn, minimize

$$\min_{g_m, \omega_m} \sum_{i=1}^{n} \left(r_i - g_m\left(\omega_m^\top X_i\right)\right)^2$$

  where $r_i = Y_i - \sum_{l \neq m} g_l\left(\omega_l^\top X_i\right)$.
- The number of terms M
  - The model building stops when the next term does not appreciably improve the fit
  - Or chosen using cross-validation.

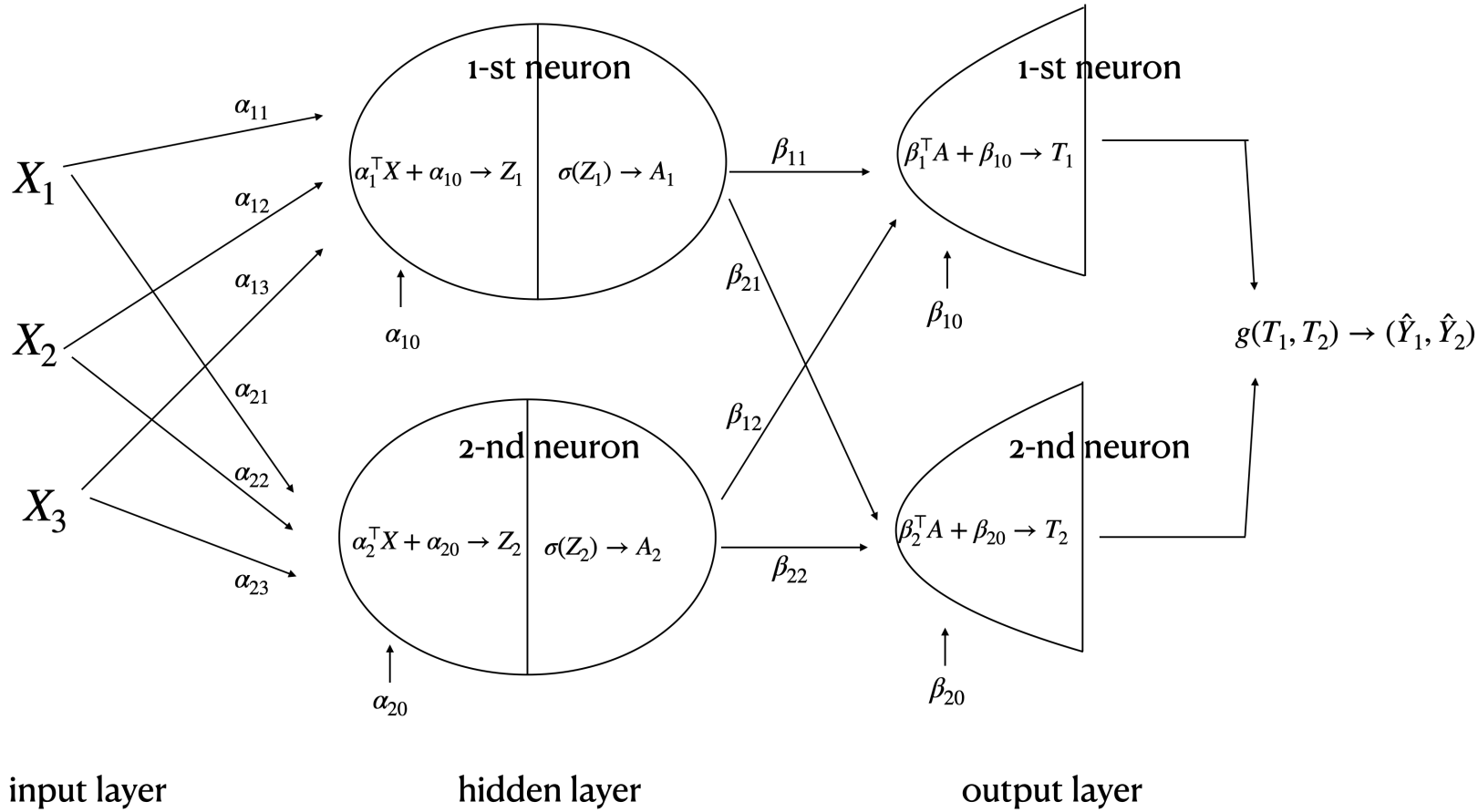
Single Hidden Layer Neural Networks

Single Hidden Layer Neural Networks

- Input: $X = (X_1, \cdots, X_p)$
- Output: $\hat{Y} = (\hat{Y}_1, \cdots, \hat{Y}_K)$
  - Continuous outcomes: typically $K = 1$, but it can handle multiple responses.
  - K -class classification: $\hat{Y}_k$ be the probability of class k, or $\hat{Y}_k \in \{0, 1\}$.

$$
\begin{aligned}
Z_m &= \alpha_{m0} + \alpha_m^\top X, m = 1, \ldots, M \\
A_m &= \sigma\left(Z_m\right), m = 1, \ldots, M \\
T_k &= \beta_{k0} + \beta_k^\top A, k = 1, \ldots, K, \text{ here } A = (A_1, \ldots, A_M) \\
\hat{Y}_k &= f_k(X) := g_k(T), k = 1, \ldots, K, \text{ here } T = (T_1, \ldots, T_K)
\end{aligned}
$$

- $Z = (Z_1, Z_2, \ldots, Z_M)$: pre-activation values (net input)
- $A = (A_1, \ldots, A_M)$: activation values (derived features)
- $T = (T_1, T_2, \ldots, T_K)$: pre-output values
- $f = (f_1(X), \ldots, f_K(X))$: output (prediction).



Example

- $p = 3$: three predictors
- $M = 2$: two hidden units in the hidden layer
- $K = 2$: two output units in the output layer
- softmax output

Activation function

$\sigma(\cdot)$ is an activation function:

i. sigmoid $\sigma(v) = 1/\left(1 + e^{-v}\right)$
ii. ReLU $\sigma(v) = \max(v, 0)$
iii. leakyReLU $\sigma(v) = v1\{v > 0\} + av1\{v \leq 0\}$ (say, $a = 0.01$)
iv. tanh (Hyperbolic Tangent) $\sigma(v) = \left(e^{v} - e^{-v}\right) / \left(e^{v} + e^{-v}\right)$
v. Gaussian radial basis function
$\sigma(x; \mu_m, \lambda_m) = \exp(-\|x - \mu_m\|^2 / 2\lambda_m)$

See next few slides for more details.

Output function g

The output $g(T) = (\ldots, g_k(T), \ldots)$ is a final transformation of the vector of outputs T.

- For regression, just an identity function $g_1(T) = T_1$, $(K = 1)$.
- Binary classification: $g_1(T) = \text{sigmoid}(T_1)$, $(K = 1)$.
- For K-class classification, the softmax function

$$g_k(T) = \mathbf{S}_k := \frac{e^{T_k}}{\sum_{\ell=1}^{K} e^{T_\ell}}, k = 1, \ldots, K$$

which gives a vector of estimated probabilities.

- The vector T: **logits**.
- The corresponding classifier: $G(X) = \arg\max_k g_k(T)$.

The complete set of parameters θ consists of

$$\{\alpha_{m0}, \alpha_m; m = 1, 2, \ldots, M\} \quad M(p+1) \text{ parameters}$$
$$\{\beta_{k0}, \beta_k; k = 1, 2, \ldots, K\} \quad K(M+1) \text{ parameters}$$

- regression: $\mathcal{L}(\theta) = \sum_{k=1}^{K} \sum_{i=1}^{n} \left(y_{ik} - f_k\left(x_i\right)\right)^2$
- classification: $\mathcal{L}(\theta) = -\sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log f_k\left(x_i\right)$, $y_{ik} := 1(y_i = k)$.
  - The corresponding classifier is $G(x) = \text{argmax}_k\, f_k(x)$.

Find minimizer of $\mathcal{L}(\theta)$ by **gradient descent**:

$$\theta \leftarrow \theta - \gamma \frac{\partial \mathcal{L}(\theta)}{\partial \theta}$$

- *gradients* derived using the chain rule of differentiation
  - called "**back-propagation**"

A single-hidden layer NN

K outputs, squared error loss

$$\mathcal{L}(\theta) \equiv \sum_{i=1}^{n} \mathcal{L}_i = \sum_{i=1}^{n} \sum_{k=1}^{K} \left(y_{ik} - f_k\left(x_i\right)\right)^2,$$

Let $\tilde{x}_i = \left(1, x_i^\top\right)^\top$, $a_{mi} = \sigma\left(\alpha_m^\top \tilde{x}_i\right)$,

$a_i = \left(a_{1i}, a_{2i}, \ldots, a_{Mi}\right)^\top$, $\tilde{a}_i = \left(1, a_{1i}, a_{2i}, \ldots, a_{Mi}\right)^\top$.

$\alpha_m := \{\alpha_{m0}, \alpha_{m1}, \alpha_{m2}, \ldots, \alpha_{mp}\}$

$\beta_k := \{\beta_{k0}, \beta_{k1}, \beta_{k2}, \ldots, \beta_{kM}\}$

The derivatives are given by, for $i = 1, \ldots, n$,

$$\frac{\partial \mathcal{L}_i}{\partial \beta_{km}} = -2\left(y_{ik} - f_k\left(x_i\right)\right) g_k'\left(\beta_k^\top \tilde{a}_i\right) \tilde{a}_{mi}$$

$$\frac{\partial \mathcal{L}_i}{\partial \alpha_{ml}} = -\sum_{k=1}^{K} 2\left(y_{ik} - f_k\left(x_i\right)\right) g_k'\left(\beta_k^\top \tilde{a}_i\right) \beta_{km} \sigma'\left(\alpha_m^\top \tilde{x}_i\right) \tilde{x}_{il}$$

The "errors" (wrt net input) at the output layer and hidden layer

$$\partial t_{ki} := \partial \mathcal{L}_i / \partial T_k = -2 \left(y_{ik} - f_k \left(x_i \right) \right) g_k' \left(\beta_k^\top \tilde{a}_i \right)$$

$$\partial z_{mi} := \partial \mathcal{L}_i / \partial Z_m = \sigma' \left(\alpha_m^\top \tilde{x}_i \right) \sum_{k=1}^{K} \beta_{km} \partial t_{ki}$$

The gradients w.r.t parameters can be written as

$$\frac{\partial \mathcal{L}_i}{\partial \beta_{km}} = (\partial t_{ki}) \tilde{a}_{mi}, \qquad \frac{\partial \mathcal{L}_i}{\partial \alpha_{ml}} = (\partial z_{mi}) \tilde{x}_{il}$$

In the r-th iteration,

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma^{(r)} \sum_{i=1}^{n} \frac{\partial \mathcal{L}_i}{\partial \beta_{km}^{(r)}}, \quad \alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma^{(r)} \sum_{i=1}^{n} \frac{\partial \mathcal{L}_i}{\partial \alpha_{ml}^{(r)}}$$

Forward and Backpropagation Algorithm

At the r-th iteration:

1. Forward pass: Given current estimate $\beta_k^{(r)}, \alpha_m^{(r)}$, compute $a_{mi}^{(r)} = \sigma\left(\tilde{x}_i^\top \alpha_m^{(r)}\right)$ and $f_k^{(r)}(x_i)$.

2. Backward pass:

$$\partial t_{ki}^{(r)} = -2\left(y_{ik} - f_k^{(r)}(x_i)\right) g_k'\left(\beta_k^{(r)\top} \tilde{a}_i^{(r)}\right)$$

$$\partial z_{mi}^{(r)} = \sigma'\left(\tilde{x}_i^\top \alpha_m^{(r)}\right) \sum_{k=1}^{K} \beta_{km}^{(r)} \partial t_{ki}^{(r)}.$$

3. Update

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma^{(r)} \sum_{i=1}^{n} (\partial t_{ki}^{(r)}) \tilde{a}_{mi}^{(r)},$$

$$\alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma^{(r)} \sum_{i=1}^{n} (\partial z_{mi}^{(r)}) \tilde{x}_{il}$$

Issues concerning activation functions

When there are multiple hidden layers (*deeper network*)...

Exploding gradients: large error gradients accumulate, resulting in very large updates; may be alleviated through *gradient clipping*.

Vanishing gradients: small error gradients accumulate, resulting in very small (or zero!) updates; may be alleviated through careful choice of activation functions.

- sigmoid: the output values between $(0, 1)$, would be very near 0 when the input values are strongly negative and vice versa; gradient almost near to zero.
- tanh: the output values between $(-1, 1)$, has stronger gradients than sigmoid, still have vanishing gradient issues
- Relu: preserves the gradient for positive Z, thus alleviate the vanishing gradient problem; only saturates when the input is negative
- leaky Relu: improves upon Relu by recovering the negative region

activiation functions

Sigmoid

$$\sigma(Z) = \frac{1}{1+e^{-Z}}, \quad \frac{d}{dZ}\sigma(Z) = \sigma(Z)(1-\sigma(Z))$$

tanh

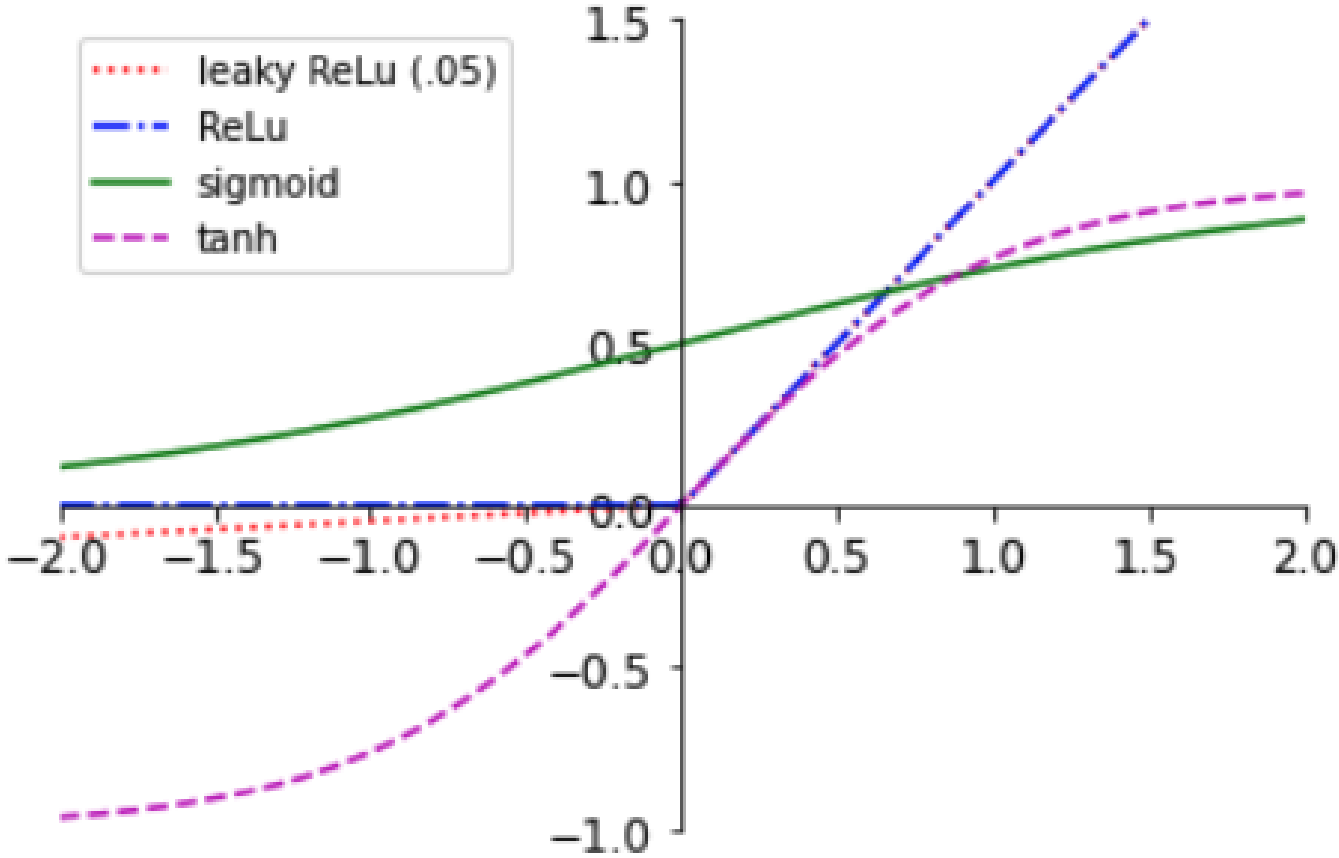
$$\tanh(Z) = \frac{e^{Z}-e^{-Z}}{e^{Z}+e^{-Z}}, \quad \frac{d}{dZ}\tanh(Z) = 1-\tanh^2(Z)$$

Rectified Linear Unit

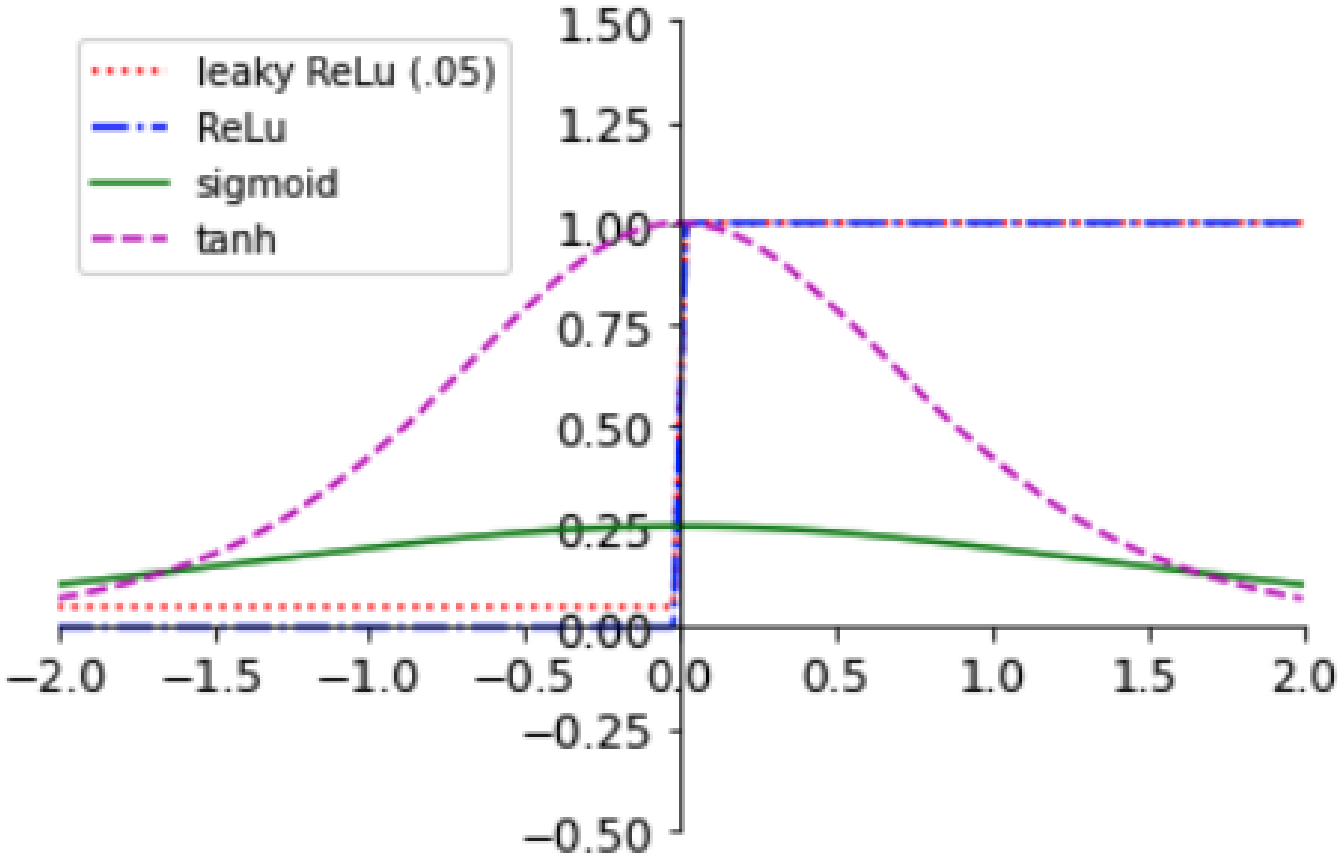
$$\mathrm{ReLu}(Z) = \max(Z,0), \quad \frac{d}{dZ}\mathrm{relu}(Z) = \begin{cases} 1 & \text{if } Z>0 \\ 0 & \text{otherwise} \end{cases}$$

Leaky Rectified Linear Unit

$$\mathrm{LReLu}(Z) = \begin{cases} Z & \text{if } Z>0 \\ aZ & \text{otherwise} \end{cases}, \quad \frac{d}{dZ}\mathrm{LReLu}(Z) = \begin{cases} 1 & \text{if } Z>0 \\ a & \text{otherwise} \end{cases}$$



Plots of sigmoid, tanh, ReLu and leaky ReLu.



Plots of the derivatives of sigmoid, tanh, ReLu and leaky ReLu.

See here for more options: https://en.wikipedia.org/wiki/Activation_function

softmax activation

- K-categories
- an K-dimensional vector $z = (z_1, z_2, \ldots z_K)$ (**logits**)
- the softmax function produces another K-dimensional vector with values in the range [0,1]

$$z \mapsto \mathbf{S}(z) = (p_1, \ldots, p_K)$$

where $p_i := P(y = i|z) = \mathbf{S}(z)_i := \frac{\exp^{z_i}}{\sum_{k=1}^{K} \exp^{z_k}}, \forall j \in 1, \ldots K.$

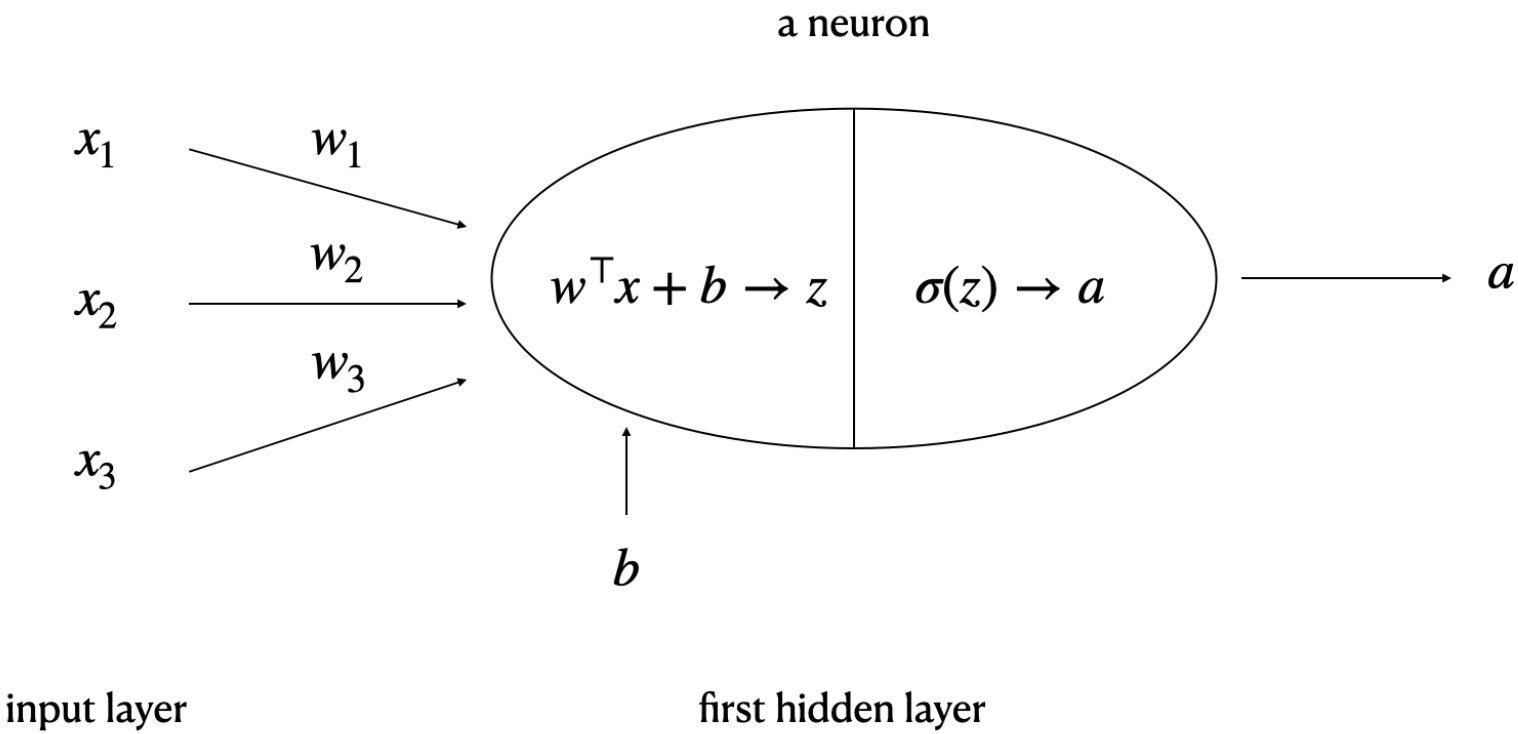
Derivatives are

$$\frac{\partial p_i}{\partial z_j} = \begin{cases} p_i (1 - p_j) & \text{if } i = j \\ -p_i p_j & \text{if } i \neq j \end{cases}$$

Note: softmax activation is one example of the so-called *vector activation*, as opposed to the elementwise activations. It is most commonly used in the output layer for multi-class classification.

Deep Neural Networks

Deep Neural Networks



a neuron: 3 input features

- parameters
  - weights: w_1, w_2, w_3
  - "bias": b

notations

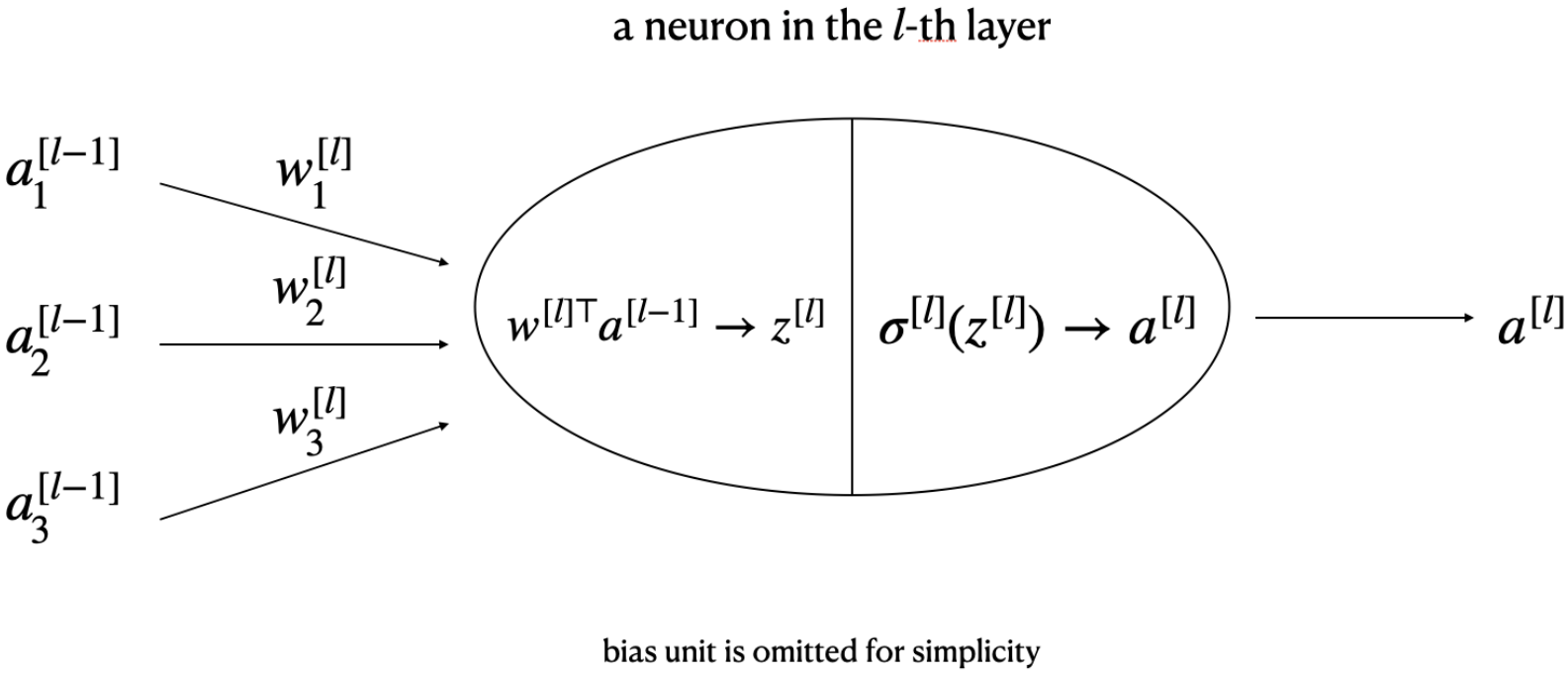
1. For inputs $x \in \mathbb{R}^p$ (p features)

- superscript i: is a reference to the i th observation; i.e., $x^{(1)}$ is the input value of the first observation.
- subscript j : is a reference to the j-th feature number; i.e., $x_2^{(1)}$ is the first observation of the second feature.

2. For network layers:

- superscript $[l]$: refers to layer l; i.e., $z^{[1]}$ is the net input at layer 1.
- subscript j : is a reference to the node number; i.e., $z_1^{[2]}$ is the net input at the first node in layer 2.

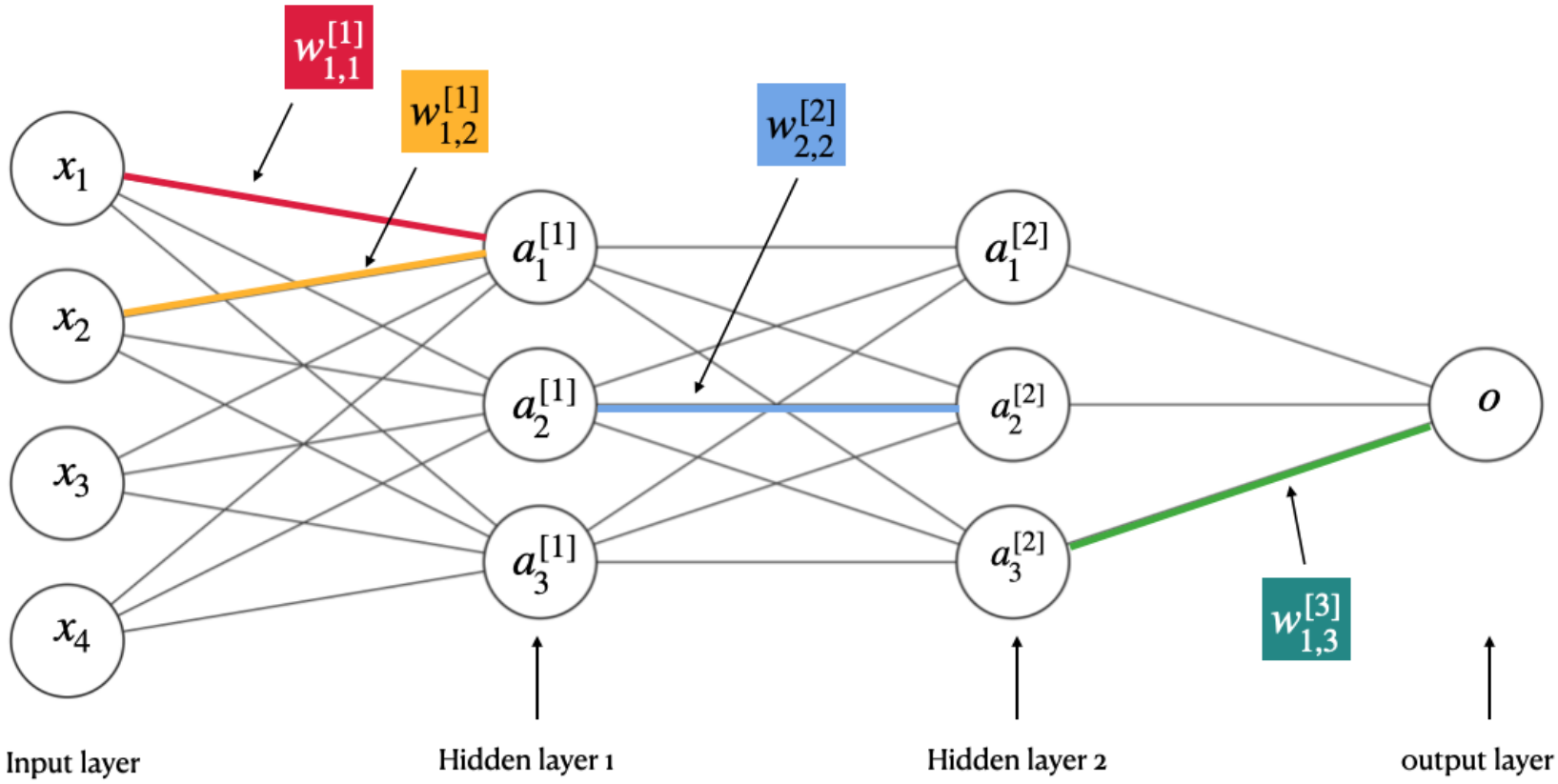
3. $n^{[\ell]}$ denotes the number of units in the ℓ-th layer.



a neuron in the ℓ-th layer: 3 (derived) input features

Example

Assume four features ($p = 4$), two observations ($n = 2$)



A three-layer neural network (two-hidden-layer neural network)

- $n^{[0]} = p, n^{[1]} = 3, n^{[2]} = 3, n^{[3]} = 1.$

example: bias in layer 1

There are 3 nodes in hidden layer 1. The shape of the bias matrix $b^{[1]}$ are (number of nodes in layer 1).

The bias matrix:

$$b^{[1]} = \begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ b_3^{[1]} \end{bmatrix}$$

example: weights in layer 1

A general data matrix X $(n \times p)$:

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \dots & x_p^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots & x_p^{(3)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(n)} & x_2^{(n)} & \dots & x_p^{(n)} \end{bmatrix}$$

The weights matrix can be represented as

$$W^{[1]} = \begin{bmatrix} w_1^{[1]\top} \\ w_2^{[1]\top} \\ w_3^{[1]\top} \end{bmatrix} = \begin{bmatrix} w_{1,1}^{[1]} & w_{1,2}^{[1]} & w_{1,3}^{[1]} & w_{1,4}^{[1]} \\ w_{2,1}^{[1]} & w_{2,2}^{[1]} & w_{2,3}^{[1]} & w_{2,4}^{[1]} \\ w_{3,1}^{[1]} & w_{3,2}^{[1]} & w_{3,3}^{[1]} & w_{3,4}^{[1]} \end{bmatrix}$$

- $w_i^{[\ell]}$ to denote the vector of weights for the i-th node in the layer ℓ
- $w_{i,j}^{[\ell]}$ to denote the j-th coordinate of $w_i^{[\ell]}$, i.e., the weight for the connection from the j-th node in the layer $\ell - 1$ to the i-th node in the layer ℓ.

example: pre-activation in layer 1

We have

$$\mathbf{X}W^{[1]\top} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & x_4^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & x_4^{(2)} \end{bmatrix} \begin{bmatrix} w_{1,1}^{[1]} & w_{1,2}^{[1]} & w_{1,3}^{[1]} & w_{1,4}^{[1]} \\ w_{2,1}^{[1]} & w_{2,2}^{[1]} & w_{2,3}^{[1]} & w_{2,4}^{[1]} \\ w_{3,1}^{[1]} & w_{3,2}^{[1]} & w_{3,3}^{[1]} & w_{3,4}^{[1]} \end{bmatrix}^{\top}$$

The pre-activation at layer-1 can be written as

$$\mathbf{Z}^{[1]} = \mathbf{X}W^{[1]\top} + b^{[1]\top}, \quad (2 \times 3)$$

$$\mathbf{Z}^{[1]} = \begin{bmatrix} z_{1,1}^{[1]} & z_{1,2}^{[1]} & z_{1,3}^{[1]} \\ z_{2,1}^{[1]} & z_{2,2}^{[1]} & z_{2,3}^{[1]} \end{bmatrix}.$$

example: activation in layer 1

The activation is applied *elementwise*:

The activation matrix $\mathbf{A}^{[1]}$ has the same shape as $\mathbf{Z}^{[1]}$

$$\mathbf{A}_{[1]} = \varphi(\mathbf{Z}) = \begin{bmatrix} \varphi(z_{1,1}^{[1]}) & \varphi(z_{1,2}^{[1]}) & \varphi(z_{1,3}^{[1]}) \\ \varphi(z_{2,1}^{[1]}) & \varphi(z_{2,2}^{[1]}) & \varphi(z_{2,3}^{[1]}) \end{bmatrix},$$

where φ is an activation function (i.e., sigmoid, etc.)

example: output layer

Layer-2 can be similarly written...

Turn to output, considering a binary classification (sigmoid activation in the output layer).

- input to the output layer is $\mathbf{A}^{[2]}$, i.e., $(2, 3)$.
- for some W of shape 1×3 :

$$\mathbf{Z}^{[3]} = \mathbf{A}^{[2]} W^{[3]\top}$$
$$g^{[3]} = \sigma(\mathbf{Z}^{[3]})$$

$g^{[3]}$ produces a vector of two predicted values, one for each observation.

example: in summary

All layers can be generalized as

$$\mathbf{Z}^{[\ell]} = \mathbf{A}^{[\ell-1]} W^{[\ell]\top} + b^{[\ell]\top}$$

where

$$W^{[\ell]} = \begin{bmatrix} w_1^{[\ell]\top} \\ w_2^{[\ell]\top} \\ \vdots \\ w_{n^{[\ell]}}^{[\ell]\top} \end{bmatrix}.$$

- shape of $W^{[\ell]}$ is $(n^{[\ell]}, n^{[\ell-1]})$
- shape of $\mathbf{Z}^{[\ell]}$ (or $\boldsymbol{A}^{[\ell]}$) is $n \times n^{[\ell]}$

In summary: 3 layers

The forward propagation equations for a three-layer network for a *single observation* can be represented as

$$
\begin{aligned}
z^{[1](i)} &= W^{[1]} a^{[0](i)} + b^{[1](i)}, a^{[0](i)} := x^{(i)} \\
a^{[1](i)} &= g^{[1]}\left(z^{[1](i)}\right) \\
z^{[2](i)} &= W^{[2]} a^{[1](i)} + b^{[2](i)} \\
a^{[2](i)} &= g^{[2]}\left(z^{[2](i)}\right) \\
z^{[3](i)} &= W^{[3]} a^{[2](i)} + b^{[3](i)} \\
a^{[3](i)} &= \hat{y}^{(i)} = g^{[3]}\left(z^{[3](i)}\right), g^{[3]}(\cdot) = \text{sigmoid}(\cdot)
\end{aligned}
$$

The shape of $W^{[\ell]}$ is $(n^{[\ell]}, n^{[\ell-1]})$.

In summary: general (L layers)

- A multilayer perceptron with $L-1$ hidden layers (L layers):
  - Input $a^{[0]}(x) = x$.
  - For $\ell = 1, \cdots, L-1$ (hidden layers),

$$z^{[\ell]}(x) = b^{[\ell]} + W^{[\ell]} a^{[\ell-1]}(x)$$
$$a^{[\ell]}(x) = g^{[\ell]}\left(z^{[\ell]}(x)\right)$$

    where $g^{[\ell]}$ is the activation function.
  - For $\ell = L$ (output layer),

$$z^{[L]}(x) = b^{[L]} + W^{[L]} a^{(L-1)}(x)$$
$$f(x, \theta) \equiv a^{[L]}(x) = g^{[L]}\left(z^{[L]}(x)\right)$$

    where $g^{[L]}$ is the output activation function.
  - Parameters $\theta : b^{[\ell]}$(biases) and $W^{[\ell]}$(weights), $\ell = 1, \cdots, L$. $\{b^{[\ell]}, W^{[\ell]}\}$ called parameters in the ℓ-th layer.

Combing n observations (using matrices),

	W	b	Pre-activation	Z	# of paras
Layer 1	$(n^{[1]}, p)$	$(n^{[1]}, 1)$	$Z^{[1]} = XW^{[1]\top} + b^{[1]\top}$	$(n, n^{[1]})$	$n^{[1]}(1+p)$
Layer ℓ	$(n^{[\ell]}, n^{[\ell-1]})$	$(n^{[\ell]}, 1)$	$Z^{[\ell]} = A^{[\ell-1]}W^{[\ell]\top} + b^{[\ell]\top}$	$(n, n^{[\ell]})$	$n^{[\ell]}(1+n^{[\ell-1]})$
Layer L	$(n^{[L]}, n^{[L-1]})$	$(n^{[L]}, 1)$	$Z^{[L]} = A^{[L-1]}W^{[L]\top} + b^{[L]\top}$	$(n, n^{[L]})$	$n^{[L]}(1+n^{[L-1]})$

- In L-th layer (the output layer), then $\hat{y} = g^{[L]}(Z^{[L]})$ is of shape $n \times n^{[L]}$.
- Depending on the output function A
  - for LS and binary classification, $n^{[L]} = 1$
  - for K-class classification, $n^{[L]} = K$.

Penalized empirical risk

For $\ell = L$ (output layer),

$$z^{[L]}(x) = b^{[L]} + W^{[L]} a^{(L-1)}(x)$$
$$f(x, \theta) \equiv a^{[L]}(x) = g^{[L]}\left(z^{[L]}(x)\right)$$

where $g^{[L]}$ is the output activation function.

$$\mathcal{L}_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}, \theta\right), y^{(i)}\right) + \lambda \Omega(\theta)$$

where $\Omega(\theta)$ is some penalty function of θ, say ℓ_1 or ℓ_2-penalty of the weights.

Loss functions (classification)

Cross-entropy (CE) loss, or log-loss, measures the performance of a classification model whose output has a probability value between 0 and 1.

As the predicted probability diverges from the actual value the CE loss consequently increases.

The cross-entropy loss is

$$H(p, \hat{p}) = \sum_{k}^{K} p_k \log \frac{1}{\hat{p}_k} = -\sum_{k} p_k \log (\hat{p}_k)$$

where, p_k is the true probability distribution and $\hat{p}_k$ is the computed probability distribution.

Binary classification:

$CE_{\text{Loss}} = H(p, \hat{p}) = -(p \log(\hat{p}) + (1-p) \log(1-\hat{p}))$ binary classification

Multi-class classification: $K(\geq 2)$-labels,

$$CE_{Loss} = H(p, \hat{p}) = -\sum_{k=1}^{K} p_k \log(\hat{p}_k) \text{ multiclass classfication}$$

Minimize the CE loss is closely related to minimizing negative log-likelihood.

Negative Log-likelihood (deviance)

The **binomial deviance** (negative loglikelihood) is

$$\mathcal{L}_n = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}^{(i)} = -\frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)}\log\left(\hat{y}^{(i)}\right) + \left(1-y^{(i)}\right)\log\left(1-\hat{y}^{(i)}\right)\right)$$

The K-class **multinomial deviance** (negative loglikelihood) is

$$\mathcal{L}_n = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}^{(i)} = -\frac{1}{n}\sum_{i}^{n}\sum_{k}^{K} y_k^{(i)}\log\left(\hat{y}_k^{(i)}\right)$$

where $y_k^{(i)} = 1(y^{(i)} = k)$ and $\hat{y}^{(i)} = (\hat{y}_1^{(i)}, \ldots, \hat{y}_K^{(i)})$ is a vector of estimated probabilities for i-th observation.

Some authors simply called them binary cross-entropy and K-class cross-entropy respectively.

For the binary CE loss with sigmoid output function $\hat{y} = \sigma(z)$,

$$\mathcal{L}_{\text{sigmoid}} = -(y \log(\hat{y}) + (1-y) \log(1-\hat{y}))$$

$$\frac{\partial \mathcal{L}_{\text{sigmoid}}}{\partial z} = \frac{\partial \mathcal{L}_{\text{sigmoid}}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} = -\left(\frac{y}{\hat{y}} - \frac{(1-y)}{1-\hat{y}} \right) \sigma(z)(1-\sigma(z))$$

For K-class CE loss with the softmax output $\hat{y} = \text{softmax}(z)$:

$$\mathcal{L}_{\text{softmax}} = -\sum_{k}^{K} y_k \log\left(\hat{y}_k\right)$$

$$\frac{\partial \mathcal{L}_{\text{softmax}}}{\partial z_j} = -\sum_{k} y_k \frac{\partial \log\left(\hat{y}_k\right)}{\partial z_j} = \hat{y}_j - y_j$$

Note that y is a one-hot encoded K-dim vector.

Stochastic Gradient Descent

Stochastic Gradient Descent

$$\mathcal{L}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}, \theta\right), y^{(i)}\right) + \lambda\Omega(\theta)$$

- Let $\theta := \left(W^{[1]}, b^{[1]}, \cdots, W^{[L]}, b^{[L]}\right)$. Initialize $\theta^{<0>}$.
- GD update: at the t-th iteration

$$\theta^{<t+1>} = \theta^{<t>} - \epsilon_t \frac{1}{B}\sum_{i\in\mathcal{B}} \left\{\nabla_\theta \mathcal{L}\left(f\left(x^{(i)}, \theta^{<t>}\right), y^{(i)}\right) + \lambda\nabla_\theta\Omega\left(\theta^{<t>}\right)\right\}$$

- $\mathcal{B}$ is a subset or a batch of cardinality B (**batch size**)
  - (taken at random without replacement from training data)
- **(full batch) gradient descent**: $B = n$.
- **stochastic gradient descent**: $B = 1$.
- **mini batch learning**: the number of batches $= n/B > 1$.

In the **mini-batch gradient descent** method, the parameters are updated based only on the current mini-batch (*one step*), and continue iterating over *all* the mini-batches till we have seen the entire data set.

The process of iterating through the *whole* training dataset is referred to as an **epoch**.

- **number of epochs**: the number of times the algorithm "sees" the entire training data.
  - So one epoch would take n/B steps.
- **total number of steps**: the total number of epochs multiplies the number of batches (n/B).

In mini-batch gradient descent, within each epoch, the following steps are used to create minibatches

- Shuffle - Shuffle the data set (X, Y) values randomly.
- Partition - Partition the data set into the defined mini-batch size set.

The general rule for mini-batch size is

- use $64, 128, 256, 512, \ldots$, i.e., a power of 2

Shuffle is usually required during the training stage, but often not required during the test stage (or *inference*).

For more details:
https://weili-code.github.io/StatisticalSimulation/7_modern_optimization.html

Backpropagation

Backpropagation

To compute $\nabla_\theta \mathcal{L}\left(f\left(X,\theta\right),Y\right)$. Define **error gradient**

$$\nabla_{z^{[\ell]}}\mathcal{L} = \nabla_{z^{[\ell]}}\mathcal{L}(\hat{f},y), \quad n^{[\ell]}\times 1$$

- For output layer L, we compute $\nabla_{z^{[L]}}\mathcal{L} = \nabla_{z^{[L]}}\mathcal{L}(\hat{f},y)$ by direct computation, or by applying chain rule (if $g^{[L]}$ is elementwise function)

$$\nabla_{z^{[L]}}\mathcal{L} = \left(g^{[L]}\right)'\left(z^{[L]}\right)\otimes\nabla_{\hat{f}}\mathcal{L}(\hat{f},y)$$

  Note $\left(g^{[L]}\right)'\left(z^{[L]}\right)$ denotes the elementwise derivative of $g^{[L]}$ w.r.t. $z^{[L]}$ elementwise.
- For $\ell = L, L-1,\ldots,1$, we have

$$\begin{aligned}
\nabla_{W^{[\ell]}}\mathcal{L} &= (\nabla_{z^{[\ell]}}\mathcal{L})(a^{[\ell-1]})^\top, \quad n^{[\ell]}\times n^{[\ell-1]}\\
\nabla_{b^{[\ell]}}\mathcal{L} &= \nabla_{z^{[\ell]}}\mathcal{L}, \quad n^{[\ell]}\times 1\\
\nabla_{a^{[\ell-1]}}\mathcal{L} &= (W^{[\ell]})^\top\nabla_{z^{[\ell]}}\mathcal{L}\\
\nabla_{z^{[\ell-1]}}\mathcal{L} &= \left(g^{[\ell-1]}\right)'\left(z^{[\ell-1]}\right)\otimes\nabla_{a^{[\ell-1]}}\mathcal{L}, \text{ if } \ell\geq 2
\end{aligned}$$

vector form

The vectorized form to include **all** observations for gradients of $\mathcal{L}_n = \frac{1}{n}\sum_i \mathcal{L}^{(i)}$ (denoted by $d\cdot$):

- $d\mathbf{Z}^{[\ell]}$ be defined so that the i-th row of $d\mathbf{Z}^{[\ell]}$ is $\left(\nabla_{z^{[\ell](i)}}\mathcal{L}^{(i)}\right)^\top$
- similarly for $d\mathbf{A}^{[\ell-1]}$

$$
\begin{aligned}
d\mathbf{Z}^{[\ell]} &= d\mathbf{A}^{[\ell]} \otimes \left(g^{[\ell]}\right)'\left(\mathbf{Z}^{[\ell]}\right), \text{ shape } (n, n^{[\ell]}) \\
dW^{[\ell]} &= \frac{1}{n}(d\mathbf{Z}^{[\ell]})^\top \mathbf{A}^{[\ell-1]}, \text{ shape } (n^{[\ell]}, n)\times(n, n^{[\ell-1]}) \\
db^{[\ell]} &= \frac{1}{n}\,\text{row Sums}\left((d\mathbf{Z}^{[\ell]})^\top\right), \text{ shape } (n^{[\ell]}, 1) \\
d\mathbf{A}^{[\ell-1]} &= d\mathbf{Z}^{[\ell]} W^{[\ell]}, \text{ shape } (n, n^{[\ell-1]})
\end{aligned}
$$

$\otimes$: elementwise operation

Some issues in training deep NN

The objective function $\mathcal{L}(\theta)$ is nonconvex, possessing many local minima; with deep networks, vanishing/exploding gradients are also issues

- the choice of activation functions (seen before)
- the choice of learning rates (and optimization algorithm)
- standardization of the inputs (and activations)
- the initialization of the weights

The complexity of the model needs special attention to avoid overfitting,

- early stopping
- regularization via penalty
- dropout
- residual connection
- data augmentation
- the architecture of the network (width/depth)