M2177.003100
Deep Learning

[2: Neuron Modeling]

Electrical and Computer Engineering
Seoul National University

(last compiled at 22:10:00 on 2018/09/05)

Outline

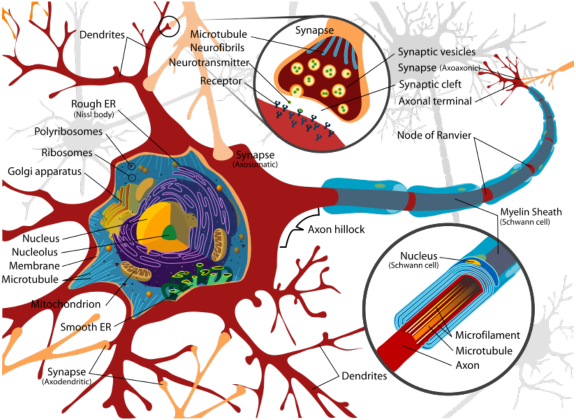
References

- *Deep Learning* by Goodfellow, Bengio and Courville ▸ Link
  - Chapter 6
- *Pattern Recognition and Machine Learning* by Bishop
  - Chapter 5: Neural Networks
- online resources:
  - *Deep Learning Specialization (coursera)* ▸ Link
  - *Stanford CS231n: CNN for Visual Recognition* ▸ Link
  - *Machine Learning Yearning* ▸ Link

Outline

Neuron

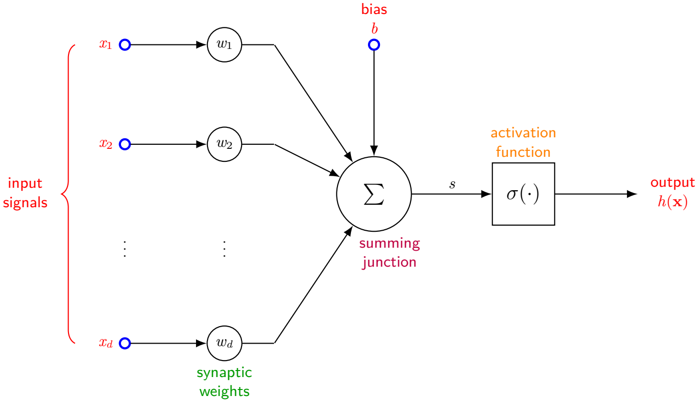
- electrically excitable cell in animal brains
  - processes and transmits information through electrical/chemical signals



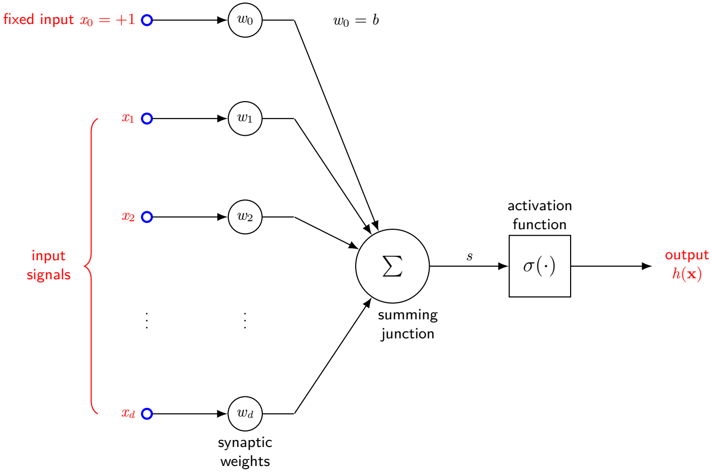
(source: http://en.wikipedia.org/wiki/Neuron)

Modeling a neuron

- three basic elements
  1. synapses (with weights)
  2. adder (input vector $\rightarrow$ scalar) adder => 가중치 계산
  3. __activation__ function (possibly nonlinear)

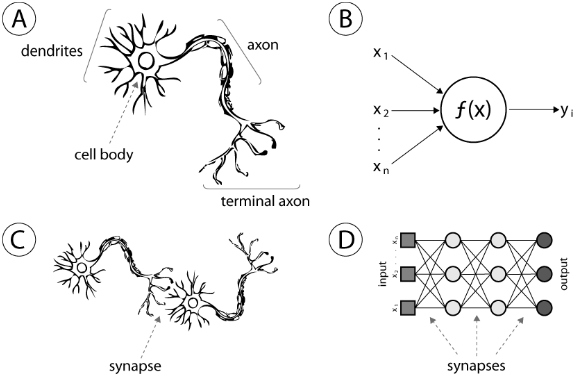


- alternative representation (w_0 for bias b):



Human neuron vs artificial neuron

1개의 hidden layer가 여러개의 neuron으로 이루어져 있음



(a) human neuron (b) artificial neuron

(c) biological neural net (d) artificial neural net

(source: Maltarollo, 2013)

Outline

Linear models

- core of linear models
  W transpose * X(행렬 곱)
  - signal (weighted sum) $z =$ ____ : combines input variables linearly
  - we have seen two models based on this

1. linear regression linear regression => 연속적결과
   - signal itself = output
   - for predicting real (unbounded) response
2. linear classification linear classification => 0 or 1 결과
   - signal is thresholded at zero to produce ± 1 output
   - for binary decisions

Logistic regression as a neuron model

- we review the third linear model:
  - outputs *probability* of a binary response

  e.g. heart attack or not, dead or alive
  - returns 'soft labels' (probability)

- this model: called *logistic* regression
  - output: real (like regression) but bounded (like classification)

- comparison: linear classification vs logistic regression
  - both deal with a binary event
  - logistic regression: allowed to be uncertain

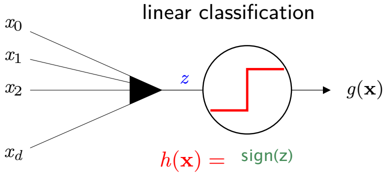
  $\Rightarrow$ intermediate values between 0 and 1 reflect this uncertainty

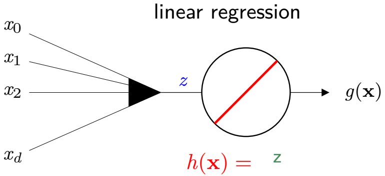
- in early neural nets: $\boxed{\text{logistic regression unit} \stackrel{\text{neuron}}{=}}$

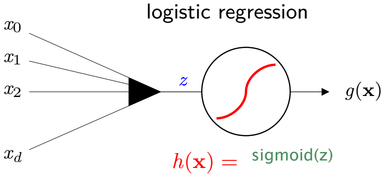
Recall: linear models

- based on "signal" z:

$$z = \sum_{i=0}^{d} w_i x_i$$







Outline

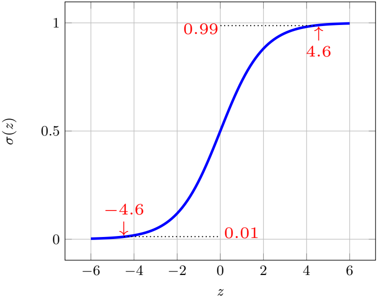
Formulation

- problem
  - given: $\boldsymbol{x} \in \mathbb{R}^{n_x}$
  - want: $\hat{y} = P(y = 1 \mid \boldsymbol{x})$
- model
  - $\hat{y} =$ P(y=1|x)
  - parameters:

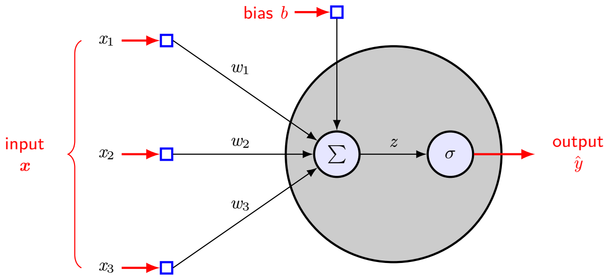
$$\boldsymbol{w} \in \mathbb{R}^{n_x}$$
$$b \in \mathbb{R}$$

  - (logistic) sigmoid:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$
$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$



- computational graph (simplified)



$$\hat{y} = \sigma(\underbrace{\boldsymbol{w}^\top \boldsymbol{x} + b}_{\triangleq z})$$

- weighted sum z: "signal"

$$\begin{aligned} z &= \sum_{i=1}^{n_{\boldsymbol{x}}} w_i x_i + b \\ &= \boldsymbol{w}^\top \boldsymbol{x} + b \end{aligned}$$

Probabilistic interpretation

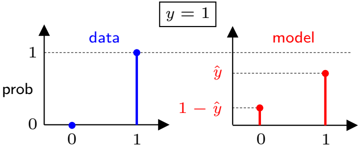
- given training set drawn independently from p_{data}

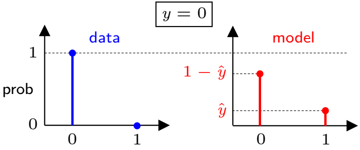
$$\mathbb{X} = \left\{ (\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \ldots, (\boldsymbol{x}^{(m)}, y^{(m)}) \right\}$$

  - consider label $y^{(i)} \in \{0, 1\}$ as (hard) probability

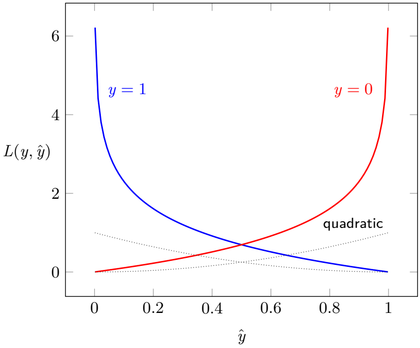
$$y \equiv P(y = 1 \,|\, \boldsymbol{x}) \quad \Rightarrow \quad P(y = 0 \,|\, \boldsymbol{x}) = 1 - P(y = 1 \,|\, \boldsymbol{x}) = 1 - y$$

- then
  - observed pmf $\hat{p}_{\text{data}} \in \{ \underbrace{y}_{P(y=1|\boldsymbol{x})} , \underbrace{1 - y}_{P(y=0|\boldsymbol{x})} \}$ $\leftarrow$ training $\underline{\text{data}}$
  - fitted pmf $p_{\text{model}} \in \{ \underbrace{\hat{y}}_{P(y=1|\boldsymbol{x})} , \underbrace{1 - \hat{y}}_{P(y=0|\boldsymbol{x})} \}$ $\leftarrow$ predicted by $\underline{\text{model}}$





Loss (= pointwise error)



- cross entropy for two pmfs p and q

$$H(p, q) = -\mathbb{E}_p[\log q]$$
$$= -\sum_k p(k) \log q(k)$$

- we use $\underline{\text{log loss}}$ (= logistic loss, cross-entropy loss):

$$L(y, \hat{y}) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

  - if $y = 1 \quad \Rightarrow \quad L(y, \hat{y}) = -\log \hat{y} \quad \Rightarrow$ want $\hat{y}$ large $\quad (\hat{y} \to 1)$
  - if $y = 0 \quad \Rightarrow \quad L(y, \hat{y}) = -\log(1 - \hat{y}) \quad \Rightarrow$ want $\hat{y}$ small $\quad (\hat{y} \to 0)$

Cost function

- simply $\underline{\text{average}}$ pointwise loss:

$$
\begin{aligned}
J(\boldsymbol{w}, b) &= -\mathbb{E}_{\mathrm{y} \sim \hat{p}_{\mathrm{data}}(y \mid \boldsymbol{x})} \log p_{\mathrm{model}}(y \mid \boldsymbol{x}) \\
&= \frac{1}{m} \sum_{i=1}^{m} L(y^{(i)}, \hat{y}^{(i)}) \\
&= -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \qquad (1)
\end{aligned}
$$

- bad news: no known closed-form equation to optimize
- good news: this cost function is convex $\Rightarrow$ global minimum exists
- we will show:

$$
\frac{\partial J}{\partial w_j} = \frac{1}{m} \sum_{i=1}^{m} \left(\sigma(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) - y^{(i)} \right) x_j^{(i)}
$$

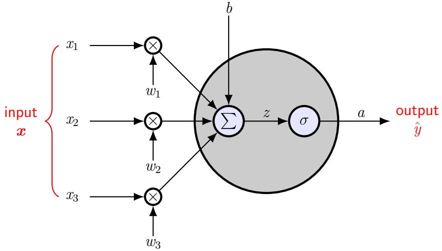
$$
\frac{\partial J}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} \left(\sigma(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) - y^{(i)} \right)
$$

Outline

Training a neuron

- find $\boldsymbol{w}$ and b that minimize cost function $J(\boldsymbol{w}, b)$ in (1)
  - use iterative optimization

  i.e. gradient descent



- repeat the following:

1. forward propagation
   - pick an example $(\boldsymbol{x}, y)$ and feed $\boldsymbol{x}$ to the neuron
   - the net returns $\hat{y} \Rightarrow$ generates loss $L(y, \hat{y})$

2. backward propagation ("backprop"): gradient pump
   - propagate error $L(y, \hat{y})$ at the output to $\boldsymbol{w}$ and b
   - update $\boldsymbol{w}$ and b using the propagated error

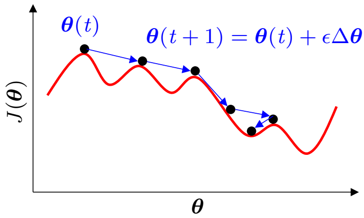
Gradient descent

- a general technique for minimizing twice-differentiable function

  e.g. cost function $J(\boldsymbol{\theta})$

- idea: $J(\boldsymbol{\theta})$ is a 'surface' in parameter space
  - start from somewhere on J (initial location is critical)
  - roll down the surface, decreasing J step by step

- two things to decide at each step
  - which direction? $\Rightarrow \quad \Delta\boldsymbol{\theta} = -\nabla J(\boldsymbol{\theta})$
  - how much? $\Rightarrow \quad \epsilon$ (learning rate)



- parameter update:

$$\begin{aligned}\boldsymbol{\theta}(t+1) &= \boldsymbol{\theta}(t) + \epsilon\Delta\boldsymbol{\theta} \\ &= \boldsymbol{\theta}(t) - \epsilon\nabla J(\boldsymbol{\theta})\end{aligned}$$

or

$$\boxed{\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon\nabla J(\boldsymbol{\theta})}$$

Gradient descent algorithm

algorithm 1 gradient descent

- initialize $\boldsymbol{\theta}$
- **while** stopping criterion not met **do**
  - sample m examples: $\mathbb{X}_m = \{(\boldsymbol{x}^{(1)}, y^{(1)}), \ldots (\boldsymbol{x}^{(m)}, y^{(m)})\}$
  - compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i=1}^{m} L(y^{(m)}, \hat{y}^{(m)})$ ▷ m forward props
  - apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$ ▷ ϵ: learning rate
- **end while**

- three variants (N: total number of examples)
  - $m = 1$: stochastic gradient descent (sgd)
  - $1 < m < N$: minibatch sgd (typical m: 64, 128, 256, 512)
  - $m = N$: batch gradient descent

Training logistic regression by backprop

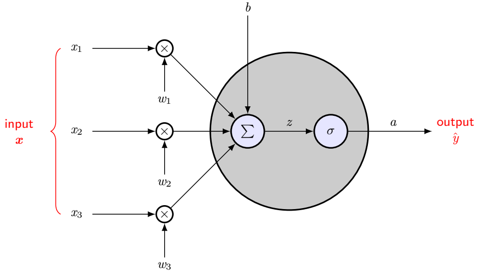
- minimize the cost function by gradient descent

$$J(\boldsymbol{w}, b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log \hat{y}^{(i)} + (1 - y^{(i)})\log(1 - \hat{y}^{(i)})\right]$$

- repeat over training examples
  - ϵ: learning rate

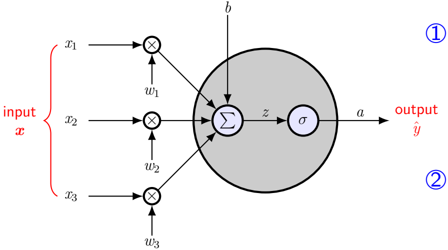
$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \epsilon \nabla_{\boldsymbol{w}} J$$
$$b \leftarrow b - \epsilon \nabla_b J$$

- forward prop:



$$z = \boldsymbol{w}^\top \boldsymbol{x} + b$$
$$\hat{y} = \sigma(z) \triangleq a$$

- some math (in the order of information flow):



① $\boxed{\text{activation } a}$

$$\hat{y} = \sigma(\boldsymbol{w}^\top \boldsymbol{x} + b) \triangleq a$$

② $\boxed{\text{cost function } J}$

$$\begin{aligned} J &= -y \log \hat{y} - (1-y)\log(1-\hat{y}) \\ &= -y \log a - (1-y)\log(1-a) \end{aligned}$$

③ $\boxed{\text{gradient at activation } a \text{ (output)}}$

$$\frac{\partial J}{\partial a} = \frac{\partial J}{\partial \hat{y}} = -\frac{y}{a} + \frac{(1-y)}{1-a}$$

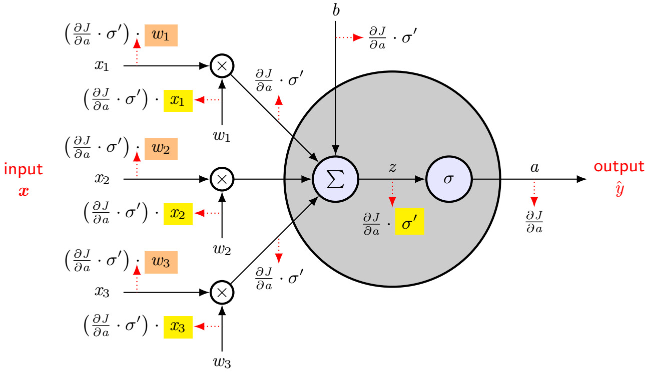
④ $\boxed{\text{local gradient at sigmoid } \sigma}$

$$\sigma' = \sigma(1-\sigma) = a(1-a)$$

⑤ $\boxed{\text{gradient at signal } z}$

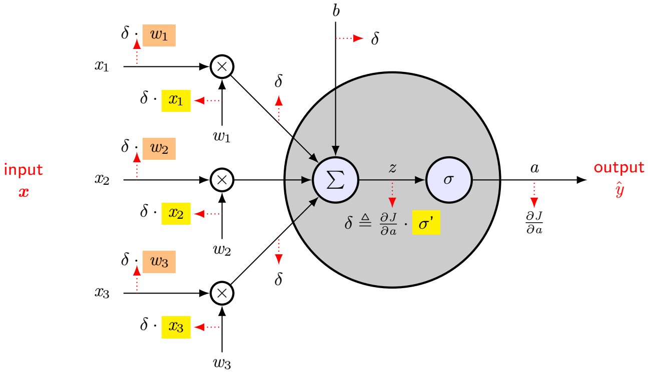
$$\begin{aligned} \color{red}{\frac{\partial J}{\partial z}} &= \frac{\partial J}{\partial a}\frac{\partial a}{\partial z} = \frac{\partial J}{\partial a} \cdot \sigma' \\ &= \left(-\frac{y}{a} + \frac{(1-y)}{1-a}\right) \cdot a(1-a) \\ &= a - y \triangleq \color{red}{\delta} \qquad [\text{“ data error”}] \end{aligned}$$

- backprop:



$$\frac{\partial J}{\partial z} = \frac{\partial J}{\partial a} \cdot \sigma' = a - y \triangleq \delta$$

- backprop (simplified):



$$\frac{\partial J}{\partial z} = \frac{\partial J}{\partial a} \cdot \sigma' = a - y \triangleq \delta$$

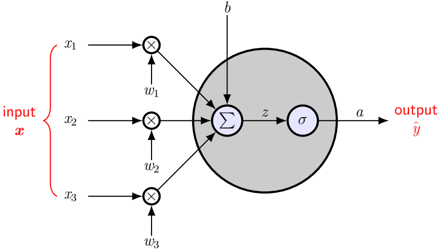
SGD equations (1 example)

- cost function

$$J(\boldsymbol{w}, b) = L(y, a) = -y \log a - (1 - y) \log(1 - a)$$

- compute gradient:

$$\begin{aligned}
\frac{\partial J}{\partial w_1} &= x_1 \cdot \frac{\partial J}{\partial z} &&= x_1(\qquad) &&= x_1 \delta \\
\frac{\partial J}{\partial w_2} &= x_2 \cdot \frac{\partial J}{\partial z} &&= x_2(a - y) &&= x_2 \delta \\
\frac{\partial J}{\partial b} &= \quad \frac{\partial J}{\partial z} &&= \quad (a - y) &&= \delta
\end{aligned}$$



- apply update:

$$\begin{aligned}
w_i &\leftarrow w_i - \epsilon \frac{\partial J}{\partial w_i} &&= w_i - \epsilon \cdot x_i \cdot \delta &&= w_i - \epsilon x_i (a - y) \\
b &\leftarrow b - \epsilon \frac{\partial J}{\partial b} &&= b - \epsilon \cdot \delta &&= b - \epsilon (a - y)
\end{aligned}$$

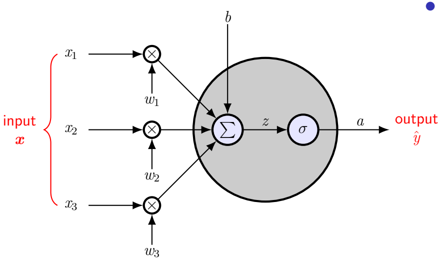
Minibatch SGD equations

- cost function

$$J(\boldsymbol{w}, b) = \frac{1}{m} \sum_{i=1}^{m} L(y^{(i)}, a^{(i)})$$

- signal, activation, delta error

$$z^{(i)} = \boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b$$
$$a^{(i)} = \sigma(z^{(i)})$$
$$\delta^{(i)} = a^{(i)} - y^{(i)}$$



- compute gradient:

$$\frac{\partial J}{\partial w_1} = \frac{1}{m} \sum_{i=1}^{m} x_1^{(i)} \delta^{(i)}$$
$$\frac{\partial J}{\partial w_2} = \frac{1}{m} \sum_{i=1}^{m} x_2^{(i)} \delta^{(i)}$$
$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} \delta^{(i)}$$

- apply update:

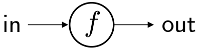
$$w_1 \leftarrow w_1 - \epsilon \frac{\partial J}{\partial w_1}$$
$$w_2 \leftarrow w_2 - \epsilon \frac{\partial J}{\partial w_2}$$
$$b \leftarrow b - \epsilon \frac{\partial J}{\partial b}$$

Outline

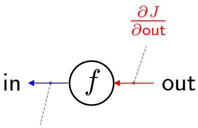
Single-gate backprop

- out $= f(\text{in})$

$\boxed{\text{forward}}$



$\boxed{\text{backprop}}$



$$\frac{\partial J}{\partial \text{in}} = \frac{\partial J}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial \text{in}}$$

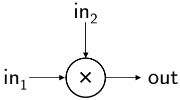
$$\frac{\partial J}{\partial \text{in}} = \underbrace{\frac{\partial J}{\partial \text{out}}}_{\substack{\text{output}\\\text{gradient}}} \cdot \underbrace{\frac{\partial \text{out}}{\partial \text{in}}}_{\substack{\text{local}\\\text{gradient}}}$$

$$= \frac{\partial J}{\partial \text{out}} \cdot f'(\text{in})$$

Multiplication

- out $=$ in$_1 \cdot$ in$_2$

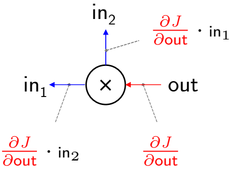
forward



$$\frac{\partial J}{\partial \text{in}_1} = \frac{\partial J}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial \text{in}_1}$$

$$= \underbrace{\frac{\partial J}{\partial \text{out}}}_{\text{output gradient}} \cdot \underbrace{\text{in}_2}_{\text{local gradient}}$$

backprop

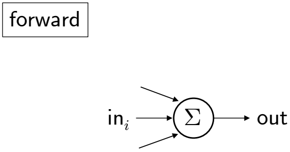


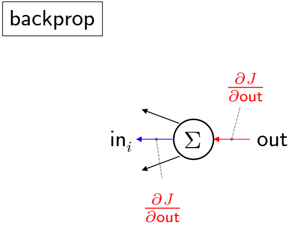
$$\frac{\partial J}{\partial \text{in}_2} = \frac{\partial J}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial \text{in}_2}$$

$$= \frac{\partial J}{\partial \text{out}} \cdot \text{in}_1$$

Summation

- $\text{out} = \sum_i \text{in}_i$





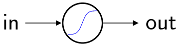
$$
\begin{aligned}
\frac{\partial J}{\partial \text{in}_i} &= \frac{\partial J}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial \text{in}_i} \\
&= \underbrace{\frac{\partial J}{\partial \text{out}}}_{\text{output gradient}} \cdot \underbrace{1}_{\text{local gradient}} \\
&= \frac{\partial J}{\partial \text{out}}
\end{aligned}
$$

- sum (forward) $\Leftrightarrow$ fan out (backprop)

Sigmoid

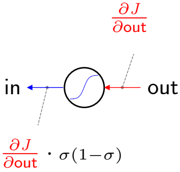
- out $= \sigma(\text{in})$

forward



$$\frac{\partial J}{\partial \text{in}} = \frac{\partial J}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial \text{in}}$$
$$= \underbrace{\frac{\partial J}{\partial \text{out}}}_{\text{output gradient}} \cdot \underbrace{\sigma'(\text{in})}_{\text{local gradient}}$$
$$= \frac{\partial J}{\partial \text{out}} \cdot [\sigma(\text{in})\,(1-\sigma(\text{in}))]$$

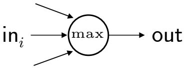
backprop



Max

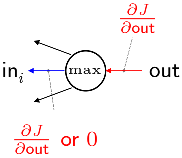
- out $= \max_i \{\text{in}_i\}$

$\boxed{\text{forward}}$



$$\frac{\partial J}{\partial \text{in}_i} = \frac{\partial J}{\partial \text{out}} \cdot \underbrace{\frac{\partial \text{out}}{\partial \text{in}}}_{1 \text{ or } 0}$$

$\boxed{\text{backprop}}$



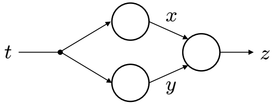
$$= \begin{cases} \frac{\partial J}{\partial \text{out}} & \text{if in}_i \text{ is max} \\ 0 & \text{otherwise} \end{cases}$$

- max (forward) $\Leftrightarrow$ mux (backprop)

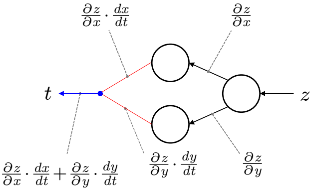
Backprop through fanout

- multivariable chain rule

forward



backprop



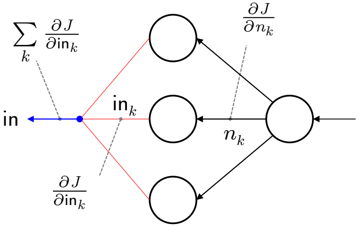
let

$$x = x(t), \;\; y = y(t)$$
$$z = f(x, y)$$

then

$$\frac{\partial z}{\partial t} = \frac{\partial z}{\partial x} \cdot \frac{\partial x}{\partial t} + \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial t}$$

- fanout



assuming

$$\mathcal{E} = f(n_1, \ldots, n_k, \ldots)$$

and

$$n_k = n_k(\text{in})$$

gives

$$\frac{\partial J}{\partial \text{in}} = \sum_k \frac{\partial J}{\partial n_k} \cdot \frac{\partial n_k}{\partial \text{in}} = \sum_k \frac{\partial J}{\partial \text{in}_k}$$

where

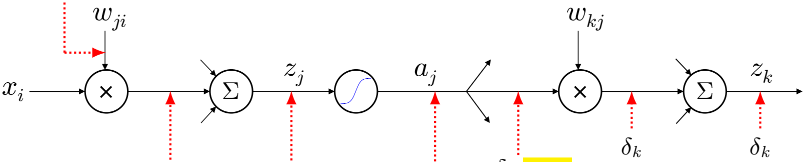
$$\text{in}_k \triangleq \text{ input to } n_k$$

- fanout (forward) $\Leftrightarrow$ sum (backprop)

Example

- computing $\dfrac{\partial J}{\partial w_{ji}}$

$$\left(\sum_k \delta_k \cdot w_{kj}\right) \cdot \sigma'(z_j) \cdot x_i \quad \Longrightarrow \quad \boxed{\frac{\partial J}{\partial w_{ji}} = \delta_j \cdot x_i = \left(\sum_k \delta_k \cdot w_{kj}\right) \cdot \sigma'(z_j) \cdot x_i}$$



$$\delta_k \cdot w_{kj}$$

$$\sum_k \delta_k \cdot w_{kj}$$

$$\delta_j = \left(\sum_k \delta_k \cdot w_{kj}\right) \cdot \sigma'(z_j)$$

$$\left(\sum_k \delta_k \cdot w_{kj}\right) \cdot \sigma'(z_j)$$

Outline

Arranging minibatch

- two options to arrange m examples
  - in columns

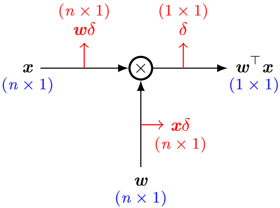
$$\boldsymbol{X}_{|||} = \begin{bmatrix} | & | & & | \\ \boldsymbol{x}^{(1)} & \boldsymbol{x}^{(2)} & \cdots & \boldsymbol{x}^{(m)} \\ | & | & & | \end{bmatrix}$$

  - in rows ("design matrix")

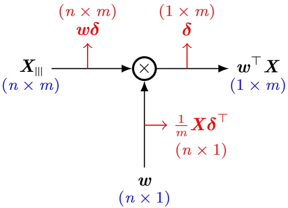
$$\boldsymbol{X}_{\equiv} = \begin{bmatrix} \text{——} & \boldsymbol{x}^{(1)\top} & \text{——} \\ \text{——} & \boldsymbol{x}^{(2)\top} & \text{——} \\ & \vdots & \\ \text{——} & \boldsymbol{x}^{(m)\top} & \text{——} \end{bmatrix}$$

Weighted sum

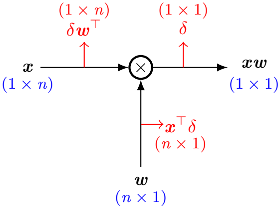
- 1 example (column):



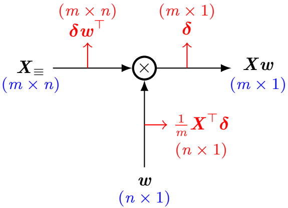
- size-m minibatch (column):



- 1 example (row):

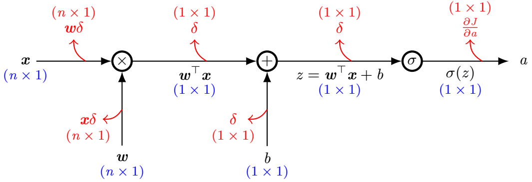


- size-m minibatch (row):

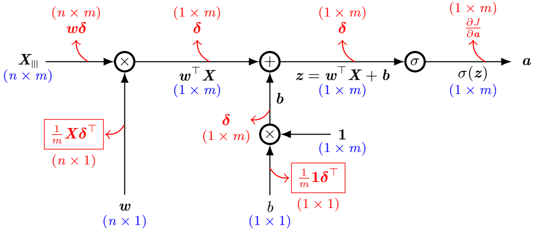


Forward/backward prop (column-wise)

- 1 example:



- size-m minibatch:

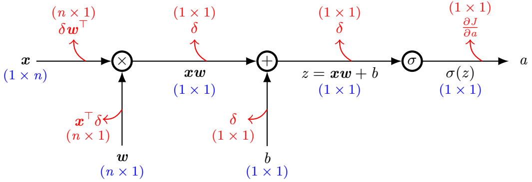


algorithm 2
logistic regression (col)

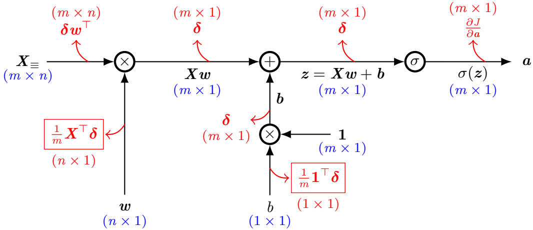
initialize $\boldsymbol{w}$, b
while necessary **do**
  $\boldsymbol{z} = \boldsymbol{w}^\top \boldsymbol{X} + \boldsymbol{b}$
  $\boldsymbol{a} = \sigma(\boldsymbol{z})$
  $\frac{\partial J}{\partial \boldsymbol{z}} \triangleq \boldsymbol{\delta} = \boldsymbol{a} - \boldsymbol{y}$
  $\frac{\partial J}{\partial \boldsymbol{w}} = \frac{1}{m}\boldsymbol{X\delta}^\top$
  $\frac{\partial J}{\partial b} = \frac{1}{m}\boldsymbol{1\delta}^\top$
  $\boldsymbol{w} \leftarrow \boldsymbol{w} - \epsilon \frac{\partial J}{\partial \boldsymbol{w}}$
  $b \leftarrow b - \epsilon \frac{\partial J}{\partial b}$
end while
return $\boldsymbol{w}$, b

Forward/backward prop (row-wise)

- 1 example:



- size-m minibatch:



algorithm 3
logistic regression (row)

initialize $\boldsymbol{w}$, b
while necessary **do**
$\quad \boldsymbol{z} = \boldsymbol{X}\boldsymbol{w} + \boldsymbol{b}$
$\quad \boldsymbol{a} = \sigma(\boldsymbol{z})$
$\quad \frac{\partial J}{\partial \boldsymbol{z}} \triangleq \boldsymbol{\delta} = \boldsymbol{a} - \boldsymbol{y}$
$\quad \frac{\partial J}{\partial \boldsymbol{w}} =$
$\quad \frac{\partial J}{\partial b} =$
$\quad \boldsymbol{w} \leftarrow \boldsymbol{w} - \epsilon \frac{\partial J}{\partial \boldsymbol{w}}$
$\quad b \leftarrow b - \epsilon \frac{\partial J}{\partial b}$
end while
return $\boldsymbol{w}$, b

Outline

Summary

- neuron: brain cell for information processing
  - model: synaptic weights, adder, nonlinear activation function
- logistic regression: a linear model to probability estimation
  - parameterized by weights and bias: $\boldsymbol{\theta} = (\boldsymbol{w}, b)$
  - used as a neuron model in early neural nets
  - log loss: $L(y, \hat{y}) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$
  - cost function $J(\boldsymbol{\theta})$: average loss from training examples
  - training: iterative optimization (such as gradient descent)
- gradient descent: a general, iterative optimization technique
  - update equation: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
  - unit of gradient estimation: batch (all), minibatch (m), stochastic (1)
  - neural nets: gradients are provided by back propagation (backprop)