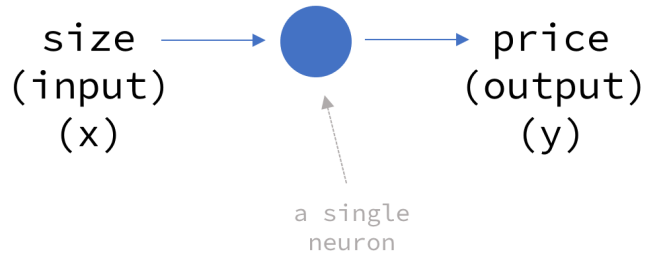
Neural Network & Deep Learning

1 Introduction

1.1 Basic concepts

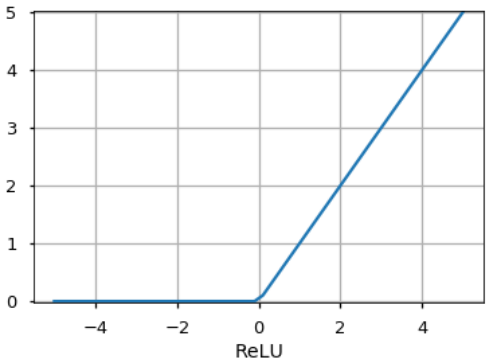
a simple neural network:

housing price prediction



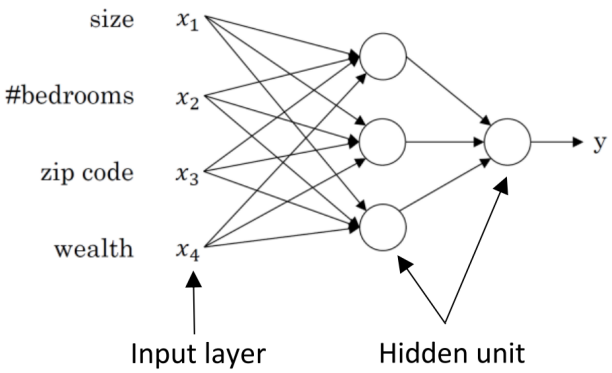
ReLU function (Rectified Linear Unit):

zero at first, then takes off as a straight line



Multiple Neural Network:

stack single neurons together → a larger neural network



- highly automated
- input layer is densely connected
- enought training examples $\overset{supervisedlearning}{\longrightarrow}$ figure out functions

1.2 Supervised Learning

input(x)	output(y)	applications	network type
home features	price	real estate	standard neural network
ad, user info	Click on ad(0/1)	online advertising	standard ...
image	object(1, ..., 1000)	photo tagging	convolutional neural network (CNN)
audio	text transcript	speech recognition	recurrent neural network (RNN)
English	Chinese	machine translation	RNN
image, radar info	position of other cars	autonomous driving	custom/ hybrid neural network

structured/ unstructured data

- structured data: databases of data (has a defined meaning)
- unstructured data: audio, image, text (relatively harder to be interpreted)

1.3 why so popular now: scale drives deep learning progress

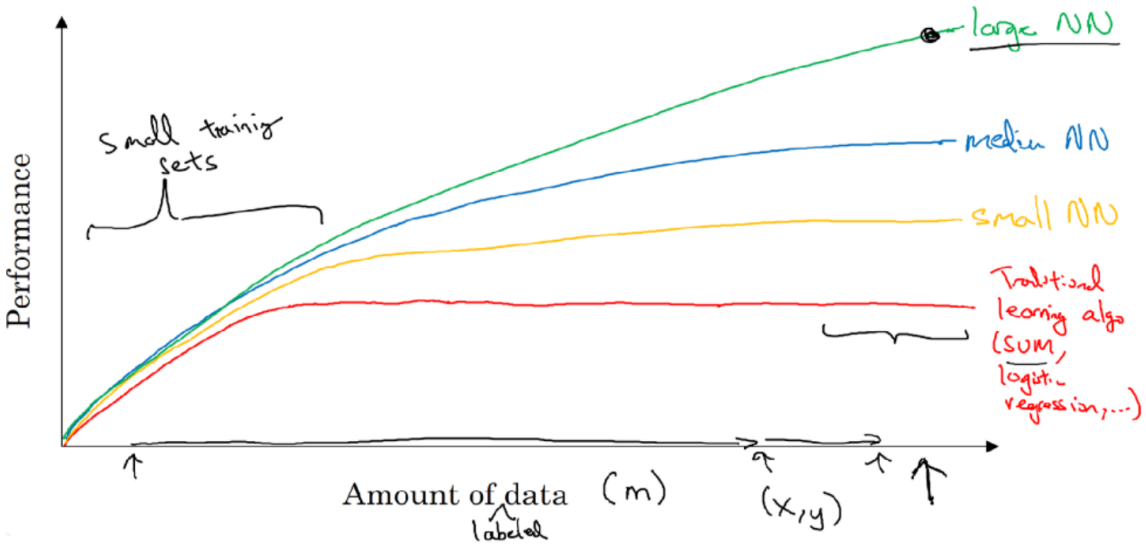
traditional learning algorithm:

support vector machine, logistic regression ...

- unable to deal with huge amounts of data
- while **digitization** of a soceity creates more data

two things to enhance the performance

1. be able to train a** big enough neural network** (hidden units, parameters, connections, data ...)
2. need **a lot of data** notation:m the size of the training set

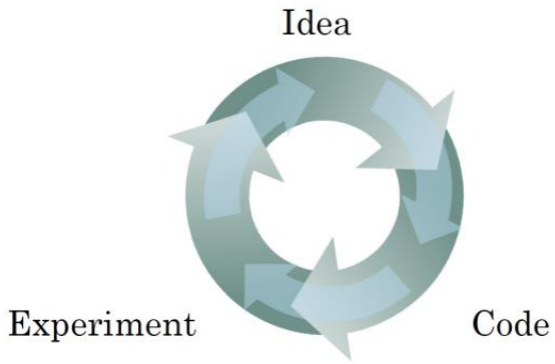


- small training sets: not very clear (your skill at hand engineering features determines the performance + some details)
- big data: large NN dominating others

the progress of deep learning includes:

data + computation + algorithms

- example of algorithm innovation: changing sigmoid to ReLU has made *gradient descent* work much faster
- computation: **hardware + algorithms**



- the process of training NN is iterative
- faster computation enables you to try more ideas and improve them

2 Basics of Neural Network programming

2.1 Binary Classification

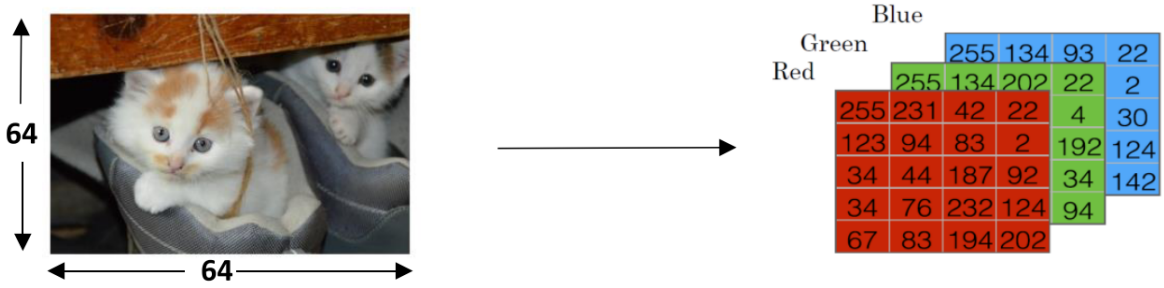
the result is a **discrete** value out put (e.g. 0/1)

- don't need a "for" loop to go over your training set
- use forward / backward propagation

a picture

→ 3 matrices of pixel intensity values (Red, Green, Blue)
→ feature vector x (n_x: dimension = total numbers of the matrices)

- example: cat / non-cat



$$x = \begin{bmatrix} 255 \\ 231 \\ 42 \\ \vdots \\ 255 \\ 134 \\ 202 \\ \vdots \\ 255 \\ 134 \\ 93 \\ \vdots \end{bmatrix} \begin{matrix} \text{red} \\ \\ \\ \\ \text{green} \\ \\ \\ \\ \text{blue} \\ \\ \\ \end{matrix}$$

$n_x = 64 \times 64 \times 3$

some notations

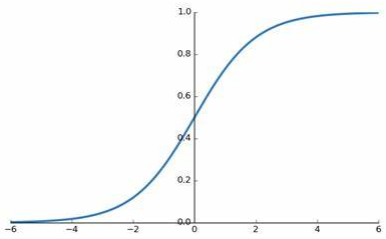
(x, y): a single training example: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)})$...
m: number of training examples
$m = m_{train}$ (training sets) / m_{test} (test sets)
$X = [x_1, x_2, \dots, x_m]$
$X.shape = (n_x, m)$
$Y = [y_1, y_2, \dots, y_m]$
$Y.shape = (1, m)$

2.2 Logistic Regression

Given x, want $\hat{y} = P(y = 1|x)$ (the probability of "y=1")
$x \in R^{n_x}$
parameters: $w \in R^{n_x}, b \in R$

if you use linear regression, you'll get $\hat{y} = w^T x + b$, which is not satisfying
then we apply it to the sigmoid function: $\hat{y} = \sigma(w^T x + b)$

- Sigmoid function:
  $\sigma(z) = \frac{1}{1+e^{-z}}$



$\hat{y} = \sigma(w^T x + b)$, where $\sigma(z) = \frac{1}{1+e^{-z}}$
Given $\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$, want $\hat{y}^{(i)} \approx y^{(i)}$

(the superscript parentheses "i" refers to data associated with the i-th training example)

Loss(error) function

(if use square error, gradient descent may not find the global optimum)
defined with respect to a **single** training example
$\mathcal{L}(\hat{y}, y) = -(y log\ \hat{y} + (1-y) log(1-\hat{y}))$
notice: "log" means "ln"

Goal: make $\mathcal{L}$ as small as possible
if $y = 1$: $\mathcal{L}(\hat{y}, y) = -log\hat{y}$
→ parameters make $\hat{y}$ close to 1
if $y = 0$: $\mathcal{L}(\hat{y}, y) = -log(1-\hat{y})$
→ parameters make $\hat{y}$ close to 0

Cost function

the cost of your parameters on the** entire** training set

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) = \frac{1}{m}\sum_{i=1}^{m} -(y^{(i)} log\ \hat{y}^{(i)} + (1-y^{(i)}) log(1-\hat{y}^{(i)}))$$

justification:

$$\left.\begin{array}{ll} if & y=1 : p(y|x) = \hat{y} \\ if & y=0 : p(y|x) = 1-\hat{y} \end{array}\right\} p(y|x) = \hat{y}^y (1-\hat{y})^{1-y}$$
$$since \quad maximizing\ p(y|x) \leftrightarrow maximizing\ log\ p(y|x)$$
$$then, \quad log\ p(y|x) = log\ \hat{y}^y (1-\hat{y})^{1-y} = (y log\ \hat{y} + (1-y) log(1-\hat{y}))$$

add the minus sign: minimizing the loss corresponds to maximizing the log of the probability

$$\begin{aligned} log\ p(labels\ in\ training\ set) &= log \prod_{i=1}^{m} p(y^{(i)}|x^{(i)}) \\ &= \sum_{i=1}^{m} p(y^{(i)}|x^{(i)}) \\ &= -\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) \\ J(w,b) &= \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}\hat{y}^{(i)}, y^{(i)}) \end{aligned}$$

$\frac{1}{m}$: for scaling
remove the minus sign: change minimizing to maximizing

2.3 Gradient Descent

want to find w, b that minimize $J(w,b)$

$J(w,b)$ is a convex function (makes this method possible)

1. initialize w, b (usually use 0) (random initialization is feasible)
2. start from the initial point and step towards the global optimum

Repeat {
$w := w - \alpha \frac{\partial J(w,b)}{\partial w}$
$b := b - \alpha \frac{\partial J(w,b)}{\partial b}$
}
notation:
α: learning rate (controls the length of each iteration)
$\frac{\partial J(w,b)}{\partial w}$: in code we use "dw"

- (suppose we only have 2 'x'):

$$x_1, x_2, w_1, w_2, b \rightarrow \boxed{z = w_1 x_1 + w_2 x_2 + b} \rightarrow \boxed{a = \sigma(z)} \rightarrow \boxed{\mathcal{L}(a, y)}$$

$$\begin{aligned} dz &= \frac{d\mathcal{L}}{dz} \\ &= \frac{d\mathcal{L}}{da} \cdot \frac{da}{dz} \\ &= (-\frac{y}{a} + \frac{1-y}{1-a}) \cdot a(1-a) \\ &= a - y \end{aligned}$$

$$\begin{aligned} then, \quad \frac{d\mathcal{L}}{dw_1} = dw_1 &= x_1 \cdot dz \\ \frac{d\mathcal{L}}{dw_2} = dw_2 &= x_2 \cdot dz \\ db &= dz \end{aligned}$$

apply them to gradient descent method (the "Repeat" part) to update the parameters

- (on m examples):
  $\frac{\partial}{\partial w_1} J(w, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial w_1} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$
- notice: when dealing with huge data sets, **avoid** using for-loops explicitly in the program (low effeciency), use **vectorization**

2.4 Vectorization

while computing $z = w^T x + b \quad (x \in R^{n_x}, w \in R^{n_x})$:

Non-vectorized	**Vectorized**
z = 0 for i in range(n_x): z += w[i]*x[i] z += b	import numpy z = np.dot(w, x) + b

- **SIMD**: single Instruction Multiple Data

  works on CPU & GPU

  numpy can take much better advantage of parallelism than for-loops thanks to SIMD

more examples:

np.exp(), np.log(), np.abs(), np.maximum(), ...

$$np.exp(): \qquad v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{bmatrix} \rightarrow u = \begin{bmatrix} e^{v_1} \\ e^{v_2} \\ \vdots \\ e^{v_m} \end{bmatrix}$$

vectorizing logistic regression & gradient descent

for iter in range(...):

$$
\begin{aligned}
Z &= [z^{(1)} \quad z^{(2)} \quad \cdots z^{(m)}] = w^T X + [b \quad b \quad \cdots b] \\
A &= [a^{(1)} \quad a^{(2)} \quad \cdots a^{(m)}] = \sigma(Z) \\
dz &= A - Y = [a^{(1)} - y^{(1)} \quad a^{(2)} - y^{(2)} \quad \cdots a^{(m)} - y^{(m)}] \\
db &= \frac{1}{m} \sum_{i=1}^{m} dz^{(i)} \\
dw &= \frac{1}{m} X dz^T = \frac{1}{m} [x^{(1)} dz^{(1)} + \cdots + x^{(m)} dz^{(m)}] \quad (an \quad n_x \times 1 \quad vector) \\
w &:= w - \alpha dw \\
b &:= b - \alpha db
\end{aligned}
$$

```python
# some code
import numpy as np
Z = np.dot(w.T, X) + b
db = np.sum(dz)
```

notice(broadcasting): here "b" is a real number, but Python will process it as a 1×m vector

2.5 About Python & NumPy: Some tricks

broadcasting

- duplicate the contents in the matrix (or a real number) to make its size appropriate
  code: [matrix].reshape(m, n)
- automated in Python, but you can use the reshape function to ensure the size of the matrix

data structure

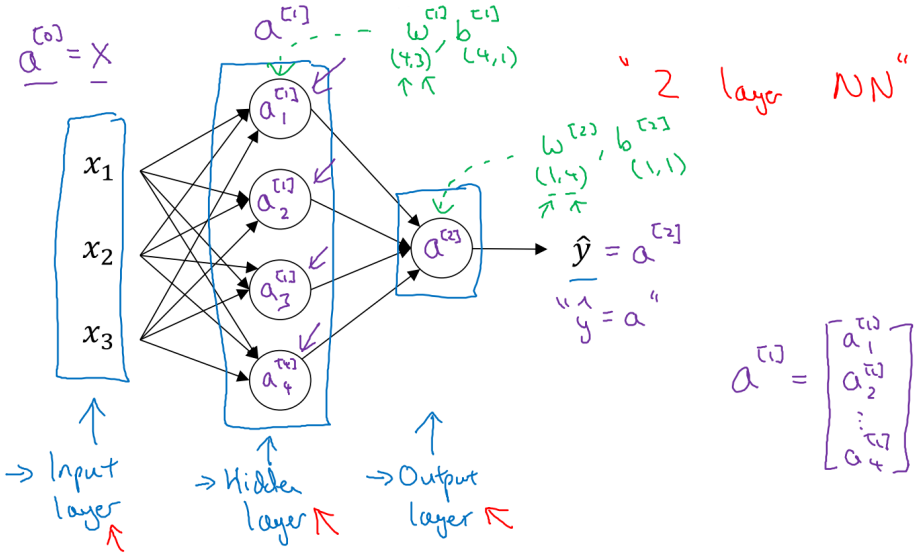
```python
import numpy as np

# avoid such data structure!
a = np.random.randn(5) # rank 1 array
print(a)
print(a.T) # looks the same as a
print(np.dot(a, a.T))  # a real number

# use this↓
b = np.random.randn(5,1) # 5*1 column vector
print(np.dot(b, b.T)) # a 5*5 matrix

assert(a.shape == (5,1)) # to make sure
```

3 One Hidden Layer Neural Network

3.1 Overview

- 2-layer NN
  repeat the logistic regression several times
  [i]: imply the number of different layers

the input layer is **not** counted



3.2 Computing the output

stack data into a matrix/vector to compute them simultaneously

- horizontally: different training examples
- vertically: different nodes in the NN

$$
\begin{aligned}
Z^{[1]} &= W^{[1]} X + b^{[1]} \\
A^{[1]} &= g(Z^{[1]}) \\
Z^{[2]} &= W^{[2]} A^{[1]} + b^{[2]} \\
A^{[2]} &= g(Z^{[2]})
\end{aligned}
\qquad
W^{[1]} = \begin{bmatrix} w_1^{[1]T} \\ w_2^{[1]T} \\ w_3^{[1]T} \\ w_4^{[1]T} \end{bmatrix}
$$

$$
X = A^{[0]} = \begin{bmatrix} x^{(1)} & x^{(2)} & \cdots & x^{(m)} \end{bmatrix}
$$

3.3 Activation Functions

activation functions can be different for different layers

Sigmoid function

$$
\begin{aligned}
a &= \frac{1}{1+e^{-z}} \\
\frac{da}{dz} &= a(1-a)
\end{aligned}
$$

only use this in the output layer while doing binary classification

Tanh function

$$
\begin{aligned}
a &= \frac{e^{z}-e^{-z}}{e^{z}+e^{-z}} \\
\frac{da}{dz} &= 1-a^2
\end{aligned}
$$

a shifted version of sigmoid function
works better than sigmoid function
problem: when z is either too large or too small, the slope is close to 0, which slows down the gradient descent process

ReLU function

$$a = max(0, z)$$

$$\frac{da}{dz} = \begin{cases} 0 & \text{if z} < 0 \\ 1 & \text{if z} > 0 \\ undefined & \text{if z} = 0 \end{cases}$$

$$leaky\ ReLU:\ a = max(0.01z, z)$$

default function of activation function
problem: derivative doesn't exist when z=0, but in practice it doesn't matter (the chance of z being precisely 0.000... is so small, and you can manually set the derivative 1 or 0;)

why we need a non-linear activation function?

if we use the linear activation function (identity activation function), then the output is just a linear function of the input, then the hidden layer becomes useless
sometimes, we use linear function, but it is very rare

3.4 Gradient Descent for Neural Networks

Parameters: $w^{[1]}, b^{[1]}, w^{[2]}, b^{[2]}, n_x = n^{[0]}, n^{[1]}, n^{[2]} = 1$

Cost function: $J(w^{[1]}, b^{[1]}, w^{[2]}, b^{[2]}) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}, y)$

Gradient Descent:

$$\begin{aligned}
&\text{Repeat } \{ \\
&\quad \text{Compute Predictions} \quad (\hat{y}^{(i)}, i = 1, 2, \dots, m) \\
&\quad dw^{[1]} = \frac{\partial J}{\partial w^{[1]}} \\
&\quad db^{[1]} = \frac{\partial J}{\partial b^{[1]}} \\
&\quad dw^{[2]} = \dots, \quad db^{[2]} = \dots \\
&\quad w^{[1]} := w^{[1]} - \alpha dw^{[1]} \\
&\quad b^{[1]} := b^{[1]} - \alpha db^{[1]} \\
&\quad w^{[2]} := \dots, \quad b^{[2]} := \dots \\
&\quad \}
\end{aligned}$$

Forward Propagation:

$$\begin{aligned}
Z^{[1]} &= W^{[1]} X + b^{[1]} \\
A^{[1]} &= g(Z^{[1]}) \\
Z^{[2]} &= W^{[2]} A^{[1]} + b^{[2]} \\
A^{[2]} &= g(Z^{[2]})
\end{aligned}$$

Backward Propagation:

$$\begin{aligned}
dZ^{[2]} &= A^{[2]} - Y \\
dW^{[2]} &= \frac{1}{m} dZ^{[2]} A^{[1]T} \\
db^{[2]} &= \frac{1}{m} np.sum(dZ^{[2]},\ axis = 1,\ keepdims = True) \\
dZ^{[1]} &= W^{[2]T} dZ^{[2]} * g^{[1]'}(Z^{[1]}) \quad * : \text{element-wise product} \\
dW^{[1]} &= \frac{1}{m} dZ^{[1]} X^T \\
db^{[1]} &= \frac{1}{m} np.sum(dZ^{[1]},\ asix = 1,\ keepdims = True)
\end{aligned}$$

3.5 Random Initialization

if you initialize hidden units of the same layer with the same **W** parameter, then they become symmetric and end up with the same result
parameter **b** doesn't have the symmetric problem

- solution:
  $W^{[1]}$=np.random.rand((2,2))*0.01
  $b^{[1]}$=np.zero((2,1))

"*0.01": if **W** is too large, it will result in very large values of **z** and causes the activation function to be saturated, thus slowing down the learning process.

4 Deep Neural Networks

4.1 Deep L-layer Neural Network

notations

L: number of layers
$n^{[l]}$: units in layer l
$a^{[l]}$: activations in layer l ($a^{[l]}=g^{[l]}(z^{[l]})$)
$w^{[l]}$: weights for $z^{[l]}$

$$Z^{[l]} = W^{[l]} A^{[l-1]} + b^{[l]}$$
$$A^{[l]} = g^{[l]}(Z^{[l]})$$

- use explicit for-loops to compute **each layer**

dimensions

$$z^{[i]} = W^{[i]} a^{[i-1]} + b^{[i]}$$

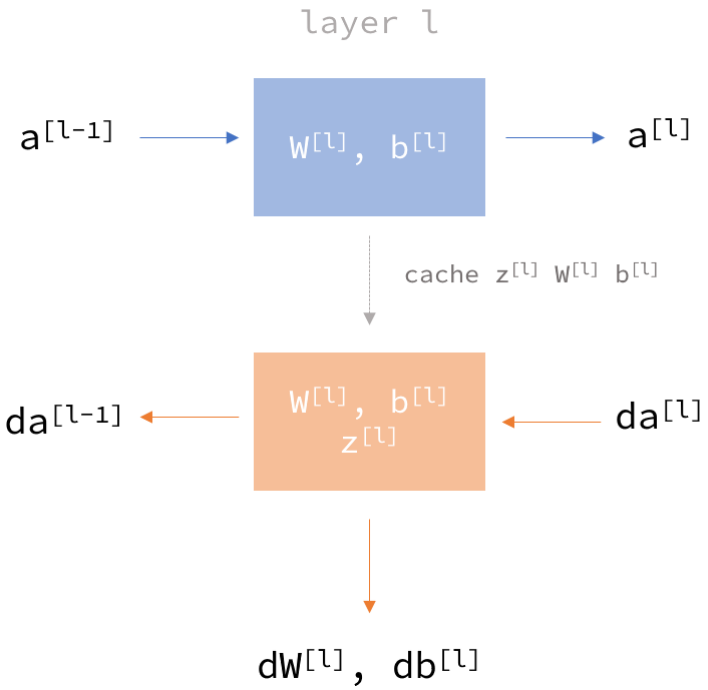
$W^{[i]}$.shape = ($n^{[i]}$, $n^{[i-1]}$)
$z^{[i]}$.shape = ($n^{[i]}$, 1),
$a^{[i-1]}$.shape = ($n^{[i-1]}$, 1)
$b^{[i]}$.shape = ($n^{[i]}$, 1)

- dW / db should have the same dimension as W / b
- after vectorization, the "1" becomes "m"

intuition about deep NN

- different layers have different functions (from simple to complex)
  earlier layers find simple things (edges, ...)
  deeper layers compose them together to detect more complex things (eyes, noses)
- circuit theory & deep learning
  There are functions you can compute with a "small" L-layer deep neural network that shallower networks require exponentially more hidden units to compute

4.2 Building Blocks of Deep Neural Networks



connecting blocks like this together makes up the forward & backward propagation

4.3 Parameters & Hyper Parameters

- Parameters: $W^{[1]}$, $b^{[1]}$, $W^{[2]}$, $b^{[2]}$, ...
- Hyper parameters: control parameters like W, b, ...
  α: learning rate
  L: number of hidden layers
  $n^{[i]}$: hidden units
  choice of activation function, momentum, minibatch size, regularization, ...

applied deep learning is a very **empirical** process
try out different values for parameters, iterate and find what works

2020.08
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Written with Typora