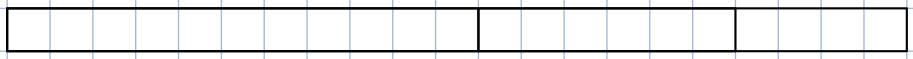
Train / Dev / Test Sets



Training | Hold-out Cross-Validation Development "Dev" set | Test

100 — 7000 — 10000 samples: 70 / 30 / 10

1 million — 10 millions samples: 98 / 1 / 1

Mismatched Train / Test Distribution / Sources

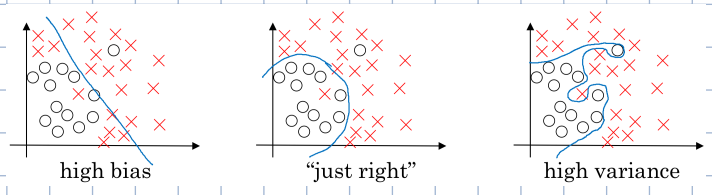
Training set:	Dev / Test set:
Cat pictures from webpages	Cat pictures from users using my app.
Low resolution satellite imagery	High resolution satellite imagery

The Rule of Thumb: Make sure the Dev and Test come from the same distribution.

Why not also training set comes from the same distribution? Well, it could be or it doesn't have to. I mean during the development of a model, the evaluation is done on the Dev set. So, the model is good as long as the evaluation on Dev set is good. That's why The Rule of Thumb is talking about Dev set and Test set.

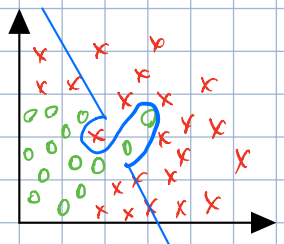
It might be OK to not have a test set. So, only train and dev set. In this case, the dev set is also called test set.

Bias and Variance



Underfitting

Overfitting



What is this?
High Bias & Variance

Cat classification

$y = 1$ Cat

$y = 0$ Non-Cat

Ideally, Train set error should be small and Dev set error should only be a bit ~~of~~ larger than Train set error.

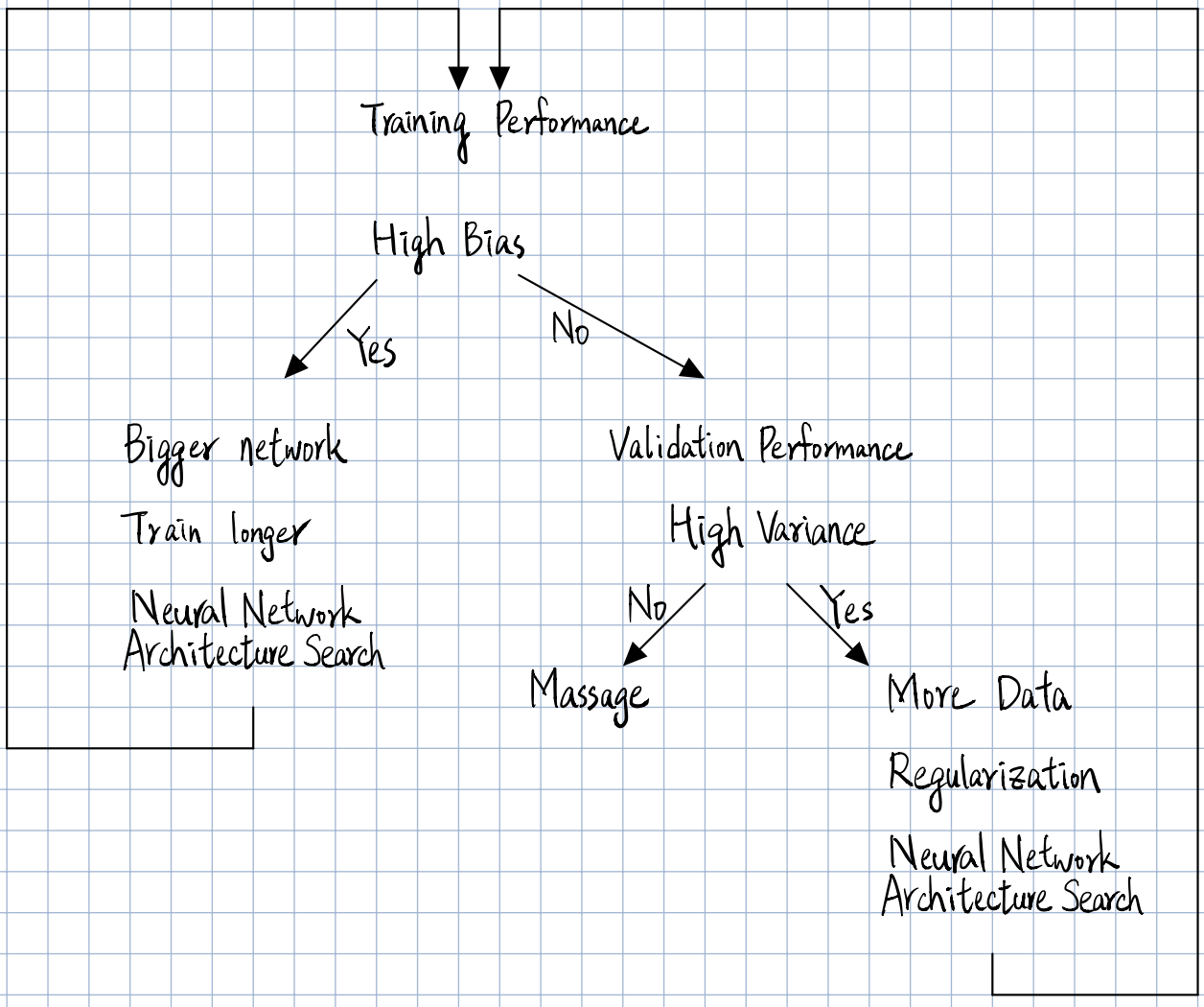
Train set error:	1%	15%	15%	0.5%
Dev set error:	11%	16%	30%	1%
	High Variance	High Bias	High Variance High Bias The Worst	Just Right Low Bias & Variance

The analysis above is predicated on the assumption below:

Human/Optimal/Bayes error $\approx$ 0%

The reason why Human error is also important is that, e.g., if human error is 15%, then this is actually pretty good.

Basic Recipe for Machine Learning



Bias and **Variance** trade-off:

Back in the pre-deep learning era, there were discussions about the bias and variance trade-off. That's because we didn't have many tools that just reduce bias or just reduce variance without hurting the other one.

In the modern deep learning and big data era, as long as we can keep neural networks large and/or keep getting more data, then getting a bigger neural network almost always reduces the bias without hurting the variance and getting more data almost always reduces the variance without hurting the bias. Thus, no more trade-off between bias and variance. They can both be reduced properly.

Regularization for Logistic Regression

Recall logistic regression: $\min_{w,b} J(w,b) = \min_{w,b} \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}, y)$

$w \in \mathbb{R}^{n_x}$: a vector of real numbers
$b \in \mathbb{R}$: a real number

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

Omit. Why only regularize weight only? w is a high dimensional vector, while b is just a real number. Thus, the majority of information is in w but not b. Hence, it doesn't make much difference.

L2 Regularization: $\|w\|_2^2 = \sum_{j=1}^{n_x} w_j^2 = w^T w$

L1 Regularization: $\frac{\lambda}{2m}\sum_{j=1}^{n_x}|w_j| = \frac{\lambda}{2m}\|w\|_1$

w will become sparse (vector/matrix with lots of 0) if L1 is used. Why?

λ: Regularization Parameter

And this is how regularization is done on Logistic Regression.

Regularization for Neural Network

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

$\|w^{[l]}\|_F^2 = \sum_{i=1}^{n^{[l]}}\sum_{j=1}^{n^{[l-1]}} (w_{i,j}^{[l]})^2$, $w: (n^{[l]}, n^{[l-1]})$. It's called Frobenius Norm

Now, the question is how to implement gradient descent with this?

Recall before adding Regularization

$\frac{\partial J}{\partial w^{[l]}} = dw^{[l]}$: (from backpropagation)

$w^{[l]} = w^{[l]} - \alpha\, dw^{[l]}$

Add Regularization

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

$w^{[l]} = w^{[l]} - \alpha \boxed{dw^{[l]}}$

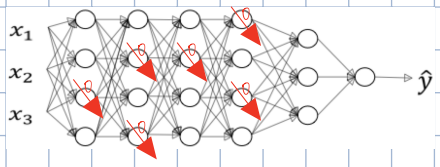
$$\rightarrow w^{[l]} = \boxed{w^{[l]} - \frac{\alpha\lambda}{m}w^{[l]}} - \alpha(\text{from backpropagation})$$

$$(1-\tfrac{\alpha\lambda}{m})w^{[l]}$$

$(1-\frac{\alpha\lambda}{m})$ will always be smaller than 1, which is why L2 Regularization is also referred to as Weight Decay.

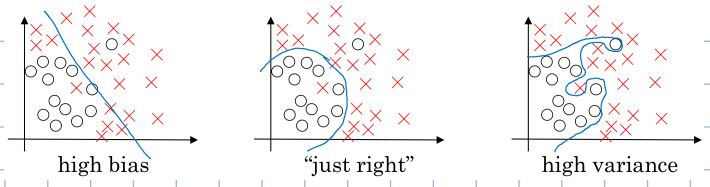
Why Regularization Reduces Overfitting?

The first intuitive explanation:



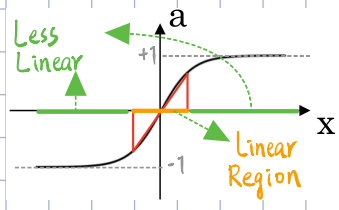
$$J(w^{[1]}, b^{[1]}, \dots, w^{[L]}, b^{[L]}) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L} \|w^{[l]}\|_F^2$$

One intuition is that if λ is very large, it will incentivize to set weights to be reasonably close to 0. If many weights for hidden units are close to 0, then it is zeroing out the impact of the hidden units. Thus, a complex neural network becomes a much simpler network. Thus, it will make it from overfitting toward underfitting. And hopefully, there will be an intermediate value of λ that results in the just-right case.



The second intuitive explanation:

The activiation function $g(z) = \tanh(z)$



$$w^{[l]} = w^{[l]} - \frac{\alpha\lambda}{m} w^{[l]} - \alpha(\text{from backpropagation})$$

$$\left(1 - \frac{\alpha\lambda}{m}\right) w^{[l]}$$

$\lambda \nearrow$, $w^{[l]} \searrow$, $z^{[l]} = w^{[l]} a^{[l-1]} + b^{[l]} \searrow$

Thus, it will use linear region in $\tanh(z)$. → $g(z)$ will become roughly linear as if it's just linear regression.

Now, recall what happens if a linear activiation function is used in a neural network.

$$\hat{y} = a^{[2]} = z^{[2]} = w^{[2]}(w^{[1]}X + b^{[1]}) + b^{[2]}$$
$$= (w^{[2]}w^{[1]})X + (b^{[2]}b^{[1]})$$
$$= w'X + b'$$

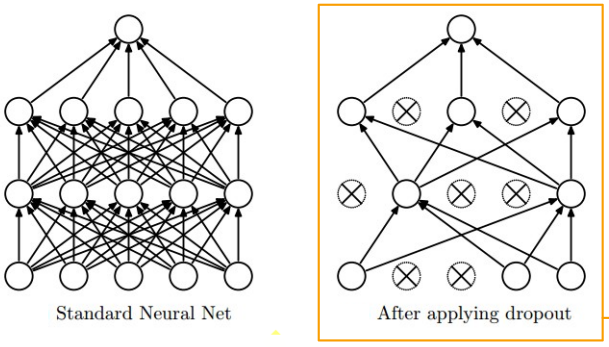
This shows that the neural network is generating a linear function of an input, which is equal to no hidden layers at all.

If every layer is a linear network, then the whole network is just a linear network, which means it can't learn the nonlinearity of data.

Thus, overfitting is reduced.

Dropout Regularization

If dropout rate is 0.5, it means for each node in hidden layers, there is 50% probability that a node will be eliminated.



For each ~~training sample~~ iteration of gradient descent, it runs through the same network but with different nodes being dropout.

→ The network becomes simpler.
Thus, overfitting is reduced.

Implementing Dropout ("Inverted Dropout") in Training time:

Hyperparameter: $l=3$, keep-prob = 0.8 (dropout rate = 0.2)

For each iteration of gradient descent (all samples)

```
d3 = np.random.rand(a3.shape[0], a3.shape[1]) < keep-prob
```

```
np.multiply(a3, d3, out=a3)
```
→ I learn it today. It's efficient code.

```
a3 /= keep-prob
```
→ Why? Assume this layer has 50 neurons. Dropout will reset 10 units to 0.
For the next layer, $z^{[4]} = w^{[4]} \cdot a^{[3]} + b^{[4]}$.
Now, $a^{[3]}$ is reduced by 20%. In order to not reduce the expected value of $z^{[4]}$, $a^{[3]}$ is divided by 0.8 because it will bump $a^{[3]}$ back by 20%, which ensures the expected value of $a^{[3]}$ is unchanged.
It's also called Inverted Dropout Technique.

Making Predictions at Testing Time: Dropout is disabled. Every units count.

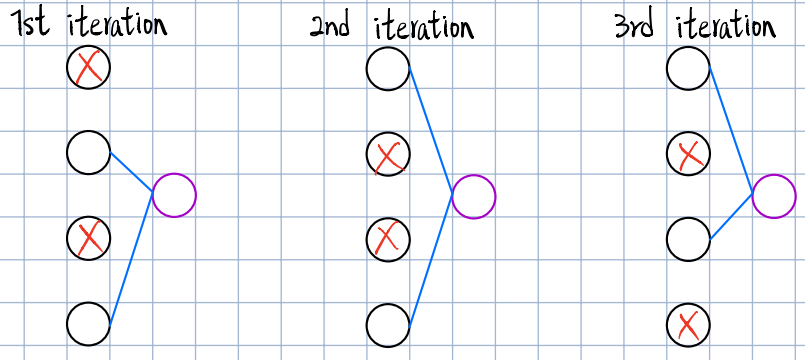
$a^{[0]} = X$
$z^{[1]} = w^{[1]} a^{[0]} + b^{[1]}$
$a^{[1]} = g^{[1]}(z^{[1]})$
⋮
$\hat{y}$

Recall that `a3 /= keep-prob` is executed in training.

In testing, we don't need to implement any value rescaling method because dropout is disabled.

Understanding Dropout

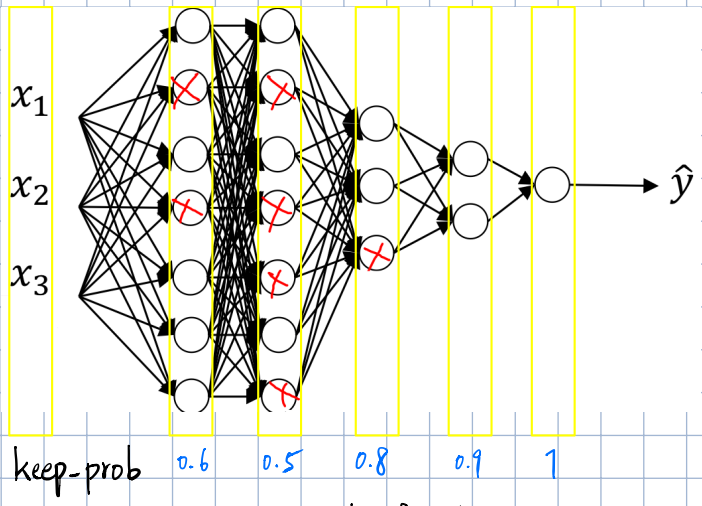
Intuition: Can't rely on any one feature, so have to spread out weights.



With dropout, the inputs can get randomly eliminated. E.g., as shown above, different units are eliminated in each iteration. So, what this means is that the unit ◯ can't rely on any one feature, because any one feature could go away at random. Thus, in particular, it will be reluctant to put all of its bets on a specific input. Hence, the unit ◯ will be more motivated to spread out the weights to four of its input units.

By spreading out the weights, it will tend to have an effect of shrinking the squared norm of the weights. The effect of implementing dropout is that it shrinks the weights and is similar to L2 Regularization. Only that L2 Regularization can be even more adaptive to the scale of different inputs.

Another important detail of dropout: keep-prob can be varied by each layer.



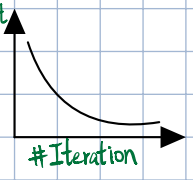
In general, the layer with more hidden units can have lower keep-prob, because more hidden units often result to overfitting.

Technically, dropout can also be applied to the input layer. But usually people don't do this. If you really want to apply dropout to the input layer, the keep-prob should be close to 1.

In Computer Vision, the feature dimension is so large such that the training data is never enough, which almost always leads to overfitting. So, dropout is frequently used in Computer Vision. However, this idea doesn't always generalize to other disciplines.

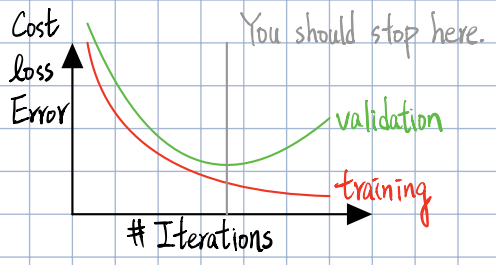
Drawback/Downside of Dropout:

Applying dropout in training will make a neural network with units being shut off randomly. Thus, the cost may not decrease monotonically. The solution is to turn off dropout when calculating cost.



Other Regularization Methods

- Data Augmentation:
- Early Stoping:



The downside of early stopping:

Machine Learning process can be seen as two tasks:

- Optimize cost function J: Gradient Descent, Momentum, RMS Prop, AdamW, etc.
- Avoid overfitting: More data, Regularization, etc.

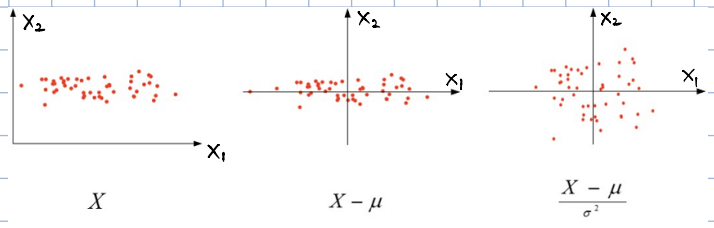
To be honest, the above two points are kind of contradicting. If I want to make cost function J as small as possible, then it's likely overfitting, and vice versa.
And we want to approach these two tasks independently. It's called Orthogonalization.

Early stopping couples these two tasks, we no longer can work on these two tasks independently, because by stopping gradient descent early, I am breaking the process of optimizing cost function J.

Andrew prefers to just use L2 Regularization and try different values of the parameter λ, so that he can just train the network as long as possible. But it's more computationlly expensive.

Normalizing Inputs

Normalizing training sets. $X \in \mathbb{R}^2$: $x^{(i)}$, $i = 1, \dots, m$



1. Subtract mean: Assume $x^{(i)} \in \mathbb{R}^n$

$$\text{mean } \mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)} \qquad \mu \in \mathbb{R}^n : (n, 1)$$

2. Normalize Variances:

$$\text{Variance: } \sigma^2 = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \mu)^2 \quad \text{(element-wise)} \qquad \sigma^2 \in \mathbb{R}^n : (n, 1)$$

$$\therefore X = \frac{X - \mu}{\sigma} \quad \because X : (n, m)$$

$\because$ It must be element-wise devision.

Note: If the mean and the variance derived from the training set is used to normalize the training data, then the Same mean and variance Must be used to normalize the test set.

X will have mean 0, variance 1. But the range is not necessarily from -1 to 1. X could still be >1 and <-1 after normalization.

In particular, you dont want to normalize the traing set and test test differently. We want the training set and test set to go through the same transformation defined by the same μ and σ^2 calculated from the traning data. Intuitively, it makes sense. But,...

OK. I dont think the normalization described above can be applied to images. If the training data is image, it doesnt make any sense to normalize this way.

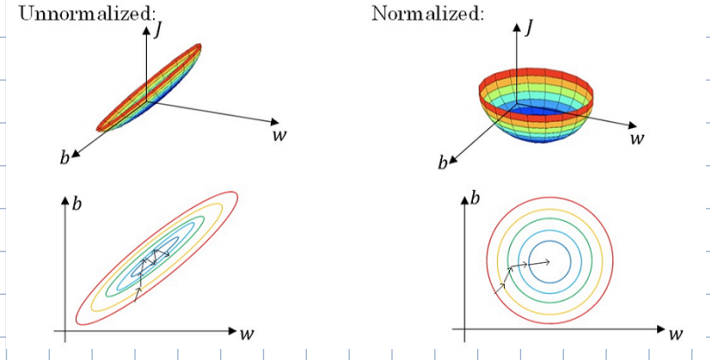
Why normalize inputs? $J(w, b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$

Assume the feature X_1's value ranges from 1 to 1000 and X_2's value ranges from 0 to 1. It needs normalization

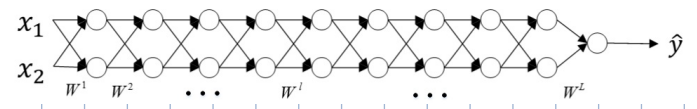
If unnormalized, then the small learning rate might be used, because it might need a lot of steps to oscillate back and forth to find its way to the minimum.

If normalized, gradient descent can go straight to the minimum.

However, if X_1 ranges from 0 to 1, X_2 ranges from -1 to 1 and X_3 ranges from 1 to 2, these features have similar ranges, they dont need to be normalized at all. Neural networks will work just fine.



Vanishing / Exploding Gradients



Given a very deep neural network, for the sake of simplicity, there are only two features, and $g(z)=z$, $b^{[l]}=0$,

Then, $\hat{y} = W^{[L]}W^{[L-1]}\cdots W^{[2]}W^{[1]}X$

$z^{[2]}$ $z^{[1]} = a^{[1]} = g^{[1]}(z^{[1]})$

For $l=1,\dots,L-1$: **Case 1**

Assume $W^{[l]} = \begin{bmatrix} 1.5 & 0 \\ 0 & 1.5 \end{bmatrix}$, $\hat{y} = W^{[L]}\begin{bmatrix} 1.5 & 0 \\ 0 & 1.5 \end{bmatrix}^{L-1}X$, If L is large, $\hat{y}$ will be exploding.

Case 2

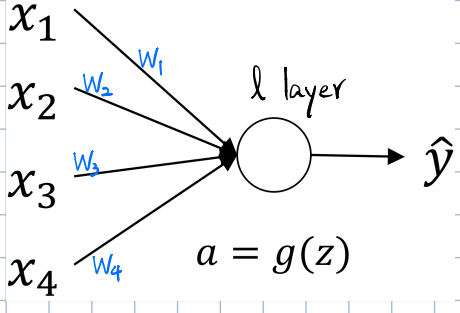
Assume $W^{[l]} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$, $\hat{y} = W^{[L]}\begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}^{L-1}X$, If L is large, $\hat{y}$ will be vanishing.

The idea is that with a very deep neural network, the activiation will increase or decrease exponentially. The similar argument can be used to show the gradient in the gradient descent is going to increase or decrease exponentially as a function of the number of layers.

Weight Initialization for Deep Networks.

It can only partially solve the problem of exploding/vanishing gradient, not entirely.

Single Neuron Example:



$z = w_1x_1 + w_2x_2 + \cdots + w_nx_n + b$ (~~b~~)

In order to not blow up z, the larger n is, the smaller we want $w_1,\dots,w_n$ to be, because $z = \sum_{i=1}^{n} w_ix_i$.

Thus, we want $\text{var}(w) = \frac{1}{n}$, n is the number of inputs for a neuron.

$w^{[l]} = \text{np.random.rand}(\text{shape}) * \text{np.sqrt}\left(\frac{1}{n^{[l-1]}}\right)$

shape: the shape of weight for l layer

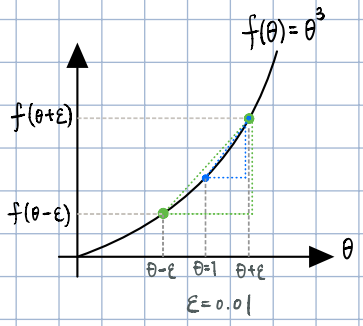
$n^{[l-1]}$: the number of neurons going into a neuron in l layer

It turns out that if $g(z) = \text{ReLU}(z)$, then it would be better to use $\text{var}(w) = \frac{2}{n}$. Thus, $\text{np.sqrt}\left(\frac{2}{n^{[l-1]}}\right)$.

Andrew mentions if $g(z) = \tanh(z)$, then $\sqrt{\frac{1}{n^{[l-1]}}}$ or $\sqrt{\frac{2}{n^{[l-1]}+n^{[l]}}}$ can be used to replace $\text{np.sqrt}\left(\frac{2}{n^{[l-1]}}\right)$.

Xavier Initialization

Numerical Approximation of Gradients



Goal: Find slope of θ. $f'(\theta)=g(\theta)=3\theta^2=3$ ← the ground truth

It turns out using the green triangle is better than using the blue triangle

$$\frac{f(\theta+\varepsilon)-f(\theta-\varepsilon)}{2\varepsilon}\approx g(\theta) \quad \text{(gradient)} \Rightarrow \frac{1.01^3-0.99^3}{2\times 0.1}=3.0001$$

$3.0001-3=0.0001$

$$\frac{f(\theta+\varepsilon)-f(\theta)}{\varepsilon}=\frac{1.01^3-1^3}{0.01}=3.0301$$

$3.0301-3=0.0301$

Gradient Checking: It's a technique to help finding bugs in the implementation of gradient descent.

Step 1: Concatenate $w^{[1]}, b^{[1]}, \dots, w^{[l]}, b^{[l]}$ and reshape into a big vector θ.

$$J(w^{[1]}, b^{[1]}, \dots, w^{[l]}, b^{[l]}) = J(\theta)$$

Step 2: Concatenate $dw^{[1]}, db^{[1]}, \dots, dw^{[l]}, db^{[l]}$ and reshape into a big vector $d\theta$.

Now the big question is: Is $d\theta$ the gradient of the cost function J?

Step 3: $J(\theta) = J(\theta_1, \theta_2, \theta_3, \dots)$

for each i:

$$d\theta_{approx}[i] = \frac{J(\theta_1, \theta_2, \dots, \theta_i+\varepsilon, \dots) - J(\theta_1, \theta_2, \dots, \theta_i-\varepsilon, \dots)}{2\varepsilon}$$

$$\text{Ideally, } d\theta_{approx}[i] \approx d\theta[i] = \frac{\partial J}{\partial \theta_i}$$

After calculating $d\theta_{approx}[i]$ for each i, now we have $d\theta_{approx}$.

Then we can calculate how close $d\theta_{approx}$ and $d\theta$ is.

Euclidean distance $dist(d\theta_{approx}, d\theta) = \dfrac{\|d\theta_{approx} - d\theta\|_2}{\|d\theta_{approx}\|_2 + \|d\theta\|_2}$

Andrew selects $\varepsilon = 10^{-7}$, if $dist(d\theta_{approx}, d\theta)$ is

- 10^{-7} great
- 10^{-5} something might go wrong
- 10^{-3} something is definitely wrong

Gradient Checking Implementation Notes

- Don't use in Traing. Only to debug.
- If algorithm fails gradient checking, check components to try to identify bugs.
- Remember Regularization.
- Don't work with dropout.
- Run at random initialization; perhaps again after some training.