Mahidol University
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Section for Clinical Epidemiology and Biostatistics

Neural Network

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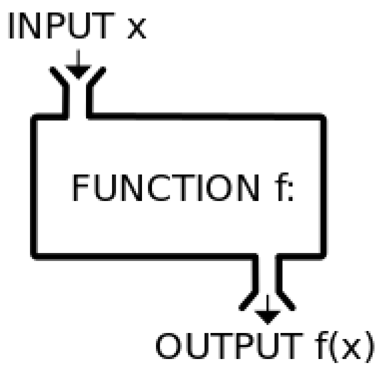
Prerequisite Mathematics

Recall your linear algebra

Linear Algebra

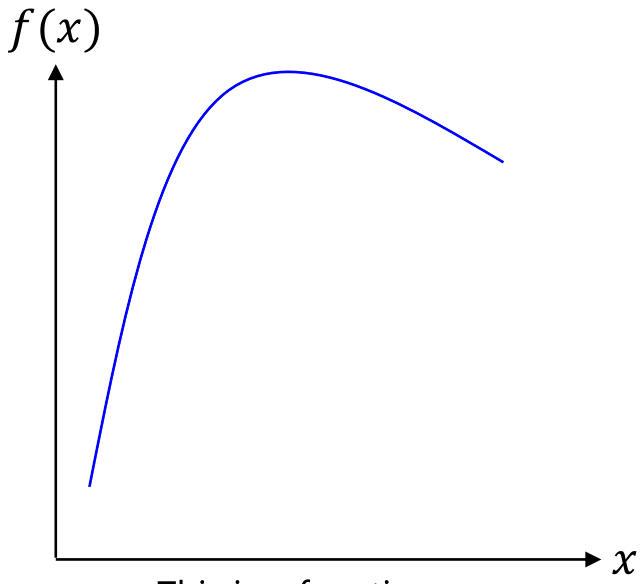
Function



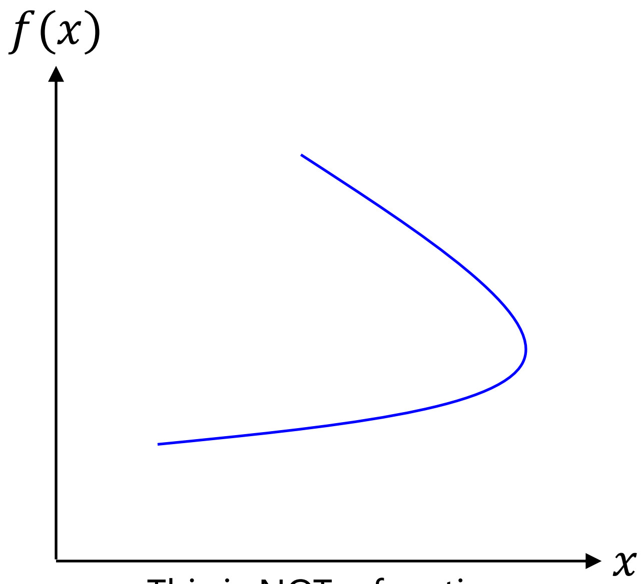
Each input must have only one output

- A function of univariate is defined as

$$x \mapsto f(x)$$



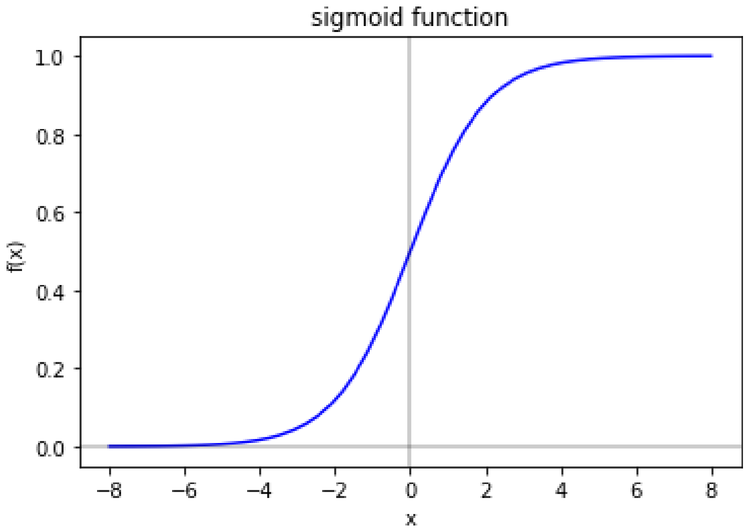
This is a function



This is NOT a function

Linear Algebra

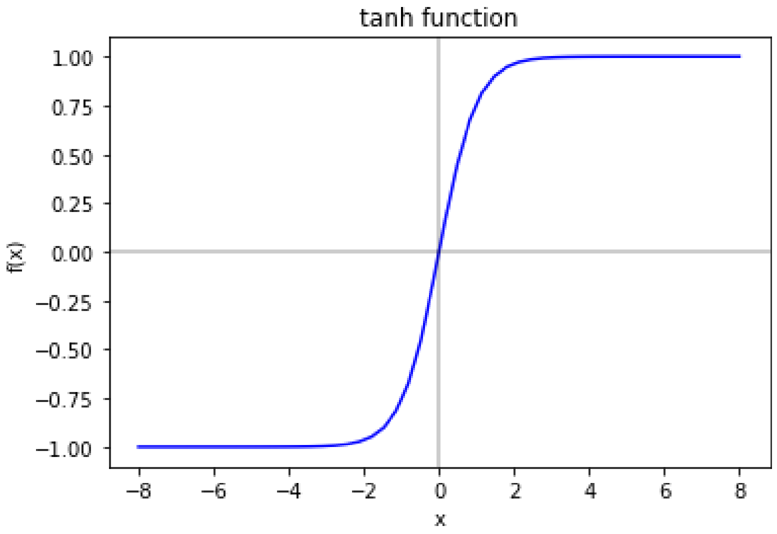
sigmoid



- Properties
  - $f(x) \in [0, 1]$
  - $x \in [-\infty, \infty]$
  - $x \to 0$, $f(x)$ becomes linear
  - $abs(x) > 4$, $f(x)$ changes slowly

Linear Algebra

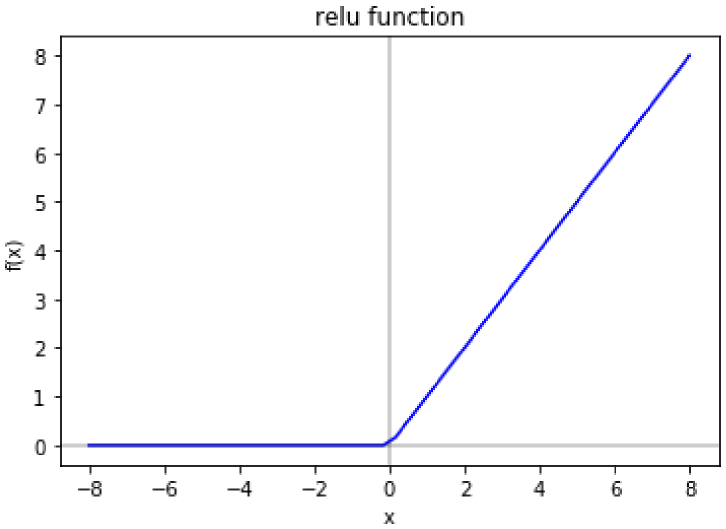
tanh



- Properties
  - f(x) ∈ [-1, 1]
  - x ∈ [-∞, ∞]
  - x → 0, f(x) becomes linear
  - abs(x) > 2, f(x) changes slowly

Linear Algebra

ReLu (Rectifier Linear Unit)

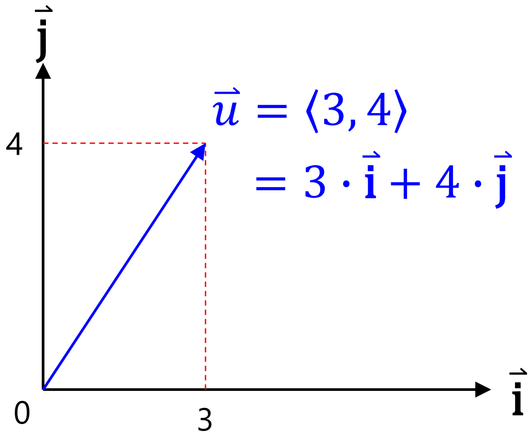



```python
def relu(x):
    y = np.maximum(0, x)
    return y
```

- Properties
  - f(x) ∈ [0, ∞]
  - x ∈ [-∞, ∞]
  - x ≤ 0, f(x) = 0
  - x > 0, f(x) = x

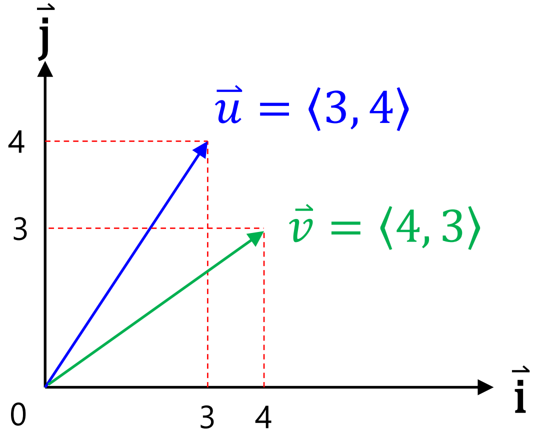
Linear Algebra

Vector



$$\|\vec{u}\| = \sqrt{3^2 + 4^2} = 5$$

- Dot product



$$\vec{u} \cdot \vec{v} = (3 \times 4) + (4 \times 3) = 24$$

- Transpose

if

$$\mathbf{u} = \begin{bmatrix} 3 & 4 \end{bmatrix}$$

then

$$\mathbf{u}^T = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

Linear Algebra

Matrix

A stack of vectors

- Pairwise multiplication

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \qquad B = \begin{bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \end{bmatrix}$$

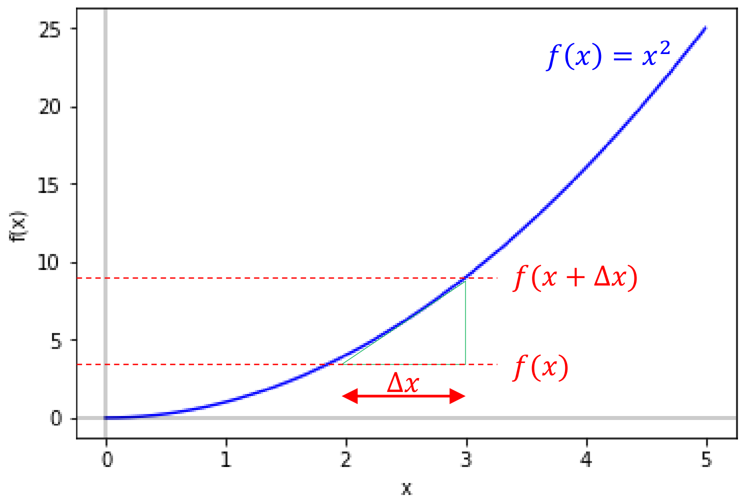
$$A \odot B = \begin{bmatrix} 1 \times 2 & 2 \times 2 & 3 \times 2 \\ 4 \times 2 & 5 \times 2 & 6 \times 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 & 6 \\ 8 & 10 & 12 \end{bmatrix}$$

- Transpose

$$A^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

Linear Algebra

Calculus (Derivative)



- Derivative

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

$\Delta x = 1$

if $x = 2$ then $f(x) = 4$

if $x = 3$ then $f(x) = 9$

$\Delta x = 0.001$

if $x = 2$ then $f(x) = 4$

if $x = 2.001$ then $f(x) \approx 4.004$

if $x = 2$ then slope $= \dfrac{\Delta f(x)}{\Delta x} = \dfrac{0.004}{0.001} = 4$

Mathematically, $\dfrac{d}{dx} f(x) = 2x = 2(2) = 4$

Linear Algebra

Derivative of sigmoid

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

$$\begin{aligned}
\frac{d}{dz}g(z) &= \frac{d}{dz}\left[\frac{1}{1+e^{-z}}\right] \\
&= \frac{d}{dz}(1+e^{-z})^{-1} \\
&= -(1+e^{-z})^{-2}\frac{d}{dz}(1+e^{-z}) \\
&= -(1+e^{-z})^{-2}\frac{d}{dz}(e^{-z})
\end{aligned}$$

$$\begin{aligned}
&= -(1+e^{-z})^{-2}(-e^{-z}) \\
&= \frac{e^{-z}}{(1+e^{-z})^2} \\
&= \frac{1}{1+e^{-z}} \cdot \frac{e^{-z}}{1+e^{-z}} \\
&= \frac{1}{1+e^{-z}} \cdot \frac{(1+e^{-z})-1}{1+e^{-z}} \\
&= \frac{1}{1+e^{-z}}\left[\frac{1+e^{-z}}{1+e^{-z}} - \frac{1}{1+e^{-z}}\right] \\
&= \frac{1}{1+e^{-z}}\left[1 - \frac{1}{1+e^{-z}}\right]
\end{aligned}$$

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

Linear Algebra

Derivative of tanh

$$g(z) = \tanh(z)$$

$$= \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$\frac{d}{dz}g(z) = \frac{(e^z + e^{-z})d(e^z - e^{-z}) - (e^z - e^{-z})d(e^z + e^{-z})}{(e^z + e^{-z})^2}$$

$$= \frac{(e^z + e^{-z})(e^z + e^{-z}) - (e^z - e^{-z})(e^z - e^{-z})}{(e^z + e^{-z})^2}$$

$$= 1 - \left(\frac{e^z - e^{-z}}{e^z + e^{-z}}\right)^2$$

$$\therefore \frac{d}{dz}g(z) = 1 - \tanh^2(z)$$

Linear Algebra

Derivative of relu

$$g(z) = \max(0, z)$$

$$\frac{d}{dz} g(z) = \begin{cases} 0 & if\ z < 0 \\ 1 & if\ z > 0 \\ undefined & if\ z = 0 \end{cases}$$

In neural network practice, z can get close to zero but never be zero, e.g. 0.00000 ...

$$\therefore \frac{d}{dz} g(z) = \begin{cases} 0 & if\ z < 0 \\ 1 & if\ z > 0 \end{cases}$$

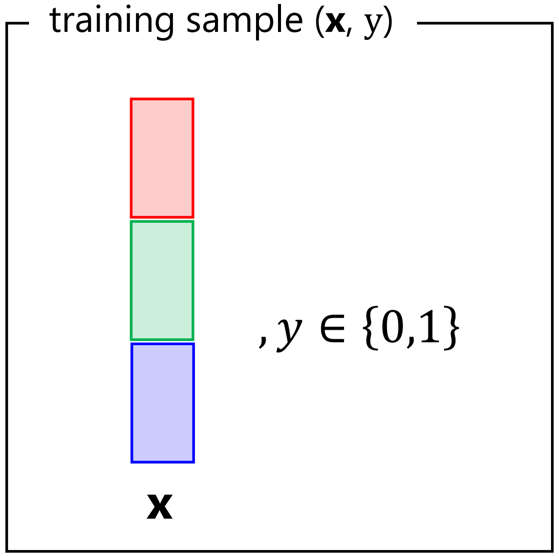
Perceptron

A smallest unit in neural network

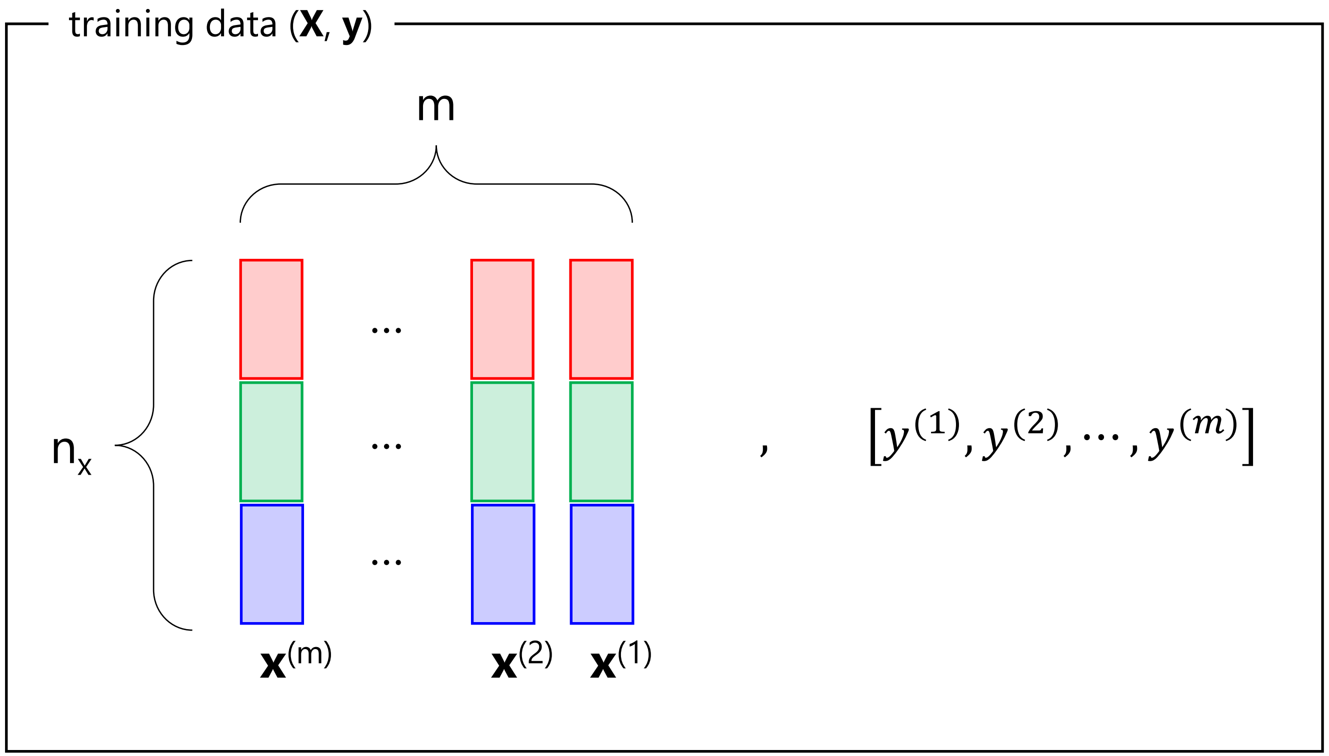
Training Sample VS Training Data

*Training sample is a pair of feature vector **x** and its class label*

$$(\mathbf{x}, y), \mathbf{x} \in \mathbb{R}^{n_x}, y \in \{0,1\}$$



*Training data is <u>m pair</u> of feature vector **x** and its class label*



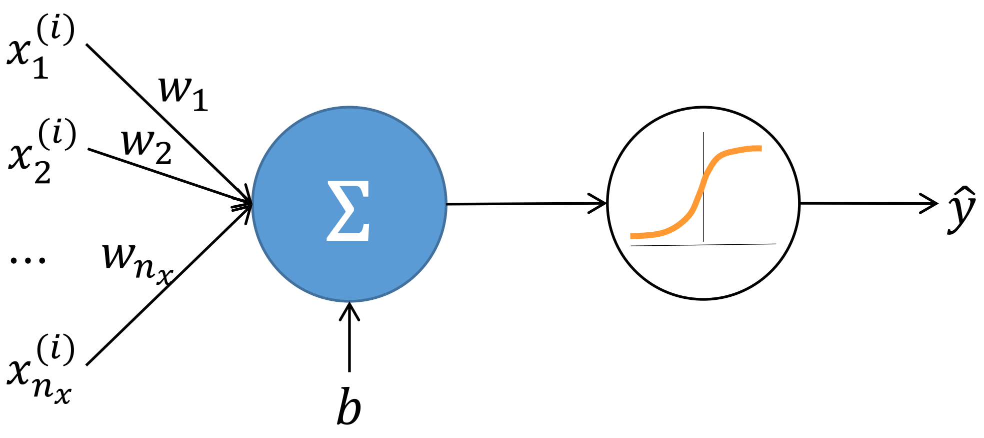
$\mathbf{x} \in \mathbb{R}^{n_x \times 1}$

$\mathbf{X} \in \mathbb{R}^{n_x \times m}$

$\mathbf{y} \in \mathbb{R}^{1 \times m}$

A Perceptron

The smallest unit of neural network

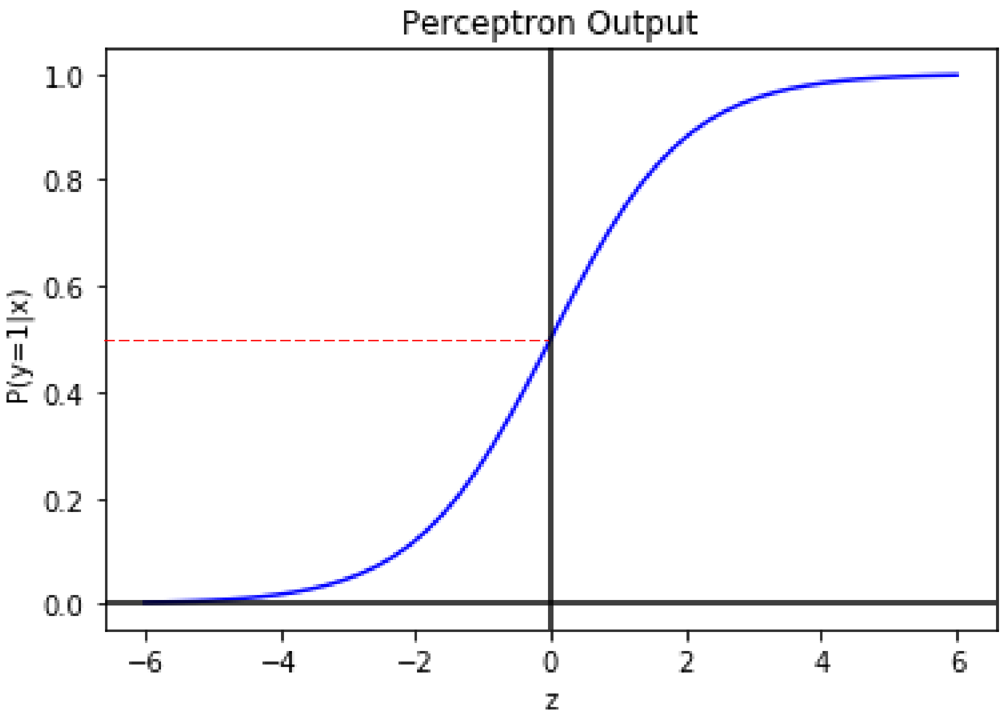


$$\hat{y} = P(y = 1|\mathbf{x}^{(i)}) = \frac{1}{1 + e^{-(\mathbf{w}^T \cdot \mathbf{x}^{(i)} + b)}}$$

- Given $\mathbf{x}^{(i)} \in \mathbb{R}^{n_x \times 1}$, determine
  - $\hat{y} = P(y = 1|\mathbf{x}^{(i)})$
- Parameters
  - $\mathbf{w} \in \mathbb{R}^{1 \times n_x}$
  - $b \in \mathbb{R}$
- Output
  - $\hat{y} = g(z) = g(\mathbf{w}^T \cdot \mathbf{x}^{(i)} + b)$

A Perceptron

The smallest unit of neural network



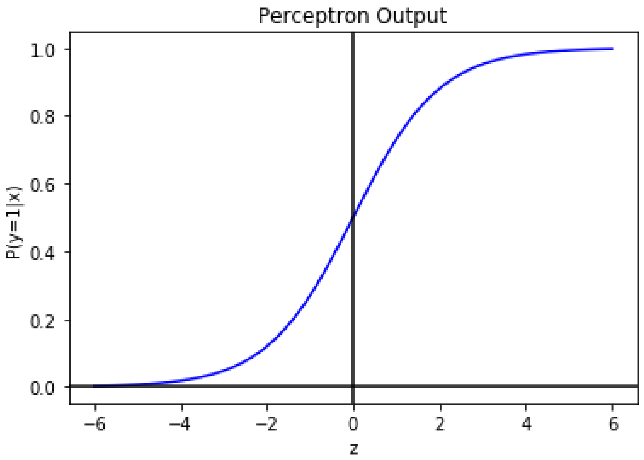
$$g(z) = \frac{1}{1 + e^{-z}}$$

- If $z \gg 0, g(z) \rightarrow 1$
- if $z \ll 0, g(z) \rightarrow 0$

Loss Function

Error of a training sample

The loss function $\mathcal{L}(\hat{y}, y)$ determines how close of $\hat{y}$ to the ground-truth y



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

Goal: $\mathcal{L}(\hat{y}, y) \rightarrow 0$

if $y = 1$,

$$\therefore z = w^T \cdot x + b, \quad \rightarrow \infty$$

$$\hat{y} = \frac{1}{1 + e^{-z}}, \quad \rightarrow 1$$

$$\mathcal{L}(\hat{y}, y) = -\log \hat{y}, \quad \rightarrow 0$$

if $y = 0$,

$$\therefore z = w^T \cdot x + b, \quad \rightarrow -\infty$$

$$\hat{y} = \frac{1}{1 + e^{-z}}, \quad \rightarrow 0$$

$$\mathcal{L}(\hat{y}, y) = -\log(1 - \hat{y}), \quad \rightarrow 0$$

Cost Function

Error of training data

The cost function $\mathcal{J}(\mathbf{w}, b)$ indicates how well the model does in entire training samples

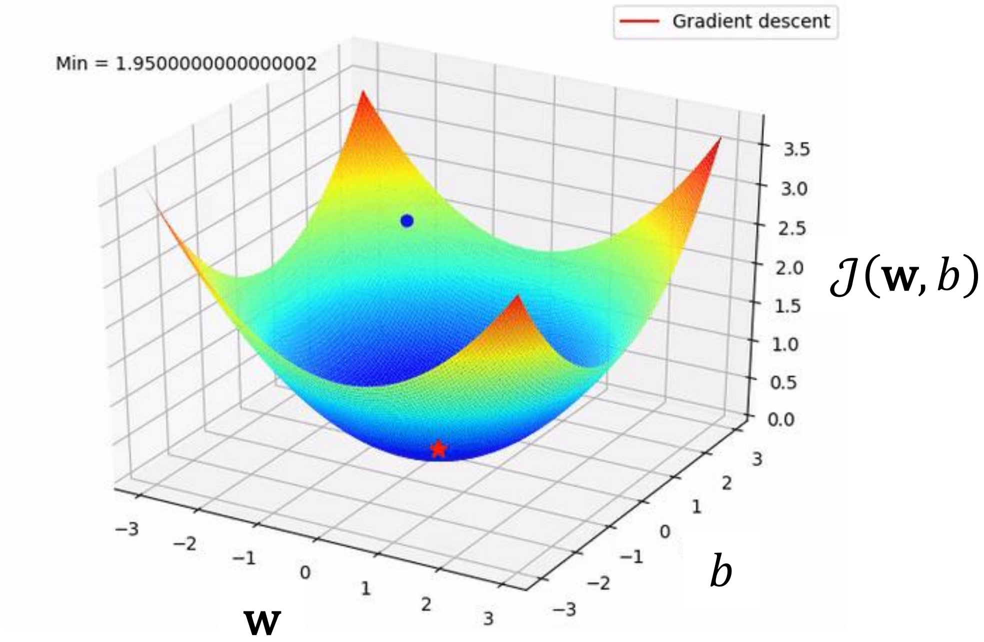
$$\mathcal{J}(\mathbf{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$

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

- Training Goal
  - Find $\mathbf{w}$, b that minimize $\mathcal{J}(\mathbf{w}, b)$

Gradient Descent

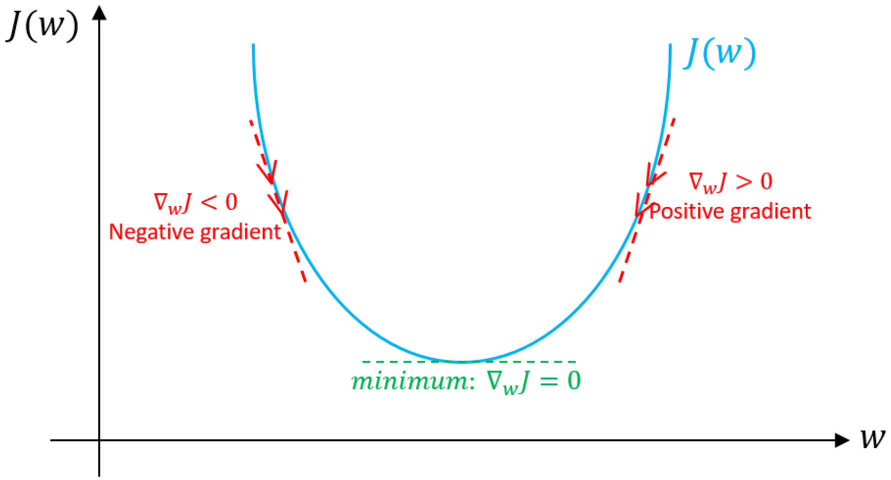
Searching for minimum point in hyperplane



- Goal
  - Determine $\mathbf{w}$, b that minimize $\mathcal{J}(\mathbf{w}, b)$

Gradient Descent

Initialize weight and adjust until the cost function approach to minimum



- Procedure

Repeat {

$$w := w - \alpha \frac{d}{dw} \mathcal{J}(w)$$

Until $\mathcal{J}(w) \rightarrow \min(\mathcal{J}(w))$

}

where α represents the learning rate (a small positive value)

On the right

$\frac{d}{dw} \mathcal{J}(w) > 0, \quad \rightarrow w$ is adjusted by decreasing $\frac{d}{dw} \mathcal{J}(w)$

On the left

$\frac{d}{dw} \mathcal{J}(w) < 0, \quad \rightarrow w$ is adjusted by increasing $\frac{d}{dw} \mathcal{J}(w)$

Gradient Descent

Summary

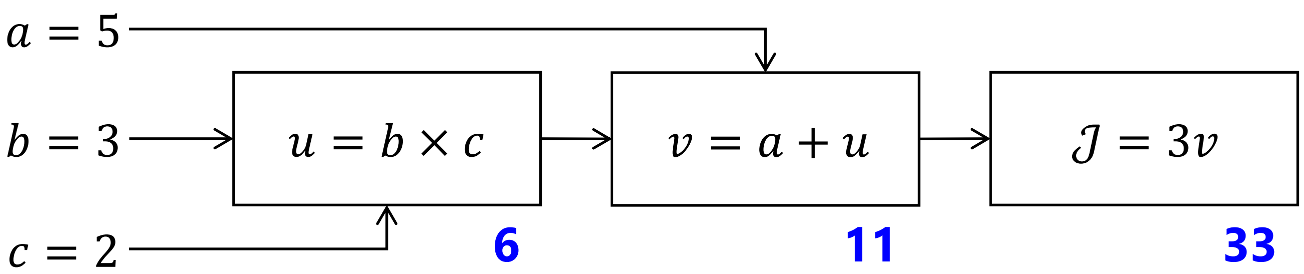
- Minimizing $\mathcal{J}(\mathbf{w}, b)$
  - $w := w - \alpha \frac{d}{dw}\mathcal{J}(w, b),$ where $w \in \mathbf{w}$
  - $b := b - \alpha \frac{d}{db}\mathcal{J}(w, b)$
- In each training iteration, we need to determine

$$\frac{d}{dw}\mathcal{J}(w, b) \quad \text{and} \quad \frac{d}{db}\mathcal{J}(w, b)$$

Computational Graph

Forward path

Given a function $\mathcal{J}(a, b, c) = 3(a + bc)$



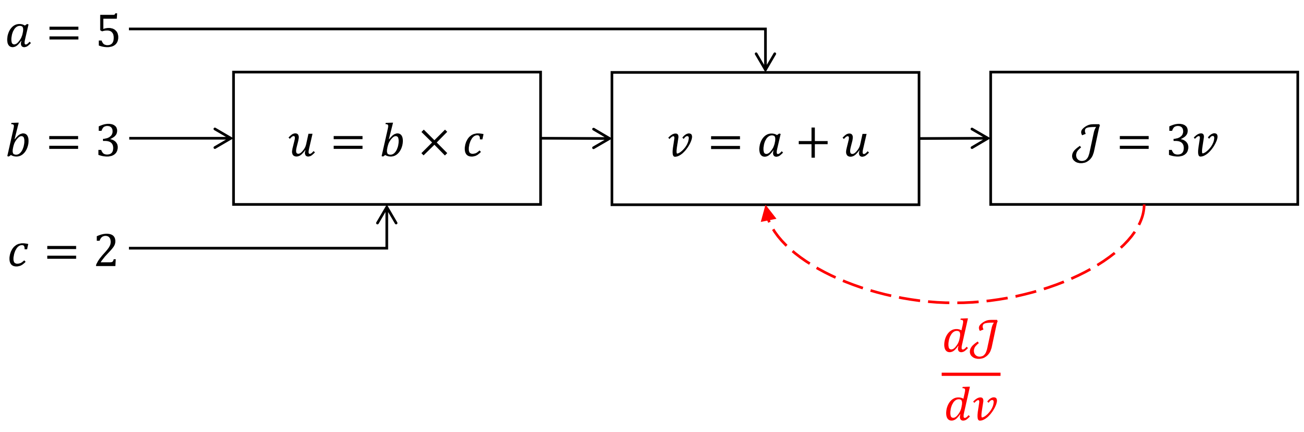
- Forward path
  - $\mathcal{J}(a, b, c)$ can be determined

- Backward path
  - Derivative of $\mathcal{J}(a, b, c)$ w.r.t. a or b or c can be determined

Computational Graph

Backward path

Given a function $\mathcal{J}(a, b, c) = 3(a + bc)$



- Finding $\frac{d\mathcal{J}}{dv}$
  - $v = 11 \xrightarrow{\text{Nudge its value}} v = 11.001$
  - $\mathcal{J} = 33 \xrightarrow{\text{Changed by } v} \mathcal{J} = 33.003$

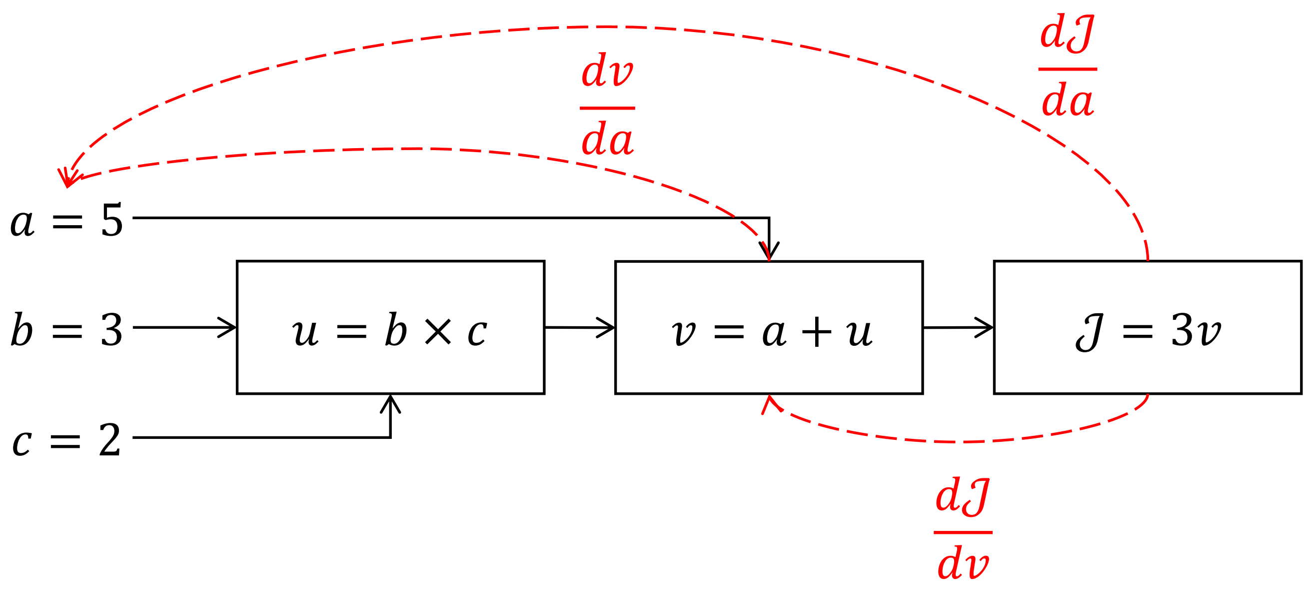
Therefore

$$\frac{d\mathcal{J}}{dv} = \frac{0.003}{0.001} = 3$$

Computational Graph

Backward path

Given a function $\mathcal{J}(a, b, c) = 3(a + bc)$



- Finding $\frac{d\mathcal{J}}{da}$
  - $a = 5 \xrightarrow{\text{Nudge its value}} a = 5.001$
  - $v = 11 \xrightarrow{\text{Changed by } a} v = 11.001$
  - $\mathcal{J} = 33 \xrightarrow{\text{Changed by } a, v} \mathcal{J} = 33.003$

Therefore

$$\frac{d\mathcal{J}}{da} = \underbrace{\frac{d\mathcal{J}}{dv} \cdot \frac{dv}{da}}_{\text{Chain rule}} = \frac{0.003}{0.001} \cdot \frac{0.001}{0.001} = 3$$

Perceptron with Gradient Descent

For a training sample

Given $\mathbf{w} = [w_1 \quad w_2]$ and b

$$
\begin{array}{l}
x_1^{(i)} \\
w_1 \\
x_2^{(i)} \\
w_2 \\
b
\end{array}
\rightarrow
\boxed{z = w_1 x_1^{(i)} + w_2 x_2^{(i)} + b}
\rightarrow
\boxed{\hat{y} = a = g(z)}
\rightarrow
\boxed{\mathcal{L}(a, y)}
$$

- Recap

$$z = \mathbf{w}^T \cdot \mathbf{x}^{(i)} + b$$

$$\hat{y} = a = g(z)$$

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

$$\mathcal{L}(a, y) = -(y \log a + (1 - y)\log(1 - a))$$

- Goal
  - To adjust $\mathbf{w} = [w_1 \quad w_2]$ and b to minimize $\mathcal{L}(a, y)$

Perceptron with Gradient Descent

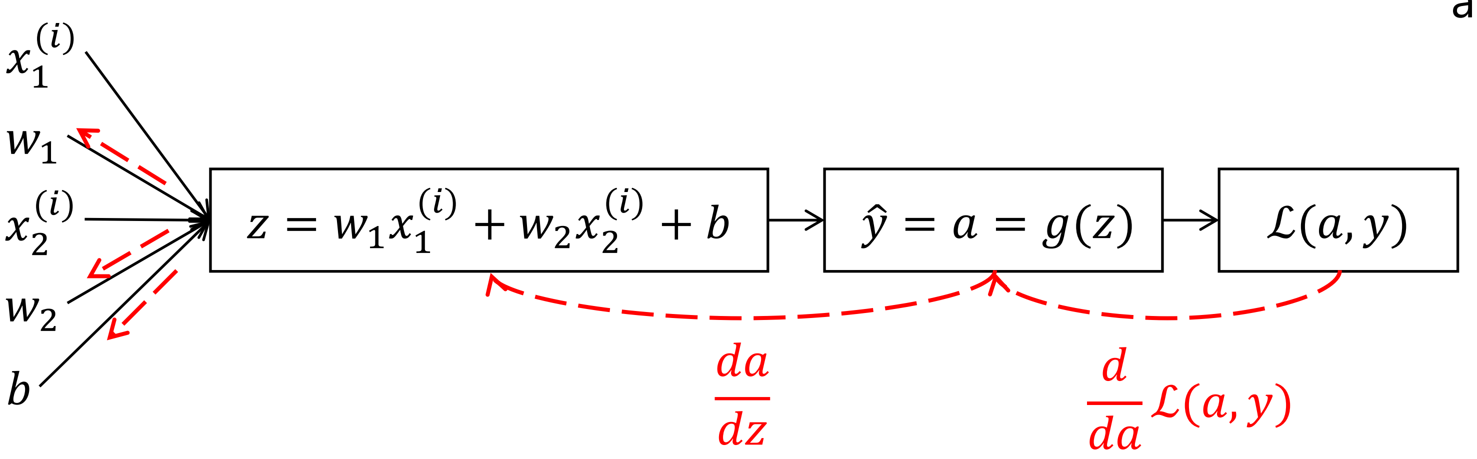
Backward Propagation

$$\Delta z = \frac{d}{dz}\mathcal{L}(a,y) = \frac{d}{da}\mathcal{L}(a,y)\cdot\frac{da}{dz}$$

since $\displaystyle \frac{d}{da}\mathcal{L}(a,y) = \frac{d}{da}\left[-y\log a-(1-y)\log(1-a)\right] = -\frac{y}{a}+\frac{1-y}{1-a}$

and $\displaystyle \frac{da}{dz} = a(1-a)$

$$\therefore \Delta z = \left(-\frac{y}{a}+\frac{1-y}{1-a}\right)\cdot a(1-a) = a-y$$



In other words, Δz is the difference between obtained output and desired output

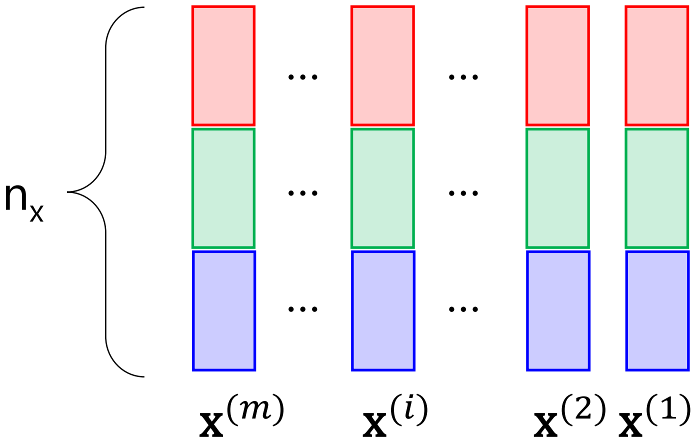
Implementation

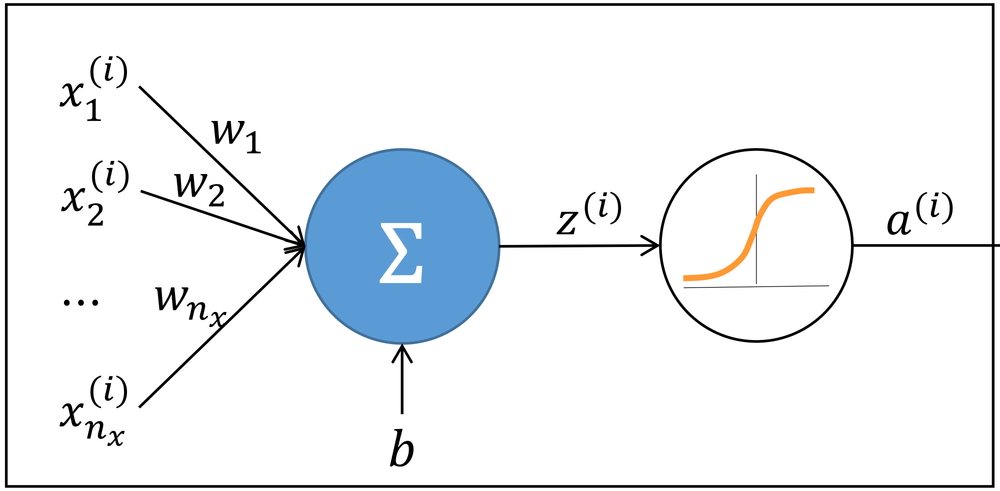
Vectorization

Applying a perceptron to m samples

Broadcasting property enable implementation without looping over training data

$$\mathbf{y} = g(\mathbf{z}) = g(\mathbf{w}^T \cdot \boldsymbol{X} + b)$$





$$[y^{(1)}, y^{(2)}, \cdots, y^{(m)}]$$

Naïve Implementation

Loop and Loop and Loop

This is NOT an efficient method

Note: Python programming does not have the Δ character. For simplicity, let's change

$$\Delta w_1 \rightarrow dw_1$$

$$\Delta w_2 \rightarrow dw_2$$

$$\Delta b \rightarrow db$$

Initialize

$$\mathcal{J} = 0, dw_1 = 0, dw_2 = 0, db = 0$$

for epoch = 1 to max_epoch:

for i = 1 to m:

compute $z^{(i)}, a^{(i)}$

$$\mathcal{J} \mathrel{+}= -\left[y^{(i)} \log a^{(i)} + \left(1 - y^{(i)}\right) \log\left(1 - a^{(i)}\right)\right]$$

compute $dz^{(i)}$

update db

for j = 1 to n_x:

update dw_j

$$\mathcal{J} /= \frac{\mathcal{J}}{m}$$

Implement with Vectorization

The efficient method

Initialize

$\mathcal{J} = 0, dw_1 = 0, dw_2 = 0, db = 0$

for epoch = 1 to max_epoch:

$$\mathbf{Z} = \mathbf{w}^T \cdot \mathbf{X} + b$$

$$\mathbf{A} = g(\mathbf{Z})$$

$$\mathcal{J} = -\frac{1}{m}\sum(\mathbf{y}\log\mathbf{A} - (1-\mathbf{y})\log(1-\mathbf{A}))$$

$$\mathbf{dz} = \mathbf{A} - \mathbf{Y}$$

$$\mathbf{dw} = \frac{1}{m}\mathbf{X} \cdot \mathbf{dz}^T$$

$$db = \frac{1}{m} \cdot np.sum(\mathbf{dz})$$

$$\mathbf{w} -= \alpha \cdot \mathbf{dw}$$

$$b -= \alpha \cdot db$$

Implement with Vectorization

The efficient method

Only loop over training iteration

for epoch = 1 to max_epoch:

$$\mathbf{Z}_{1\times m} = \underbrace{\left(\mathbf{w}_{1\times n_x}\right)^T \cdot \mathbf{X}_{n_x\times m}}_{1\times m} + b$$

$$\mathbf{A}_{1\times m} = g(\mathbf{Z}_{1\times m})$$

$$\mathcal{J} = \underbrace{-\frac{1}{m}\sum_{i=1}^{m}(\underbrace{\mathbf{y}_{1\times m}\log \mathbf{A}_{1\times m}}_{1\times m} - \underbrace{(1-\mathbf{y}_{1\times m})\log(1-\mathbf{A}_{1\times m})}_{1\times m})}_{1\times 1}$$

$$\mathbf{dz}_{1\times m} = \mathbf{A}_{1\times m} - \mathbf{y}_{1\times m}$$

$$\mathbf{dw}_{1\times n_x} = \frac{1}{m}\mathbf{X}_{n_x\times m} \cdot (\mathbf{dz}_{1\times m})^T$$

$$db = \frac{1}{m}\sum_{i=1}^{m}\mathbf{dz}_{1\times m}$$

$$\mathbf{w}_{1\times n_x} -= \alpha \cdot \mathbf{dw}_{1\times n_x}$$

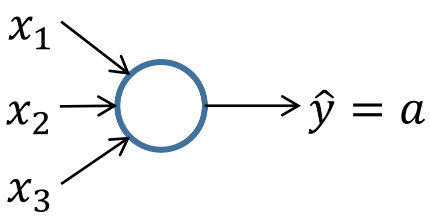
$$b -= \alpha \cdot db$$

Neural Network

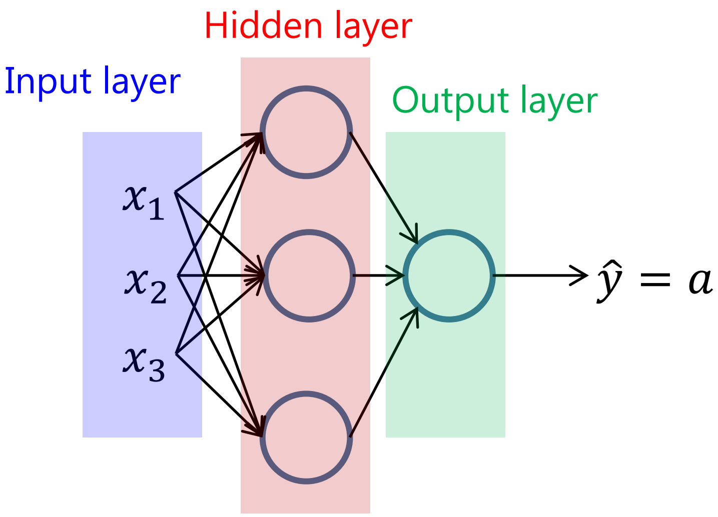
A collection of perceptrons

Shallow Neural Network

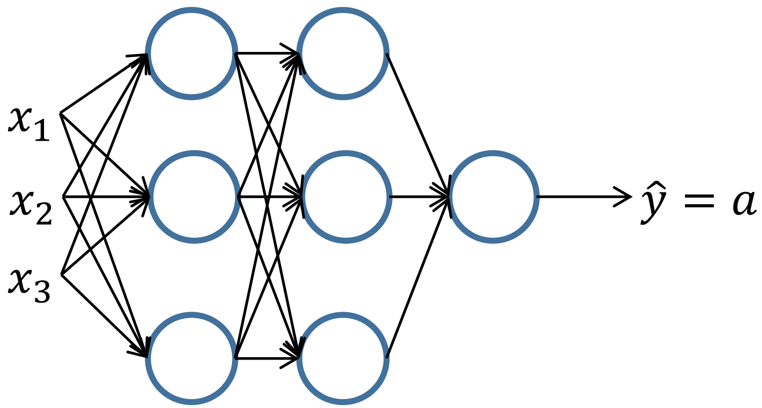
None or a few hidden layers



1-Layer Network
(0 Hidden Layer)
(perceptron or logistic regression)



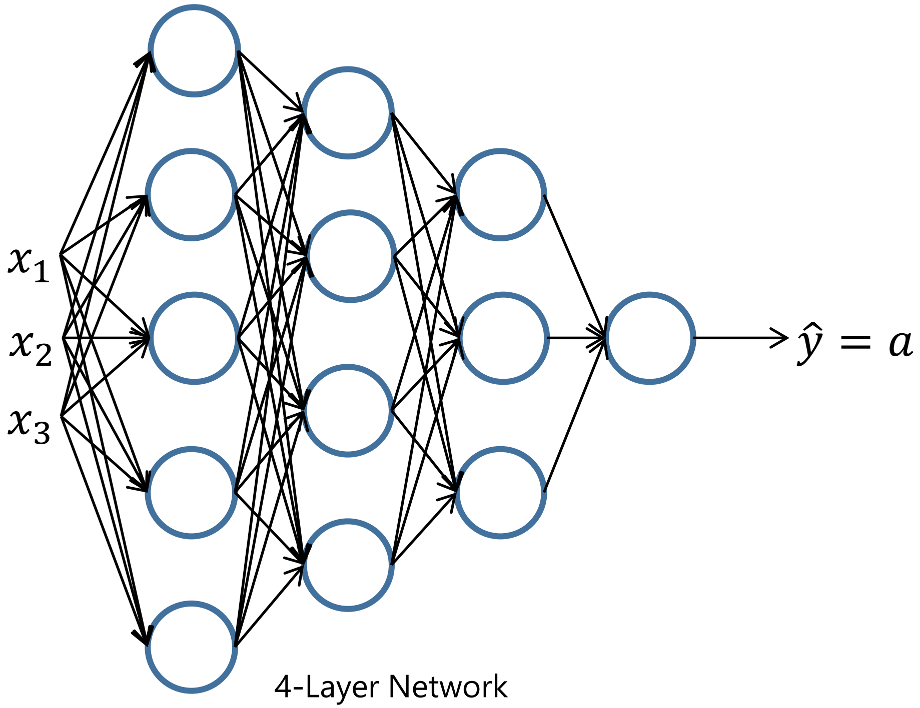
2-Layer Network
(1 Hidden Layer)



3-Layer Network
(2 Hidden Layer)

Deep Neural Network

More hidden layers



4-Layer Network
(3 Hidden Layer)

- Notations

L represents the number of layers (exclude the input layer)

$n^{[l]}$ represents the number of units in the l^{th} layer

Examples:

$n^{[1]} = 5, \quad n^{[2]} = 4, \quad n^{[3]} = 3, \quad n^{[4]} = 1$

$g^{[l]}(\cdot)$ represents the activation function in the l^{th} layer

$\boldsymbol{z}^{[l]}$ represents the linear combination in the l^{th} layer

$\boldsymbol{a}^{[l]}$ represents the activated values in the l^{th} layer

$\mathbf{W}^{[l]}$ represents the weights matrix in the l^{th} layer

$\mathbf{b}^{[l]}$ represents the bias in the l^{th} layer

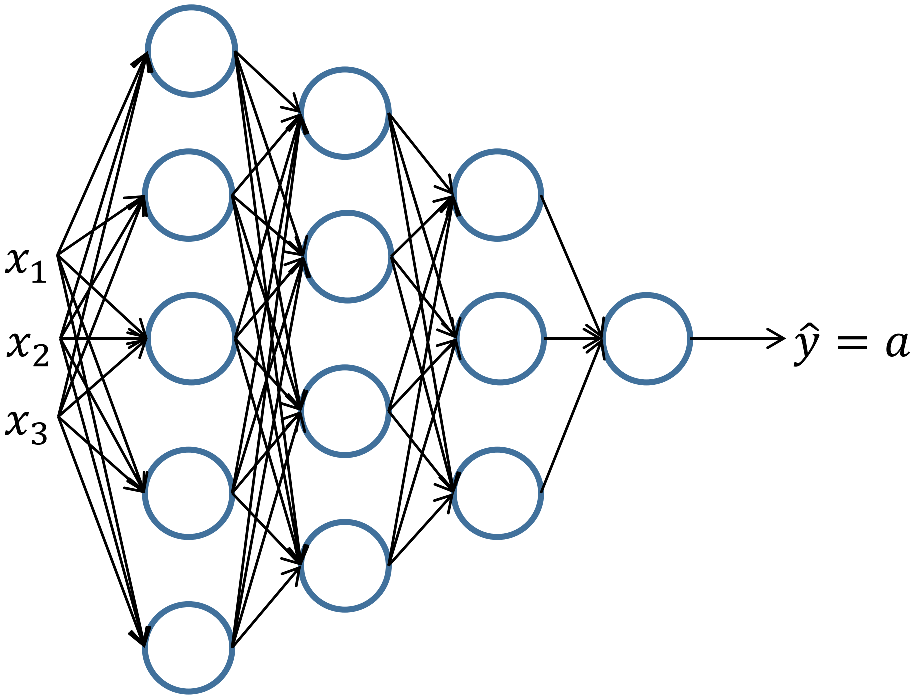
$\mathbb{W}$ represents the collection of weights matrix of all layers

$w_{i,j}$ represents the weights connecting between the i^{th} unit in the l^{th} layer to the j^{th} unit in the $(l-1)^{th}$ layer

$\mathbb{b}$ represents the collection of bias vectors of all layers

Deep Neural Network

Weights



- Weights $\mathbb{W} = \begin{bmatrix} \mathbf{W}^{[1]} \\ \mathbf{W}^{[2]} \\ \mathbf{W}^{[3]} \\ \mathbf{W}^{[4]} \end{bmatrix}$

$$\mathbf{W}^{[l]} = \begin{bmatrix} \mathbf{w}_1^{[l]} \\ \cdots \\ \mathbf{w}_{n^{[l]}}^{[l]} \end{bmatrix}_{n^{[l]},n^{[l-1]}}$$

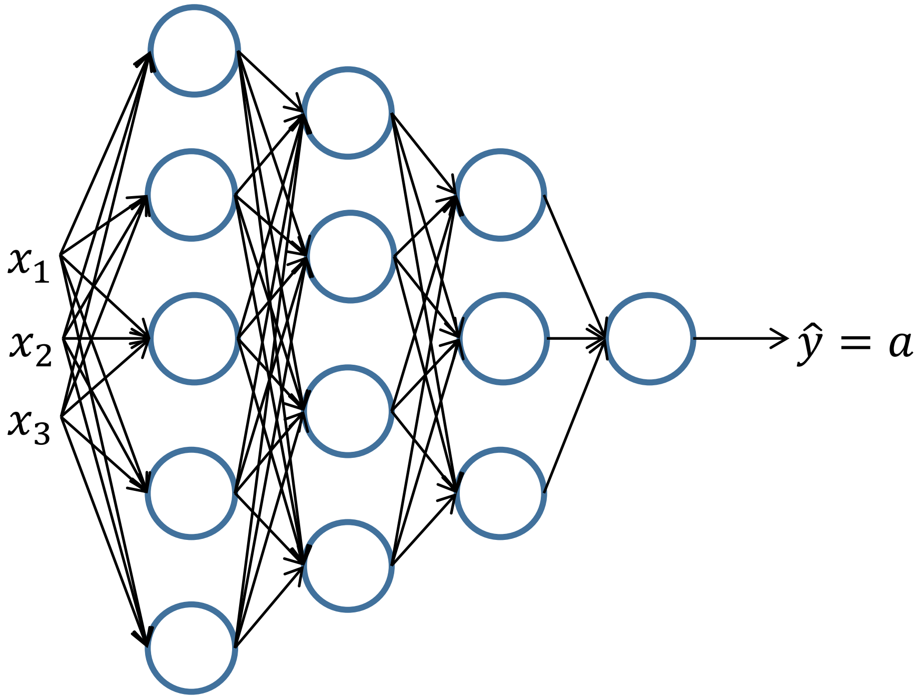
- Example

$$\mathbf{W}^{[3]} = \begin{bmatrix} w_{1,1} & \cdots & w_{1,4} \\ \vdots & \ddots & \vdots \\ w_{3,1} & \cdots & w_{3,4} \end{bmatrix}$$

Dimension of $\mathbf{W}^{[l]}$ is $\left(n^{[l]}, n^{[l-1]}\right)$

Deep Neural Network

Biases



- Biases

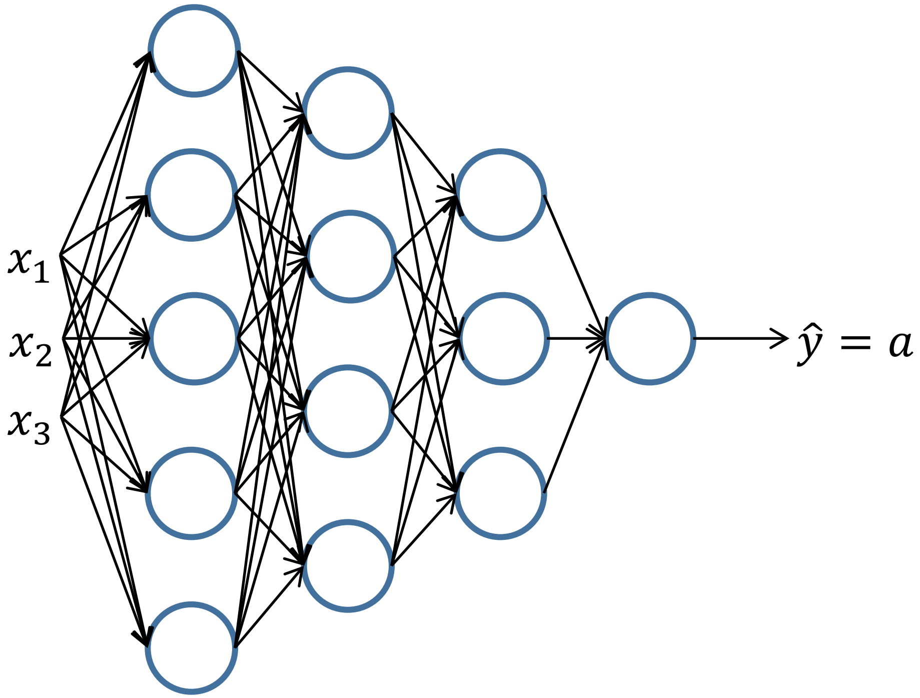
$$\mathbb{b} = [\mathbf{b}^{[1]} \quad \dots \quad \mathbf{b}^{[4]}] = \begin{bmatrix} b_1^{[1]} & \cdots & b_1^{[4]} \\ \vdots & \cdots & \vdots \\ b_5^{[1]} & \cdots & b_3^{[4]} \end{bmatrix}$$

$$\therefore \mathbf{b}^{[l]} = \begin{bmatrix} b_1^{[l]} \\ \vdots \\ b_{n^{[l]}}^{[l]} \end{bmatrix}$$

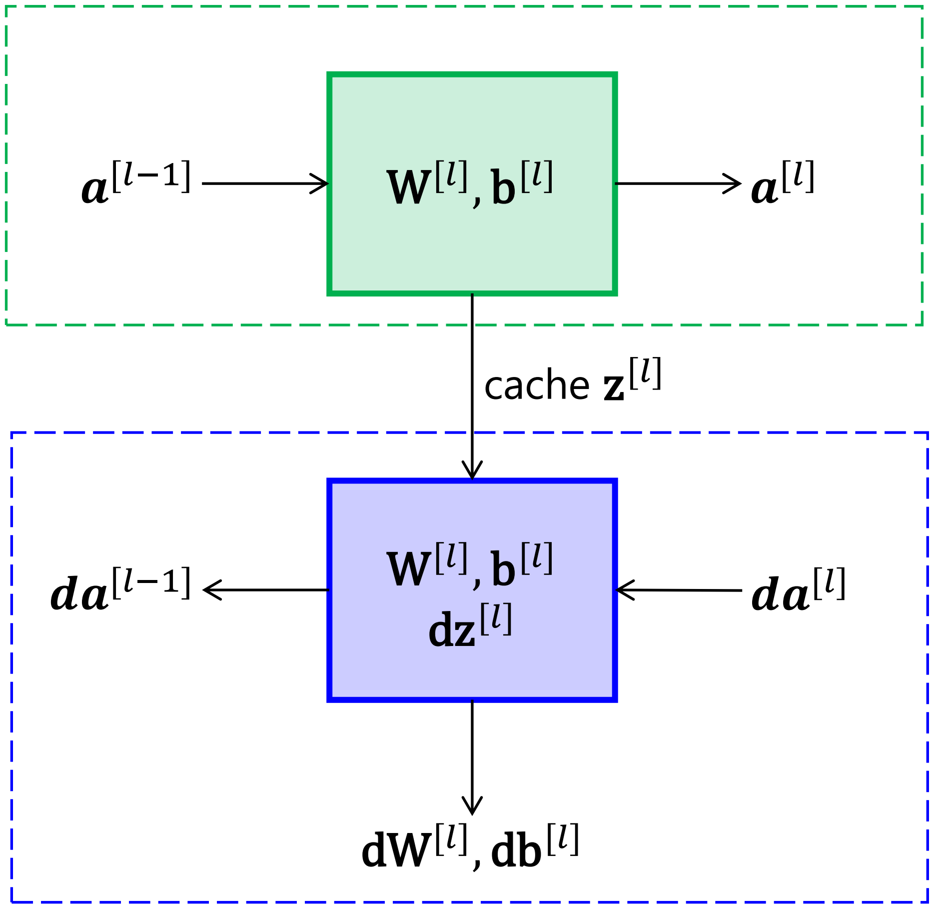
Dimension of $\mathbf{b}^{[l]}$ is $\left(n^{[l]}, 1\right)$

Implementation with Vectorization

The L layers neural network

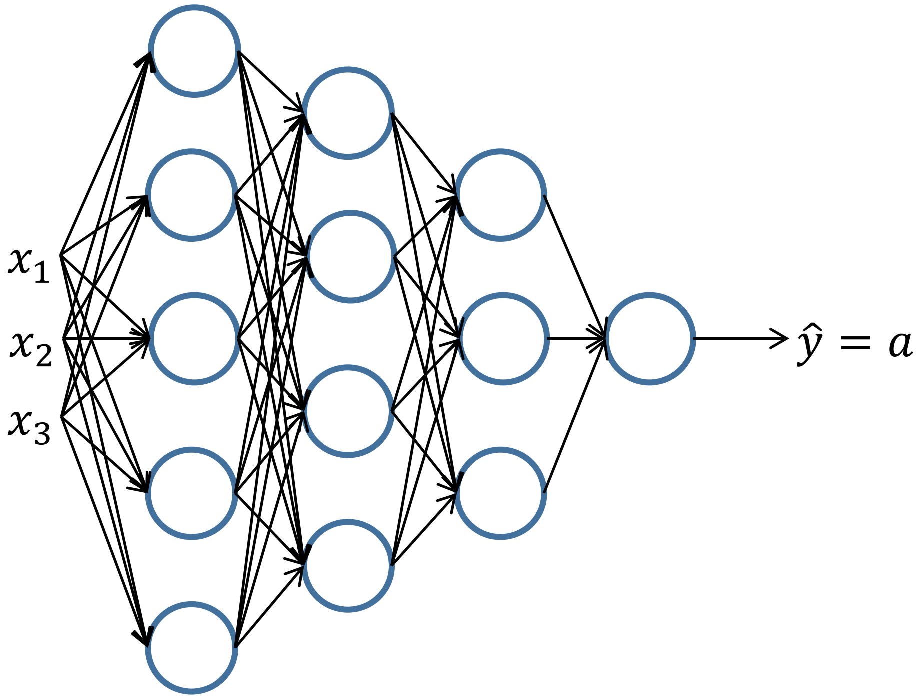


- At the layer l: $\mathbf{W}^{[l]}, \mathbf{b}^{[l]}$



Implementation with Vectorization

The L layers neural network



- At the layer l: $\mathbf{W}^{[l]}, \mathbf{b}^{[l]}$
  - Forward Propagation

$$\mathbf{z}^{[l]} = \mathbf{W}^{[l]} \cdot \boldsymbol{a}^{[l-1]} + \mathbf{b}^{[l]}$$

$$\boldsymbol{a}^{[l]} = g^{[l]}(\mathbf{z}^{[l]})$$

  - Backward Propagation

$$\mathbf{dz}^{[l]} = \mathbf{da}^{[l]} * g'^{[l]}(\mathbf{z}^{[l]})$$

$$\mathbf{dW}^{[l]} = \frac{1}{m}\mathbf{dz}^{[l]} \cdot \boldsymbol{a}^{[l-1]^T}$$

$$\mathbf{db}^{[l]} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{dz}^{[l]}$$

$$np.sum(\mathbf{dz}^{[l]}, axis = 1, keepdims = True)$$

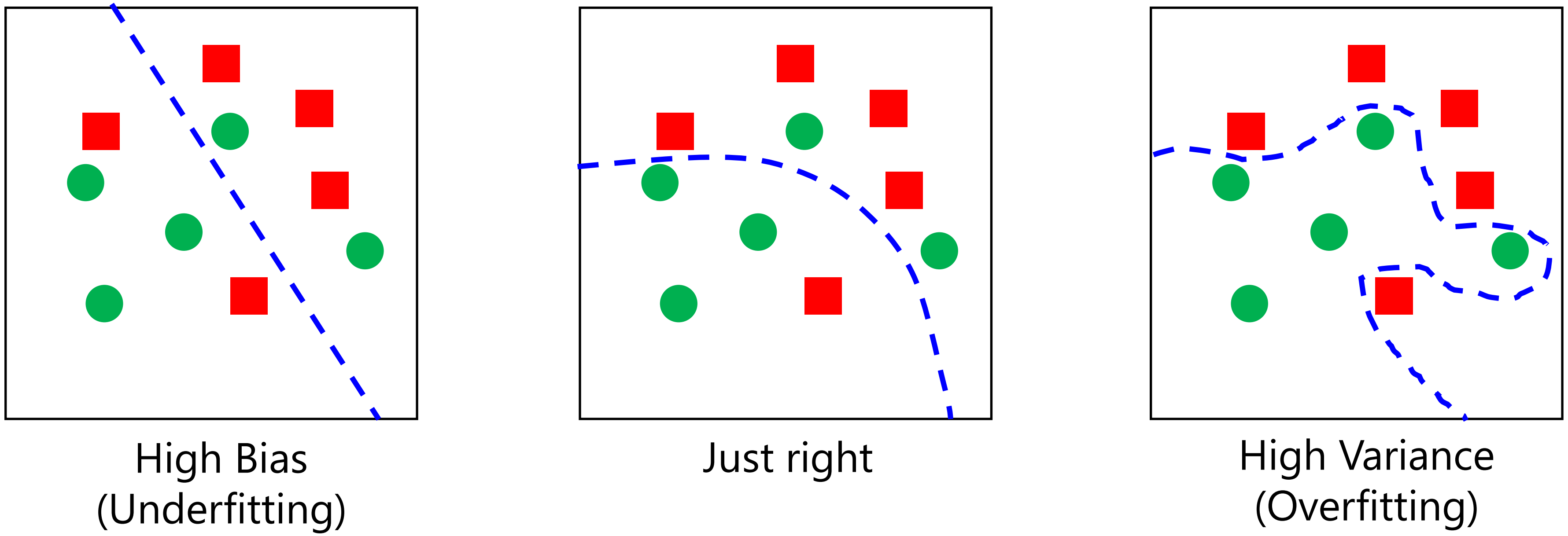
$$\mathbf{da}^{[l-1]} = \mathbf{W}^{[l]^T} \cdot \mathbf{dz}^{[l]}$$

Model Tuning

Bias and Variance Problem

Easy to learn but difficult to master

- Unable to visualize in high dimensional data



Regularization

L1 and L2

L1 and L2 Regularization

Recall the cost function of perceptron

Goal:

$\min_{\mathbf{w},b} \mathcal{J}(\mathbf{w}, b), \qquad \mathbf{w} \in \mathbb{R}^{n_x}, b \in \mathbb{R}$

- L1 regularization (Lasso)

$$\mathcal{J}(\mathbf{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \boxed{\frac{\lambda}{2m}\|\mathbf{w}\|_1}$$

Regularization term

where $\|\mathbf{w}\|_1 = \sum_{j=1}^{n_x}|w_j|$

λ represents the regularization parameter

- L1 makes many weights become zeros
- Good for compacting the model
- L1 is not often used

L1 and L2 Regularization

Recall the cost function of perceptron

Goal:

$$\min_{\mathbf{w},b} \mathcal{J}(\mathbf{w}, b), \qquad \mathbf{w} \in \mathbb{R}^{n_x}, b \in \mathbb{R}$$

- L2 regularization (Ridge)

$$\mathcal{J}(\mathbf{w}, b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \boxed{\frac{\lambda}{2m}\|\mathbf{w}\|_2^2}$$

Regularization term

where $\|\mathbf{w}\|_2^2 = \sum_{j=1}^{n_x} w_j^2 = \mathbf{w}^T \cdot \mathbf{w}$

λ represents the regularization parameter

- L2 is much more often used compared to L1

L2 Regularization

L2 of Deep Neural Network

The cost function

$$\mathcal{J}\left(\mathbf{w}^{[1]}, \mathbf{b}^{[1]}, \dots, \mathbf{w}^{[L]}, \mathbf{b}^{[L]}\right) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L}\|\mathbf{w}\|_F^2$$

where

Frobenious norm $\|\mathbf{w}\|_F^2 = \sum_{i=1}^{n^{[l-1]}}\sum_{j=1}^{n^{[l]}}\left(w_{ij}^{[l]}\right)^2$

$\mathbf{w}^{[l]}: (n^{[l]}, n^{[l-1]})$

- Modifying back propagation

$$\mathbf{dw}^{[l]} = (\cdot) + \frac{\lambda}{m}\mathbf{w}^{[l]}$$

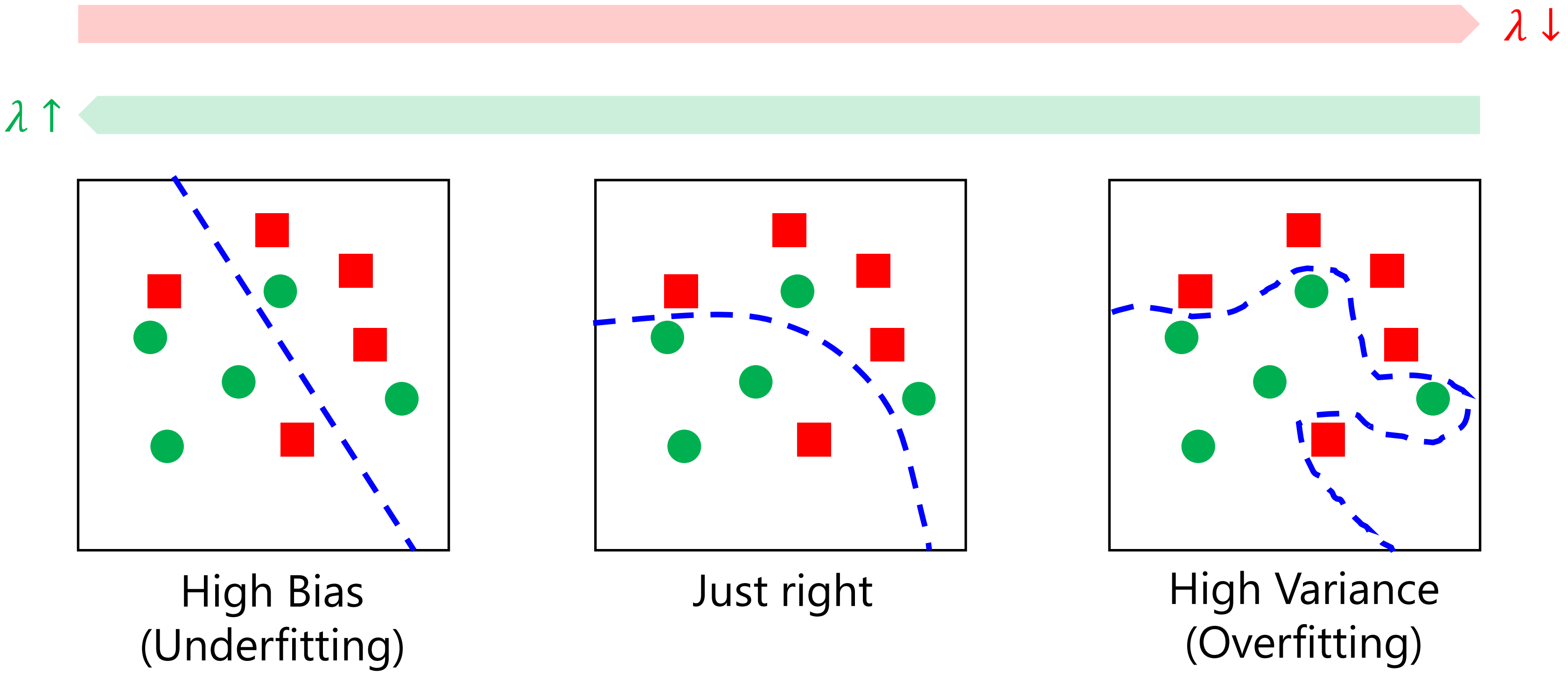
$$\begin{aligned}\mathbf{w}^{[l]} &= \mathbf{w}^{[l]} - \alpha\mathbf{dw}^{[l]} \\ &= \mathbf{w}^{[l]} - \alpha\left[(\cdot) + \frac{\lambda}{m}\mathbf{w}^{[l]}\right] \\ &= \mathbf{w}^{[l]} - \frac{\alpha\lambda}{m}\mathbf{w}^{[l]} - \alpha(\cdot) \\ &= \left(1 - \frac{\alpha\lambda}{m}\right)\mathbf{w}^{[l]} - \alpha(\cdot)\end{aligned}$$

Weight Decay

where $(\cdot)$ represents the term obtained from original back propagation

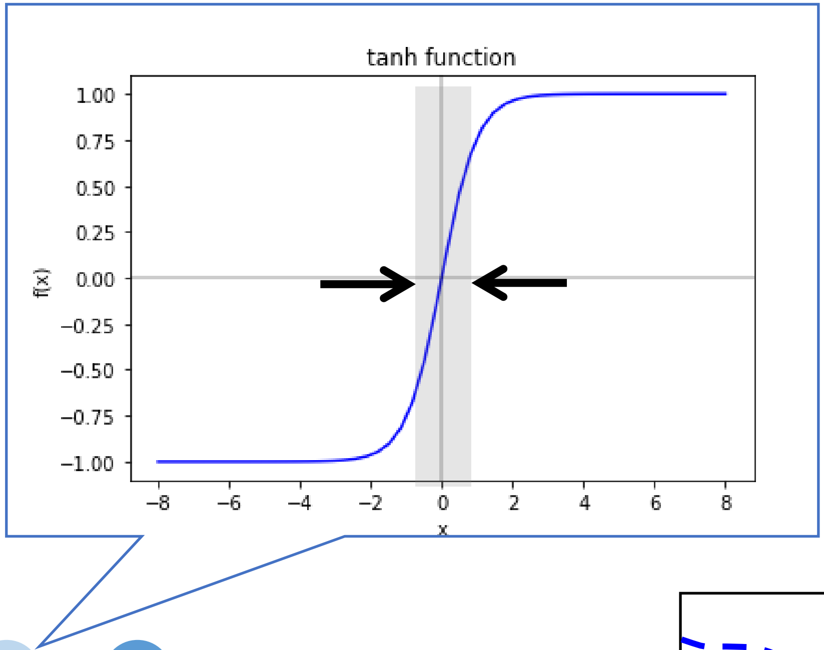
L2 Regularization

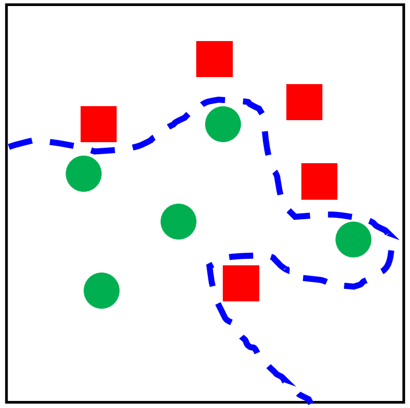
Why does L2 prevent overfitting?



L2 Regularization

Why does L2 prevent overfitting?



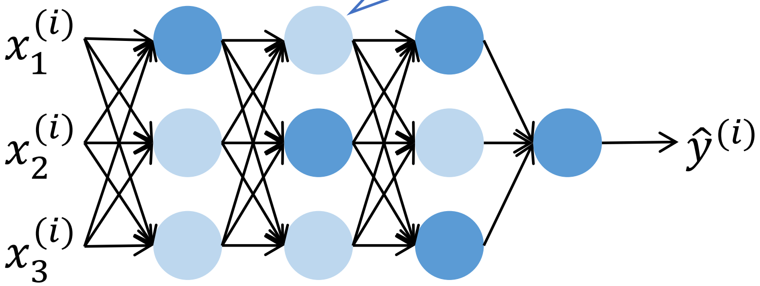


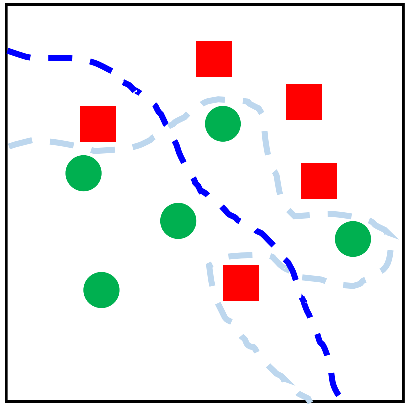
$\lambda \uparrow$

$\mathbf{w}^{[l]} \downarrow$

$\mathbf{z}^{[l]} \downarrow$

$\because \mathbf{z}^{[l]} = \mathbf{w}^{[l]} a^{[l-1]} + \mathbf{b}^{[l]}$





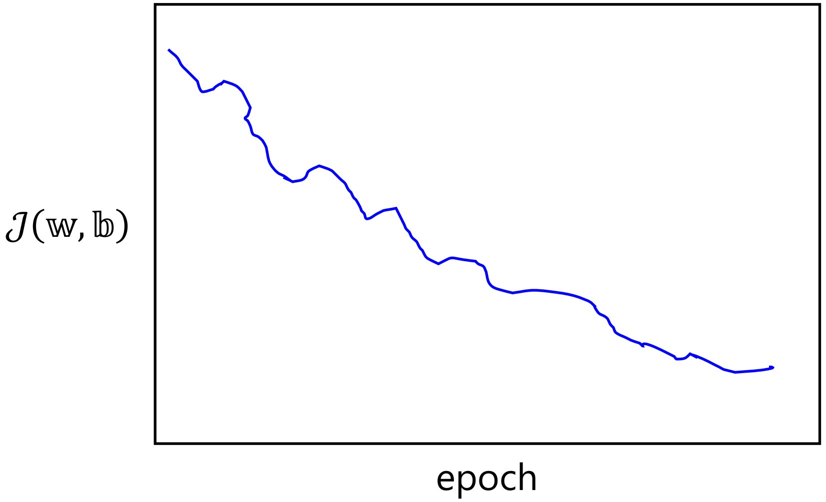
Decision boundary is stretched out

L2 Regularization

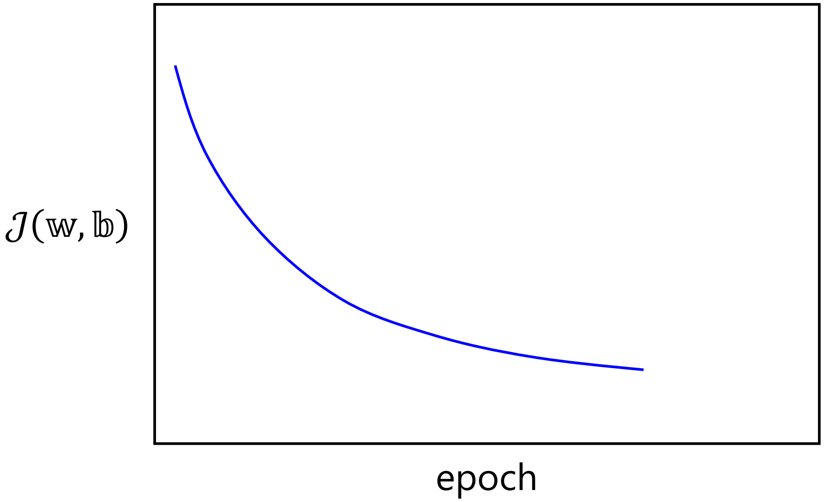
Smoother cost function

$$\mathcal{J}\left(\mathbf{w}^{[1]}, \mathbf{b}^{[1]}, \dots, \mathbf{w}^{[L]}, \mathbf{b}^{[L]}\right) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L}\|\mathbf{w}\|_F^2$$

Without regularization



With regularization



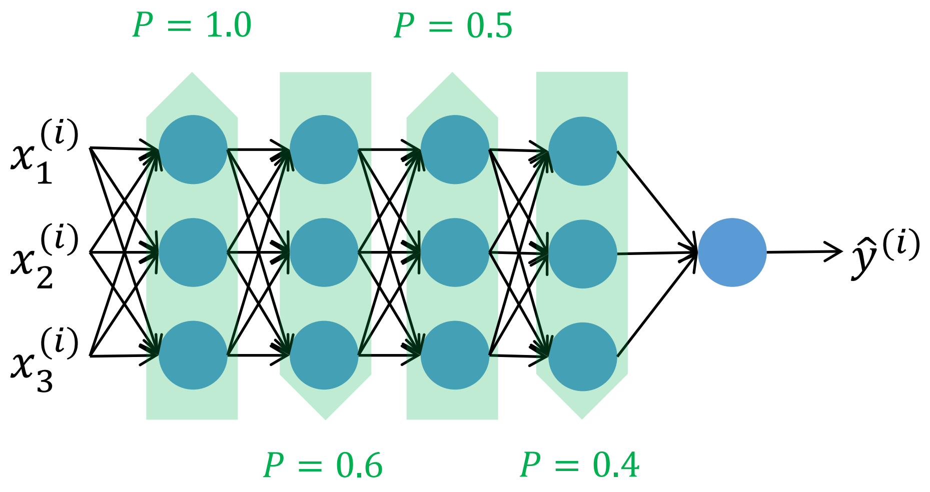
Regularization

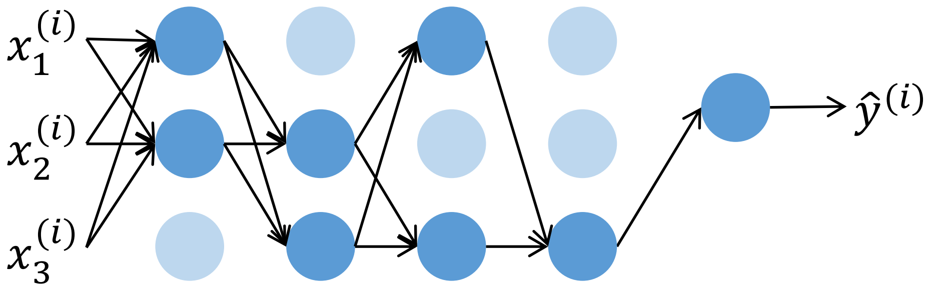
DropOut & DropConnect

DropOut

Ensemble Neural Network

- Set the probability of enable hidden units in each hidden layer
- The edges connected to any disable hidden unit will be removed
- DropOut is applied ONLY training but NOT testing
- DropOut produces many possible combination of neuron network
- DropOut is very popular in computer vision

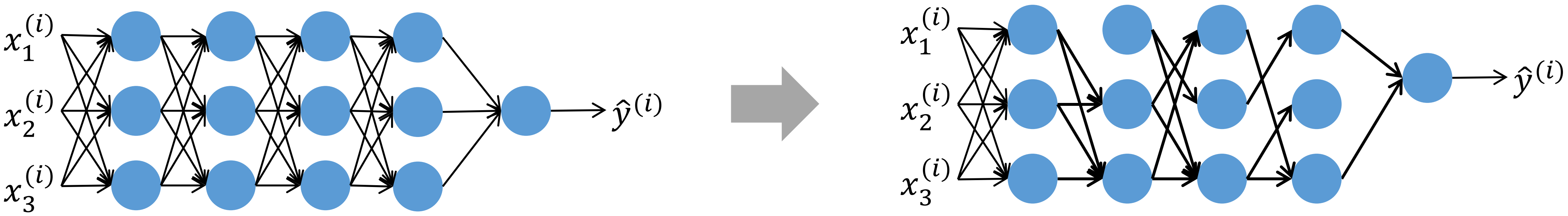




DropConnect

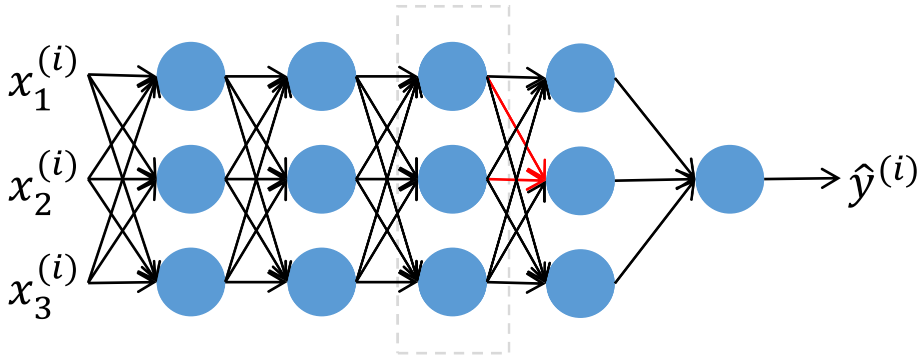
Generalization of DropOut

- Set the Boolean mask to randomly disable connections
- Rescale output on active connections
- DropConnect is applied ONLY for training but NOT testing
- DropConnect makes even more possible combination than dropout
- DropConnect is very popular in computer vision



Implementation

Illustration of DropConnect at the layer 3



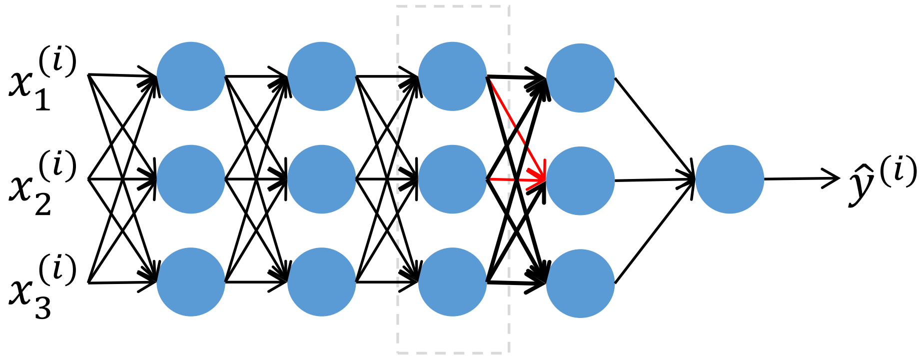
- Define theoretical variable to Python variable
  - P as keepprob
  - Create a Boolean mask to randomly disable weights

```
keepprob = 0.8
d3 = np.random.rand(a3.shape[0], a3.shape[1]) < keepprob
```

```
In [43]: d3
Out[43]:
array([[ True,  True,  True],
       [False,  True,  True],
       [ True, False,  True]])
```

Implementation

Illustration of DropConnect at the layer 3



- Rescale the $\boldsymbol{a}^{[3]}$

```
a3 /= keepprob
```

- Example: If $\boldsymbol{a}^{[3]}$ is

```
array([[1., 2., 3.],
       [4., 5., 6.],
       [7., 8., 9.]])
```

- Rescale $\boldsymbol{a}^{[3]}$ after drop connect will be

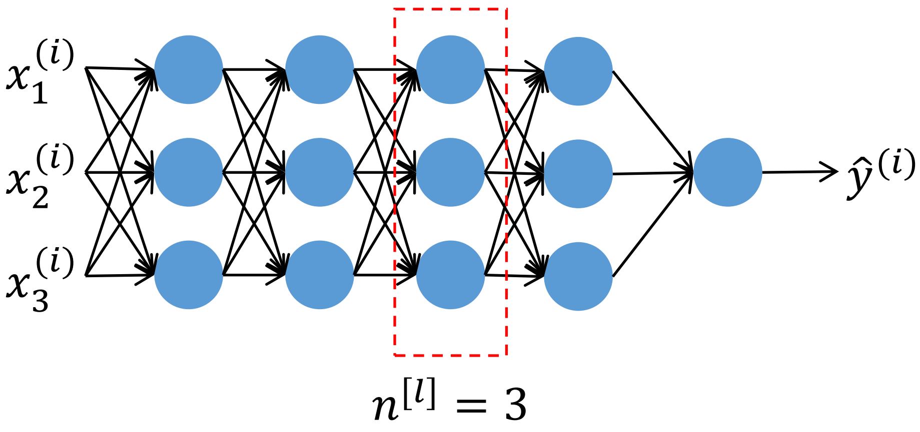
```
array([[ 1.25,  2.5 ,  3.75],
       [ 0.  ,  6.25,  7.5 ],
       [ 8.75,  0.  , 11.25]])
```

- In practice a3 is obtained from

$$\boldsymbol{a}^{[3]} = g^{[3]}\left(\mathbf{z}^{[3]}\right) = g^{[3]}(\mathbf{W}^{[3]} \cdot \boldsymbol{a}^{[2]} + \mathbf{b}^{[3]})$$

Recommended Settings

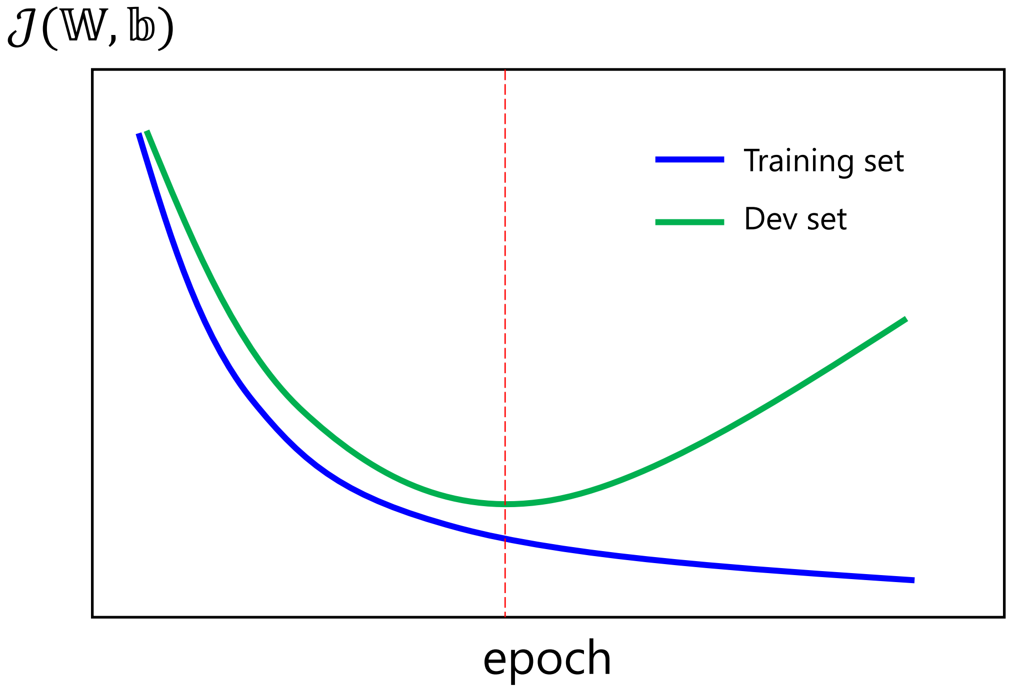
Some idea to set your keepprob



- The keepprob can be different value in different layer
- The lower $n^{[l]}$ (number of hidden units in the layer l) the higher keepprob
- Input layer has keepprob equal to 1

Other Regularizations

Early stopping



- Stop training based on the cost convergence

Gradient

Normalized Input

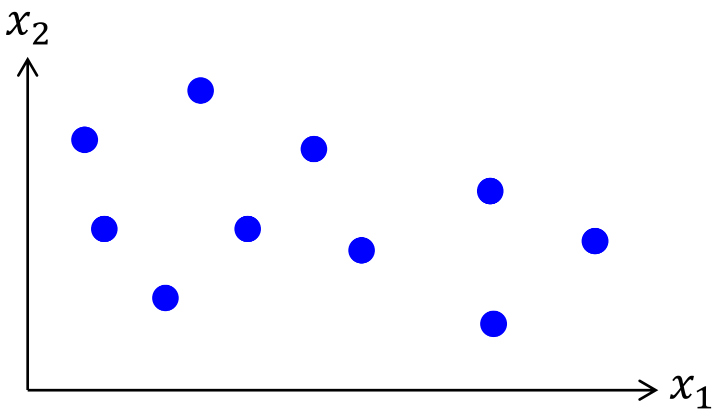
Speed up your training

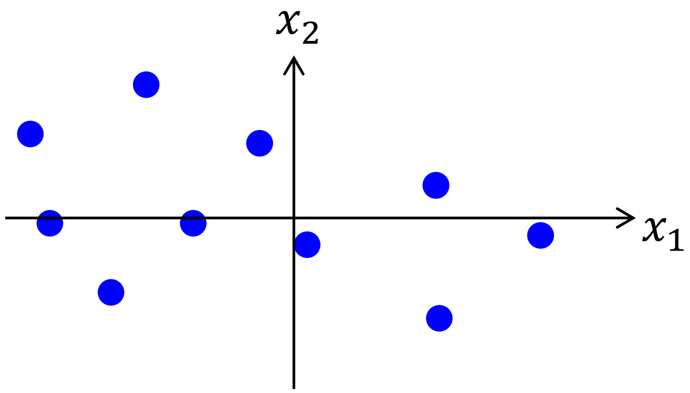
- Subtract mean

$$\mu = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}^{(i)}$$

$$\mathbf{X} \coloneqq \mathbf{X} - \mu$$

- Data will have zero mean

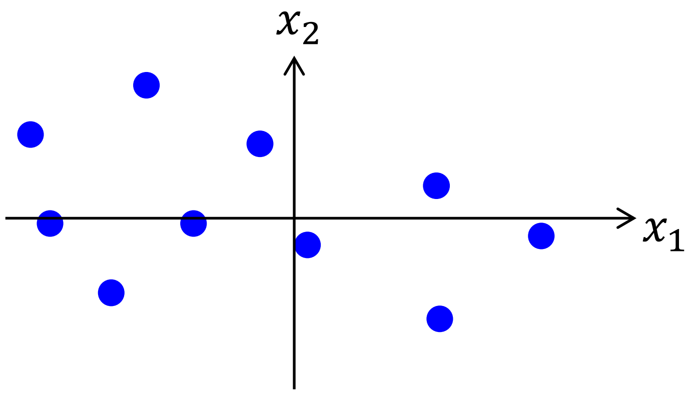




x_1 has higher variance compared to x_2

Normalized Input

Speed up your training

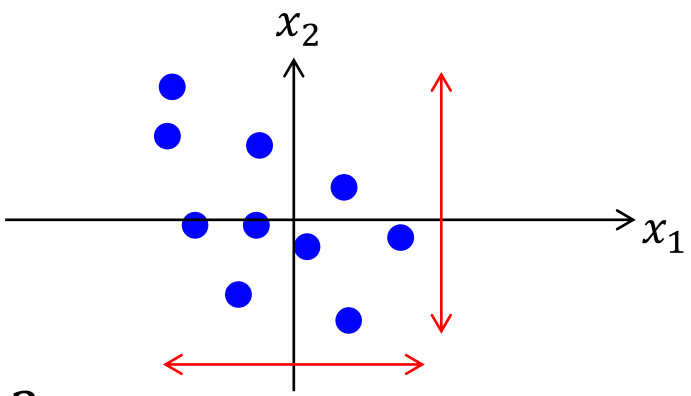


- Normalized variance

$$\sigma^2 = \frac{1}{m}\sum_{i=1}^{m}\left(\mathbf{x}^{(i)}\right)^2$$

$$\mathbf{X} = \frac{\mathbf{X}}{\sigma^2}$$

- Data will have zero mean and normalized variance



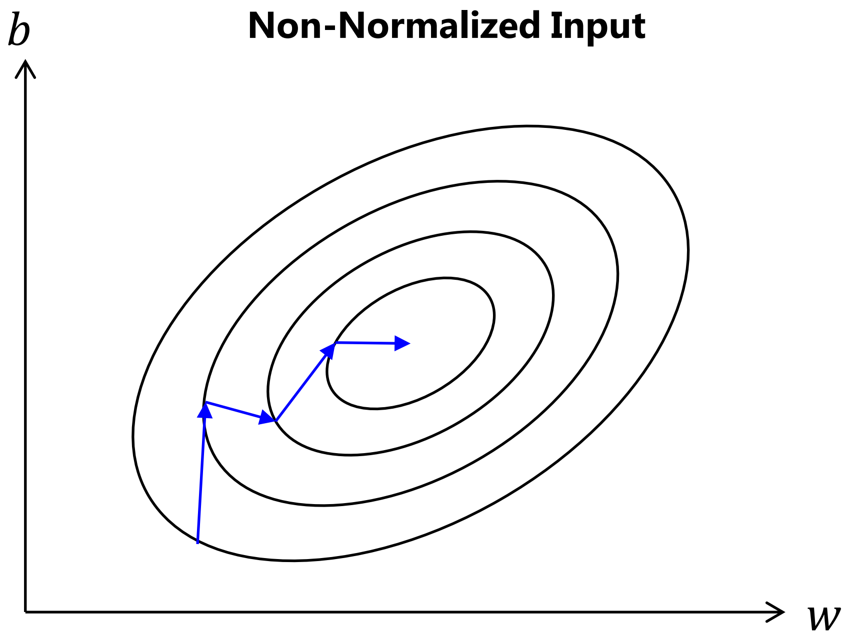
- μ and σ^2 from training set will be used in test set

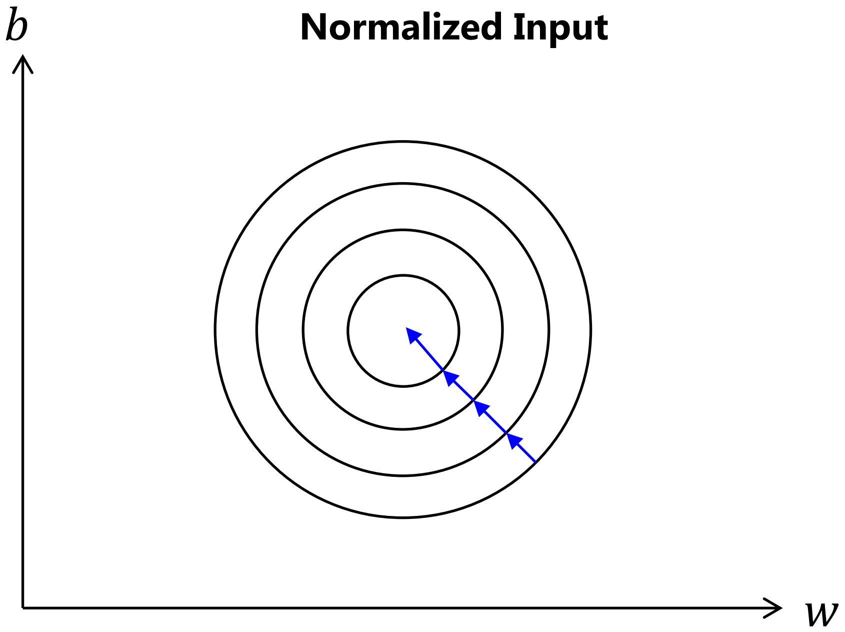
Normalized Input

Speed up your training

- Given a contour of the cost function

Gradient is oscillated and take longer time to the minimum value





Gradient moves more directly to the minimum value

Minibatch Gradient Descent

Batch VS Mini-batch

Dividing training data into minibatch

Notations

$\mathbf{X}^{\{t\}}$ and $\mathbf{y}^{\{t\}}$ for training samples of mini-batch t

- Vectorization enables effective computation over m samples

$$\mathbf{X}_{n_x \times m} = \left[\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(m)}\right]$$

$$\mathbf{y}_{1 \times m} = \left[y^{(1)}, y^{(2)}, \dots, y^{(m)}\right]$$

- What if m is extremely large, e.g. 5,000,000
  - Use mini-batch

$$\mathbf{X}_{n_x \times m} = \Big[\underbrace{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(1000)}}_{\mathbf{X}^{\{1\}}} \Big| \underbrace{\mathbf{x}^{(1001)}, \mathbf{x}^{(1002)}, \dots, \mathbf{x}^{(2000)}}_{\mathbf{X}^{\{2\}}} \Big| \cdots\cdots \Big| \underbrace{\dots\dots \mathbf{x}^{(5,000,000)}}_{\mathbf{X}^{\{5000\}}}\Big]$$

$$\mathbf{y}_{1 \times m} = \Big[\underbrace{y^{(1)}, y^{(2)}, \dots, y^{(1000)}}_{\mathbf{y}^{\{1\}}} \Big| \underbrace{y^{(1001)}, y^{(1002)}, \dots, y^{(2000)}}_{\mathbf{y}^{\{2\}}} \Big| \cdots\cdots \Big| \underbrace{\dots\dots y^{(5,000,000)}}_{\mathbf{y}^{\{5000\}}}\Big]$$

Mini-Batch Implementation

From the previous example

while {

for t in range(0, 5000):

 # Forward propagation on $X^{\{t\}}$

$$\mathbf{z}^{[1]} = \mathbf{w}^{[1]} \cdot \mathbf{X}^{\{t\}} + \mathbf{b}^{[1]}$$

$$\boldsymbol{a}^{[1]} = g(\mathbf{z}^{[1]})$$

$$\vdots$$

$$\mathbf{z}^{[L]} = \mathbf{w}^{[L]} \cdot \boldsymbol{a}^{[L-1]} + \mathbf{b}^{[L]}$$

$$\boldsymbol{a}^{[L]} = g(\mathbf{z}^{[L]})$$

Use vectorization implementation

from $\mathbf{X}^{\{t\}}, \mathbf{y}^{\{t\}}$

$$\mathcal{J}^{\{t\}} = \frac{1}{1000} \sum_{i=1}^{1000} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2 \times 1000} \sum_{l} \left\| \mathbf{w}^{[l]} \right\|_F^2$$

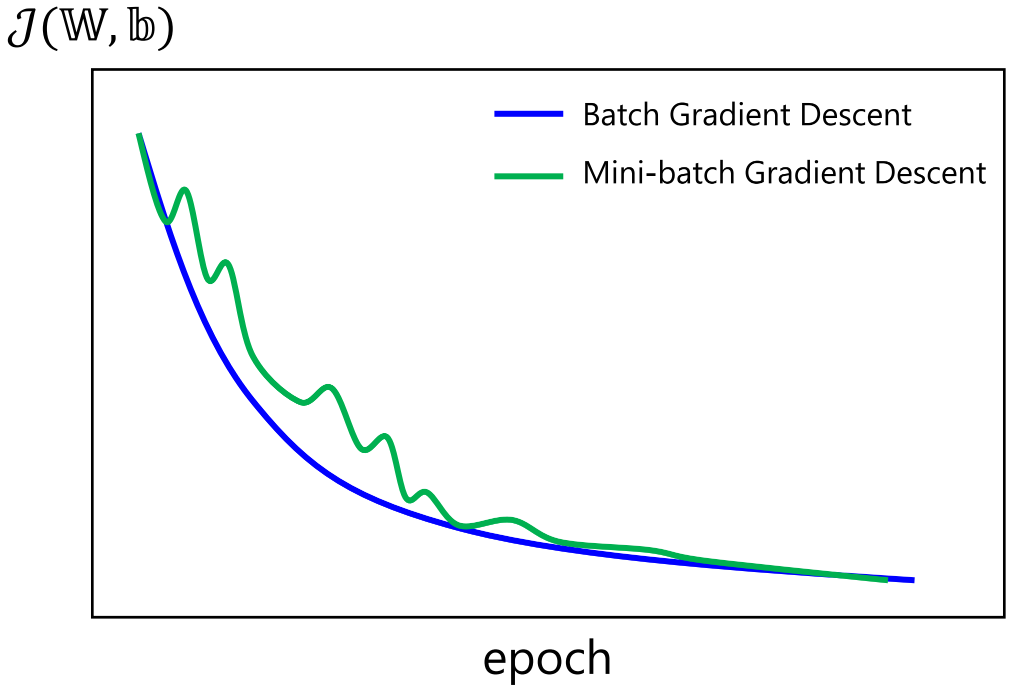
Backward propagation w.r.t. $\mathcal{J}^{\{t\}}$ using $\mathbf{X}^{\{t\}}$ and $\mathbf{y}^{\{t\}}$

$$\mathbf{w}^{[l]} = \mathbf{w}^{[l]} - \alpha \mathbf{dw}^{[l]}$$
$$\mathbf{b}^{[l]} = \mathbf{b}^{[l]} - \alpha \mathbf{db}^{[l]}$$

} until converge

Mini-batch gradient descent

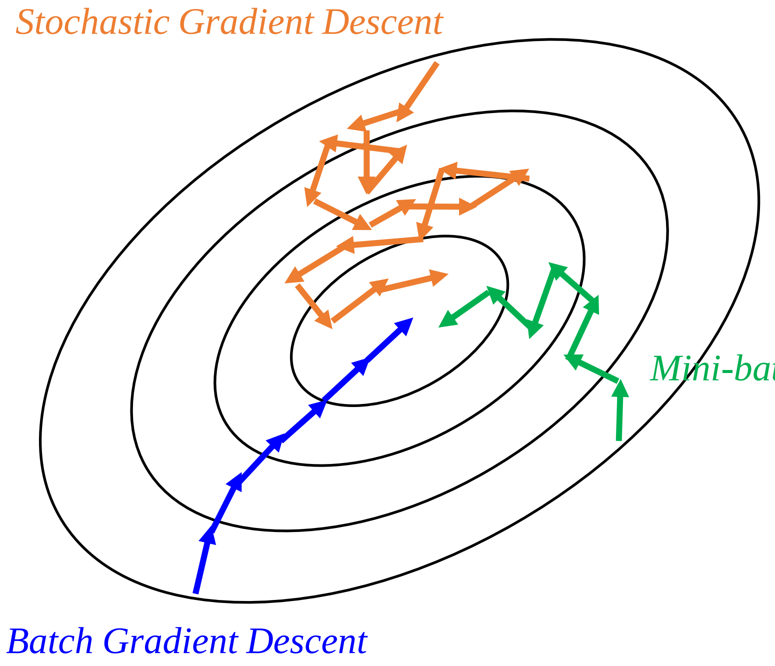
Cost function comparison



- The cost function of mini-batch gradient descent could be oscillated
  - $\mathbf{X}^{\{1\}}$, $\mathbf{y}^{\{1\}}$ might be an easy gradient
  - $\mathbf{X}^{\{2\}}$, $\mathbf{y}^{\{2\}}$ might be a harder gradient
  - Overall should be downward

Choosing Mini-batch size

The extreme cases



- Mini-batch size = m
  - Batch gradient descent

$$\left(\mathbf{X}^{\{1\}}, \mathbf{y}^{\{1\}}\right) = (\mathbf{X}, \mathbf{y})$$

- Mini-batch size = 1
  - Stochastic gradient descent

$$\left(\mathbf{X}^{\{1\}}, \mathbf{y}^{\{1\}}\right) = \left(\mathbf{x}^{(1)}, y^{(1)}\right)$$

Characteristics	Batch	Mini-batch	SGD
Speed	Very Slow	Fast	Slow *Does not leverage vectorization*
Convergence to minimum	Guarantee	Not Guarantee	Not Guarantee

Choosing Mini-batch size

Conclusion

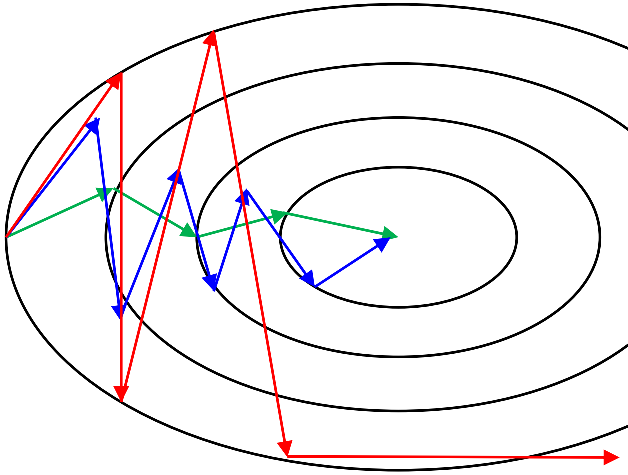
- Small Training Set ($m \leq 2000$)
  - Use Batch gradient descent
- Otherwise
  - Use Mini-batch
- Suggested mini-batch size
  - 2^k to perfectly fit in CPU/GPU memory, e.g. 64, 128, 256, 512, etc

Gradient Optimization

Momentum Gradient Descent, RMSprop, and ADAM

Momentum Gradient Descent

Idea



Gradient Descent

Momentum Gradient Descent

Overshoot (too much learning rate)

- Desired movement directions
  - Fast to the minimum point

    From our example, movement on this direction (→) should be fast

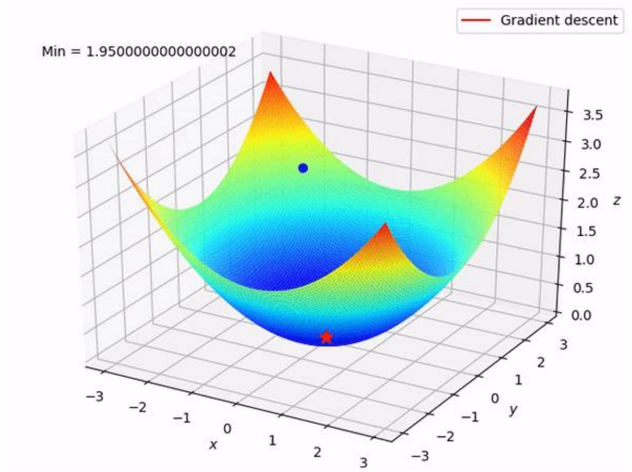
  - Slow to others

    From our example, movement on this direction (↕) should be slow

Momentum Gradient Descent

Velocity and Acceleration

Similar to a ball rolling in a bowl



- On iteration t:

  Compute **dW**, **db** on a set of mini-batch

$$\mathbf{v_{dW}} = \beta\mathbf{v_{dW}} + (1-\beta)\mathbf{dW}$$

friction velocity acceleration

$$\mathbf{v_{db}} = \beta\mathbf{v_{db}} + (1-\beta)\mathbf{db}$$

$$\mathbf{W} = \mathbf{W} - \alpha\mathbf{v_{dW}}$$

$$\mathbf{b} = \mathbf{b} - \alpha\mathbf{v_{db}}$$

Momentum Gradient Descent

Implementation

Initialize $\mathbf{v_{dW}} = 0, \mathbf{v_{db}} = 0$

Note: dimension of $\mathbf{v_{dW}} = \mathbf{dW}$

dimension of $\mathbf{v_{db}} = \mathbf{db}$

Hyper-parameters are α, β

- On iteration t:

  Compute **dW**, **db** on a set of mini-batch

  $$\mathbf{v_{dW}} = \beta \mathbf{v_{dW}} + (1-\beta)\mathbf{dW}$$

  $$\mathbf{v_{db}} = \beta \mathbf{v_{db}} + (1-\beta)\mathbf{db}$$

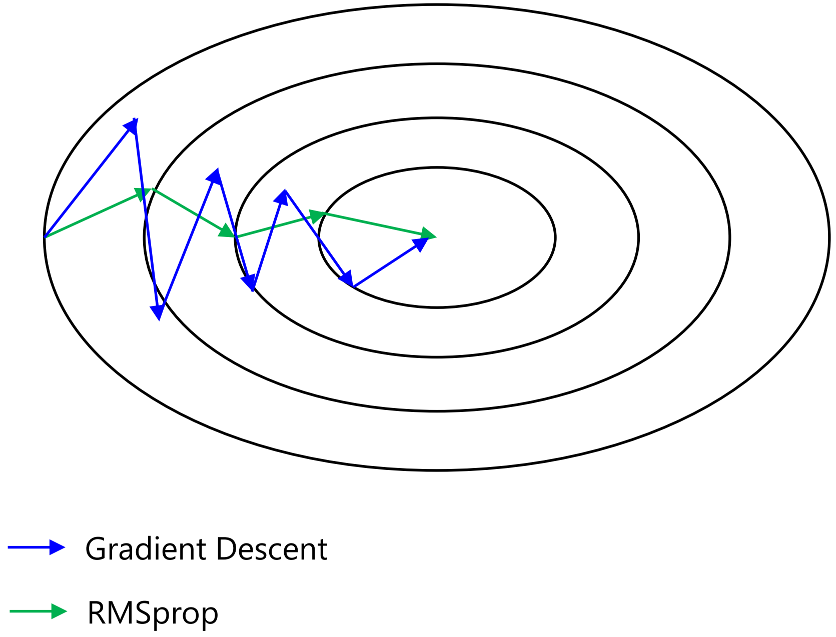
  $$\mathbf{W} = \mathbf{W} - \alpha \mathbf{v_{dW}}$$

  $$\mathbf{b} = \mathbf{b} - \alpha \mathbf{v_{db}}$$

- In practice, $\beta = 0.9$
- Some literature omitted $1 - \beta$

RMSprop

Speed up gradient descent



- On iteration t:

  Compute **dW**, **db** on a set of mini-batch

$$s_{\mathbf{dW}} = \beta s_{\mathbf{dW}} + (1-\beta)\mathbf{dW}^2$$

$$s_{\mathbf{db}} = \beta s_{\mathbf{db}} + (1-\beta)\mathbf{db}^2$$

$$\mathbf{W} = \mathbf{W} - \frac{\alpha \mathbf{dW}}{\sqrt{s_{\mathbf{dW}}} + \varepsilon}$$

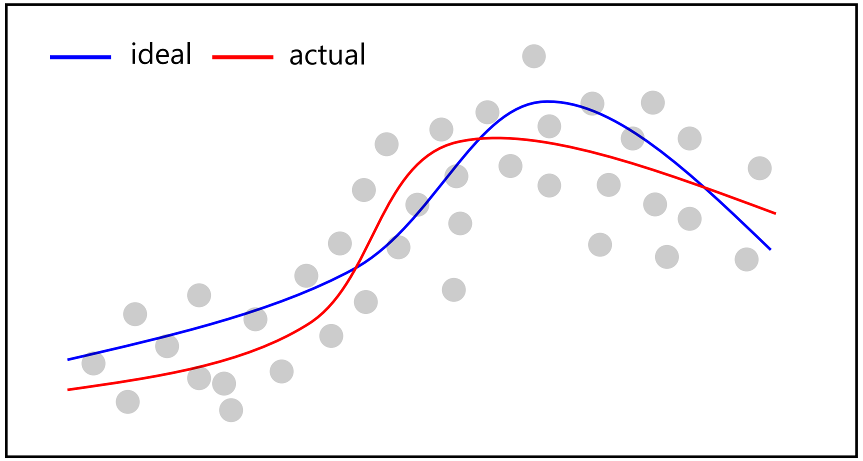
$$\mathbf{b} = \mathbf{b} - \frac{\alpha \mathbf{db}}{\sqrt{s_{\mathbf{db}}} + \varepsilon}$$

a small positive number for numerical stabilization (preventing divided by zero)

- RMSprop enables to use the larger learning rate without overshoot movement

Bias Correction

Idea



- Bias correction of data point t is defined as

$$v_t = \beta v_{t-1} + (1-\beta)\theta_t$$

data point t

$$\text{set } \beta = 0.98, \qquad v_0 = 0$$

$$v_1 = 0.98v_0 + 0.02\theta_1$$

$$v_2 = 0.98v_1 + 0.02\theta_2 = 0.0196\theta_1 + 0.02\theta_2$$

- Use $\dfrac{v_t}{1-\beta^t}$ to estimate the ideal data point t

- Not accurate at the beginning of t but later will be much more accurate

Adaptive Moment Estimation (Adam)

Combining momentum and RMSprop

Initialize $\mathbf{v}_{\mathbf{dW}} = 0, s_{\mathbf{dW}} = 0, \mathbf{v}_{\mathbf{db}} = 0, s_{\mathbf{db}} = 0$

Note: Adam works well in wide range across deep learning applications

- On iteration t:

  Compute **dw**, **db** on a set of mini-batch

$$\mathbf{v}_{\mathbf{dW}} = \beta_1 \mathbf{v}_{\mathbf{dW}} + (1-\beta_1)\mathbf{dW}$$

$$\mathbf{v}_{\mathbf{db}} = \beta_1 \mathbf{v}_{\mathbf{db}} + (1-\beta_1)\mathbf{db}$$

momentum

$$s_{\mathbf{dW}} = \beta_2 s_{\mathbf{dW}} + (1-\beta_2)\mathbf{dW}^2$$

$$s_{\mathbf{db}} = \beta_2 s_{\mathbf{db}} + (1-\beta_2)\mathbf{db}^2$$

RMSprop

$$\mathbf{v}_{\mathbf{dW}}^{\text{correct}} = \frac{\mathbf{v}_{\mathbf{dW}}}{1-\beta_1^t}, \quad \mathbf{v}_{\mathbf{db}}^{\text{correct}} = \frac{\mathbf{v}_{\mathbf{db}}^{\text{correct}}}{1-\beta_1^t}$$

$$\mathbf{s}_{\mathbf{dW}}^{\text{correct}} = \frac{\mathbf{s}_{\mathbf{dW}}}{1-\beta_2^t}, \quad \mathbf{s}_{\mathbf{db}}^{\text{correct}} = \frac{\mathbf{s}_{\mathbf{db}}^{\text{correct}}}{1-\beta_2^t}$$

bias correction

$$\mathbf{W}^{[l]} = \mathbf{W}^{[l]} - \alpha \frac{\mathbf{v}_{\mathbf{dW}}^{\text{correct}}}{\sqrt{\mathbf{s}_{\mathbf{dW}}^{\text{correct}}} + \varepsilon}$$

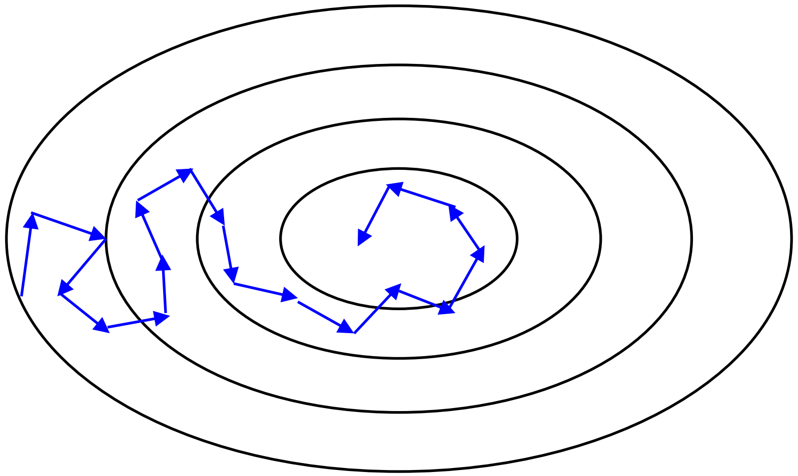
$$\mathbf{b}^{[l]} = \mathbf{b}^{[l]} - \alpha \frac{\mathbf{v}_{\mathbf{db}}^{\text{correct}}}{\sqrt{\mathbf{s}_{\mathbf{db}}^{\text{correct}}} + \varepsilon}$$

updating

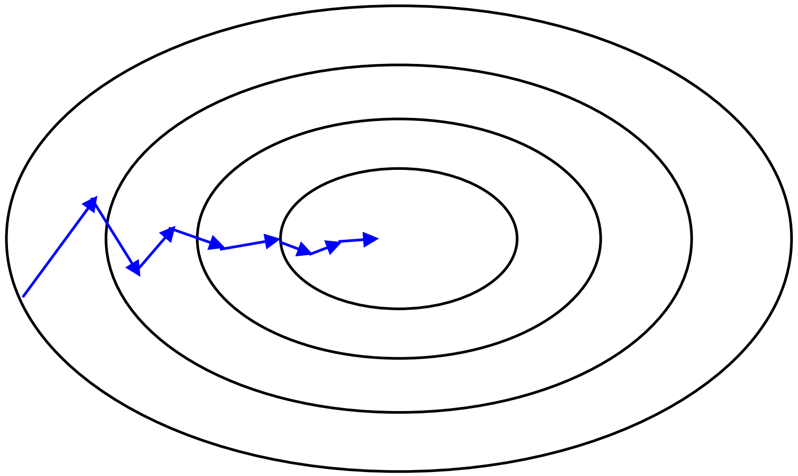
Suggested Hyper-parameters

Fixed learning rate VS Decayed Learning rate

- α: Need to be tuned
- β_1: 0.9
- β_2: 0.999
- ε: 10^{-8}



Fixed learning rate



Decayed Learning rate

Hyperparameter Tuning

Strategy to choose hyper-parameters

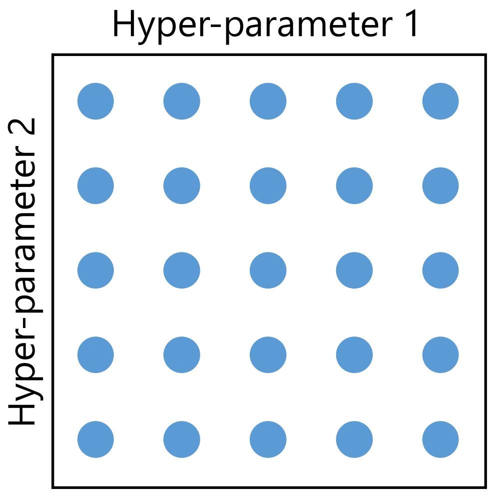
Deep learning hyperparameters

Ranked by importance

- 1st priority
  - α: Learning rate
- 2nd priority
  - β: Adam's parameters only $(\beta_1, \beta_2, \varepsilon)$ (Use default values)
  - Mini-batch size
  - $n^{[l]}$: Number of hidden units in the layer l
- 3rd priority
  - L: Number of layers
  - β: Momentum and RMSprop

Tuning Strategies

Grid approach



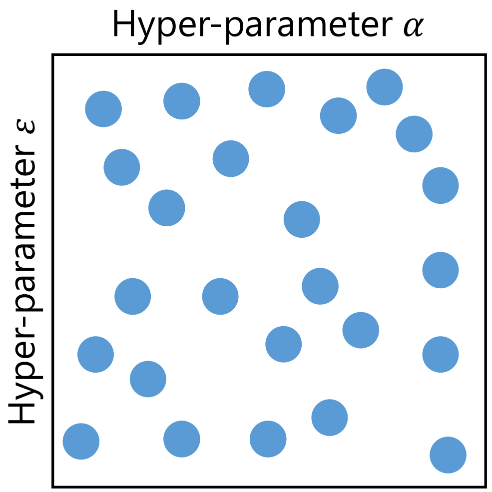
- Grid approach is acceptable for traditional ML

- Limitations
  - Important of some hyperparameters might not be fully address

  - Ex. Grid allows trial on 5 values of α and ε from 25 experiments

Tuning Strategies

For deep learning random grid is better



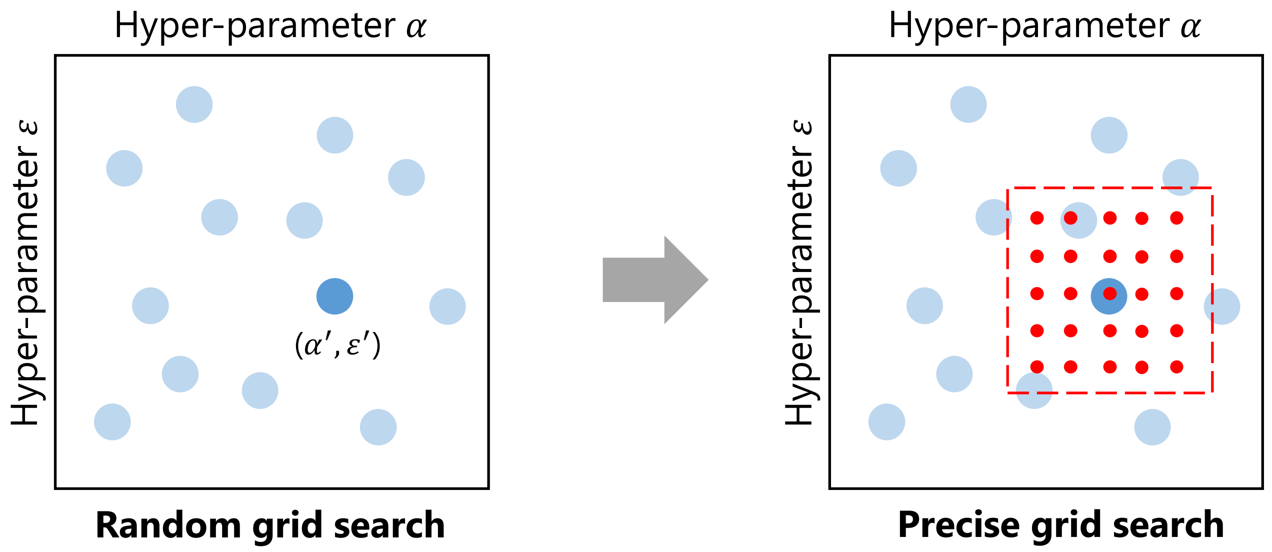
- Random grid allows trial on 25 values of α from 25 experiments

- Random grid gives us more richly to explore sets of possible hyperparameters

Tuning Strategies

Coarse to fine

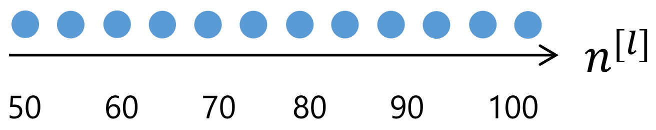
- Start from randomly coarse
- Randomly fine later



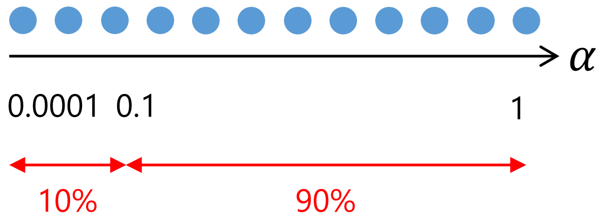
Tuning Strategies

Use the appropriate scale to pitch hyperparameters

- Normal scale works for some hyperparameters
  - $n^{[l]}$
  - L



- Log-scale is good for learning rate



Spending 10% of resource to search between 0.0001 to 0.1 whereas 90% of resources to search between 0.1 to 1