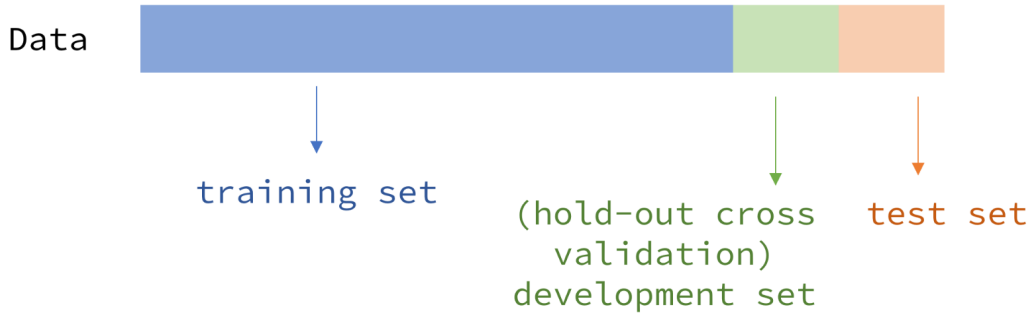
Improving Deep Neural Networks

1 Setting Up your Machine Learning application

1.1 train / dev/ test sets



- Previously: **70%** train + **30%** test // **60%** train + **20%** dev + **20%** test
- Now (big data): 1,000,000 = 980,000(**98%**) train + 10,000(**1%**) dev + 10,000(**1%**) test
  for data sets with over 1 million examples, the training set can take up 99.5%

A test set is not always necessary (depend on whether you need an unbiased estimate)

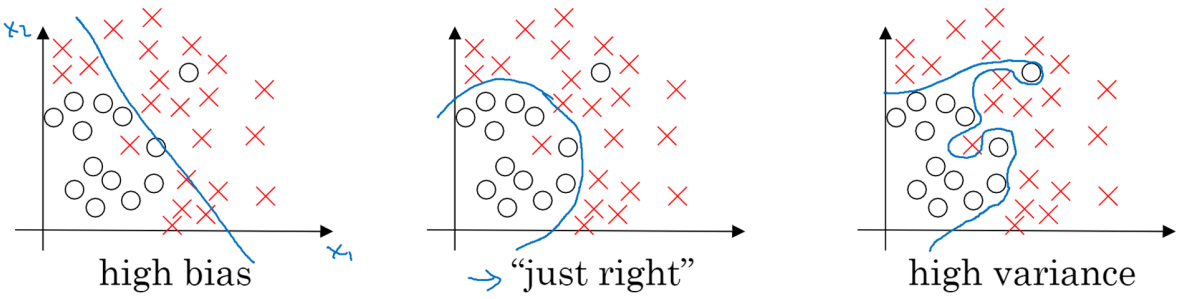
Mismatched train/test distribution

for example:

- training set: cat pictures from webpages
- dev/test sets: cat pictures from users using the app

One Rule: make sure that dev and test sets come from the same distribution

1.2 Bias & Variance

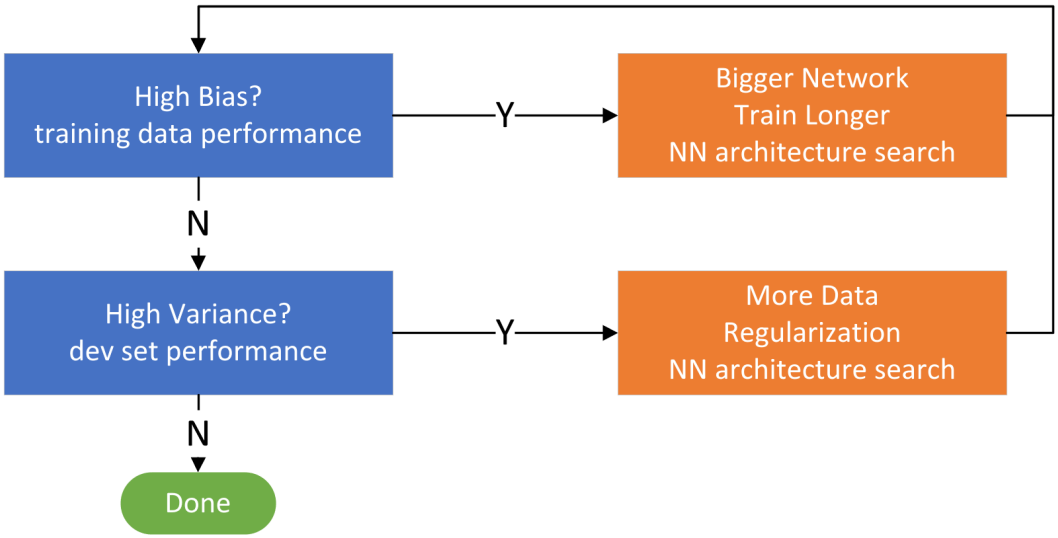


underfitting overfitting

*	High Variance	High Bias	High Bias & High Variance	Low Bias & Low Variance
Train set error	1%	15%	15%	0.5%
Dev set error	11%	16%	30%	1%

* based on the assumption that Bayesion Optimal error is close to 0%

1.3 Basic "Recipe" for ML



Bias-Variance trade-off

1.4 Regularization

in logistic regression:

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

$$L_2\ regularization:\ ||w||_2^2 = \sum_{j=1}^{n_x} w_j^2 = w^T w$$

$$\text{square Euclidean norm of the parameter vector w}$$

$$(L_1\ regularization:\ \frac{\lambda}{2m}|w|_1 = \frac{\lambda}{2m}\sum_{j=1}^{n_x}|w_j|)$$

- omitting the regularization of **b** makes little difference (w is a high dimensional parameter vector, while b is just a single number)
- if we use L_1 regularization, then **w** will end up being sparse (have a lot of zeros)

notice: "lambda" is a reserved keyword in Python, use "lambd" to represent the lambda regularization parameter

in neural network:

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

$$||w^{[l]}||_F^2 = \sum_{i=1}^{n^{[l-1]}}\sum_{j=1}^{n^{[l]}}(w_{ij}^{[l]})^2 \qquad w : (n^{[l-1]}, n^{[l]})$$

$$\text{Frobenius norm of the parameter vector w}$$

$$dw^{[l]} = (\text{from backprop}) + \boxed{\frac{\lambda}{m}w^{[l]}}$$

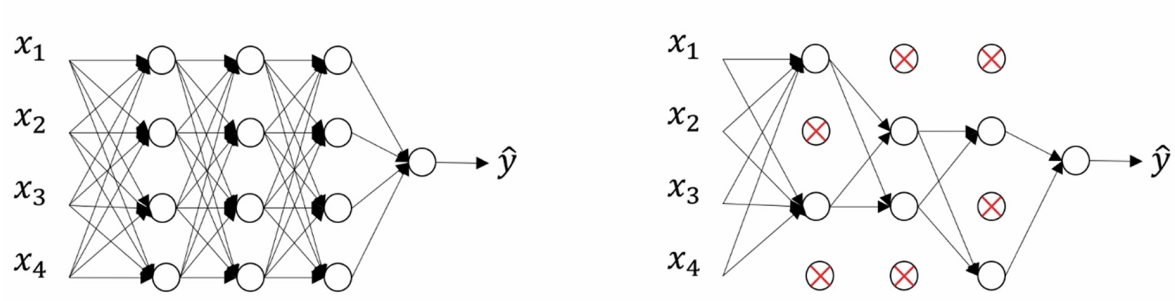
$$\begin{aligned}\text{"weight decay"} \quad w^{[l]} &:= w^{[l]} - \alpha dw^{[l]} \\ &:= w^{[l]} - \alpha[(\text{from backprop}) + \frac{\lambda}{m}w^{[l]}] \\ &:= (1 - \frac{\alpha\lambda}{m})w^{[l]} - \alpha(\text{from backprop})\end{aligned}$$

why regularization reduces overfitting?

big λ causes W close to zero
→ zero out or at least reduce the impact of many hidden units
→ a simple, but deep NN (close to logistic regression)

big λ and small W causes Z relatively small
→ the activation function (on a small range) will be relatively linear
→ the neural network will be calculating something close to a simple linear function
→ less likely to overfit

1.5 Dropout Regularization



for **each** example:

1. go through each of the layers
2. set some probability of eliminating a node in neural network
3. eliminate the selected nodes (remove all the ingoing & outgoing things from the selected nodes)
4. end up with a much smaller, diminished network

implementing dropout (inverted dropout)

L=3, keep-prob=0.8

d^3=np.random.rand(a^3.shape[0], a^3.shape[1]) < keep-prob

a^3=np.multiply(a^3, d^3)

a^3 /= keep-prob #ensure the expected value of a^3 remains the same

NO dropout at **test** time
the output shouldn't be random, it will add noise to your prediction

intuitions about dropout

why it works

- using a smaller network is like using a regularized network
- can't rely on any one feature, so have to spread out weights (onto differet units)

  tend to have an effect of shrinking the squared norm of the weights

usage:

1. lower the value of keep-prob for layers that are more likely to overfit (drawback: need to search more hyper parameters for using cross-validation)
2. apply dropout to some layers and don't apply to others

frequently used in computer vision (lack of data causes overfitting)
only use it when the function is overfitting

downside: while using dropout, the cost function **J** is not well-defined, so it becomes harder to check wheter the cost funtion **J** is declining.

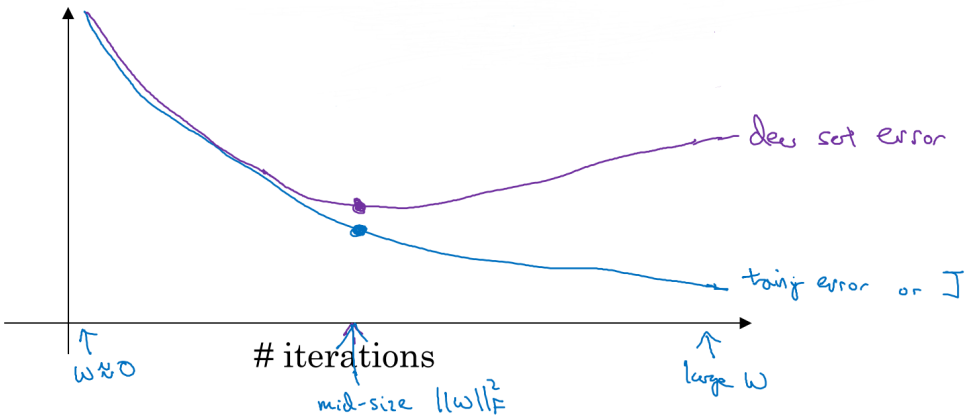
1.6 Other Regularization Methods

Data Augmentation

when having trouble obtaining new training data, augment the current training set

images: flip, distort, rotate, clip...
characters: rotate, distort...

Early Stopping



plot [dev set error] and [training error / cost function J] in the same graph
stop training **halfway**

using 1 method to solve 2 problems:

1. optimize the cost function J -- gradient descent, ...
2. not overfit -- regularization, ...

1.7 Normalizing Input

1. substract/zero out the mean:

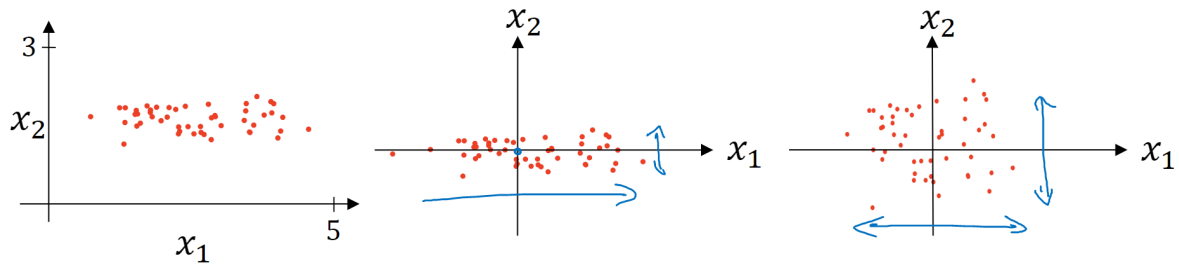
$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$
$$x = x - \mu$$

2. normalize variance

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

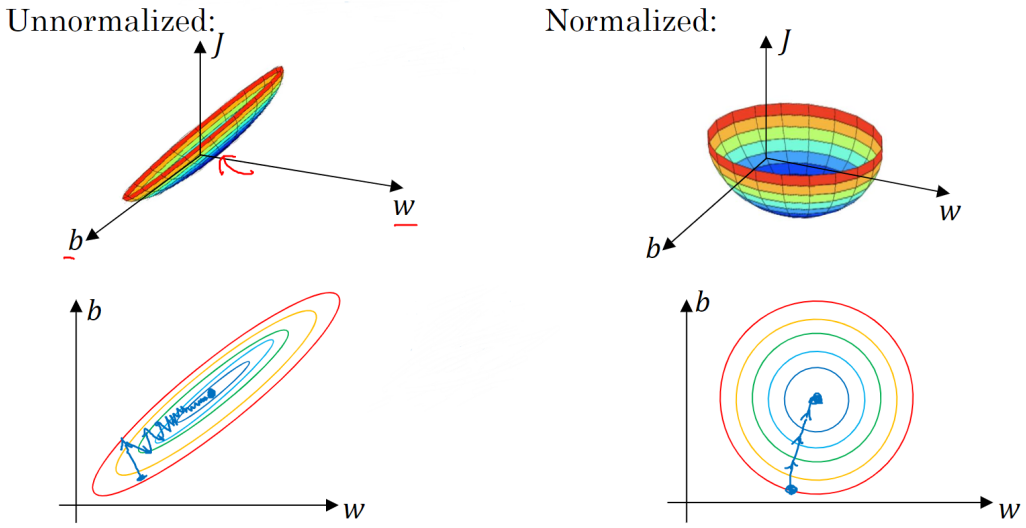
$$x/ = \sigma^2$$

$**$: element y squaring ???



- result: the variance of x1 and x2 are both equal to 1
- tip: use the **same** μ and σ to normalize the training set and the test set

why normalize?



ensure all the features on a similar scale, more symmetric, can use larger steps ...
→ easier to optimize

1.8 Vanishing/Exploding Gradients

if the weight parameter **w** is more\less than 1,
then in a very **deep** network, the activations increasing/decreasing **exponentially**

partial solution

set a reasonable **variance** of the initialization of the weight matrices

- doesn't solve but help reduce the vanishing/exploding gradients problem

for ReLU:

$$z = w_1 x_1 + w_2 x_2 + \ldots + w_n x_n$$

$$\text{larger } n \rightarrow \text{smaller } w_1$$

$$\text{in order to make} \quad Var(w_i) = \frac{2}{n}$$

$$\text{let} \quad W^{[l]} = \text{np.random.randn(shape)} * \boxed{\text{np.sqrt}(\frac{2}{n^{[l-1]}})}$$

for other activations:

tanh: $\sqrt{\frac{1}{n^{[l-1]}}}$ (Xavier Initialization), or $\sqrt{\frac{2}{n^{[l-1]}+n^{[l]}}}$

- set the variance as a hyperparameter
- tuning this parameter is not so effective

1.9 Gradient Checking

Numerical Approximation of Gradients

$$\text{two-sided:} \quad f'(\theta) = \lim_{\epsilon \to 0} \frac{f(\theta+\epsilon) - f(\theta-\epsilon)}{2\epsilon} \quad error: O(\epsilon^2)$$
$$\text{one-sided:} \quad f'(\theta) = \lim_{\epsilon \to 0} \frac{f(\theta+\epsilon) - f(\theta)}{\epsilon} \quad error: O(\epsilon)$$

use **two-sided** difference (more accurate) to check the derivatives(backprop)

Gradient Checking for a NN

- concatenate:
  take $W^{[1]}, b^{[1]}, \dots, W^{[L]}, b^{[L]}$ and reshape into a big vector θ
  take $dW^{[1]}, db^{[1]}, \dots, dW^{[L]}, db^{[L]}$ and reshape into a big vector $d\theta$

for each i:

$$d\theta^{[i]}_{approx} = \frac{J(\theta_1, \theta_2, \dots, \theta_i + \epsilon, \dots) - J(\theta_1, \theta_2, \dots, \theta_i - \epsilon, \dots)}{2\epsilon}$$
$$d\theta^{[i]} = \frac{\partial J}{\partial \theta_i}$$
$$if\ \epsilon = 10^{-7}$$
$$\text{check} \quad \frac{||d\theta_{approx} - d\theta||_2}{||d\theta_{approx}||_2 + ||d\theta||_2} \approx \begin{cases} 10^{-7} & \text{great} \\ 10^{-5} & \text{okay but double check} \\ 10^{-3} & \text{not good} \end{cases}$$

tips

- Don't use in trainin, only to debug
- If algorithm fails grad check, look at components to try to identify bug
- Remember regularization
- Doesn't work with dropout
- Run at random initialization; perhaps again after some training

2 Optimization Algorithms

2.1 Mini-batch Gradient Descent

split the training set into smaller ones → mini-batches

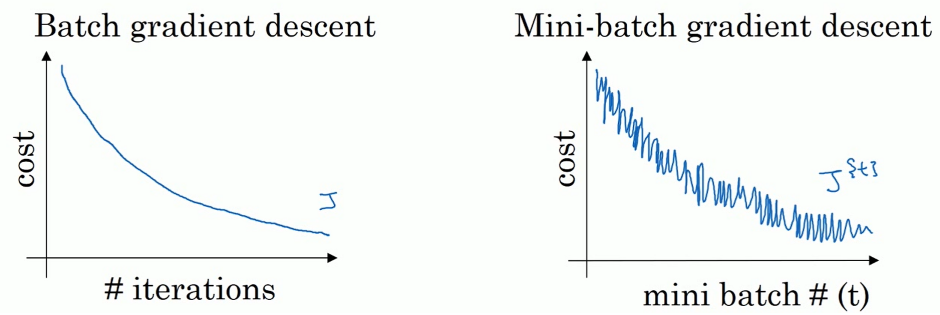
example: (m=5,000,000)

$$\underset{(n_x,m)}{X} = [\underbrace{x^{(1)} x^{(2)} \dots x^{(1000)}}_{X^{\{1\}}} | \underbrace{x^{(1001)} x^{(1002)} \dots x^{(2000)}}_{X^{\{2\}}} | \dots | \underbrace{\dots x^{(m)}}_{X^{\{5000\}}}]$$
$$\underset{(1,m)}{Y} = [\underbrace{y^{(1)} y^{(2)} \dots y^{(1000)}}_{Y^{\{1\}}} | \underbrace{y^{(1001)} y^{(1002)} \dots y^{(2000)}}_{Y^{\{2\}}} | \dots | \underbrace{\dots y^{(m)}}_{Y^{\{5000\}}}]$$

{i}: different mini-batches

use $X^{\{t\}}, Y^{\{t\}}$ to substitute X, Y in gradient descent, use a for-loop to go through

epoch: a single pass through the entire training set



more noise

choosing the mini-batch size

- if **size = m** : Batch gradient descent
  (takes too much time per iteration, especially when the training set is large)
- if **size =1** : Stochastic gradient descent
  (extremely noisy)
  (won't converge, oscillate around the region of the minium)
  (lose speedup from vectorization)
- choose a size **in between** (not too big or too small)

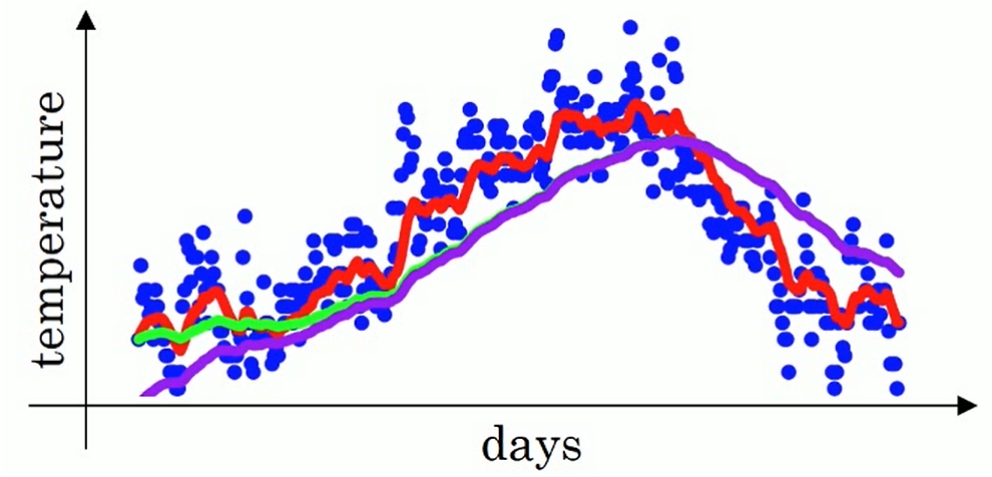
instruction:

1. small training set: use batch gradient descent
2. big training set: typical mini-batch size: 2^n (usually n=6~9, 10)

- make sure mini-batch $X^{\{t\}}, Y^{\{t\}}$ fits in CPU/GPU memory

2.2 Exponentially weighted averages

example: temperature



red: β = 0.9
purple: β = 0.98 (before bias correction)
green: β = 0.98 (after bias correction)

$$v_0 = 0 v_t = \beta v_{t-1} + (1-\beta)\theta_t = (1-\beta)\sum_{i=1}^{t} \beta^{t-i}\theta_i$$

```
v0=0
Repeat{
    get next theta_t
    v_theta := beta*v_theta + (1-beta)theta_t
}
```

- v_t as approximately average over $\frac{1}{1-\beta}$ days' temperature
- larger β adapts more slowly to changes, but smoother and less noisy
- 0.9 is a robust value for β

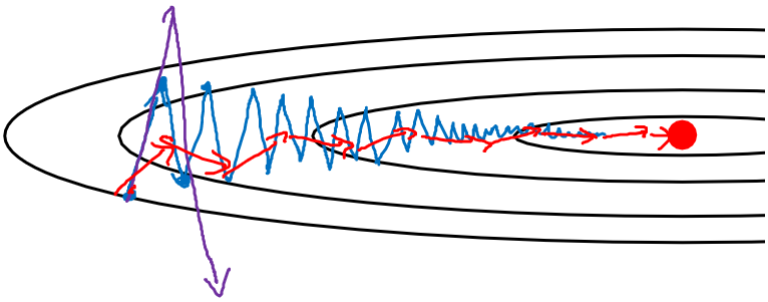
Bias correction

$$v_t = \frac{v_t}{1-\beta^t}$$

mainly in the initial period
as t gets larger, the bias correction has less effects

2.3 Gradient Descent with Momentum

Momentum



damp out oscillations in the path to the minimum

$v_{dW} = 0,\ v_{db} = 0$
on iteration t:
  compute dw, db using current mini-batch

$$\begin{aligned} v_{dW} &= \beta v_{dW} + (1-\beta)dW \\ v_{db} &= \beta v_{db} + (1-\beta)db \\ W &:= W - \alpha v_{dW} \\ b &:= b - \alpha b_{dW} \end{aligned}$$

- 2 hyperparameters: α β
- in practice, don't use bias correction when implementing gradient descent / momentum

2.4 RMSprop

Root Mean Square Propagation

$$s_{dW} = 0,\ s_{db} = 0$$

on iteration t:

compute dw, db using current mini-batch

$$s_{dW} = \beta_2 s_{dW} + (1-\beta_2)(dW)^2$$
$$s_{db} = \beta_2 s_{db} + (1-\beta_2)(db)^2$$
$$W := W - \alpha \frac{dW}{\sqrt{s_{dW}} + \epsilon}$$
$$b := b - \alpha \frac{db}{\sqrt{s_{db}} + \epsilon}$$

ϵ : a very small number$(e.g.\ 10^{-8})$

2.5 Adam Optimization Algorithm

Adam: Adaptive Moment Estimation

binding momentum and RMSprop together

$$v_{dW} = 0,\ s_{dW} = 0,\ v_{db} = 0,\ s_{db} = 0$$

on iteration t:

compute dw, db using current mini-batch

$$v_{dW} = \beta_1 v_{dW} + (1-\beta_1)dW, \quad v_{db} = \beta_1 v_{db} + (1-\beta_1)db$$
$$s_{dW} = \beta_2 s_{dW} + (1-\beta_2)(dW)^2, \quad s_{db} = \beta_2 s_{db} + (1-\beta_2)(db)^2$$
$$W := W - \alpha \frac{dW}{\sqrt{s_{dW}} + \epsilon}$$
$$b := b - \alpha \frac{db}{\sqrt{s_{db}} + \epsilon}$$
$$v_{dW}^{corrected} = \frac{v_{dW}}{1-\beta_1^t}, \quad v_{db}^{corrected} = \frac{v_{db}}{1-\beta_1^t}$$
$$s_{dW}^{corrected} = \frac{s_{dW}}{1-\beta_2^t}, \quad s_{db}^{corrected} = \frac{s_{db}}{1-\beta_2^t}$$
$$W := W - \alpha \frac{v_{dW}^{corrected}}{\sqrt{s_{dW}^{corrected}} + \epsilon}$$
$$b := b - \alpha \frac{v_{db}^{corrected}}{\sqrt{s_{db}^{corrected}} + \epsilon}$$

hyperparameters choice:

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

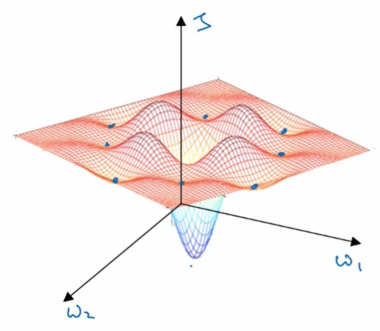
2.6 Learning Rate Decay

in order to solve the mini-batch oscillating problem

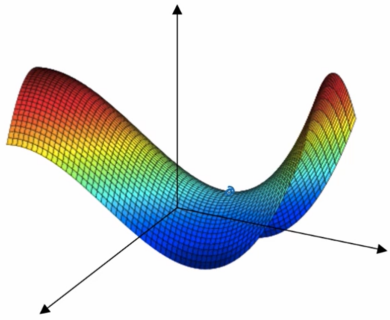
$$\alpha = \frac{1}{1 + \text{decay-rate} * \text{epoch-num}}\alpha_0$$
$$or \quad \alpha = 0.95^{\text{epoch-num}}\alpha_0 \qquad \text{——exponentially decay}$$
$$\alpha = \frac{k}{\sqrt{\text{epoch-num}}}\alpha_0 \qquad \text{——discrete staircase}$$

- manual decay: sometimes when the data set is small

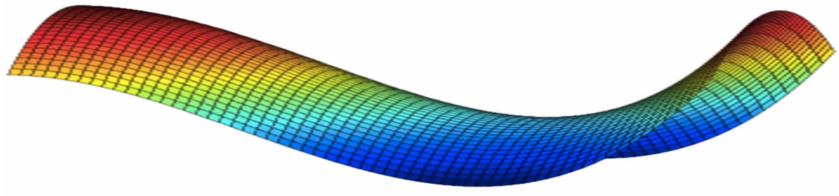
2.7 Local Optima



- Unlikely to get stuck in a bad local optima (big data set) ↑



- more likely to stuck in saddle points ↑

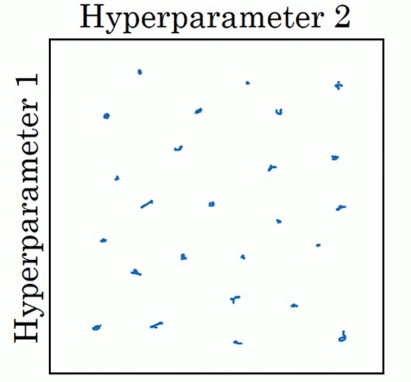


- plateau: slow down the learning process ↑ (use the optimization algorithms above)

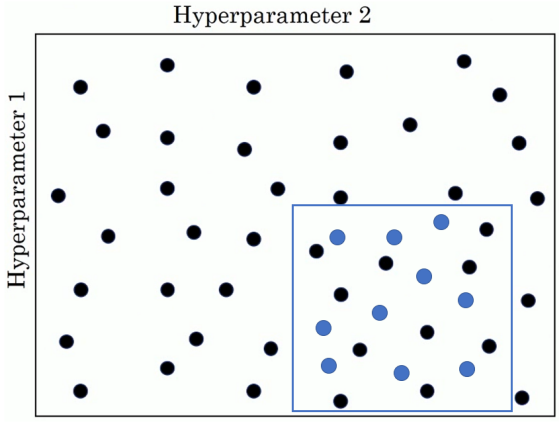
3 Hyperparameter Tuning

3.1 Tuning Process

1. don't use a grid, try **random** values (richly exploring set of possible values)



2. coarse to fine
   find a point, then zoom in to the region nearby and sample more densely



3.2 Appropriate Scale

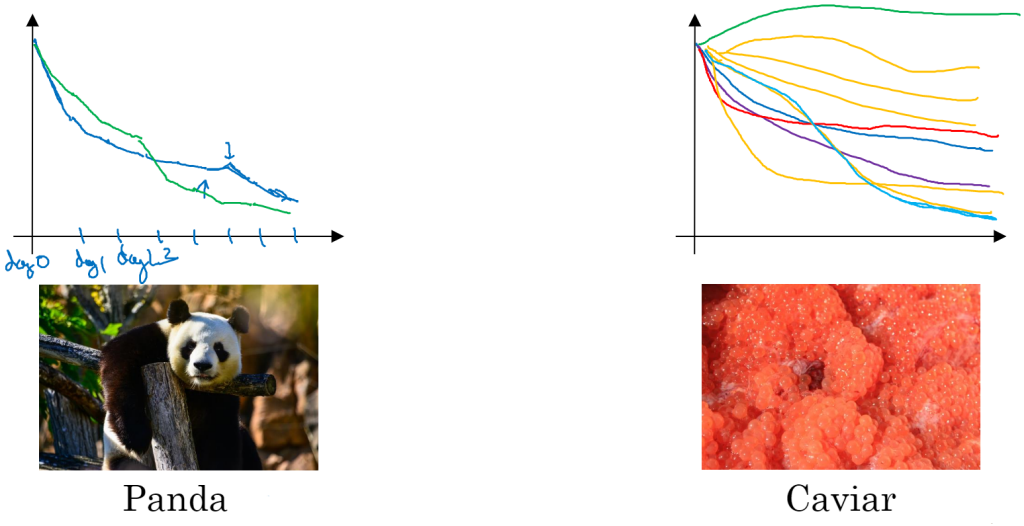
use a **logarithm scale** instead of a linear scale

search α in range 0.0001 ~ 1 :
r = -4*np.random.rand()
$\alpha = 10^r$

search β in range 0.9 ~ 0.999 :
consider 1-β
(when β comes close to 1, the result becomes very sensitive, so we need to sample more densely)

3.3 In Practice: Panda vs. Caviar

intuitions do get stale, re-evaluate hyperparameters occasionally



Panda Caviar

- PANDA: babysitting one model (when lacking computational capacity)
  keep watching the model and tune the parameters accordingly
- CAVIAR: trainin many models in parallel (when having enough computational resourses)
  pick the one that works best

3.4 Batch Normalization

normalize activations

implementing batch norm

For a deep network, after normalizing inputs (see 1.7), we can also normalize $a^{[l]}$ so as to train $w^{[l]}$, $b^{[l]}$ faster

$$\text{Given some intermediate values in NN (in layer l): } \underbrace{z^{(i)}, \ldots, z^{(n)}}_{z^{[l](i)}}$$

$$(\text{mean}): \quad \mu = \frac{1}{m}\sum_i z^{(i)}$$

$$(\text{variance}): \quad \sigma^2 = \frac{1}{m}\sum (z_i - \mu)^2$$

$$z^{(i)}_{norm} = \frac{z^{(i)} - \mu}{\sqrt{\sigma^2 + \epsilon}} \qquad (\varepsilon: \text{ in case } \sigma{=}0)$$

$$\tilde{z}^{(i)} = \gamma z^{(i)}_{norm} + \beta$$

$$if \quad \gamma = \sqrt{\sigma^2 + \epsilon},\ \beta = \mu,\ then\ \tilde{z}^{(i)} = z^{(i)}$$

use $\tilde{z^{(i)}}$ to replace $z^{(i)}$
normalize the mean and variance of these hidden unit values
controlled by 2 learnable parameters γ, β,which allow you to freely set the value of $\tilde{z}$

fitting batch norm into a neural network

the Batch Norm happens between computing **z** and computing **a**

$$x \xrightarrow{w^{[1]},b^{[1]}} z^{[1]} \xrightarrow[\text{Batch Norm}]{\beta^{[1]},\gamma^{[1]}} \tilde{z}^{[1]} \rightarrow a^{[1]} = g^{[1]}(\tilde{z}^{[1]}) \xrightarrow{w^{[2]},b^{[2]}} z^{[2]} \xrightarrow[\text{BN}]{\beta^{[2]},\gamma^{[2]}} \tilde{z}^{[2]} \rightarrow a^{[2]} \rightarrow \ldots$$

- use batch norm along with mini-batch, in which case the parameter **b** gets zeroed out (can be omitted)

$$\begin{aligned}&\text{for t=1...n use mini-batch}\\ &\quad \text{compute forward prop on } X^{\{t\}}\\ &\quad\quad \text{in each hidden layer, use BN to replace } z^{[l]} \text{with } \tilde{z}^{[l]}\\ &\quad \text{use backprop to compute } dw^{[l]}, d\beta^{[l]}, d\gamma^{[l]}\\ &\quad \text{update parameters } w^{[l]} = w^{[l]} - \alpha dw^{[l]}, \beta^{[l]} = \ldots, \gamma^{[l]} = \ldots\end{aligned}$$

- can be also used with momentum, RMSprop, Adam ...

why does batch norm work?

"covariate shift"

- **z** can change, but the mean and variance remains the same
- Reduce the amout of shifts of the distribution of these hidden units' values
- Ease the problem of input values changing, stablize the input values for each layer
- Make each layer more adaptive to changes and more independent from other layers

batch norm as regularization

- Each mini-batch is scaled by the mean/variance computed on just that mini-batch
- BN adds some noise to the values $z^{[l]}$ within that mini-batch. So similar to dropout, it adds some noise to each hidden layer's activations
- BN has a slight regularization effect

batch norm at test time

- during training time, μ and σ^2 are computed on an entire mini-batch
- but at test time, the network process a single example at a time
  need to estimate μ and σ^2 (implement exponentially weighted average or others)

3.5 Softmax Regression

multi-class classification

activation function

C : number of classes (C=2, softmax → logistic regression)
output: a (C,1) vector

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

$$\text{softmax activation function:}$$

$$t = e^{z^{[l]}}$$

$$a^{[l]} = \frac{e^{z^{[l]}}}{\sum_{j=1}^{C} t_i}, \quad a_i^{[l]} = \frac{t_i}{\sum_{j=1}^{C} t_i}$$

$$\text{example:}$$

$$z^{[L]} = \begin{bmatrix} 5 \\ 2 \\ -1 \\ 3 \end{bmatrix} \qquad \text{t} = \begin{bmatrix} e^5 \\ e^2 \\ e^{-1} \\ e^3 \end{bmatrix}$$

$$a^{[L]}_{\text{softmax}} = g^{[L]}\left(z^{[L]}\right) = \begin{bmatrix} e^5 / \left(e^5 + e^2 + e^{-1} + e^3\right) \\ e^2 / \left(e^5 + e^2 + e^{-1} + e^3\right) \\ e^{-1} / \left(e^5 + e^2 + e^{-1} + e^3\right) \\ e^3 / \left(e^5 + e^2 + e^{-1} + e^3\right) \end{bmatrix} = \begin{bmatrix} 0.842 \\ 0.042 \\ 0.002 \\ 0.114 \end{bmatrix}$$

$$a^{[L]}_{\text{hardmax}} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

hardmax: the biggest element outputs 1, others 0

Loss function

$$\mathcal{L}(\hat{y}, y) = -\sum_{j=1}^{C} y_j \, log\hat{y}_j$$

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

$$Y = [y^{(1)}, y^{(2)}, \dots, y^{(m)}] \quad (C, m) \text{ matrix}$$

gradient descent with softmax

$$\text{forward} \quad z^{[L]} \to a^{[L]} = \hat{y} \to \mathcal{L}(\hat{y}, y)$$

$$\text{backprop} \quad dz^{[L]} = \hat{y} - y$$

3.6 Deep Learning Frameworks

Caffe/Caffe2, CNTK, DL4J, Keras, Lasagne, mxnet, PaddlePaddle, TensorFlow, Theano, Torch ...

Choosing deep learning frameworks

- Ease of programming (development and deployment)
- Running speed
- Truly open (open source with good governance)

TensorFlow

```
# tensorflow ver 1.2.1

import numpy as np
import tensorflow as tf

coefficients = np.array([[1.], [-10.], [25.]])

w = tf.Variable(0,dtype=tf.float32)  #the parameter we are trying to optimize
x = tf.placeholder(tf.float32, [3,1]) #put data into it
# only need to implement the forward prop, tensorflow has built-in backward functions
# cost = tf.add(tf.add(w**2, tf.multiply(-10.,w)), 25)
# cost = w**2 - 10*w + 25 #tensorflow overloads the functions
cost = x[0][0]*w**2 + x[1][0]*w + x[2][0]
train = tf.train.GradientDescentOptimizer(0.01).minimize(cost)
init = tf.global_variables_initializer()
session = tf.Session()
session.run(init)
print(session.run(w))
# with tf.Session() as session:
#   session.run(init)
#   print(session.run(w))

for i in range(1000):
    session.run(train, feed_dict={x:coefficients})
print(session.run(w))
```

2020.08
Marcus
Written with Typora