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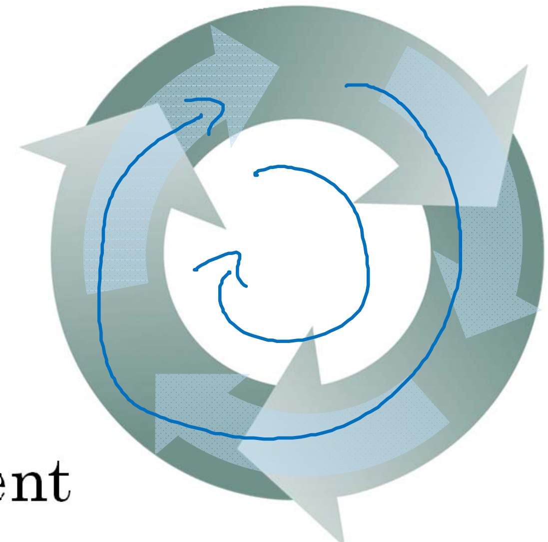
Setting up your ML application

Train/dev/test sets

Applied ML is a highly iterative process

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

Idea



Experiment

Code

NLP, Vision, Speech, Structural data

Ads search Security logistics ....

Andrew Ng

Train/dev/test sets

training set

- Hold-out cross validation
- Development set "dev"

test

Previous era: 70/30% (train / test)

60/20/20%

100 - 1000 - 10000

Big data: 1,000,000 10,000 10,000

98/1/1%

99.5/ ~~.25~~ .4 / ~~.25~~ .1%

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Mismatched train/test distribution

Cats

Training set:
Cat pictures from webpages

Dev/test sets:
Cat pictures from users using your app

→ Make sure dev and test come from same distribution.

"test"

train / dev

train / test

→ train / dev

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

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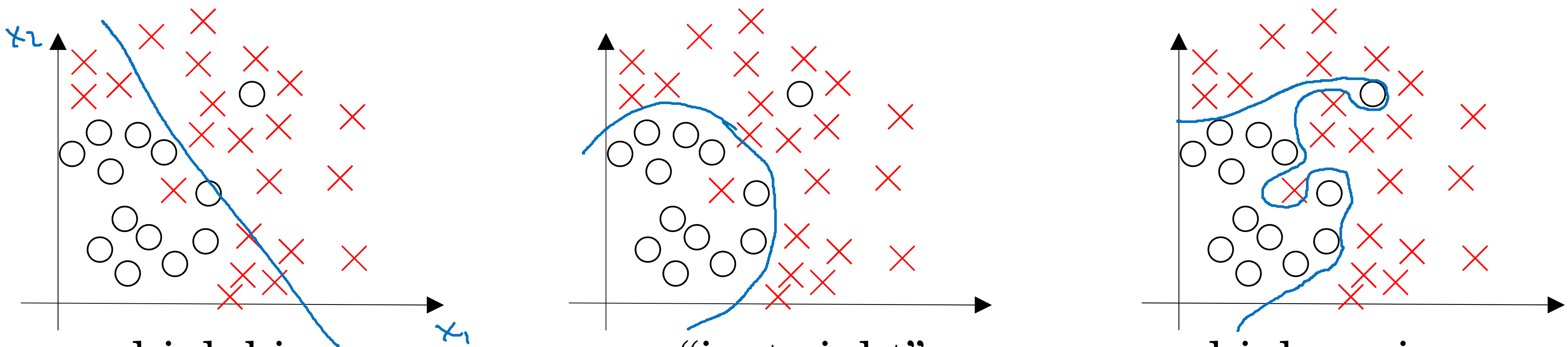
Setting up your ML application

Bias/Variance

Bias and Variance



high bias — "just right" — high variance

Underfitting — Overfitting

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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 variance	low bias low variance

Human: ≈0%

Optimal (Bayes) error: ~~≈0%~~ 15%

Blurry images

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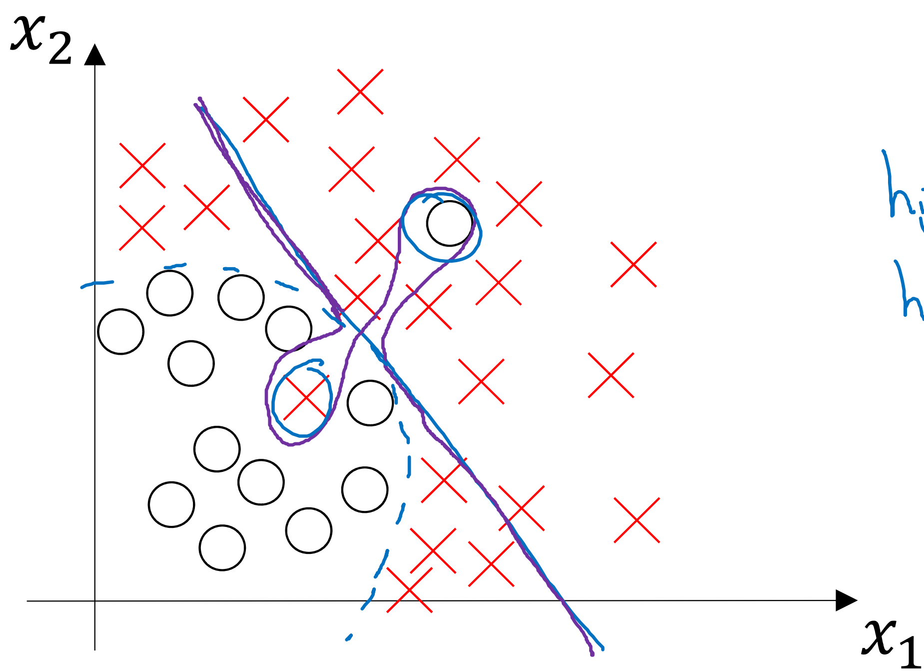
High bias and high variance



high bias
high varian

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Setting up your ML application

Basic “recipe” for machine learning

Basic "recipe" for machine learning

Basic recipe for machine learning

High bias?
(training data performance)

Y

- Bigger network
- Train longer
- (NN architecture search)

N

High variance?
(dev set performance)

Y

- More data
- Regularization
- (NN architecture search)

N

Done

Bias variance "tradeoff"

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Regularizing your neural network

Regularization

Logistic regression

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

λ = regularization parameter

lambda   lambd

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

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

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

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

w will be sparse

Neural network

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

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

"Frobenius norm" $\qquad \|\cdot\|_2^2 \qquad \|\cdot\|_F^2$

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

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

"Weight decay"

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

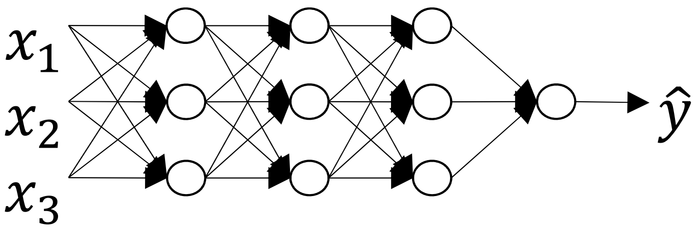
$$= w^{[l]} - \frac{\alpha\lambda}{m} w^{[l]} - \alpha(\text{from backprop})$$

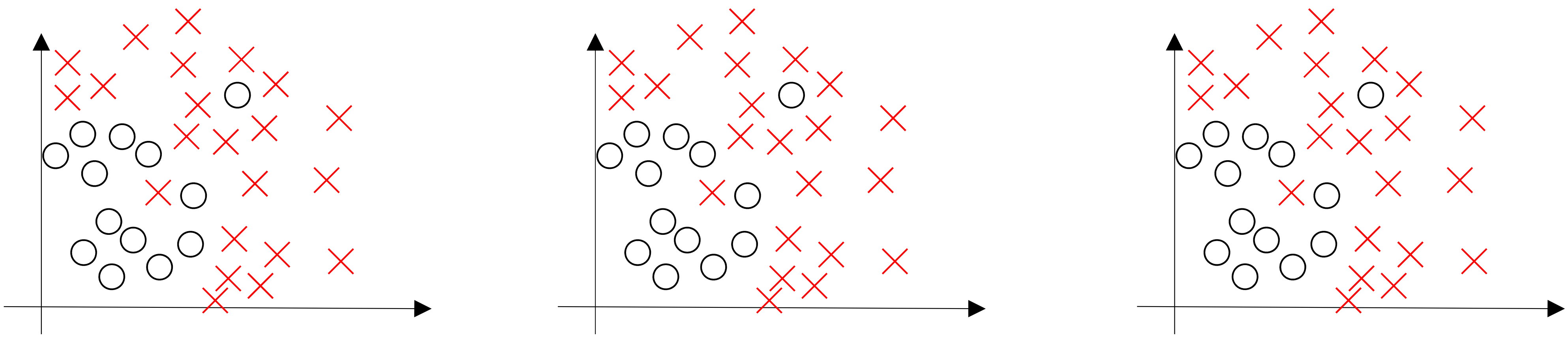
$$= \underbrace{\left(1 - \frac{\alpha\lambda}{m}\right)}_{<1} \underbrace{w^{[l]} - \alpha(\text{from backprop})}$$

Neural network

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

How does regularization prevent overfitting?





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How does regularization prevent overfitting?

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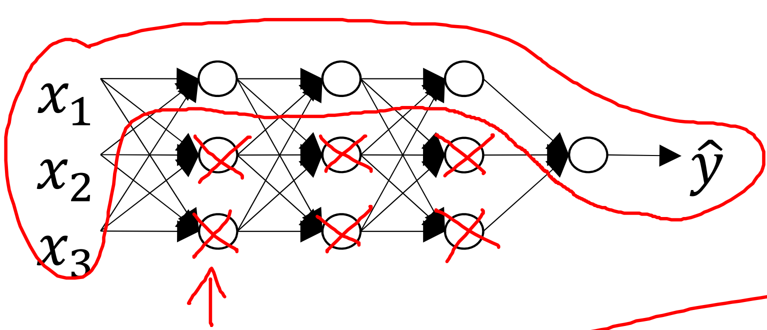
Regularizing your neural network

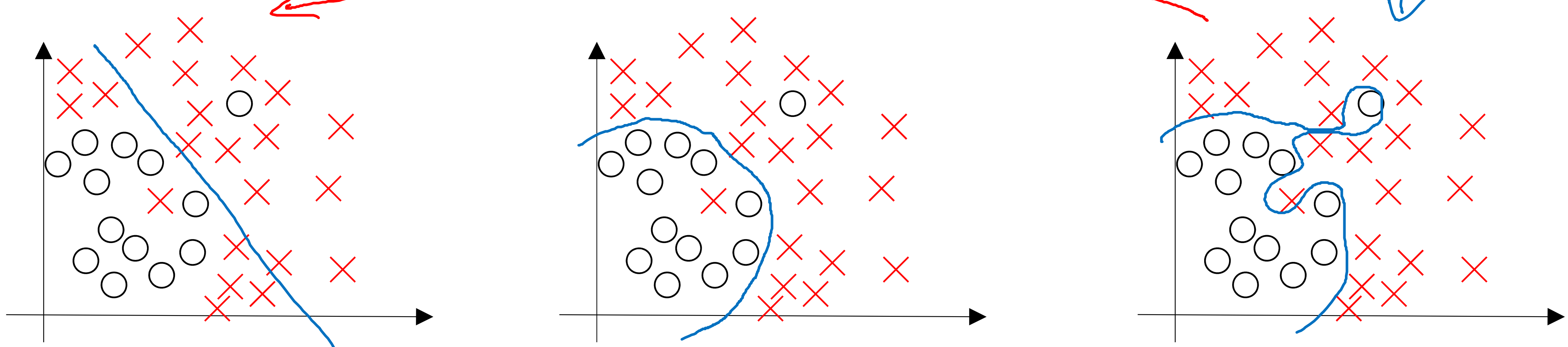
Why regularization reduces overfitting

How does regularization prevent overfitting?



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

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



high bias "just right" high variance

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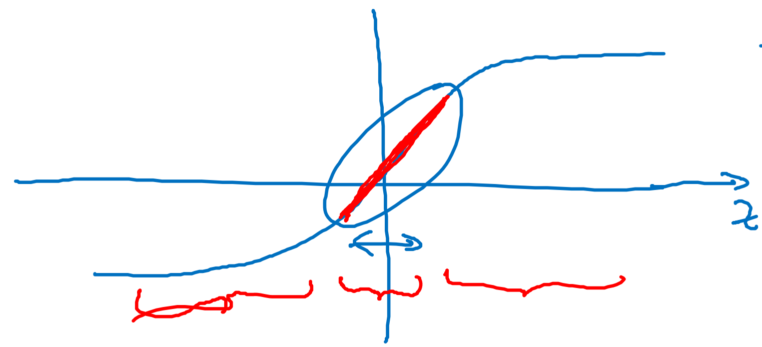
How does regularization prevent overfitting?

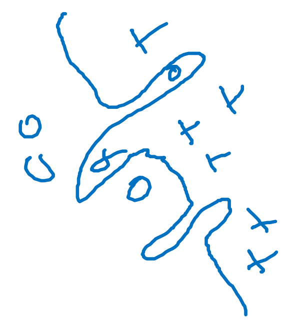


tanh

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

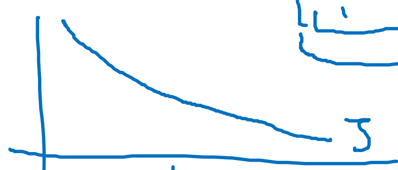
$\lambda \uparrow$ $\quad W^{[l]} \downarrow$

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



Every layer ≈ linear.

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



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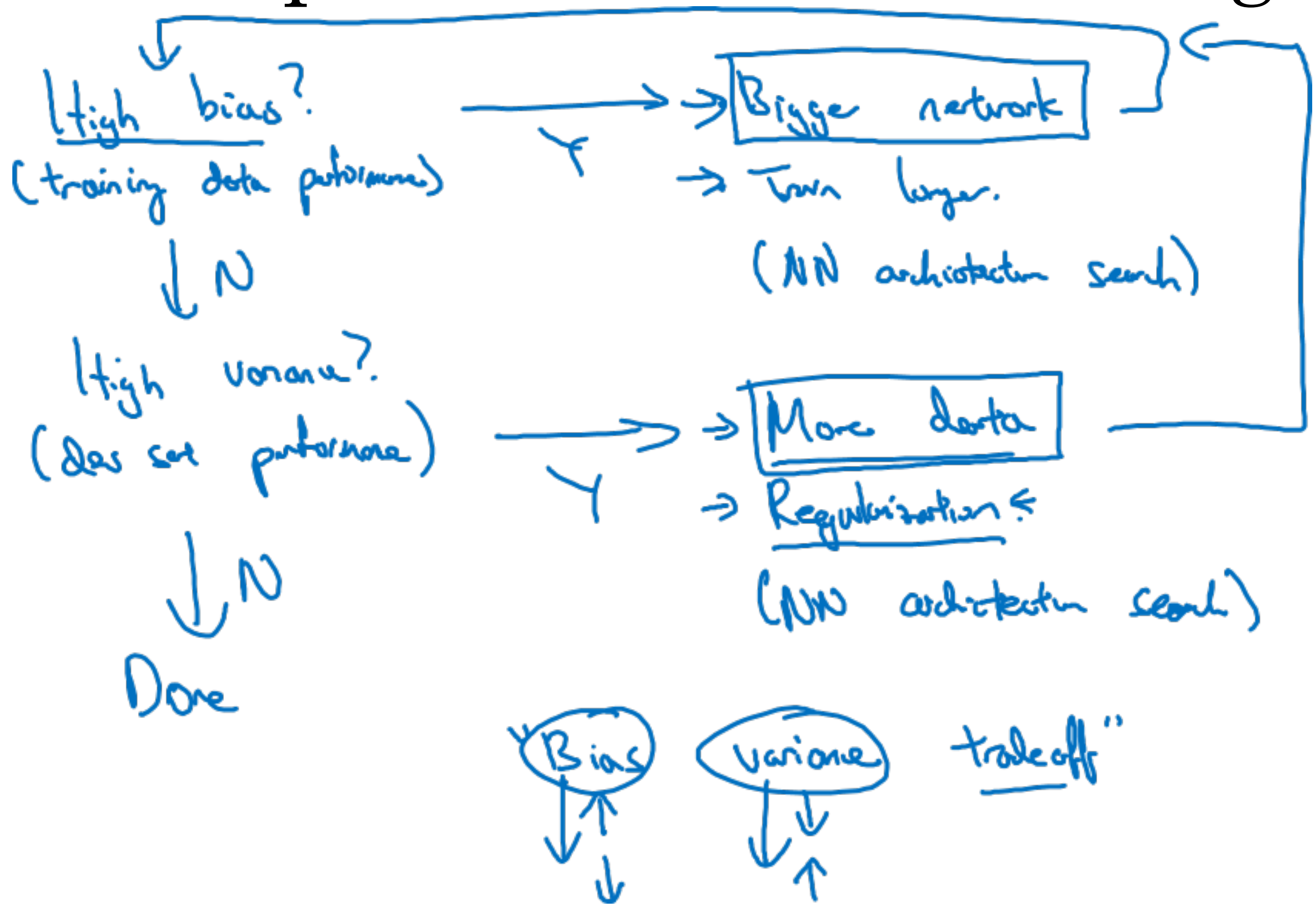
Setting up your ML application

Basic “recipe” for machine learning

Basic "recipe" for machine learning

Basic recipe for machine learning



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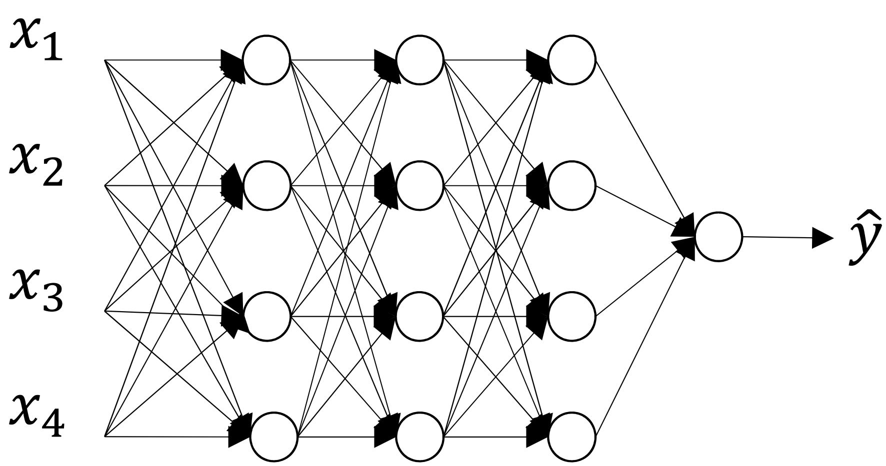
Regularizing your neural network

Dropout regularization

Dropout regularization



0.5 0.5 0.5

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Implementing dropout ("Inverted dropout")

Illustrate with layer $l = 3$. keep-prob = 0.8 0.2

$\rightarrow$ $\boxed{d3}$ = np.random.rand(a3.shape[0], a3.shape[1]) < keep-prob

a3 = np.multiply(a3, d3) # a3 *= d3.

$\rightarrow$ $\boxed{\text{a3 /= } \cancel{0.8} \text{ keep-prob}}$ $\leftarrow$

50 units. $\rightsquigarrow$ 10 units shut off

$$z^{[4]} = w^{[4]} \cdot a^{[3]} + b^{[4]}$$

reduced by 20%.

Test

/= 0.8

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Making predictions at test time

$a^{[0]} = X$

No drop out.

$z^{[1]} = W^{[1]} \underline{a^{[0]}} + b^{[1]}$

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

$z^{[2]} = W^{[2]} \underline{a^{[1]}} + b^{[2]}$

$a^{[2]} = \ldots$

$\downarrow$

$\hat{y}$

$/=$ keep-prob

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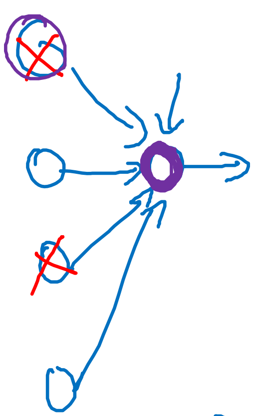
Regularizing your neural network

Understanding dropout

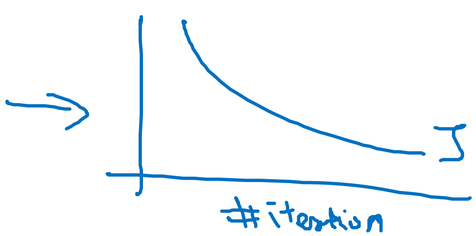
Why does drop-out work?

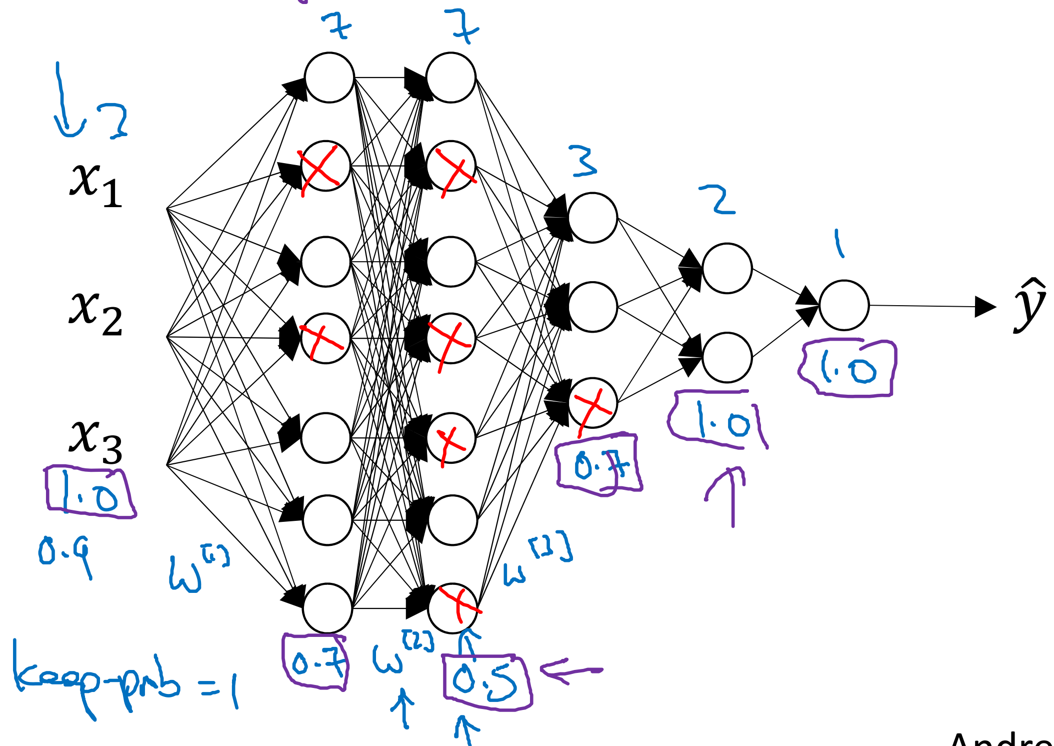
Intuition: Can't rely on any one feature, so have to spread out weights. → Shrink weights. L_2



→ Computer Vision

Downside: J





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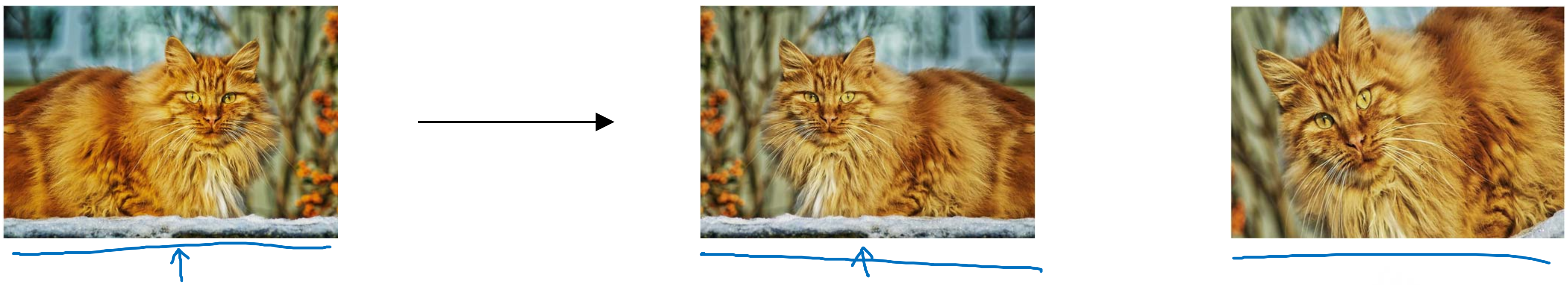
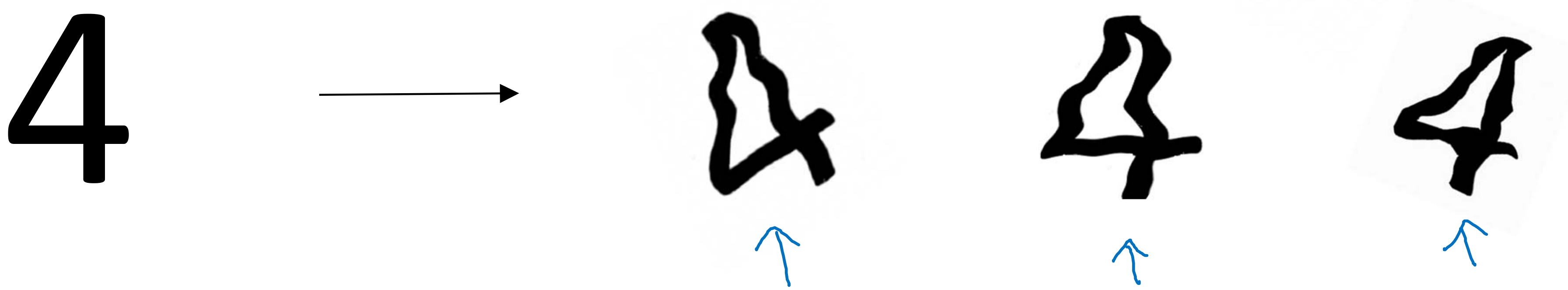
Regularizing your neural network

Other regularization methods

Data augmentation





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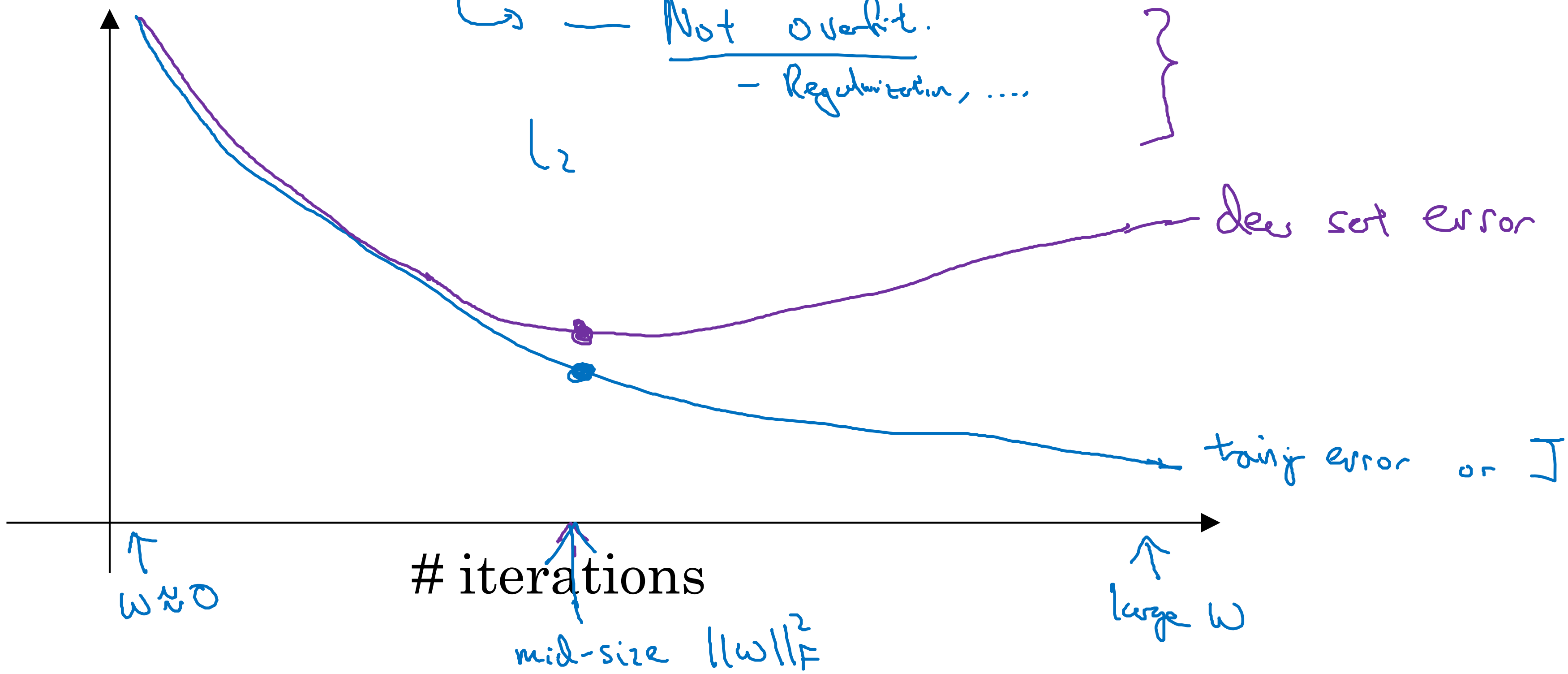
Early stopping

Orthogonalization

- Optimize cost function J
  - Gradient, ...
- Not overfit
  - Regularization, ...

L_2

$J(w,b)$



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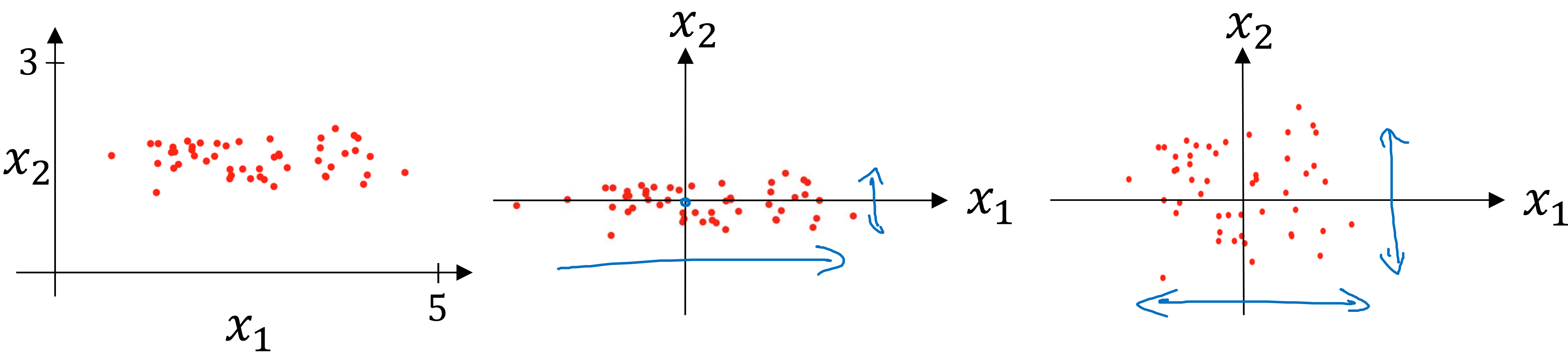
Setting up your optimization problem

Normalizing inputs

Normalizing training sets

$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$



Subtract mean:

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

$$\boxed{x := x - \mu}$$

Normalize variance

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

element-wise

$$\boxed{x \mathrel{/}= \sigma^2}$$

Use same μ, σ^2 to normalize test set.

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Why normalize inputs?

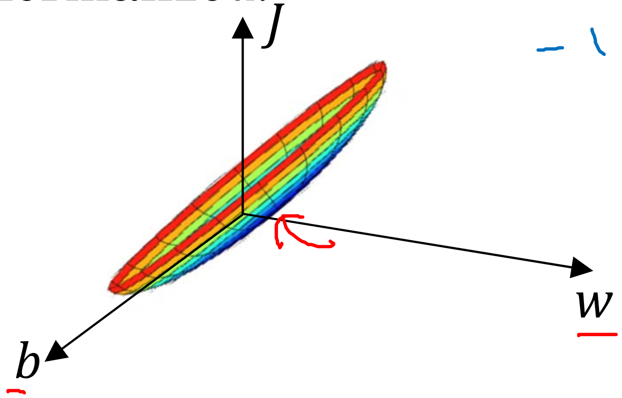
$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$

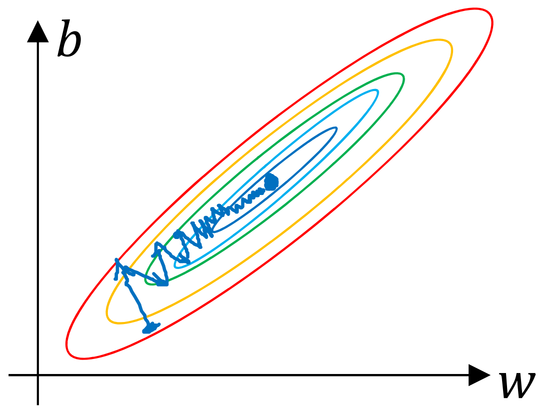
w_1 x_1: 1 ... 1000 ←

w_2 x_2: 0 ... 1 ←

−1 ... 1

Unnormalized:



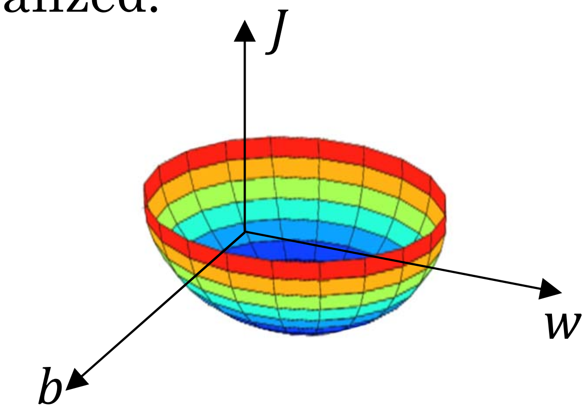


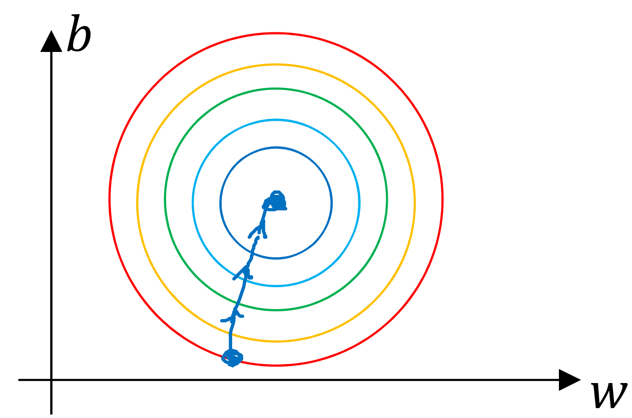
x_1 : 0 ... 1

x_2 : −1 ... 1

x_3 : 1 ... 2

Normalized:





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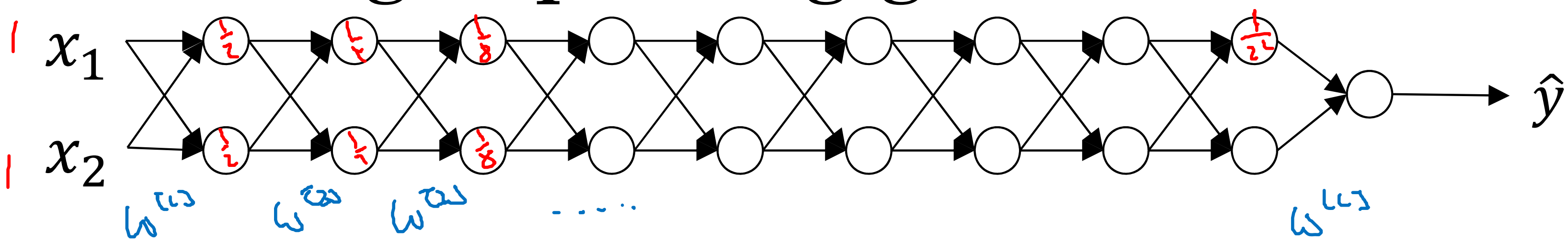
Setting up your optimization problem

Vanishing/exploding gradients

Vanishing/exploding gradients

$L = 150$



L

$g(z) = z$. $b^{[l]} = 0$.

$\hat{y} = W^{[L]} W^{[L-1]} W^{[L-2]} \cdots \underbrace{W^{[3]} W^{[2]} W^{[1]} x}_{a^{[3]}}$

1.5^L

0.5^L

$z^{[1]} = W^{[1]} x$

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

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

$W^{[l]} > I$

$W^{[l]} < I \quad \begin{bmatrix} 0.9 & \\ & 0.9 \end{bmatrix}$

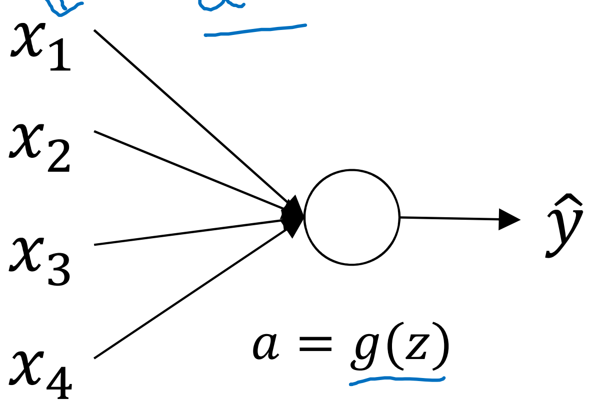
$W^{[l]} = \begin{bmatrix} \cancel{1.5}\ 0.5 & 0 \\ 0 & \cancel{1.5}\ 0.5 \end{bmatrix}$

$\hat{y} = W^{[L]} \begin{bmatrix} \cancel{1.5}\ 0.5 & 0 \\ 0 & \cancel{1.5}\ 0.5 \end{bmatrix}^{L-1} x$

$1.5^{L-1} x$

$0.5^{L-1} x$

Single neuron example



$a^{[l]}$

$w^{[l]}$

$z = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + \cancel{b}$

Large $n \rightarrow$ Smaller w_i

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

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

ReLU $\qquad g^{[l]}(z) = \mathrm{ReLU}(z)$

Other variants:

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

Xavier initialization

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

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Setting up your optimization problem

Numerical approximation of gradients

Checking your derivative computation

$f(\theta) = \theta^3$

$\theta \in \mathbb{R}$.

J

$g(\theta) = \frac{d}{d\theta} f(\theta) = f'(\theta)$

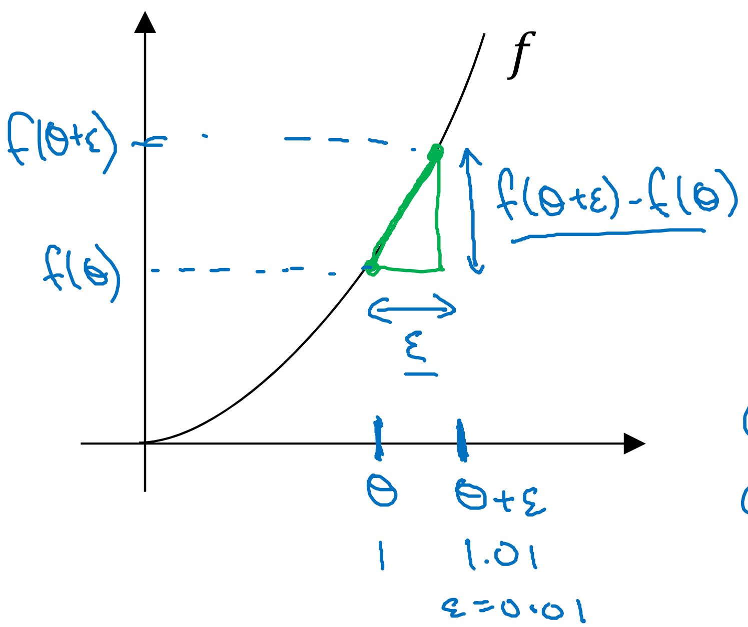
dw

db

$g(\theta) = 3\theta^2$.

$g(\theta) = 3\cdot(1)^2 = 3$ when $\theta = 1$

$$\boxed{\frac{f(\theta+\varepsilon) - f(\theta)}{\varepsilon} \approx g(\theta)}$$



$$\frac{(1.01)^3 - 1^3}{0.01} = 3.0301 \approx 3$$

$\theta = 1$

$\theta + \varepsilon = 1.01$

0.0301

3.1

3.2

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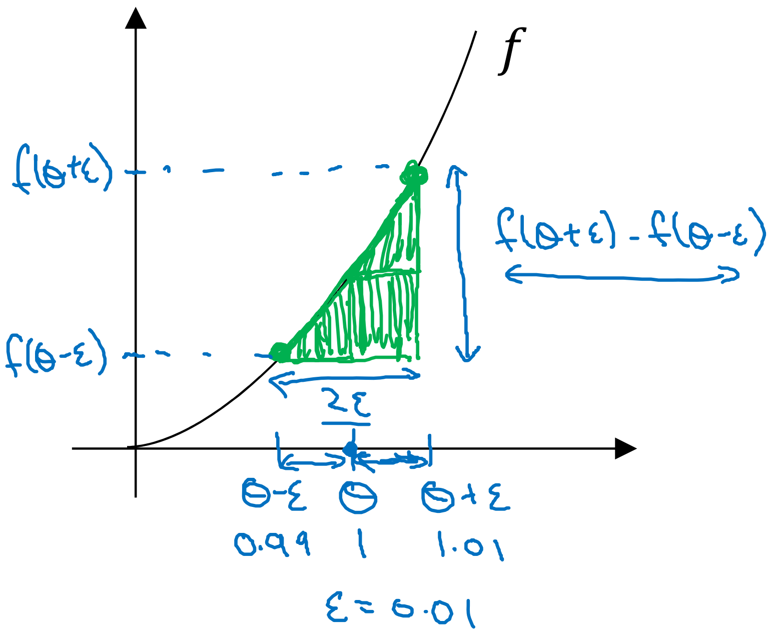
Checking your derivative computation

$f(\theta) = \theta^3$



$$\boxed{\frac{f(\theta+\varepsilon) - f(\theta-\varepsilon)}{2\varepsilon} \approx g(\theta)}$$

$$\frac{(1.01)^3 - (0.99)^3}{2(0.01)} = 3.0001 \approx 3$$

$$g(\theta) = 3\theta^2 = 3$$

approx error: 0.0001

(prev slide: 3.0301. error: 0.03)

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

0.01

0.0001

$$\frac{f(\theta+\varepsilon) - f(\theta)}{\varepsilon} \qquad \text{error}: O(\varepsilon)$$

0.01

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Setting up your optimization problem

Gradient Checking

Gradient check for a neural network

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

concatenate

$J(W^{[1]}, b^{[1]}, \ldots, W^{[L]}, b^{[L]}) = J(\theta)$

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

concatenate

Is $d\theta$ the gradient of $J(\theta)$?

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Gradient checking (Grad check)

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

for each i:

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

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

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

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

10^{-5}

$\rightarrow 10^{-3}$ – worry.

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

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Setting up your optimization problem

Gradient Checking implementation notes

Gradient checking implementation notes

- Don't use in training – only to debug

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

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

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

- Remember regularization.

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

$d\theta$ = gradient of J w.r.t. θ

- Doesn't work with dropout.

J $\underline{\text{keep-prob} = 1.0}$

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

$\underline{w, b \approx 0}$

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