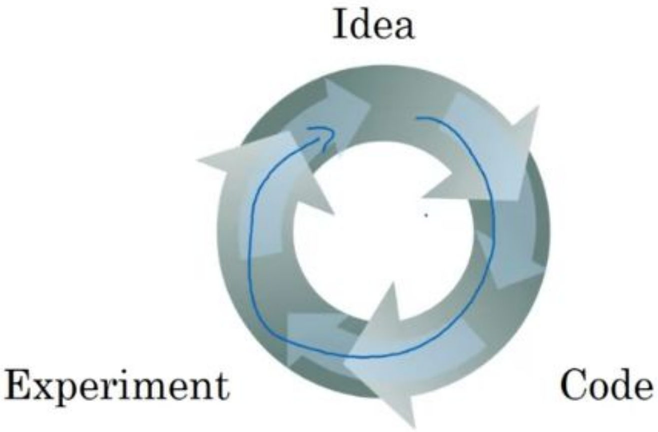
Improving Deep Neural Networks: Hyperparameter Tuning, Regularization and Optimization

27/03/2021 Minsung Kim

Setting up your machine learning application

Applied ML is a highly iterative process

- # layers
- # hidden units
- learning rates
- activation functions
- ...



NLP, Vision, Speech, Structural data

Ads   Search   Security   logistic ....

Setting up your machine learning application

Test/dev/test sets

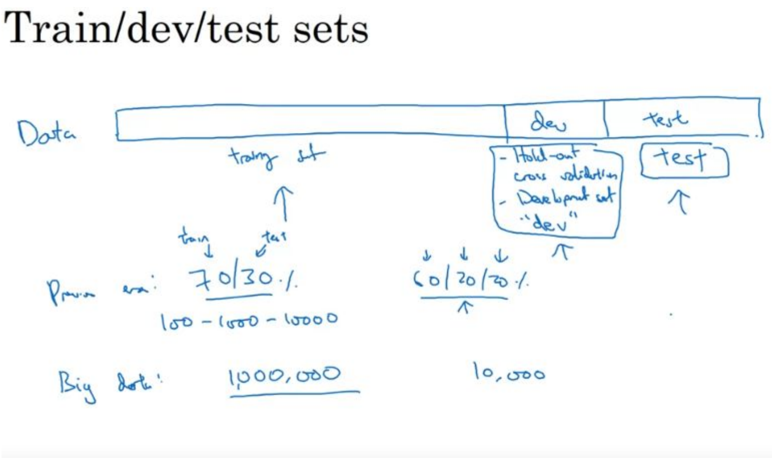
Previous era: 70/30 or 60/20/20 - 데이터의 양이 작았기에

Modern era: dev/test -> 데이터가 많아서 굳이 이전처럼 나눌필요 없이 적당히

ex) total 1,000,000 -> Dev 10,000 Test 10,000

98/1/1

99/0.5/0.5



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Mismatched train/test distribution

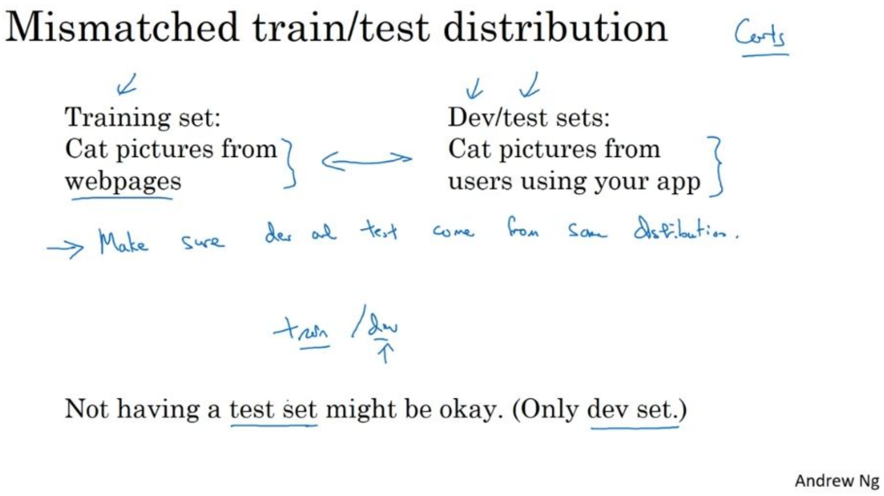
Training vs. Dev/Test

서로 다른 분포에서 나오는 데이터들을 다룸.

Test와 Dev는 같은 분포에서 나오도록 할것.

Training은 상관없나?

Not having a test set might be okay. (only dev set)



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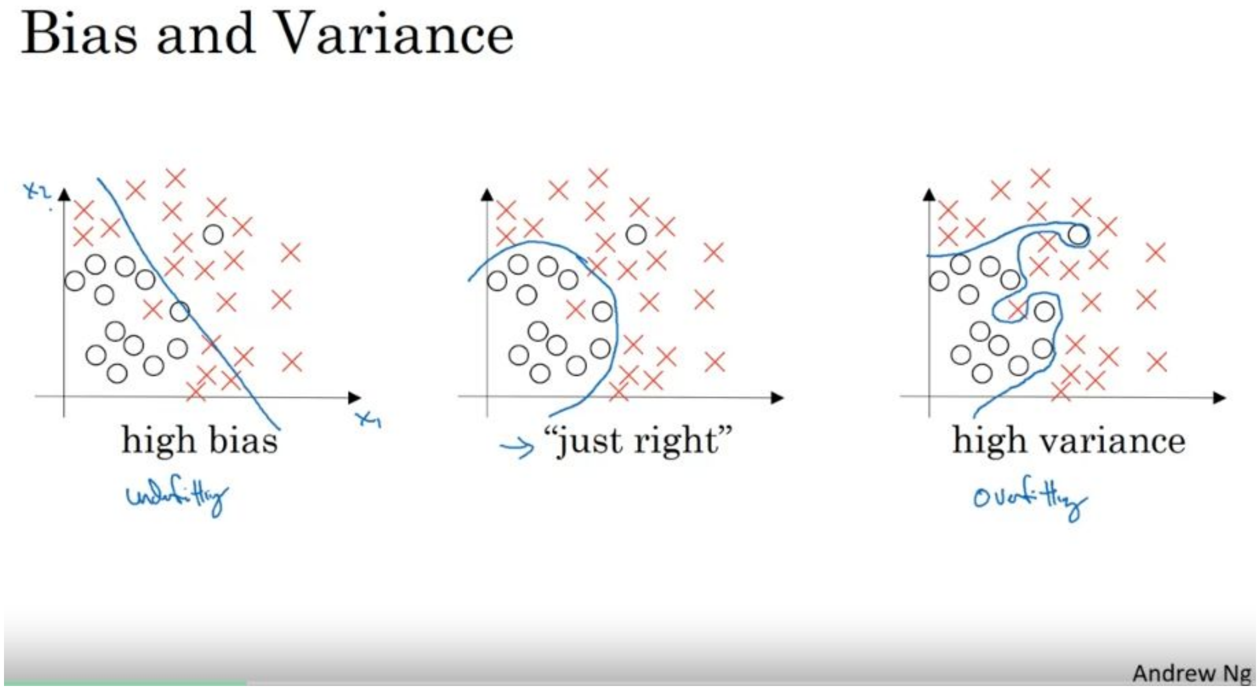
Bias/Variance



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Bias/Variance

Bias and Variance

Cat classification

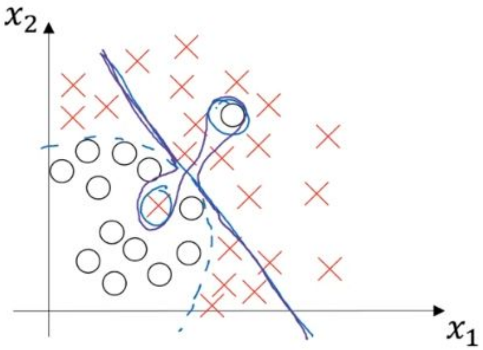
$y=1$

$y=0$

Train set error:	1%	15%	15%	0.5%
Dev set error:	11%	16%	30%	1%
	high variance	high bias	high bias & high varian	low bias low variance

Human: ≈0%

Optimal (Bayes) error: ~~≈0%~~ 15%   Blurry images



High bias and high variance

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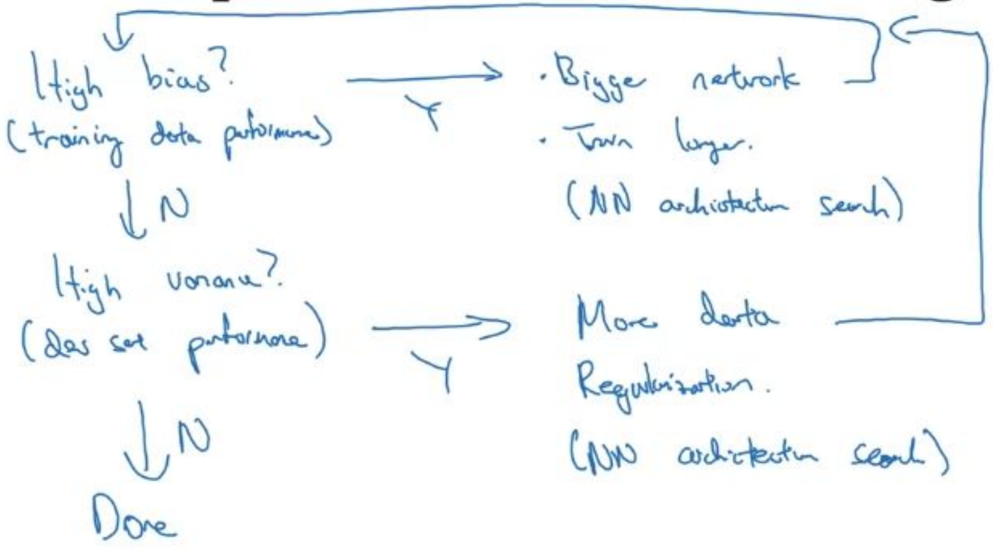
Basic recipe for machine learning



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Basic recipe for machine learning

High bias?
(training data performance)

Y →
→ $\boxed{\text{Bigger network}}$
→ Train longer.
(NN architecture search)

↓ N

High variance?
(dev set performance)

Y →
→ $\boxed{\text{More data}}$
→ Regularization
(NN architecture search)

↓ N

Done

Bias variance "tradeoff"

Regularizing your neural network

Logistic regression

$w \in \mathbb{R}^{n_x}, \quad b \in \mathbb{R}$

λ = regularization parameter

lambda lambd

$$\min_{w,b} J(w,b)$$

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

omit

L2 regularization $\quad \|w\|_2^2 = \sum_{j=1}^{n_x} w_j^2 = w^T w \longleftarrow$

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

w will be sparse

Regularizing your neural network

Neural network

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

"Frobenius norm"

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

Regularizing your neural network

Gradient descent?

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

$$\rightarrow W^{[l]} := W^{[l]} - \alpha \, dW^{[l]}$$

Before regularization

$$W^{[l]} := W^{[l]} - \alpha \left[(\text{from backprop}) + \frac{\lambda}{m} W^{[l]} \right]$$

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

$$\left(1 - \frac{\alpha\lambda}{m}\right)$$

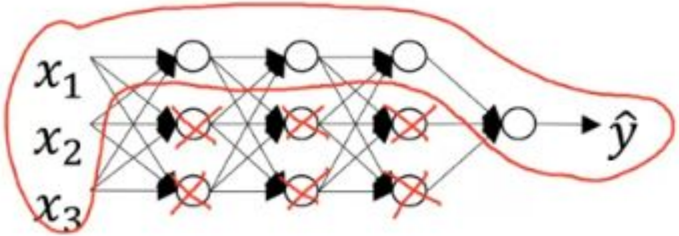
After regularization

Regularizing your neural network

Regularization은 왜 오버피팅을 감소시킬까?

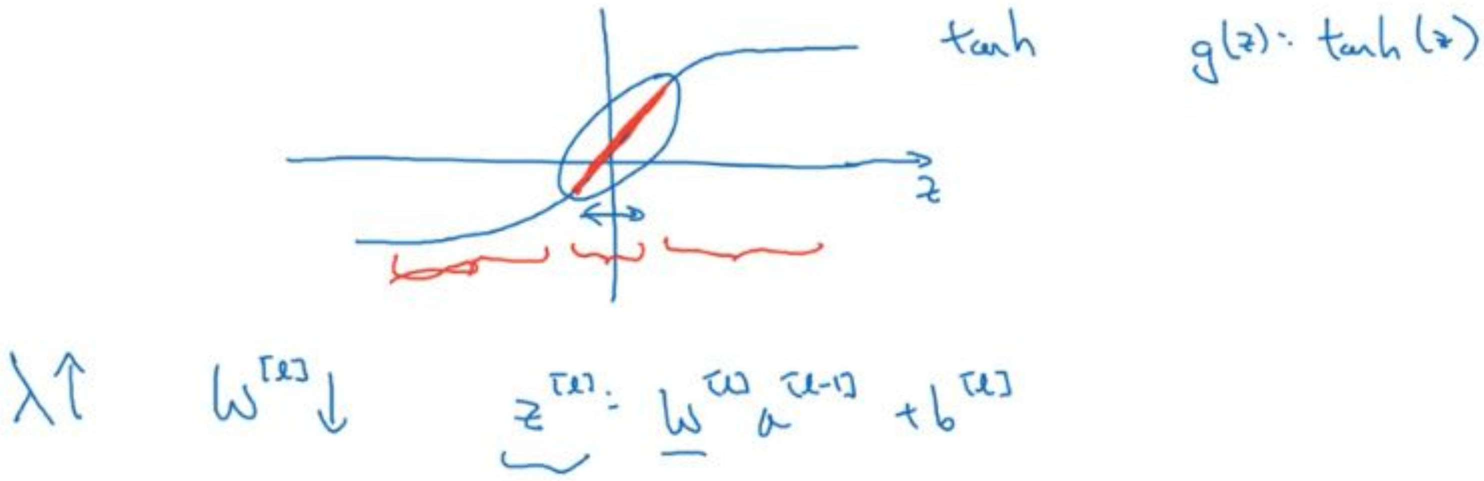
$$J(w^{[l]}, b^{[l]}) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L} \underbrace{\|w^{[l]}\|_F^2}$$

$$w^{[l]} \approx 0$$



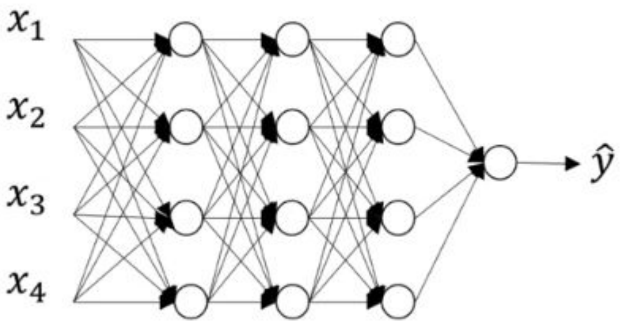
Regularizing your neural network

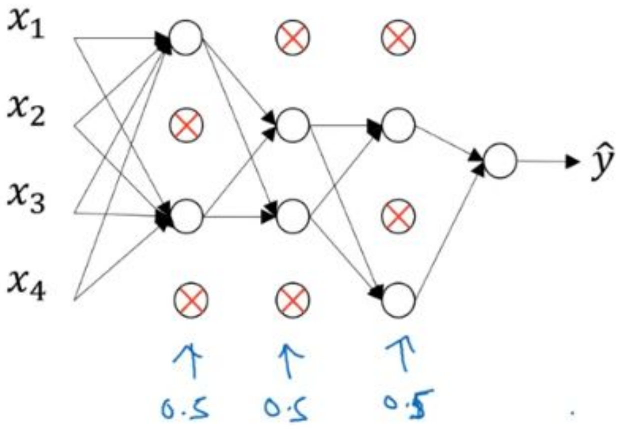
Regularization은 왜 오버피팅을 감소시킬까?



Regularizing your neural network

Dropout regularization





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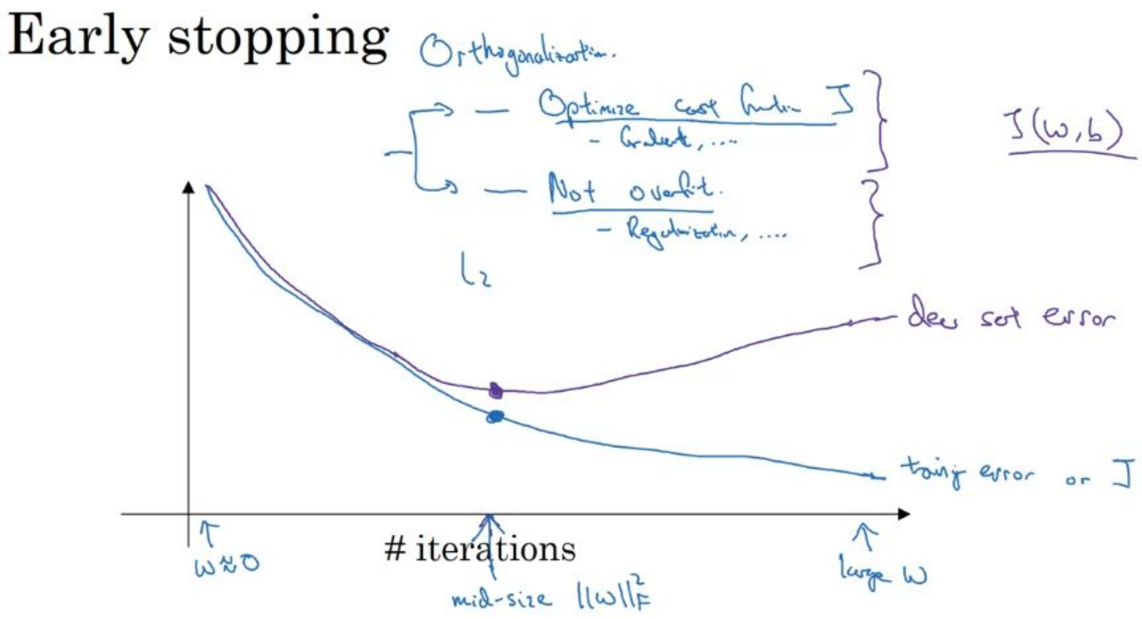
Regularizing your neural network

다른 Regularization 방법들

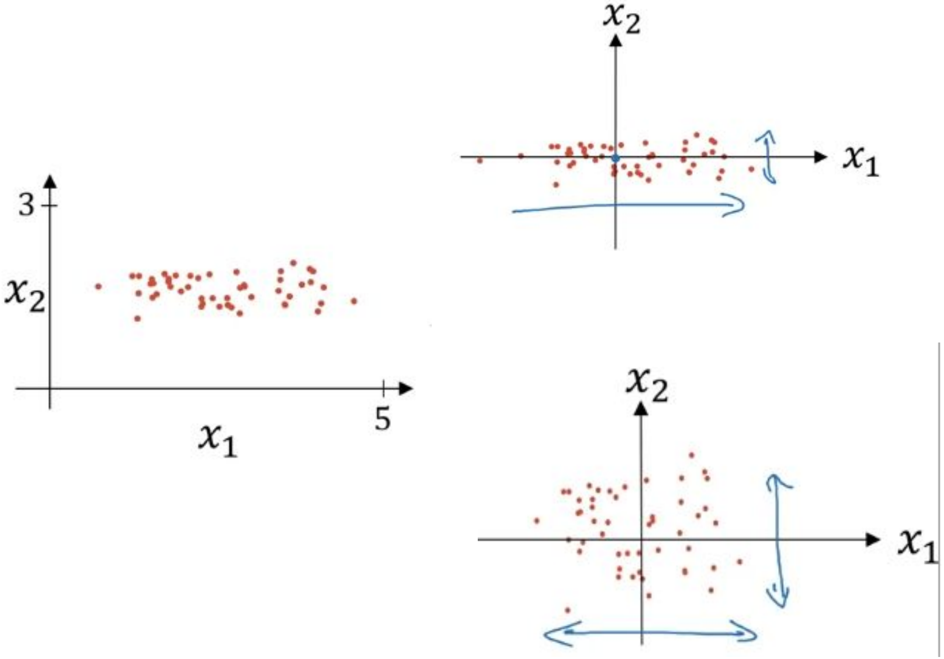
Data augmentation

Regularizing your neural network

다른 Regularization 방법들



Setting up your optimization problem



Subtract mean:

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

$$x := x - \mu$$

Normalize variance

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

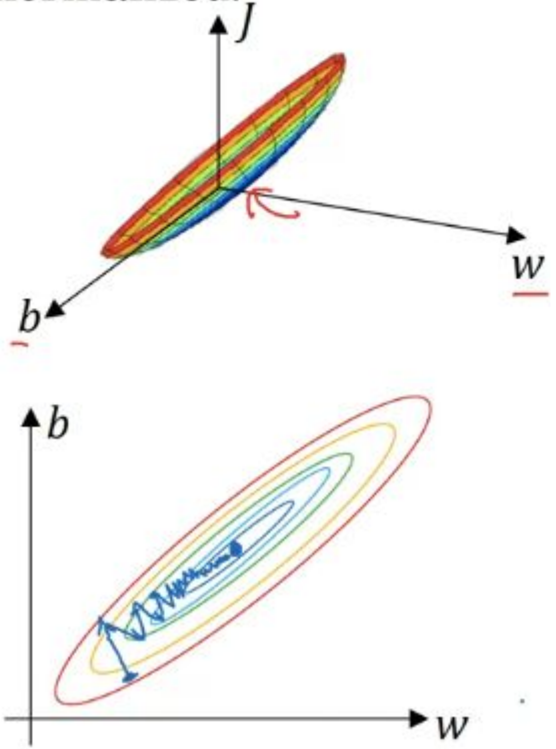
← element-wise

$$\frac{x - \mu}{\sigma}$$

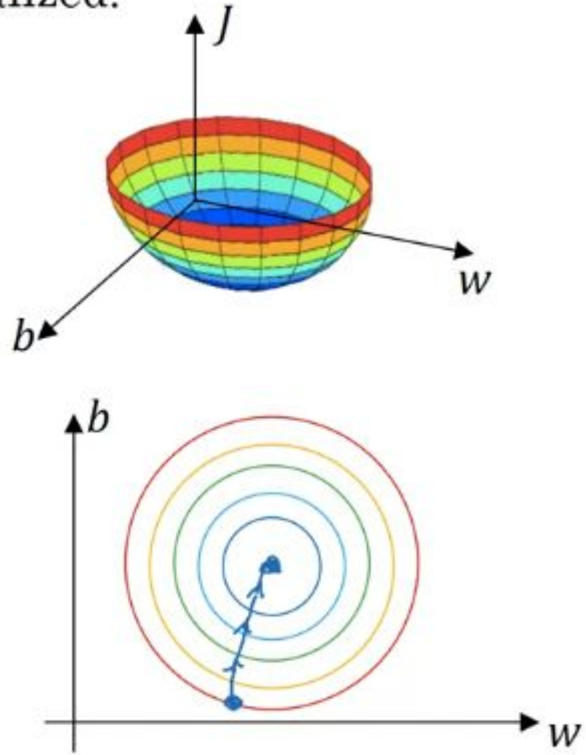
Setting up your optimization problem

w_2 x_2, 0...1

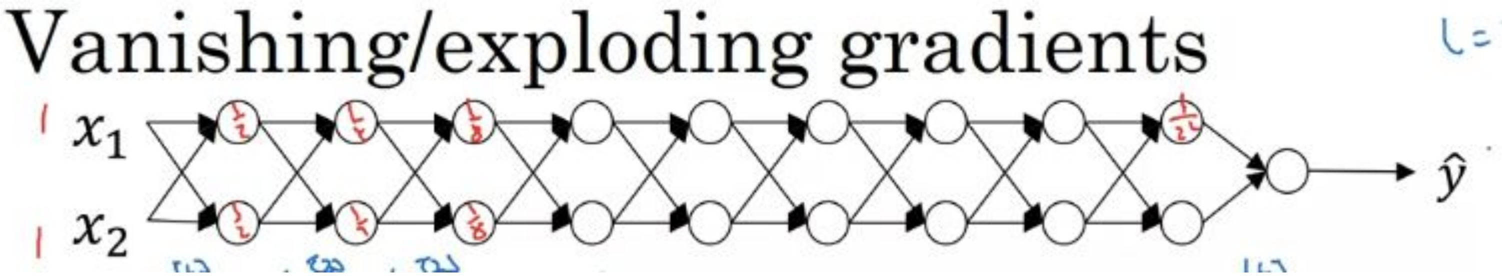
Unnormalized:



Normalized:



Setting up your optimization problem



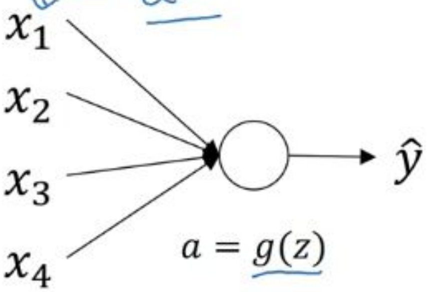
$W^{[l]} > I$ -> W 커지면서 Exploding

$W^{[l]} < I$ -> W가 작아지면서 Vanishing

Setting up your optimization problem

Single neuron example

$a^{[l-1]}$



$w^{[l]}$

$z = w_1x_1 + w_2x_2 + \cdots + w_nx_n \cancel{+b}$

Large n $\rightarrow$ Smaller w_i

$Var(w_i) = \cancel{\frac{1}{n}} \; \frac{2}{n}$

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

ReLU $\quad g^{[l]}(z) = \text{ReLU}(z)$

Other variants:

tanh $\boxed{\sqrt{\frac{1}{n^{[l-1]}}}}$

Xavier initialization

$\sqrt{\frac{2}{n^{[l-1]} + n^{[l]}}}$

Setting up your optimization problem

Checking your derivative computation

$$f'(\theta) = \lim_{\varepsilon \to 0} \frac{f(\theta+\varepsilon) - f(\theta-\varepsilon)}{2\varepsilon}$$

Take $\boxed{W^{[1]}}, \boxed{b^{[1]}}, \dots, W^{[L]}, b^{[L]}$ and reshape into a big vector θ.

Take $\boxed{dW^{[1]}}, \boxed{db^{[1]}}, \dots, dW^{[L]}, db^{[L]}$ and reshape into a big vector $d\theta$.

Is $d\theta$ the gradient of J

Setting up your optimization problem

for each i:

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

$$\approx \underline{d\theta}[i] = \underline{\frac{\partial J}{\partial \theta_i}}$$

$$d\theta_{approx} \overset{?}{\approx} d\theta$$

Check $\rightarrow \dfrac{\| d\theta_{approx} - d\theta \|_2}{\| d\theta_{approx} \|_2 + \| d\theta \|_2}$ $\approx 10^{-7}$ – great!

10^{-5}

$\rightarrow 10^{-3}$ – worry.

$\underline{\varepsilon = 10^{-7}}$

Setting up your optimization problem

Gradient checking implementation notes

- Don't use in training – only to debug

$d\theta_{approx}[i] \longleftrightarrow d\theta[i]$

- If algorithm fails grad check, look at components to try to identify bug.

$db^{[l]}$ $dw^{[l]}$

- Remember regularization.

$J(\theta) = \frac{1}{m} \sum_i \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \underbrace{\frac{\lambda}{2m} \sum_l \|w^{[l]}\|_F^2}$

$d\theta$ = grad of J w.r.t. θ

- Doesn't work with dropout. J keep-prob = 1.0

- Run at random initialization; perhaps again after some training.

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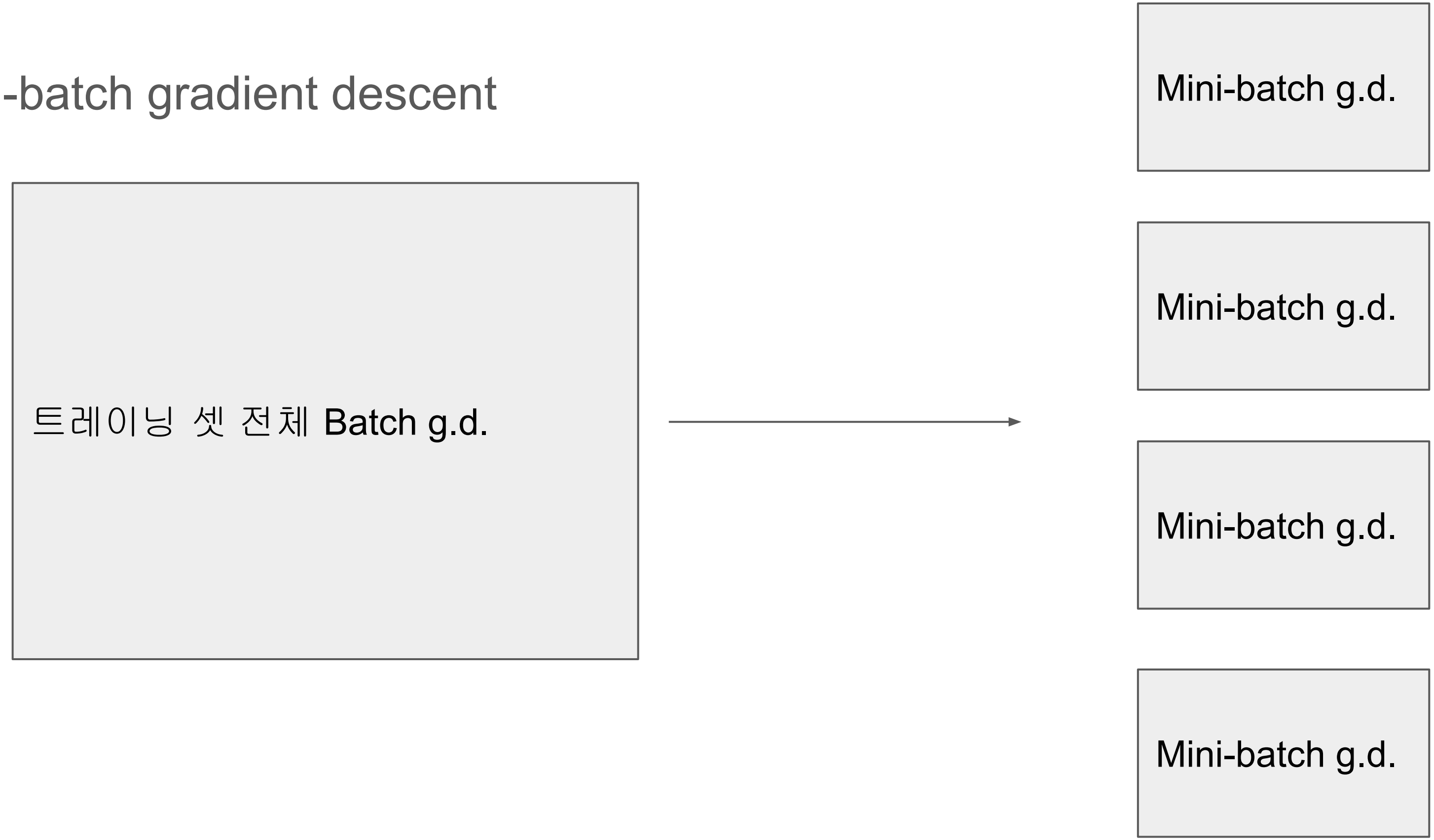
Optimization algorithms

Mini-batch gradient descent



Optimization algorithms

Mini-batch gradient descent

repeat {
for $t = 1, \ldots, 5000$ {

Forward prop on $X^{\{t\}}$.

$$Z^{[1]} = W^{[1]} X^{\{t\}} + b^{[1]}$$

$$A^{[1]} = g^{[1]}(Z^{[1]})$$

$$\vdots$$

$$A^{[L]} = g^{[L]}(Z^{[L]})$$

Vectorized implementation (1000 examples)

1 step of grad descent using $X^{\{t\}}, Y^{\{t\}}$. (as if m=1000)

X, Y

Compute cost $J^{\{t\}} = \frac{1}{1000} \sum_{i=1}^{l} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2 \cdot 1000} \sum_{l} \|W^{[l]}\|_F^2$.

from $X^{\{t\}}, Y^{\{t\}}$.

Backprop to compute gradients wrt $J^{\{t\}}$ (using $(X^{\{t\}}, Y^{\{t\}})$)

$W^{[l]} := W^{[l]} - \alpha dW^{[l]}$, $b^{[l]} := b^{[l]} - \alpha db^{[l]}$

}

}

"1 epoch"

pass through training set.

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Optimization algorithms

Mini-batch gradient descent

repeat { for $t = 1, \dots, 5000$ {

Forward prop on $X^{\{t\}}$.

$$\left.\begin{aligned} Z^{[1]} &= W^{[1]} X^{\{t\}} + b^{[1]} \\ A^{[1]} &= g^{[1]}(Z^{[1]}) \\ &\vdots \\ A^{[L]} &= g^{[L]}(Z^{[L]}) \end{aligned}\right\} \text{Vec}$$

Compute cost $J^{\{t\}} = \frac{1}{1000} \sum_{i=1}^{l} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2 \cdot 1000} \sum_{l} \|W^{[l]}\|_F^2$.

Backprop to compute gradients wrt $J^{\{t\}}$ (using $(X^{\{t\}}, Y^{\{t\}})$)

$W^{[l]} := W^{[l]} - \alpha dW^{[l]}$, $b^{[l]} := b^{[l]} - \alpha db^{[l]}$

}

}

1 step of gradient descent using $X^{\{t\}}, Y^{\{t\}}$. (as if $m = 1000$)

X, Y

"1 epoch" – pass through training set.

- Epoch means one pass over the full training set
- Batch means that you use all your data to compute the gradient during one iteration.
- Mini-batch means you only take a subset of all your data during one iteration.

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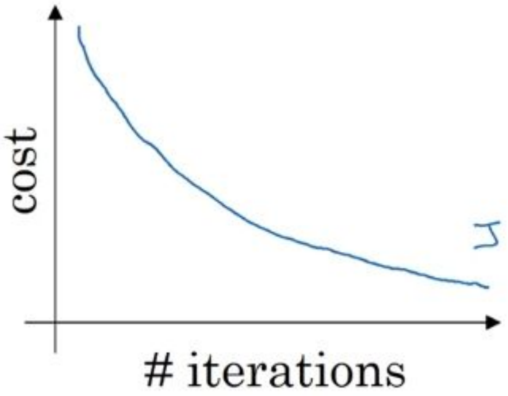
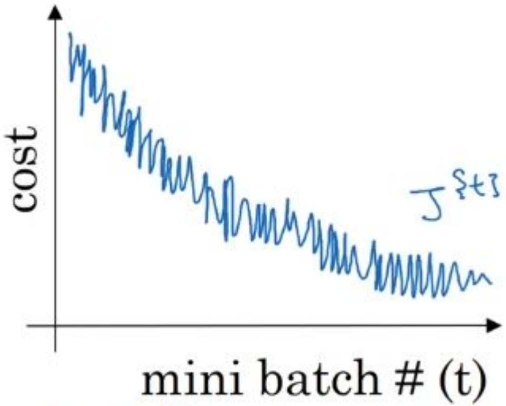
Optimization algorithms

Training with mini batch gradient descent

Batch gradient descent



Mini-batch gradient descent



Plot $J^{\{t\}}$ computed using $X^{\{t\}}, Y^{\{t\}}$

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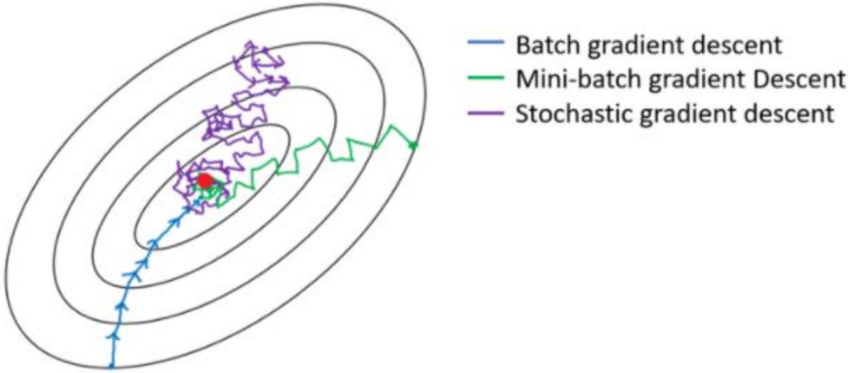
Optimization algorithms



Stochastic gradient Descent

Lose speedup from vectorization

In-between (mini-batch size not too big/small)

Fastest learning.

- Vectorization. (~1,000)

Batch gradient descent (mini-batch size = m)

Too long per iteration

Typical mini-batch sizes:

$\underbrace{\underset{2^6}{64}, \underset{2^7}{128}, \underset{2^8}{256}, \underset{2^9}{512}}$ $\quad \underset{2^{10}}{1024}$

Make sure mini-batch fit in CPU/GPU memory.

$X^{\{t\}}, Y^{\{t\}}$.

Optimization algorithms

Exponentially weighted averages

$$V_t = \beta V_{t-1} + (1-\beta)\theta_t$$

$\beta = 0.9$: ≈ 10 days' temperature.

$\beta = 0.98$: ≈ 50 days

V_t as approximately average over $\approx \frac{1}{1-\beta}$ days' temperature.

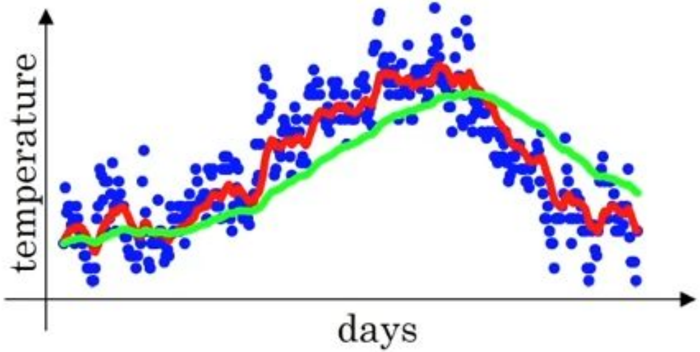
$$\frac{1}{1-0.98} = 50$$

$$SMA = \frac{A_1 + A_2 + \ldots + A_n}{n}$$

where:

A = Average in period n

n = Number of time periods



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Optimization algorithms

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$$SMA = \frac{A_1 + A_2 + \ldots + A_n}{n}$$

where:

A = Average in period n

n = Number of time periods

What Is an Exponential Moving Average (EMA)?

An exponential moving average (EMA) is a type of moving average (MA) that places a greater weight and significance on the most recent data points. The exponential moving average is also referred to as the exponentially weighted moving average.

Optimization algorithms

Exponentially weighted averages

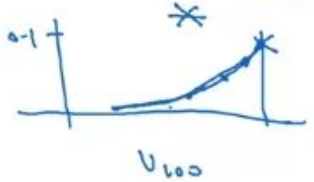
$$v_t = \beta v_{t-1} + (1-\beta)\theta_t$$

$$v_{100} = 0.9v_{99} + 0.1\theta_{100}$$

$$\boxed{v_{99} = 0.9v_{98} + 0.1\theta_{99}}$$

$$\boxed{v_{98} = 0.9v_{97} + 0.1\theta_{98}}$$

$$\cdots$$



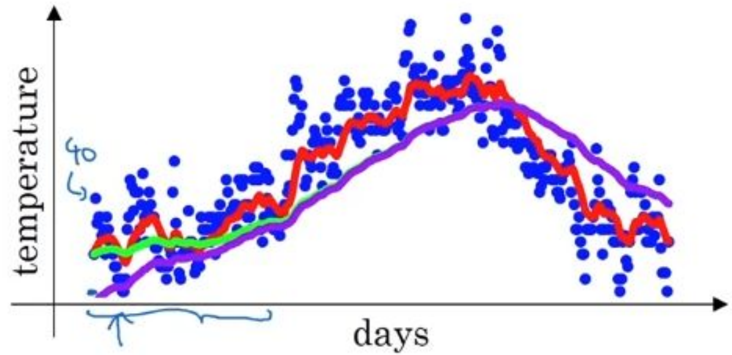
$$0.1\,\theta_{98} + 0.9\,v_{97}$$

$$V_{100} = 0.1\,\theta_{100} + 0.9\,\cancel{v_{99}}\,(0.1\,\theta_{99} + 0.9\,\boxed{\cancel{v_{98}}})$$

$$= 0.1\,\theta_{100} + 0.1 \times 0.9 \cdot \theta_{99} + 0.1\,(0.9)^2\,\theta_{98} + 0.1\,(0.9)^3\,\theta_{97} + 0.1\,(0.9)^4\,\theta_{96} + \cdots$$

Optimization algorithms

Bias correction



$\beta = 0.98$

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

$V_0 = 0$

$V_1 = \cancel{0.98 V_0 +} \; 0.02\,\theta_1$

$V_2 = 0.98\,V_1 + 0.02\,\theta_2$

$= 0.98 \times 0.02 \times \theta_1 + 0.02\,\theta_2$

$= 0.0196\,\theta_1 + 0.02\,\theta_2$

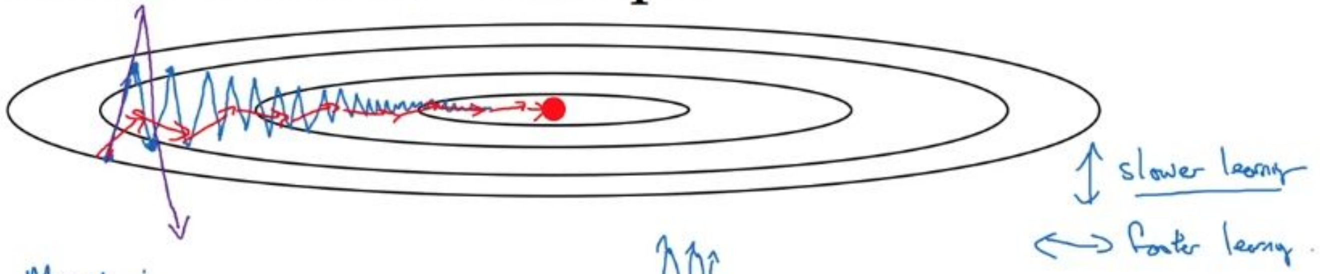
$\dfrac{V_t}{1-\beta^t}$

$t=2: \quad 1-\beta^t = 1-(0.98)^2 = 0.0396$

$\dfrac{V_2}{0.0396} = \dfrac{0.0196\,\theta_1 + 0.02\,\theta_2}{0.0396}$

Optimization algorithms

Gradient descent example



Momentum:

On iteration t:

Compute dW, db on current mini-batch.

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

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

"$V_\theta = \beta V_\theta + (1-\beta) \theta_t$"

$$W := W - \alpha V_{dW}, \quad b := b - \alpha V_{db}$$

Optimization algorithms

Implementation details

On iteration t:

Compute dW, db on the current mini-batch

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

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

$$W = W - \alpha v_{dW}, \;\; b = b - \alpha v_{db}$$

Hyperparameters: α, β $\beta = 0.9$

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