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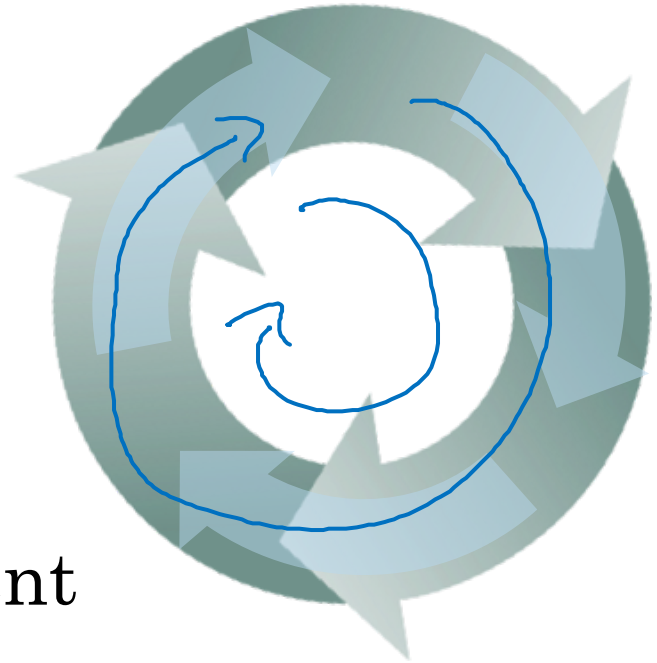
Setting up your ML application

Train/dev/test sets

Applied ML is a highly iterative process

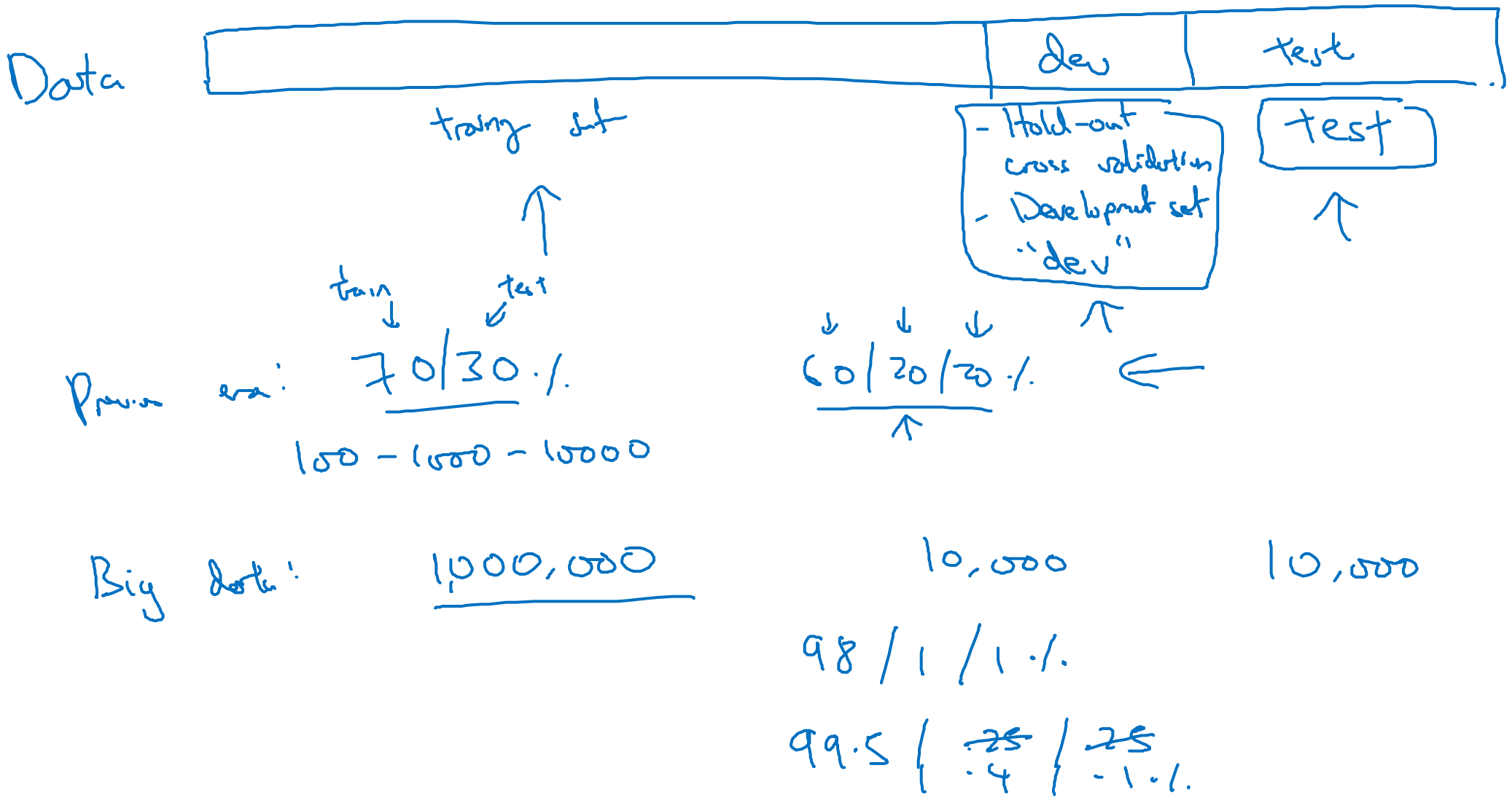
- # layers
- # hidden units
- learning rates
- activation functions
- ...



NLP, Vision, Speech, Structured data

Ads Search Security Logistic ....

Train/dev/test sets



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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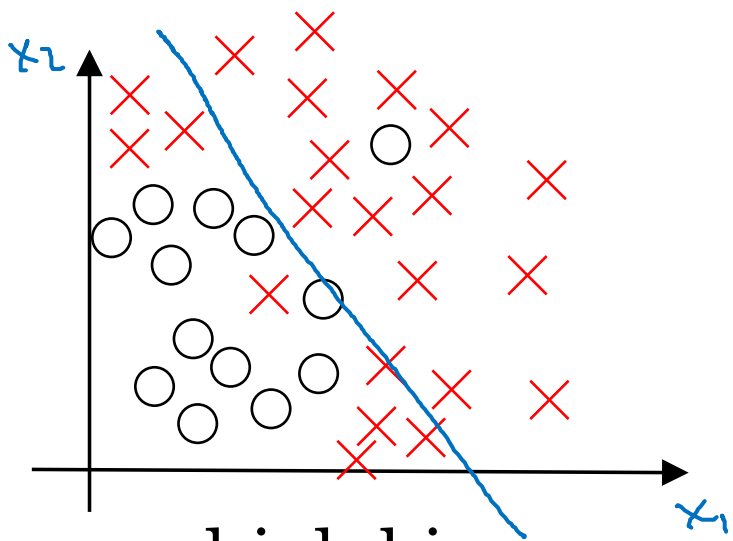
Setting up your ML application

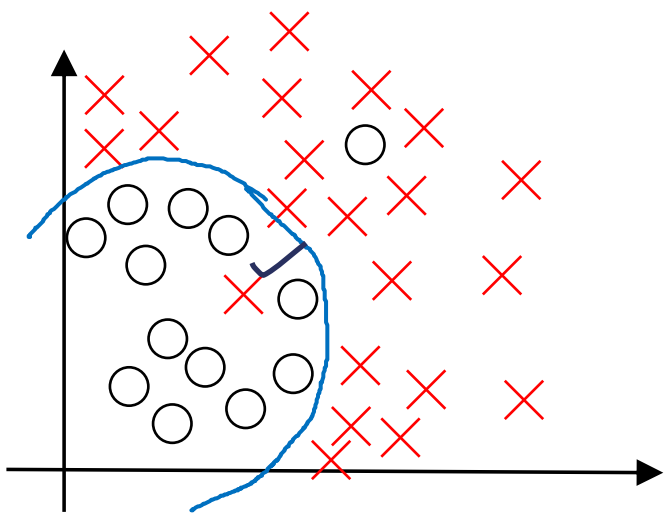
Bias/Variance

Bias and Variance

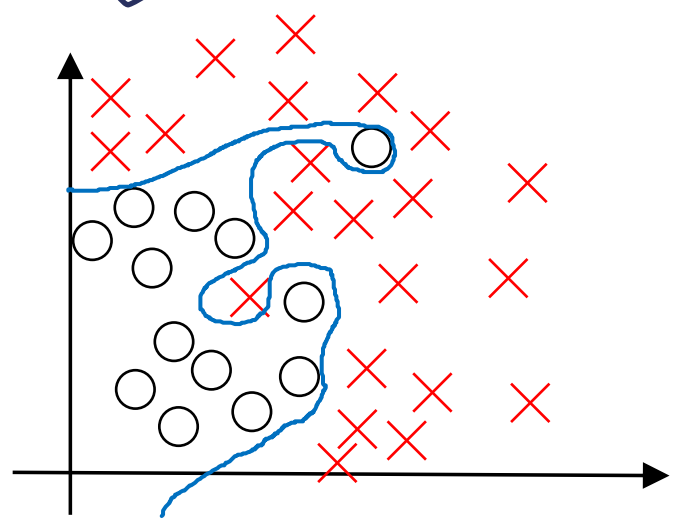


high bias

Underfitting



"just right"

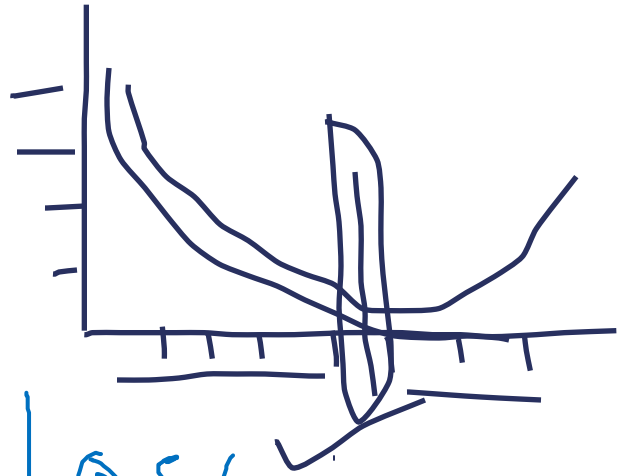


high variance

Overfitting

Bias and Variance

Cat classification



Train set error: 1% | 15% | 15% | 0.5%

Dev set error: 11% | 16% | 30% | 1%

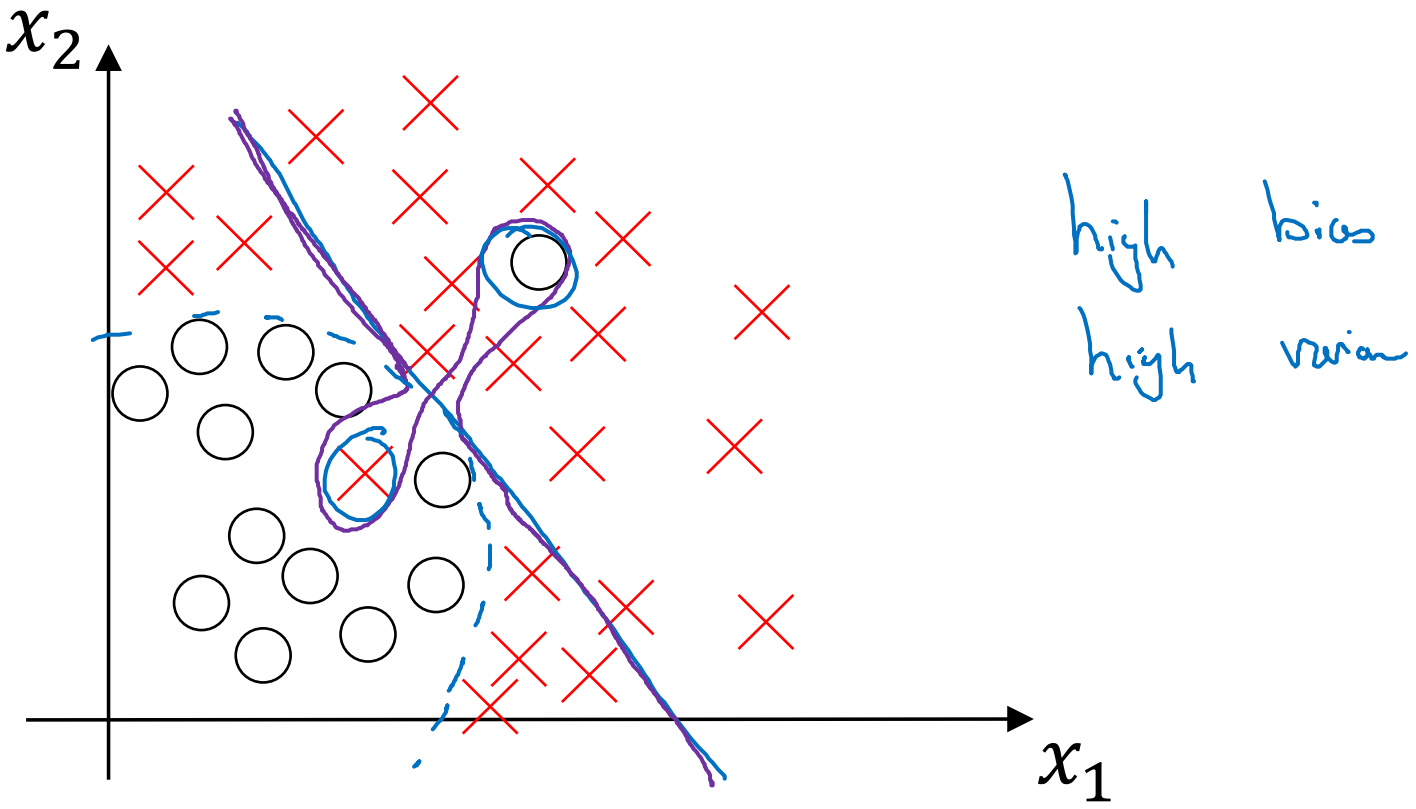
high variance | high bias | high bias & high variance | low bias, low variance

Human: ≈0%

Optimal (Bayes) error: ~~≈0%~~ 15%

Blurry images

High bias and high variance



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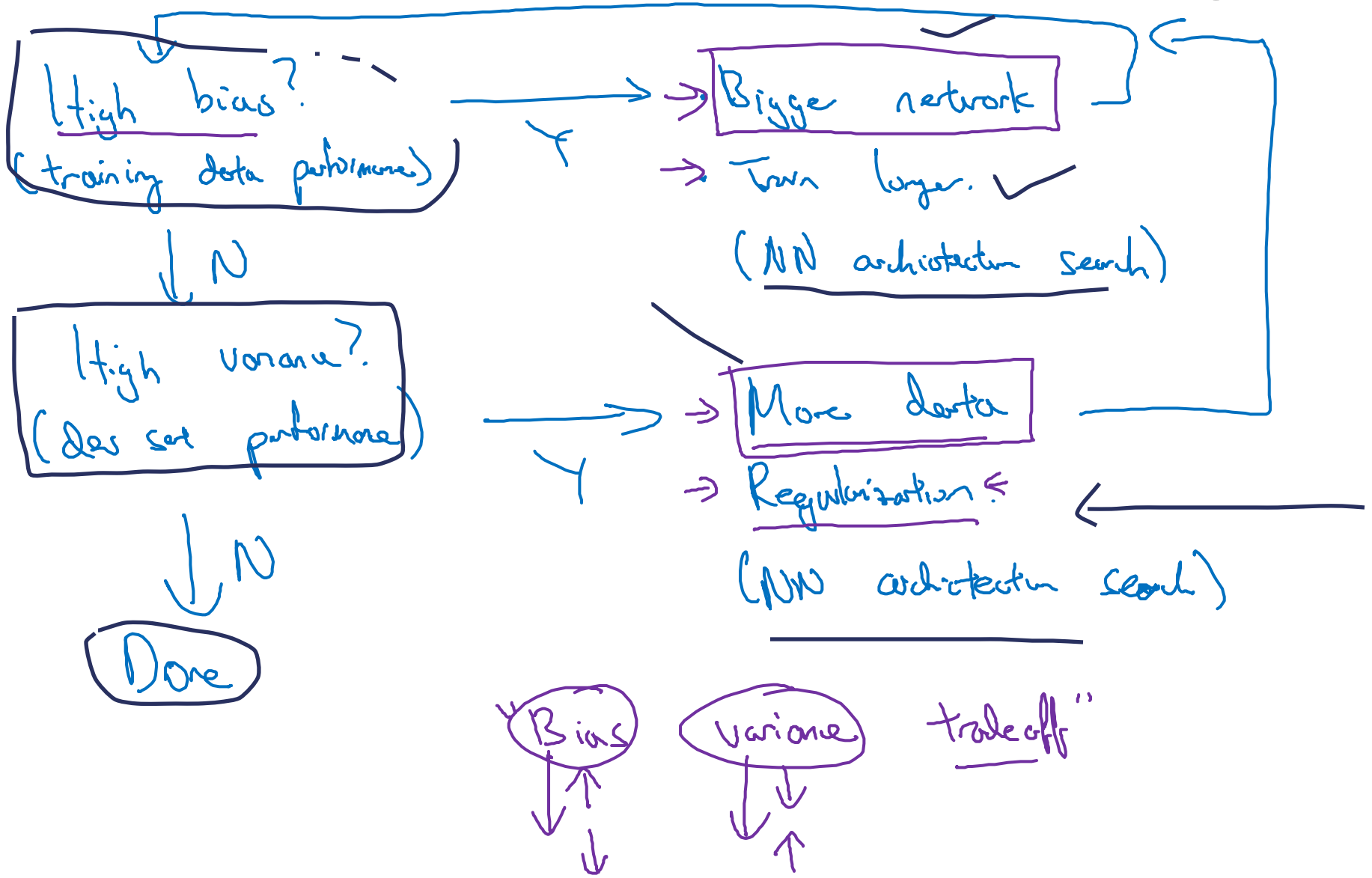
Setting up your ML application

Basic “recipe” for machine learning

Basic recipe for machine learning



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Regularizing your neural network

Regularization

Logistic regression

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

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

λ = regularization parameter

lambda lambd

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

$+ \frac{\lambda}{2m} b^2$

omit

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 be sparse

Neural network

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

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

$w^{[l]}: (n^{[l]}, n^{[l-1]})$

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

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

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

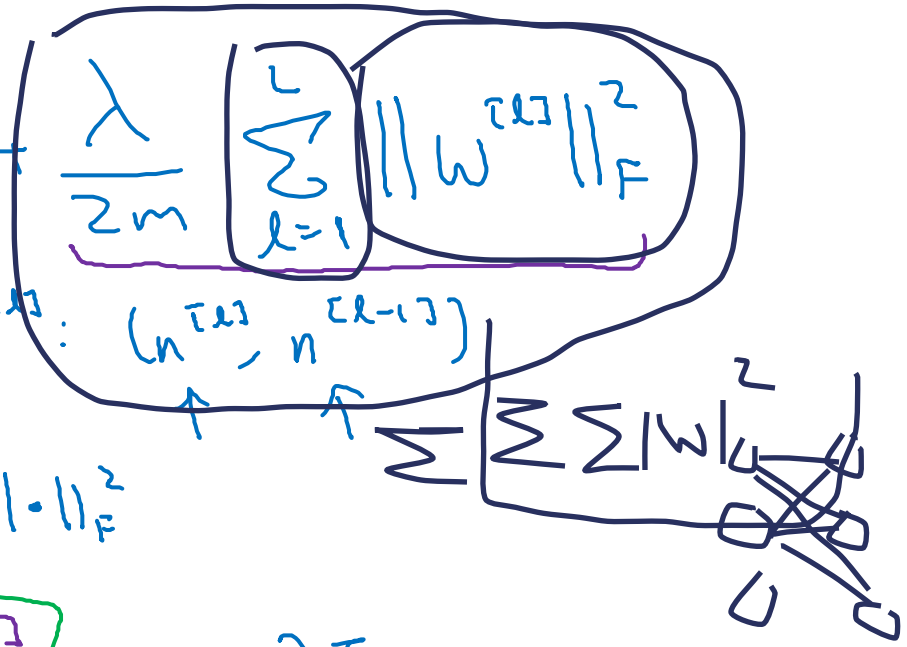
$$\frac{\partial J}{\partial w^{[l]}} = dw^{[l]}$$

"Weight decay"

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

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

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



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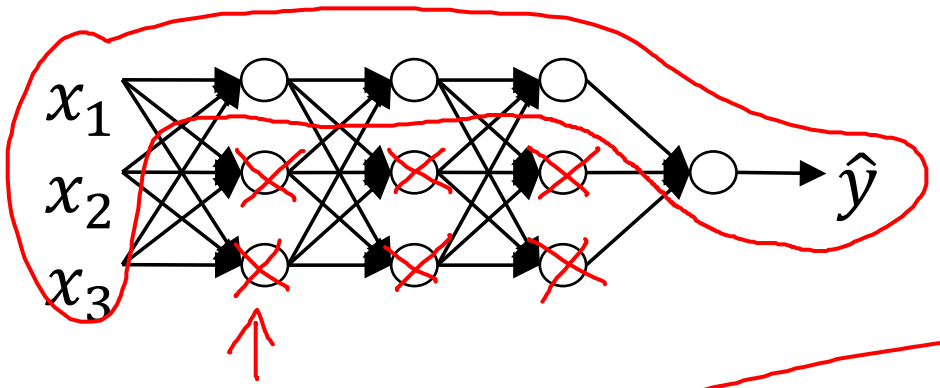
Regularizing your neural network

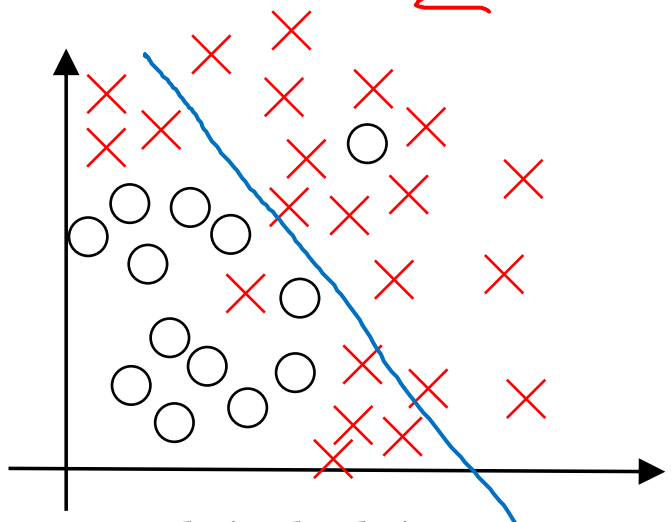
Why regularization reduces overfitting

How does regularization prevent overfitting?

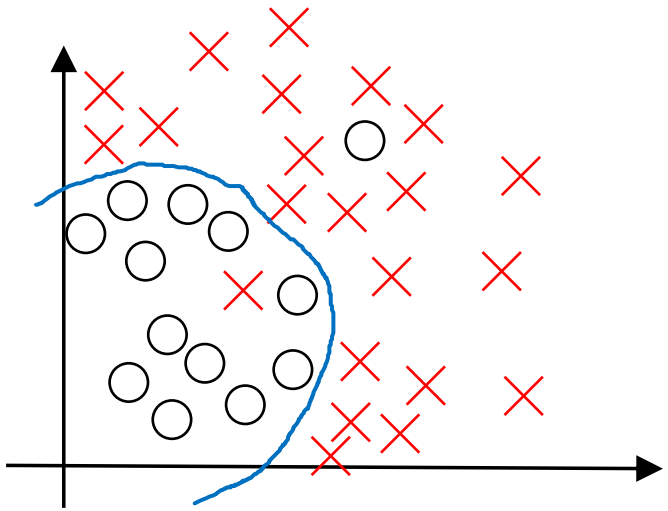


$$J(w^{[l]}, b^{[l]}) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L} \|w^{[l]}\|_F^2$$

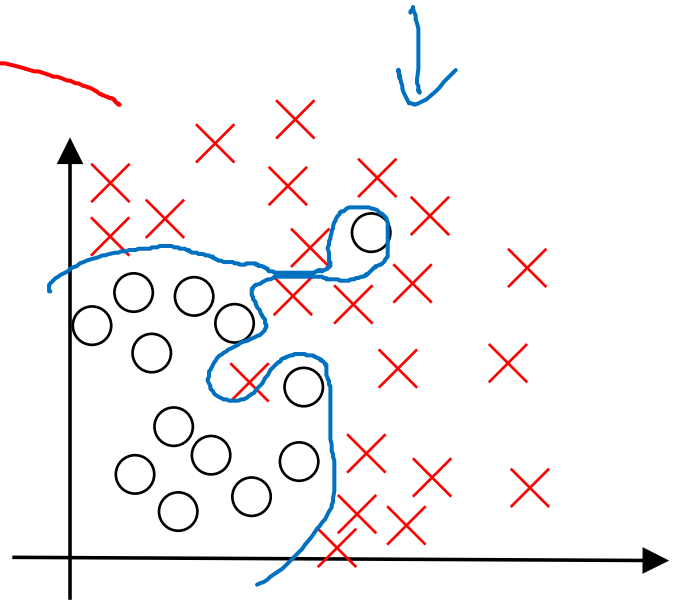
$w^{[l]} \approx 0$



high bias



"just right"



high variance

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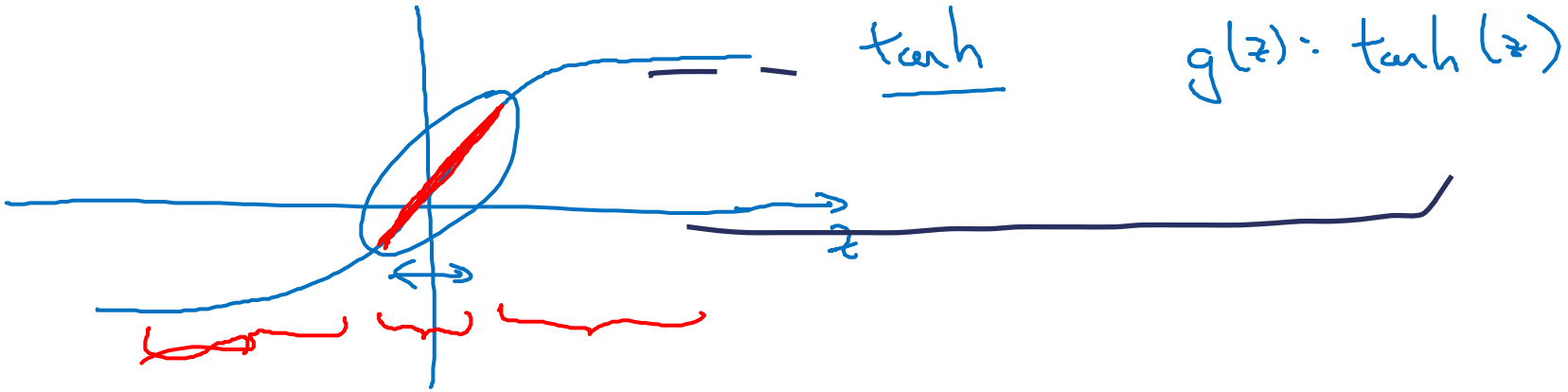
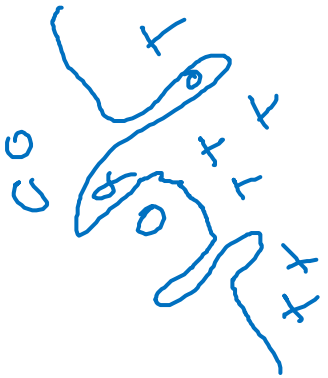
How does regularization prevent overfitting?

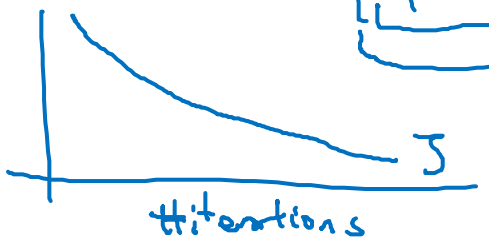


$\lambda \uparrow$ $\quad W^{[l]} \downarrow$ $\quad z^{[l]} = W^{[l]} a^{[l-1]} + b^{[l]}$



Every layer $\approx$ 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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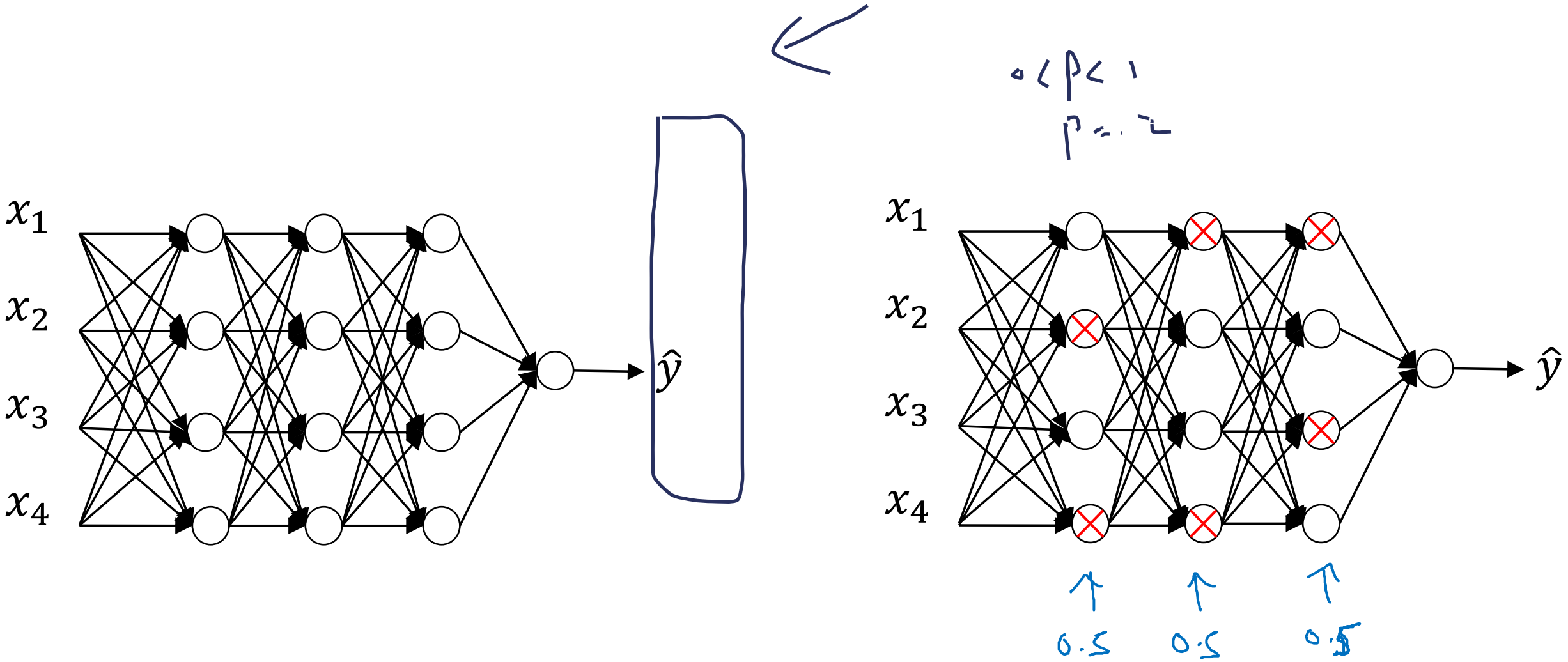
Regularizing your neural network

Dropout regularization

Dropout regularization



Implementing dropout ("Inverted dropout")

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

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

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

$a3 /= keep\text{-}prob$

50 units. ⇝ 10 units shut off

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

$a^{[3]}$ reduced by 20%.

Test

$/= 0.8$

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Making predictions at test time

$a^{[0]} = X$

No drop out.

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

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

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

$a^{[3]} = \ldots$

$\downarrow$

$\hat{y}$

/= keep-prob

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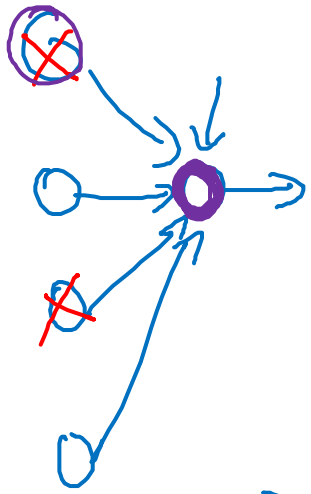
Regularizing your neural network

Understanding dropout

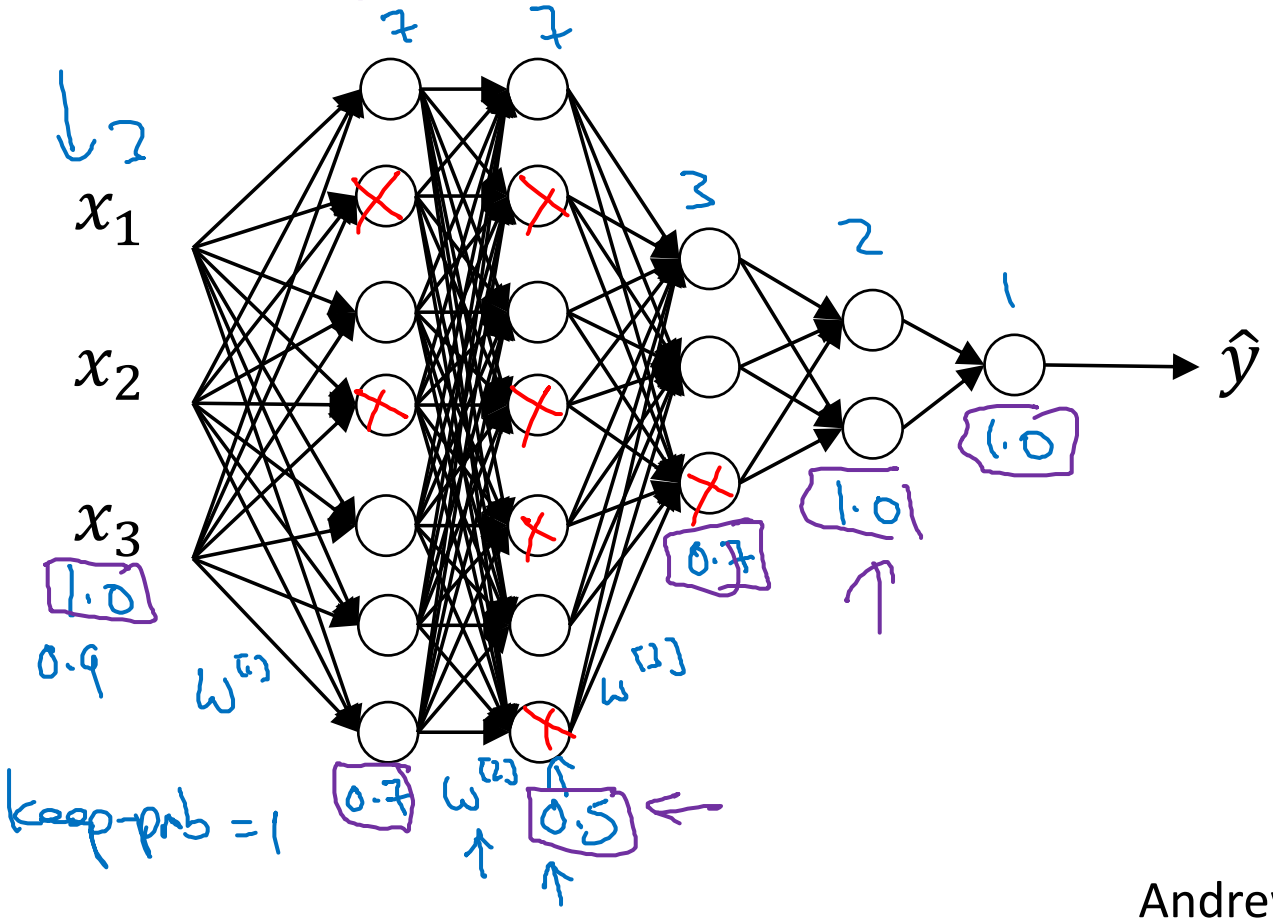
Why does drop-out work?

Intuition: Can't rely on any one feature, so have to spread out weights. ⇝ Shrink weights. b_2



→ Computer Vision

Downside: J



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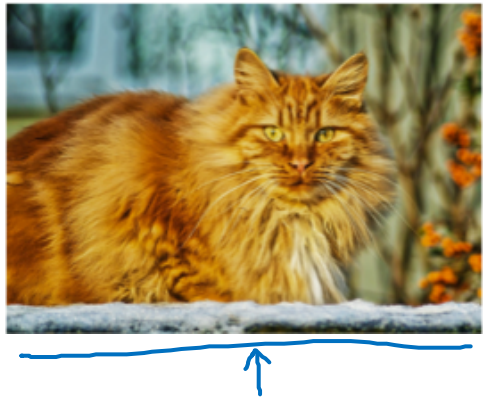
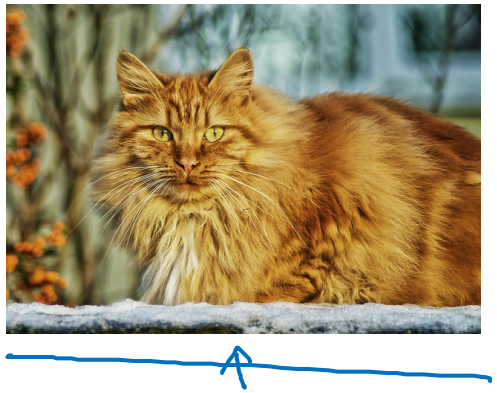
Regularizing your neural network

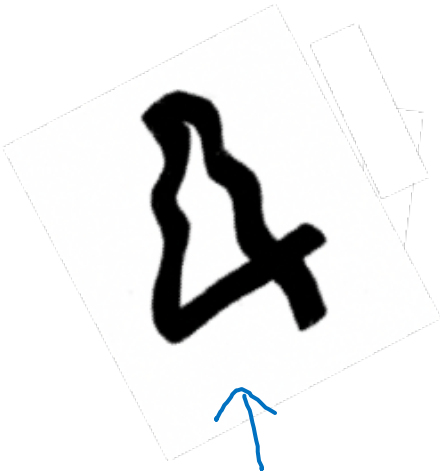
Other regularization methods

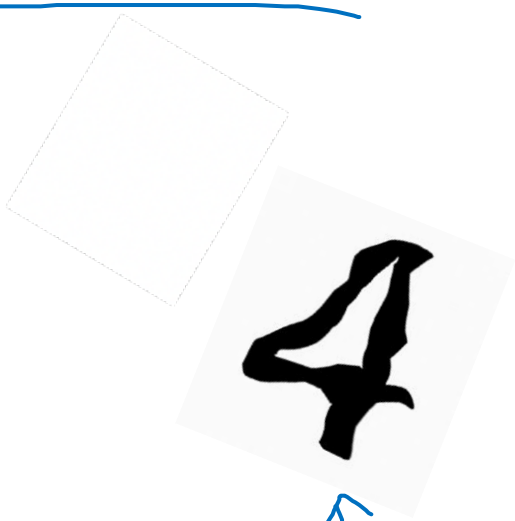
Data augmentation





4





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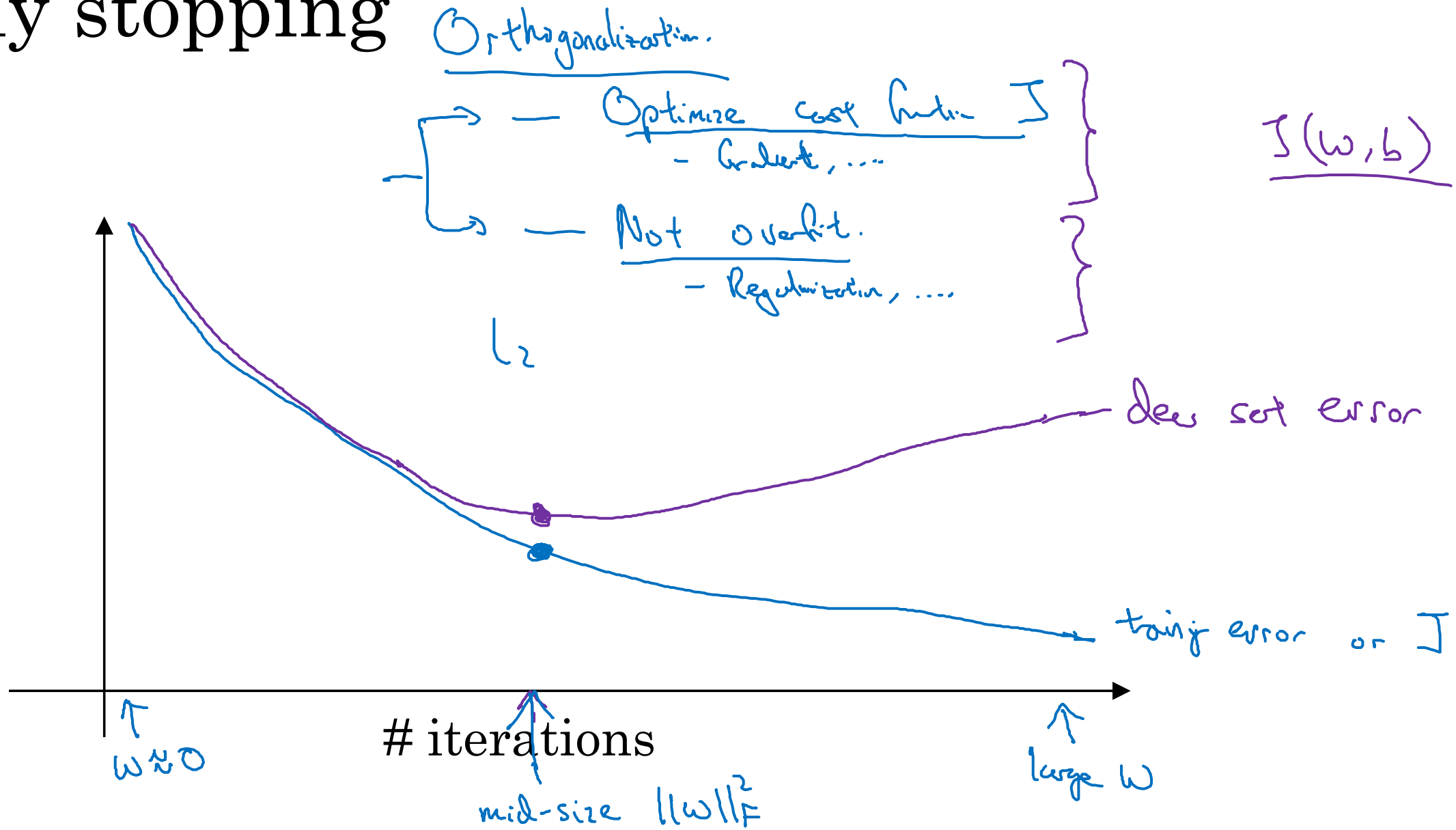
Early stopping



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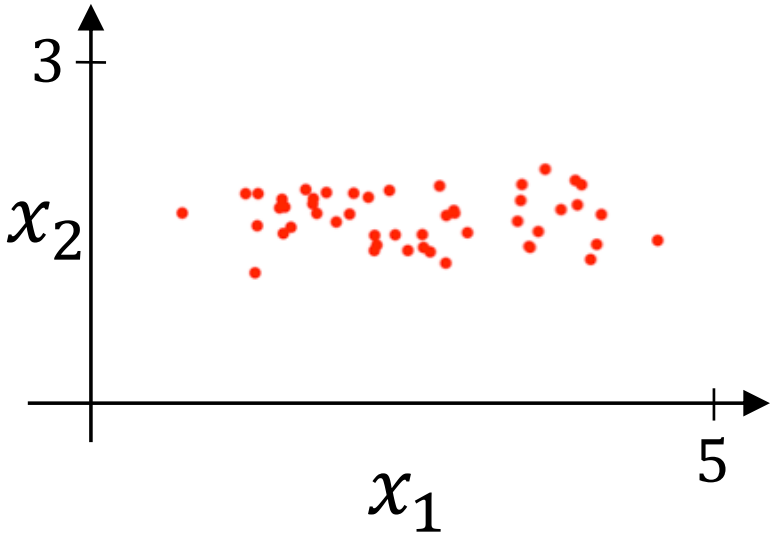
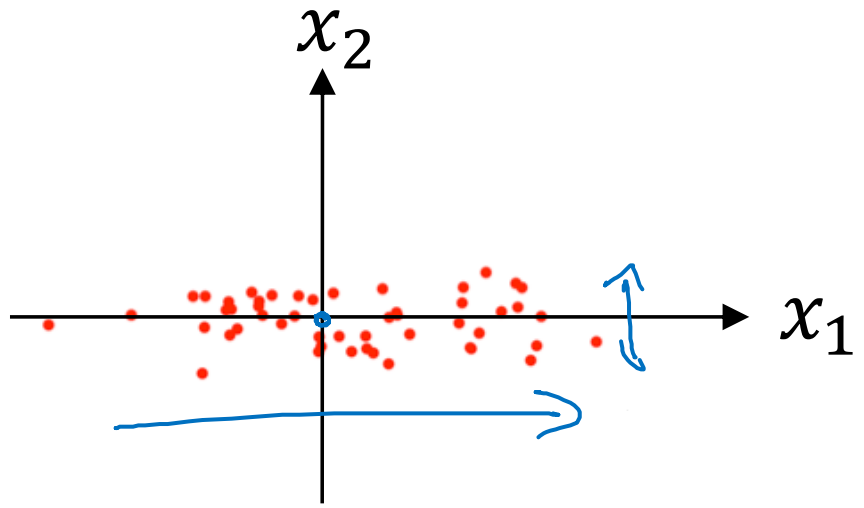
Setting up your optimization problem

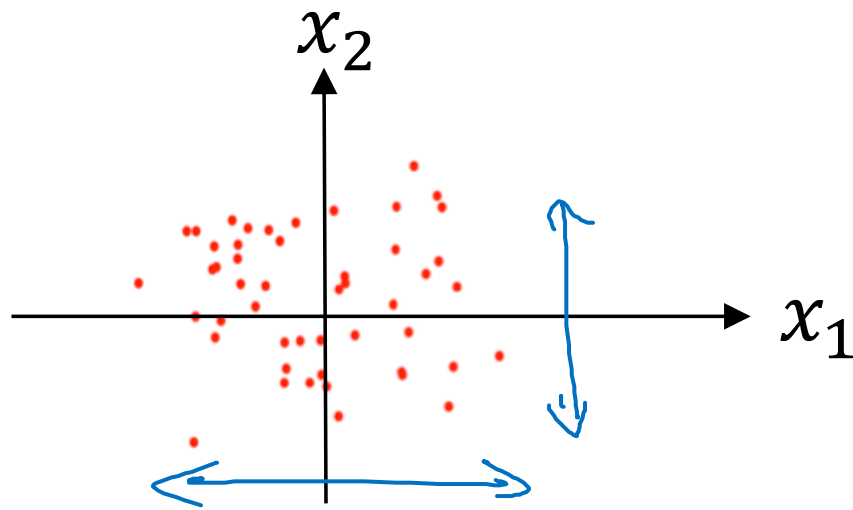
Normalizing inputs

Normalizing training sets

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







Subtract mean:

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

$x := x - \mu$

Normalize variance

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

↑ element-wise

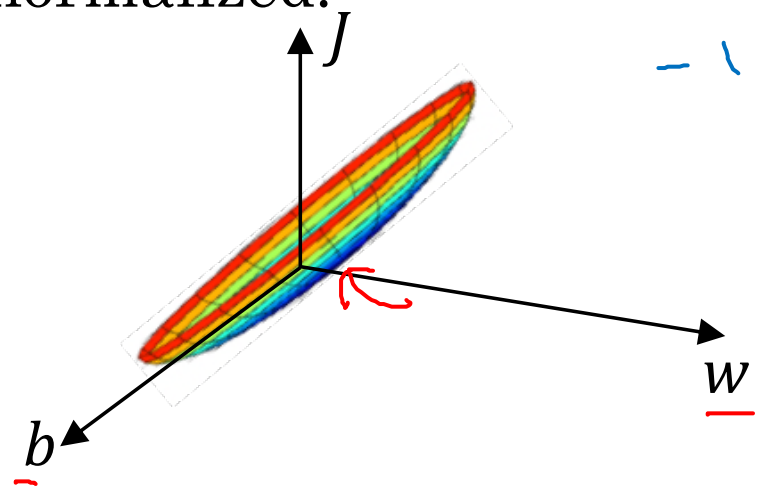
$x /= \sigma^2$

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

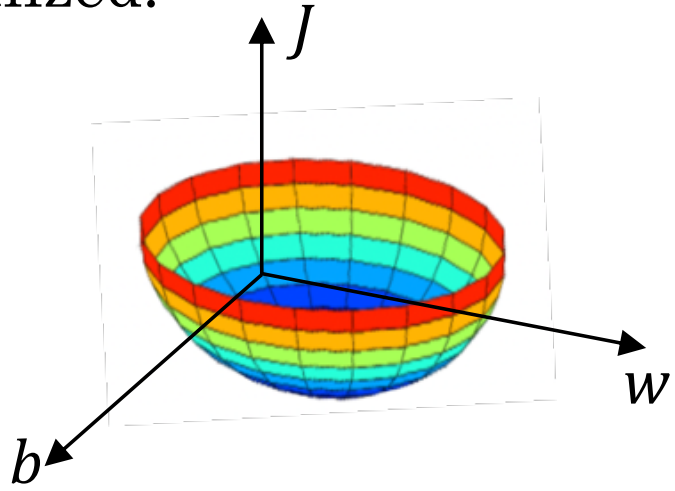
Why normalize inputs?

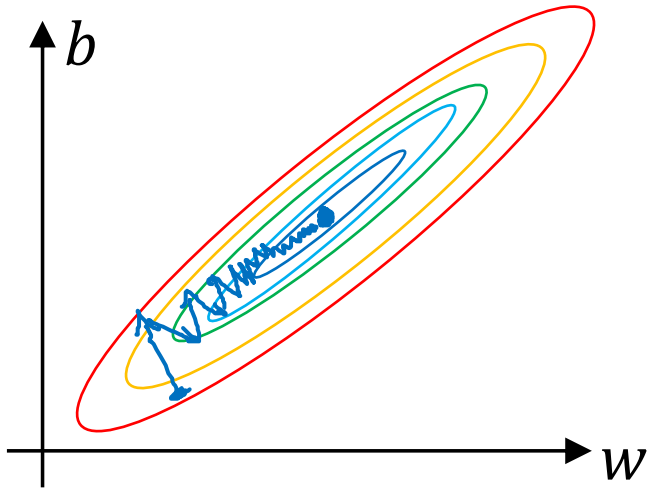
$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$

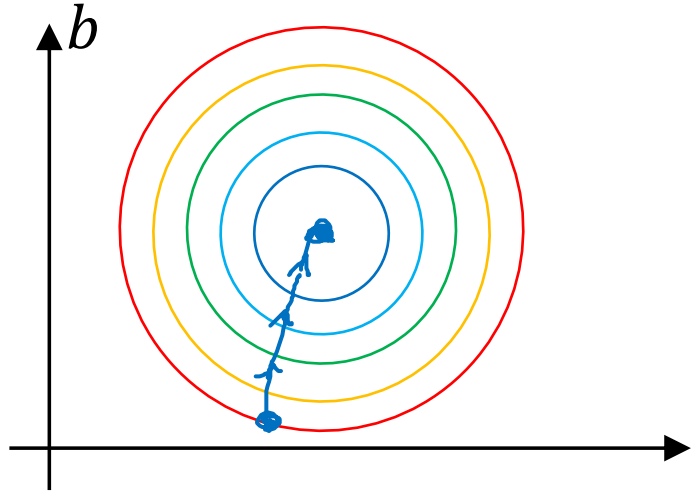
Unnormalized:



Normalized:







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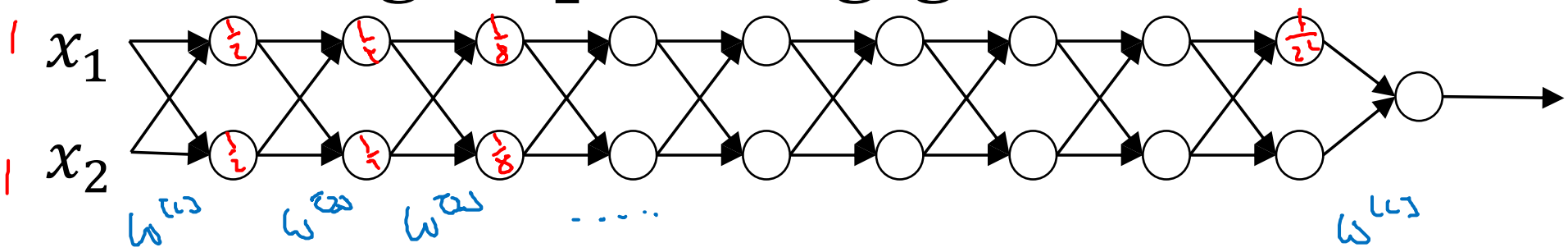
Setting up your optimization problem

Vanishing/exploding gradients

Vanishing/exploding gradients



$L = 150$

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

$\hat{y} = w^{[L]} w^{[L-1]} w^{[L-2]} \cdots w^{[3]} w^{[2]} w^{[1]} x$ $\quad a^{[3]}$

1.5^L

0.5^L

$w^{[l]} > I$

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

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

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

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

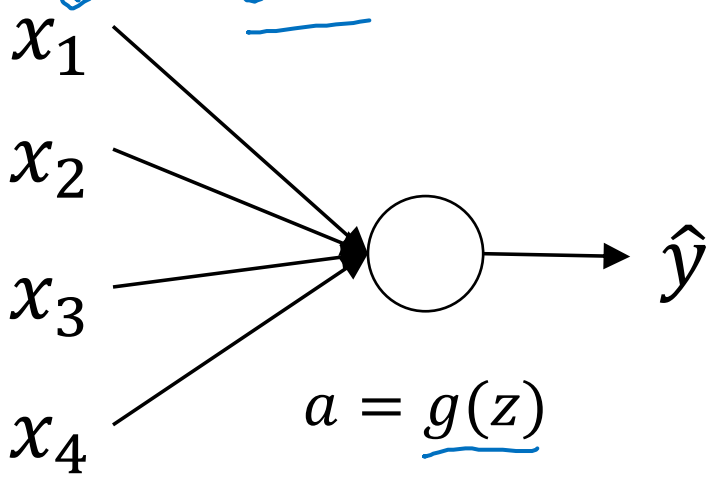
$w^{[l]} = \begin{bmatrix} 1.5 & 0 \\ 0 & 1.5 \end{bmatrix}$ $\quad 0.5$ $\quad 0.5$

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

$1.5^{L-1} x$

$0.5^{L-1} x$

Single neuron example



$w^{[l]}$

$z = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$ ~~+b~~

large n → smaller w_i

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

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

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

Other variants:

tanh

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

Xavier initialization

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

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Setting up your optimization problem

Numerical approximation of gradients

Checking your derivative computation

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

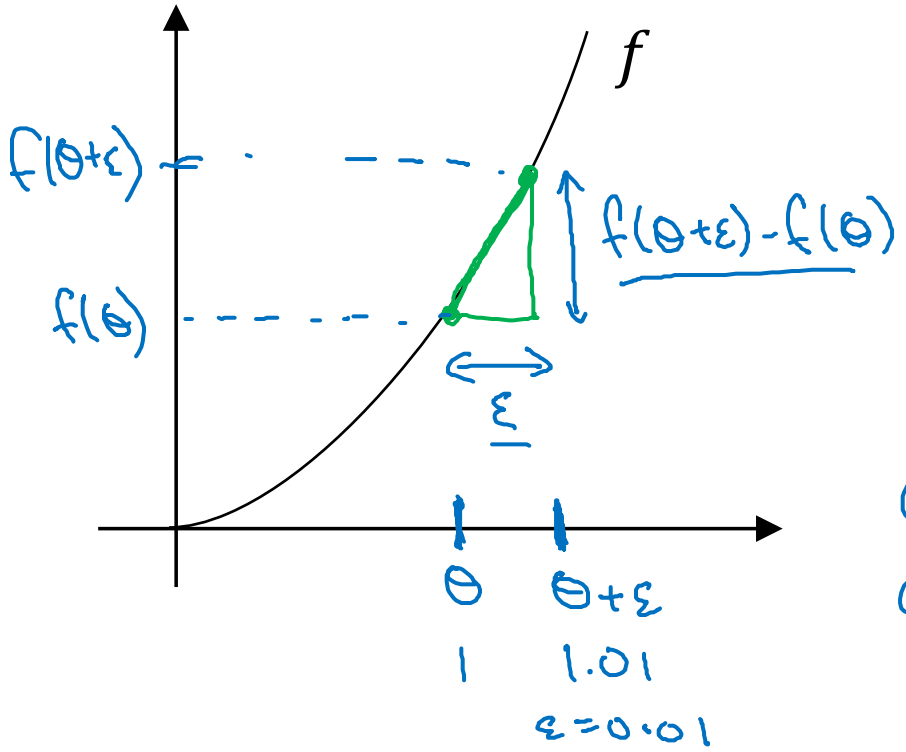
$\theta \in \mathbb{R}$.

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

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

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

$\frac{dw}{db}$



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

$\theta = 1$

$\theta + \varepsilon = 1.01$

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

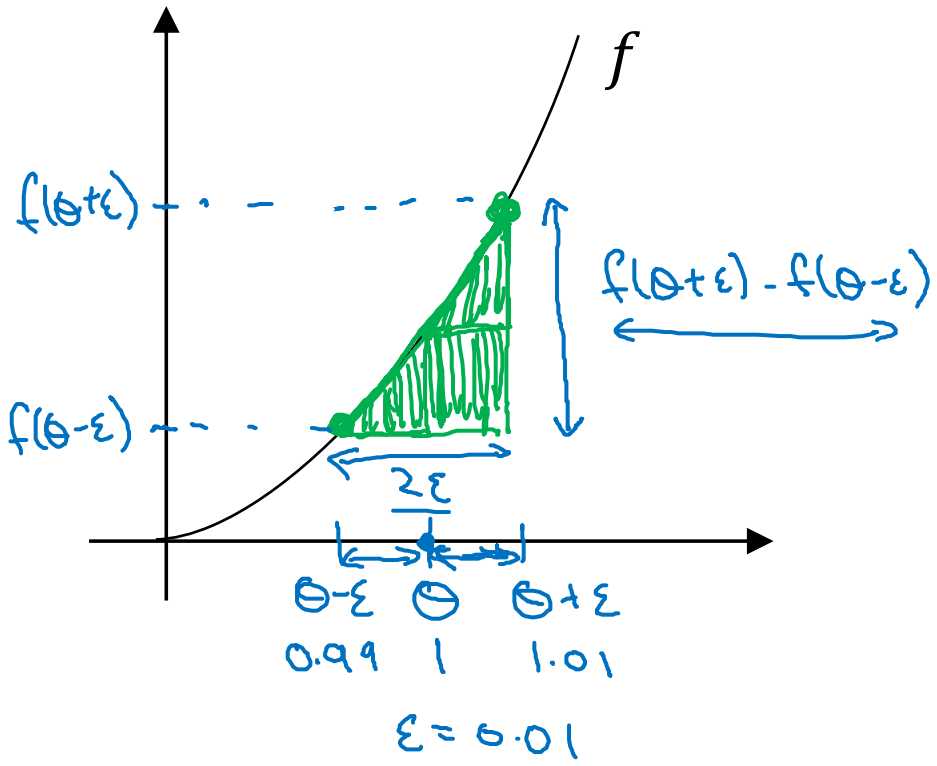
0.0301

3.1

3.2

Checking your derivative computation

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



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

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

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

approx error: 0.0001

(prev slide: 3.0301. error: 0.03)

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

$O(\varepsilon^2)$

0.01

0.0001

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

0.01

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Setting up your optimization problem

Gradient Checking

Gradient check for a neural network

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

concatenate

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

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

concatenate

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

Gradient checking (Grad check)

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

for each i:

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

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

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

Check $\frac{\|d\theta_{approx} - d\theta\|_2}{\|d\theta_{approx}\|_2 + \|d\theta\|_2}$

$\varepsilon = 10^{-7}$

$\approx 10^{-7}$ — great! ←

10^{-5}

$\rightarrow 10^{-3}$ — worry. ←

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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

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

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

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

- Remember regularization.

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

$d\theta$ = gradient of J wrt. θ

- Doesn't work with dropout.

J keep-prob = 1.0

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

$W, b \approx 0$