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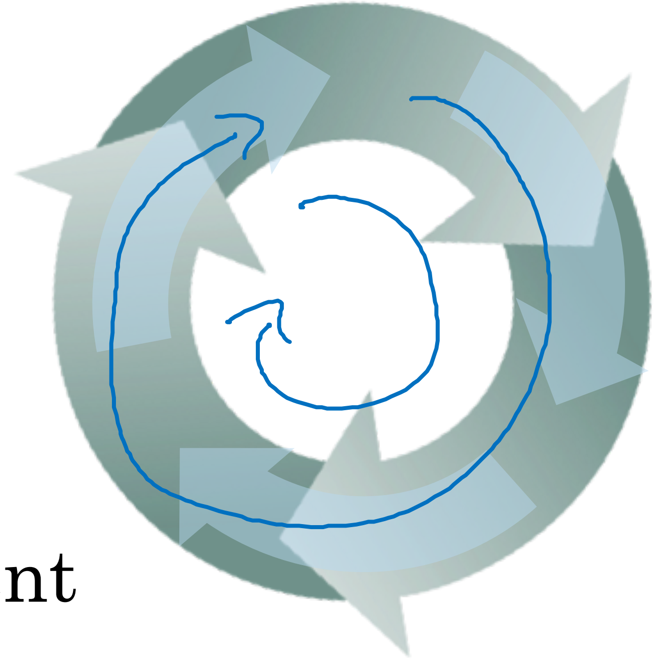
Setting up your ML application

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 ....

Train/dev/test sets

training set

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

test

train test

Previous era: 70/30 %

100 - 1000 - 10000

60/20/20 %

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

98/1/1 %

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

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.

train / dev "test"

train / test

→ train / dev

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

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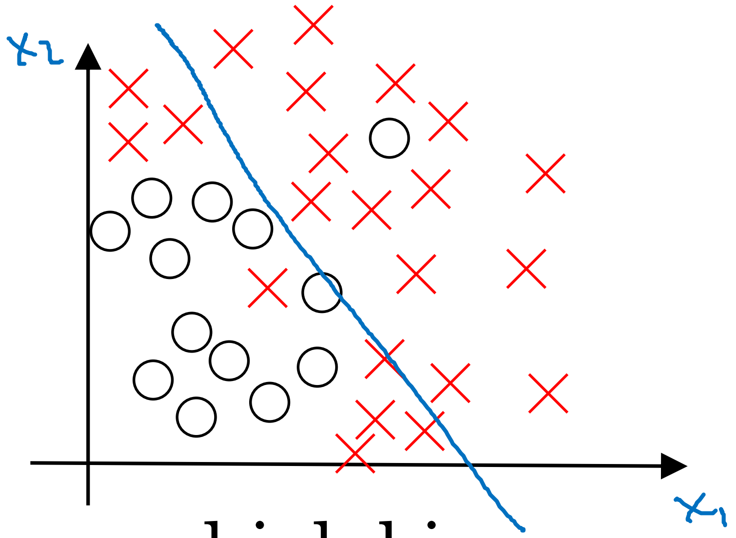
Setting up your ML application

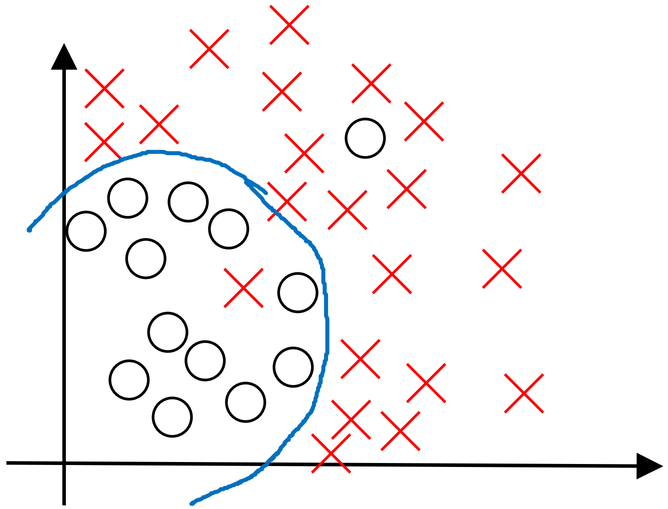
Bias/Variance

Bias and Variance

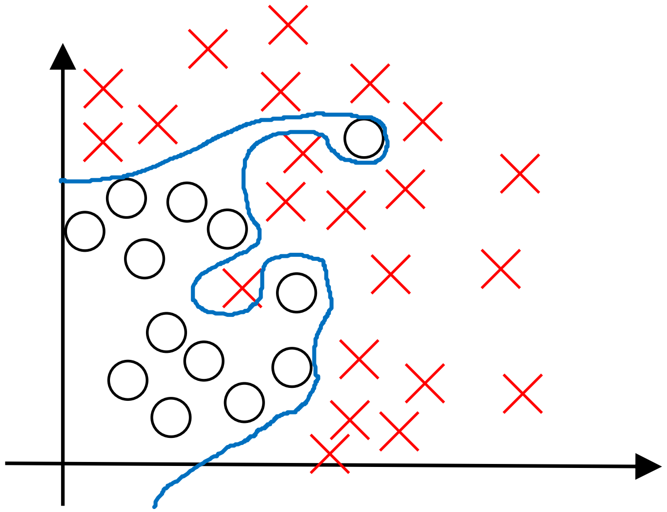


high bias

Underfitting



→ “just right”



high variance

Overfitting

Bias and Variance

Cat classification

y=1

y=0

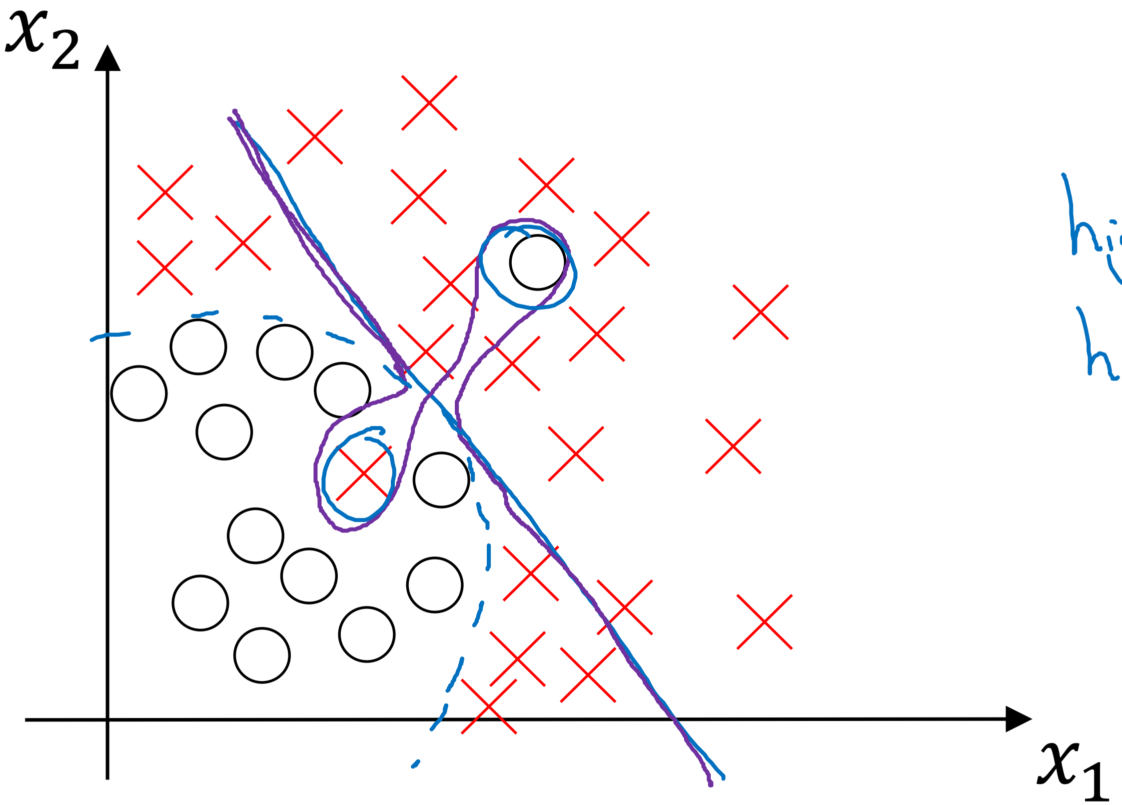
Train set error:	1%	15%	15%	0.5%
Dev set error:	11%	16%	30%	1%
	high variance	high bias	high bias & high varian	low bias low variance

Human: ≈0%

Optimal (Bayes) error: ~~≈0%~~ 15%

Blurry images

High bias and high variance



high bias
high varian

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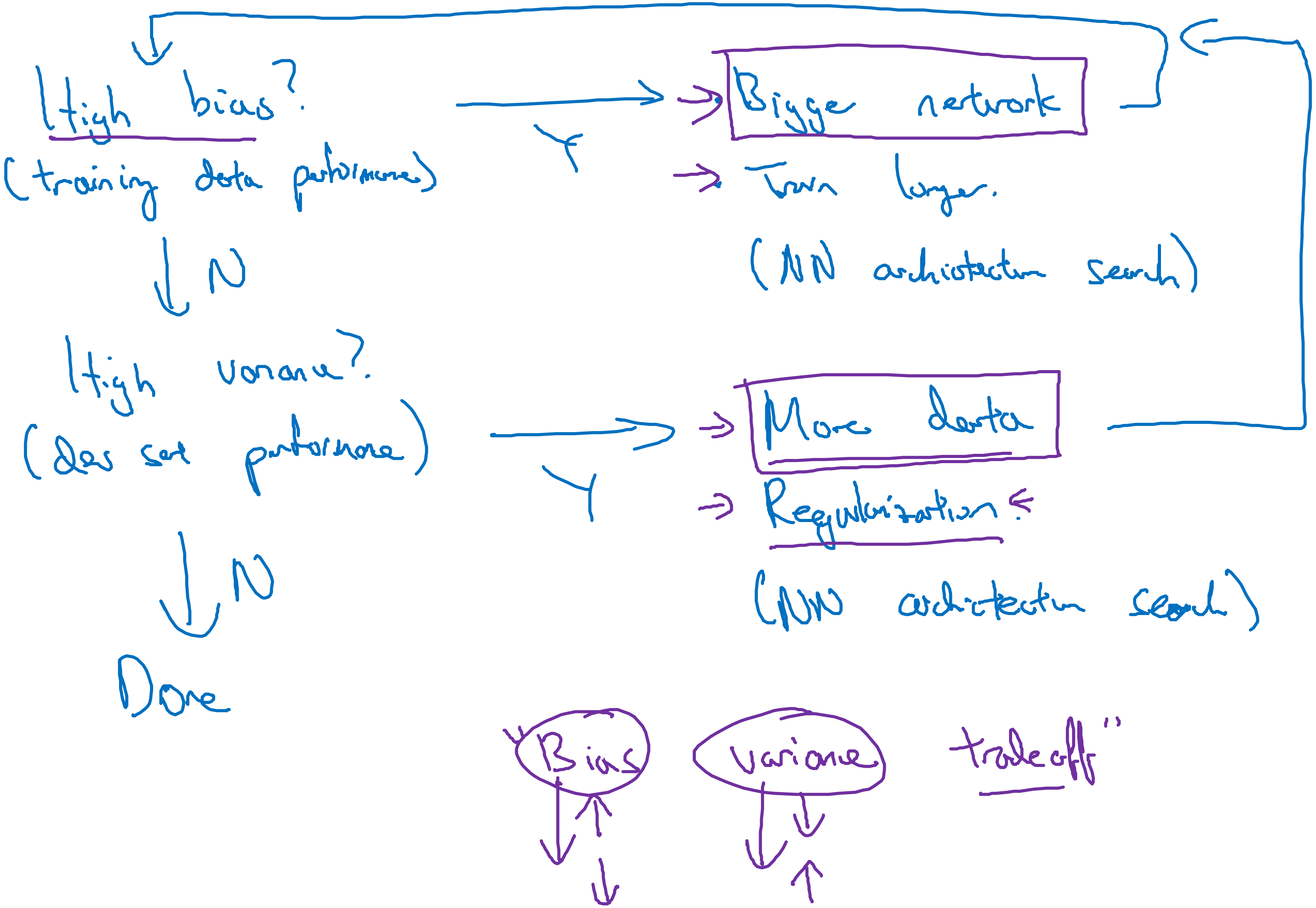
Setting up your ML application

Basic “recipe” for machine learning

Basic recipe for machine learning



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Regularizing your neural network

Regularization

Logistic regression

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

λ = regularization parameter

lambda   lambd

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

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

omit

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

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

w will be sparse

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Neural network

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

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

"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"

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

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

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

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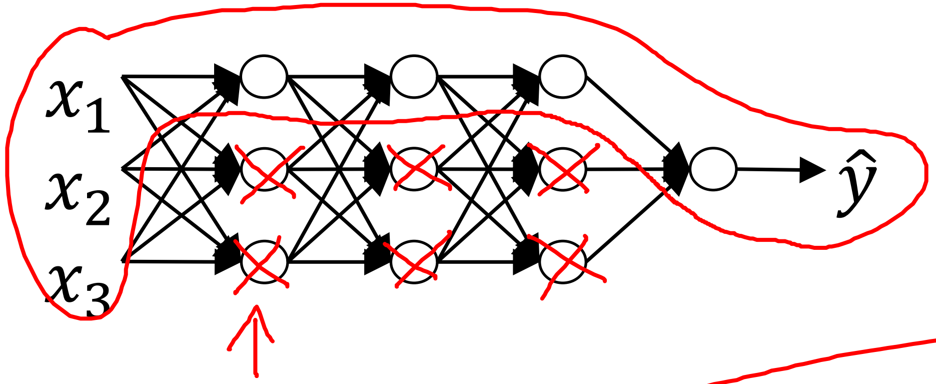
Regularizing your neural network

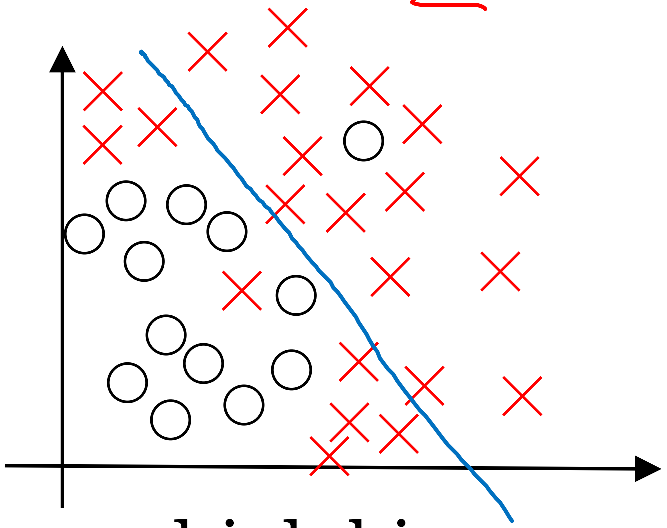
Why regularization reduces overfitting

How does regularization prevent overfitting?

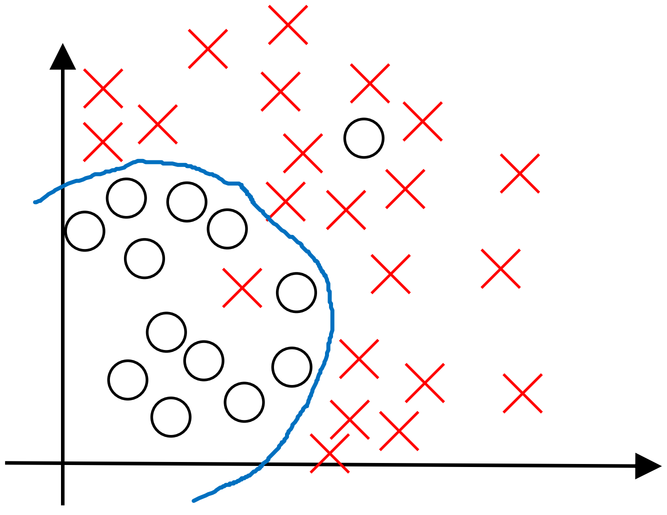


$$J(w^{[l]}, b^{[l]}) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(y^{(i)}, y^{(i)}) + \frac{\boxed{\lambda}}{2m}\sum_{l=1}^{L} \underbrace{\|w^{[l]}\|_F^2}$$

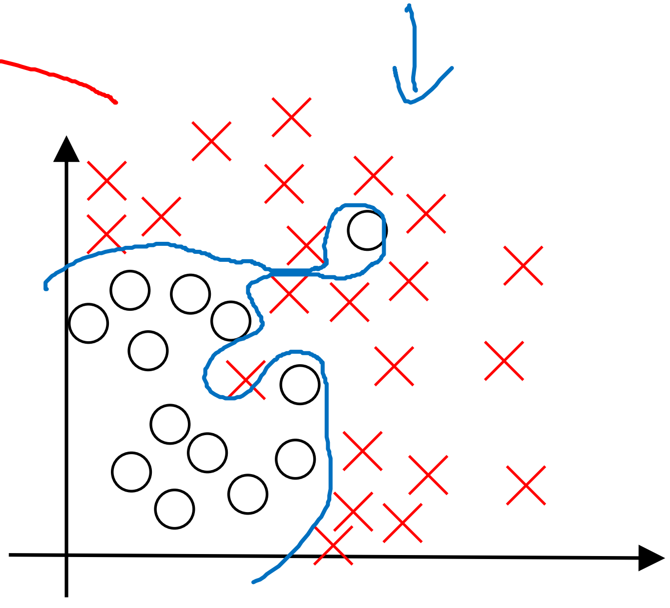
$$\underline{w^{[l]} \approx 0}$$



high bias



"just right"



high variance

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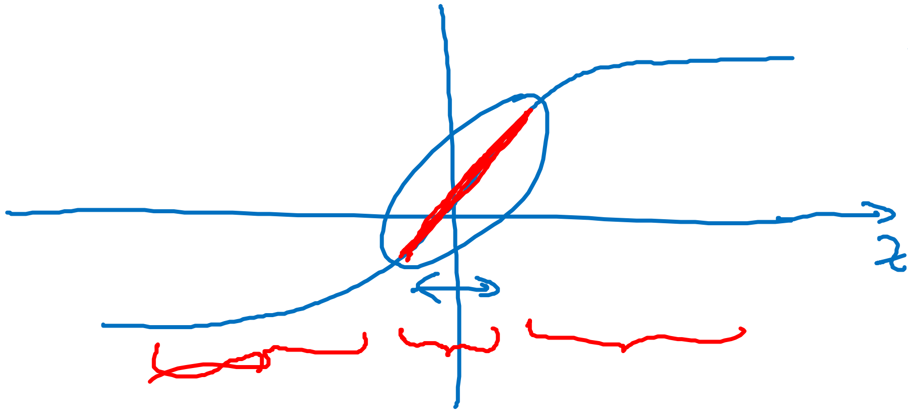
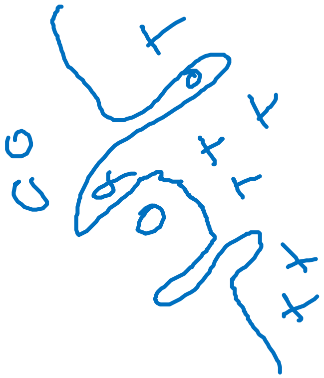
How does regularization prevent overfitting?



$\underline{\tanh}$

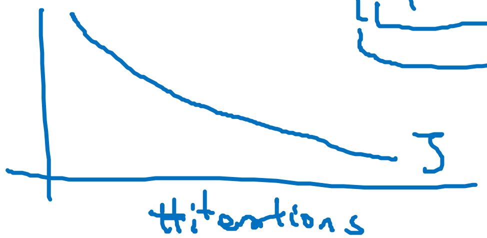
$g(z) = \tanh(z)$

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



Every layer ≈ linear.

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



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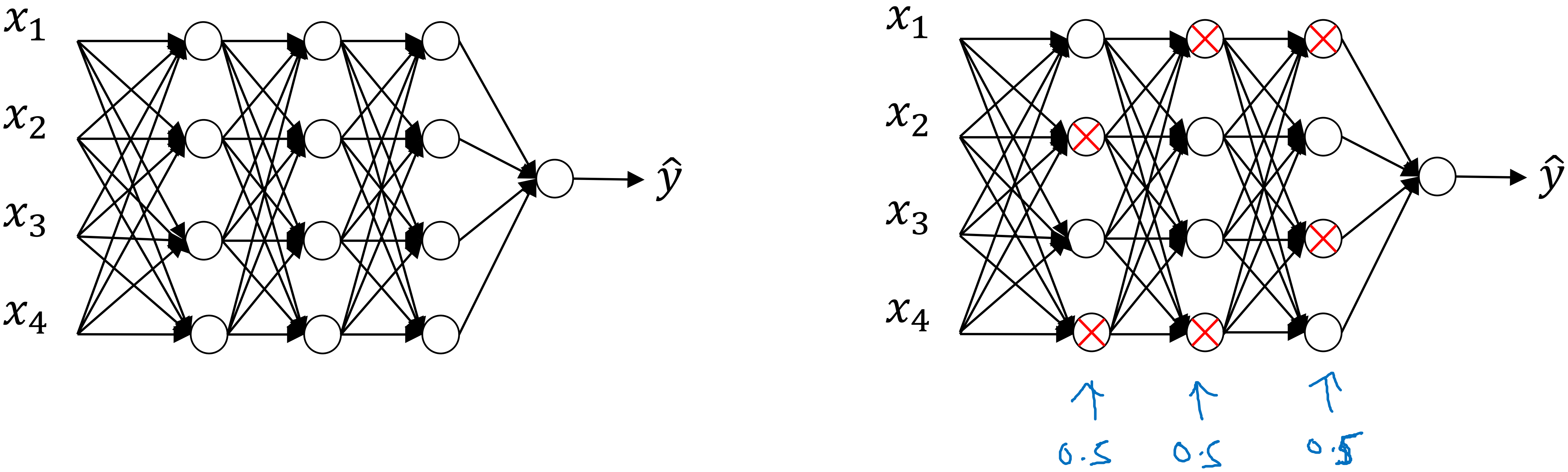
Regularizing your neural network

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-prob

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

→ a3 /= ~~0.8~~ keep-prob ←

50 units. ⇝ 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.

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

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

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

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

$$\downarrow$$

$$\hat{y}$$

$/= \text{keep-prob}$

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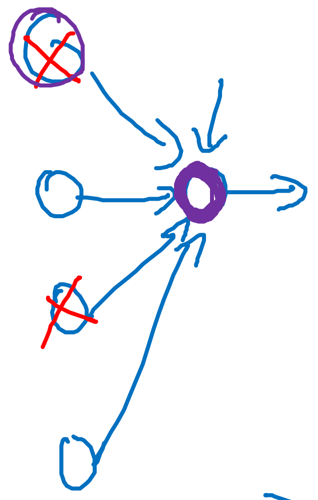
Regularizing your neural network

Understanding dropout

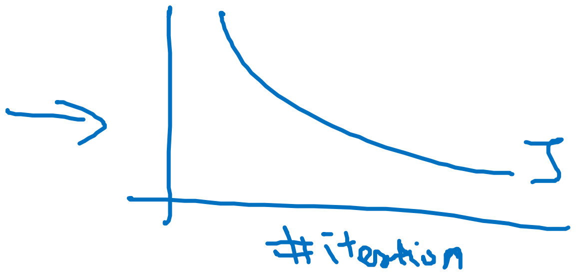
Why does drop-out work?

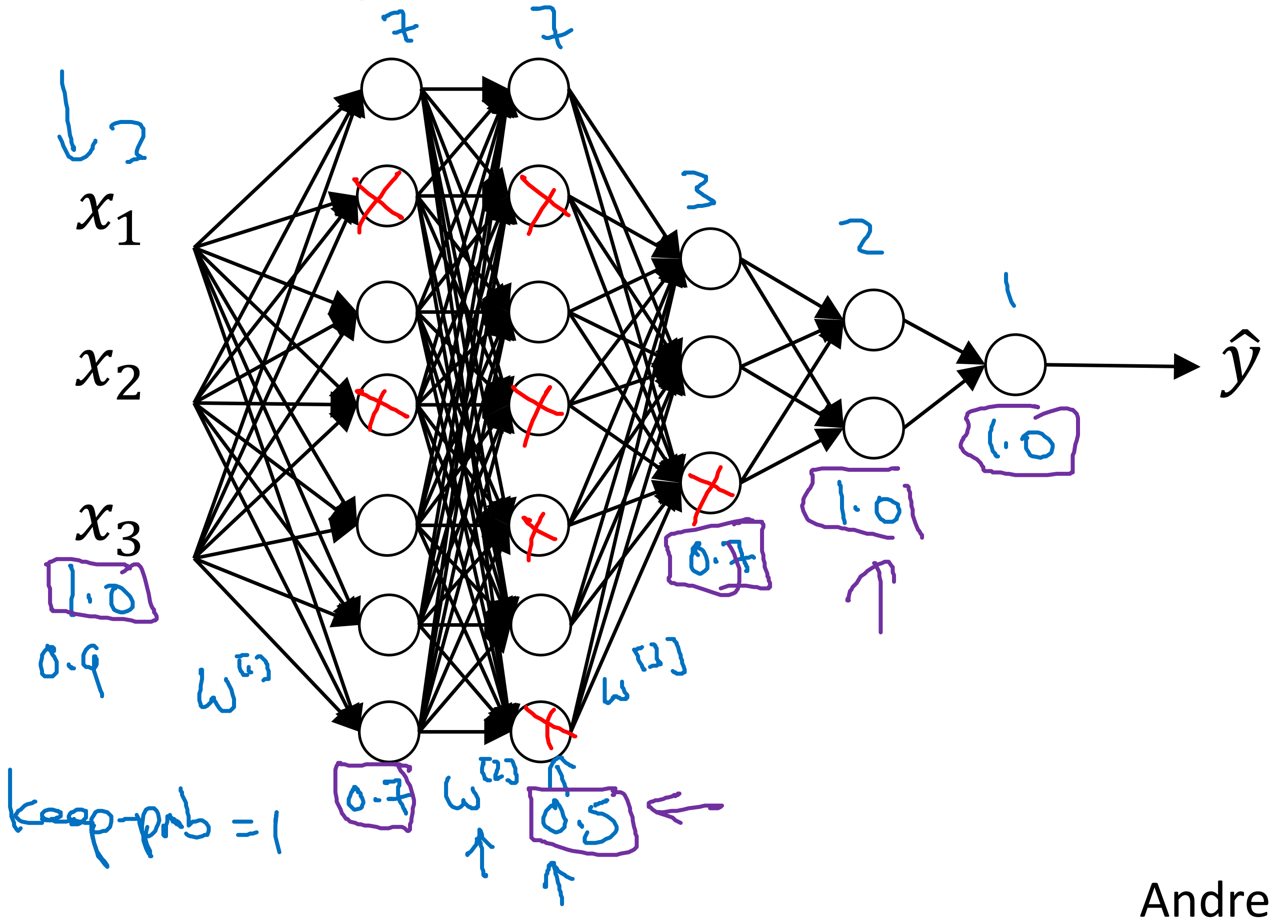
Intuition: Can't rely on any one feature, so have to spread out weights. → Shrink weights. L_2



→ Computer Vision

Downside: J





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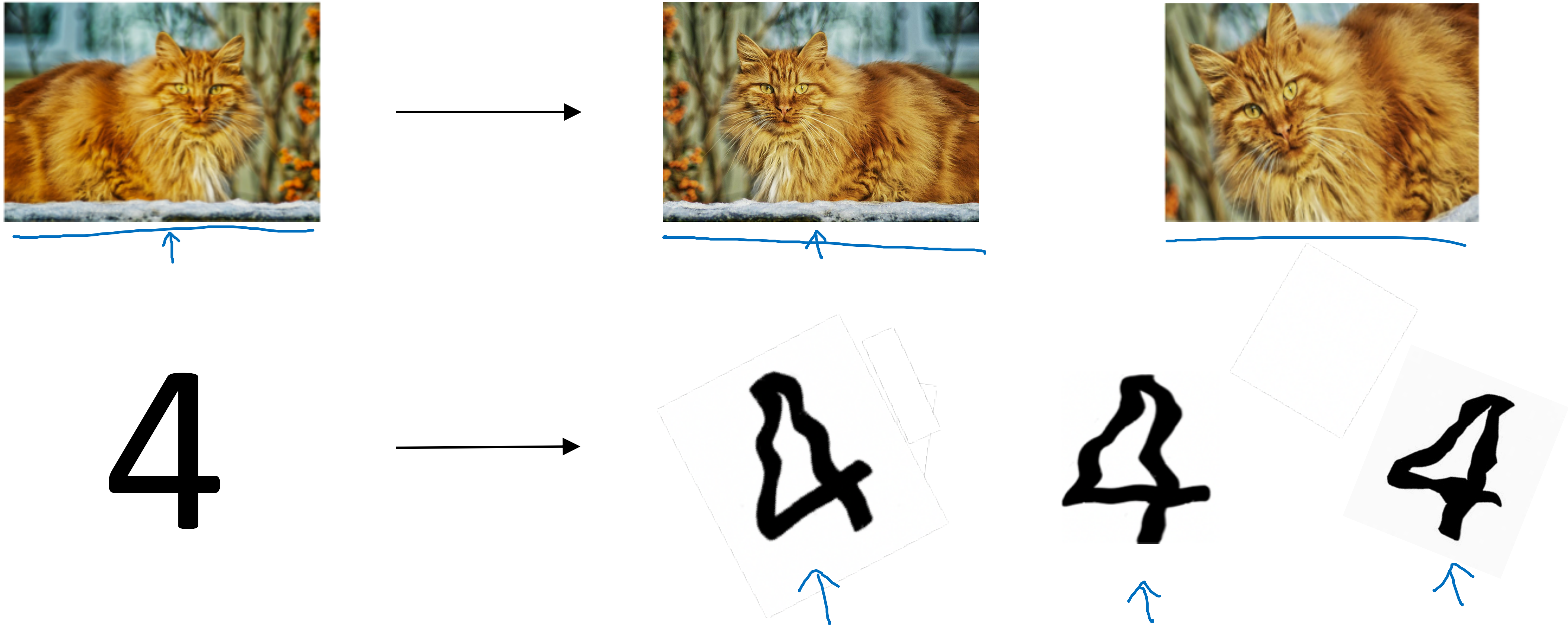
Regularizing your neural network

Other regularization methods

Data augmentation



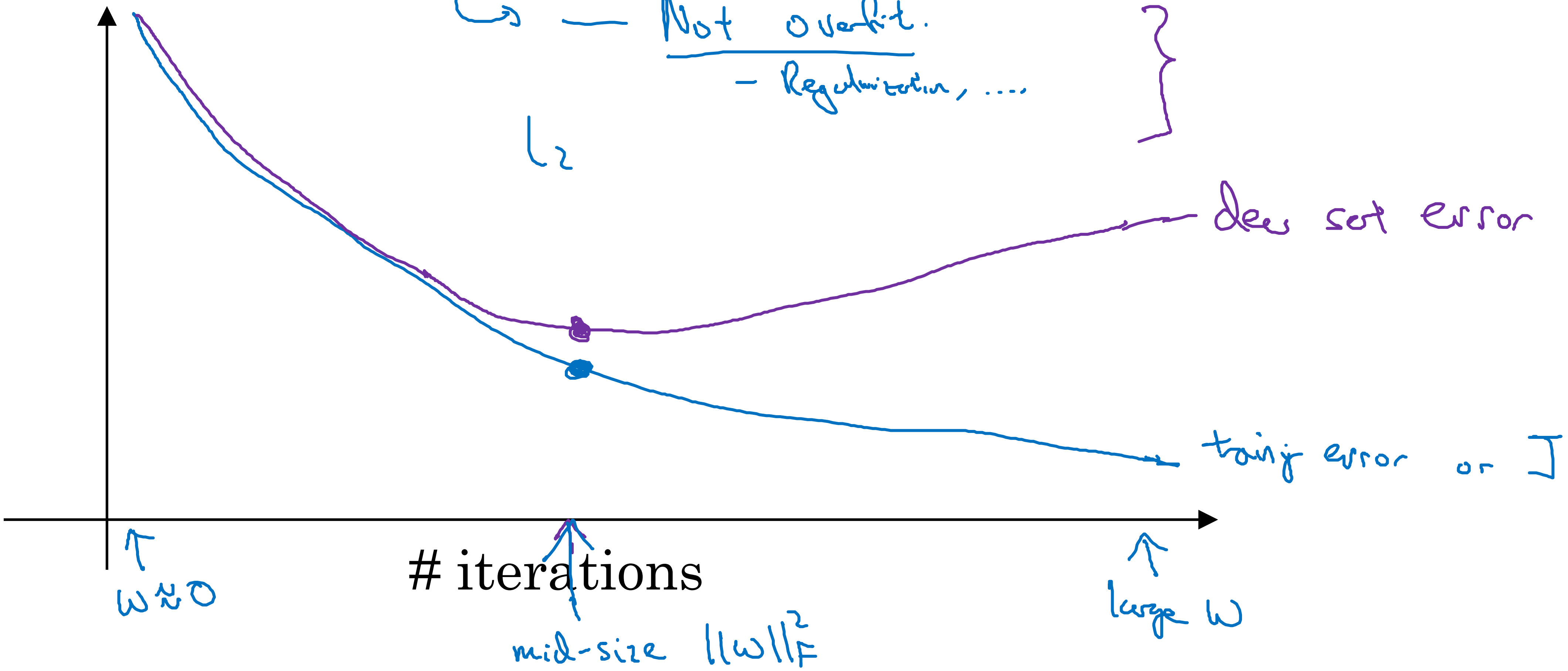
Early stopping

Orthogonalization.

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

L_2

$J(w,b)$



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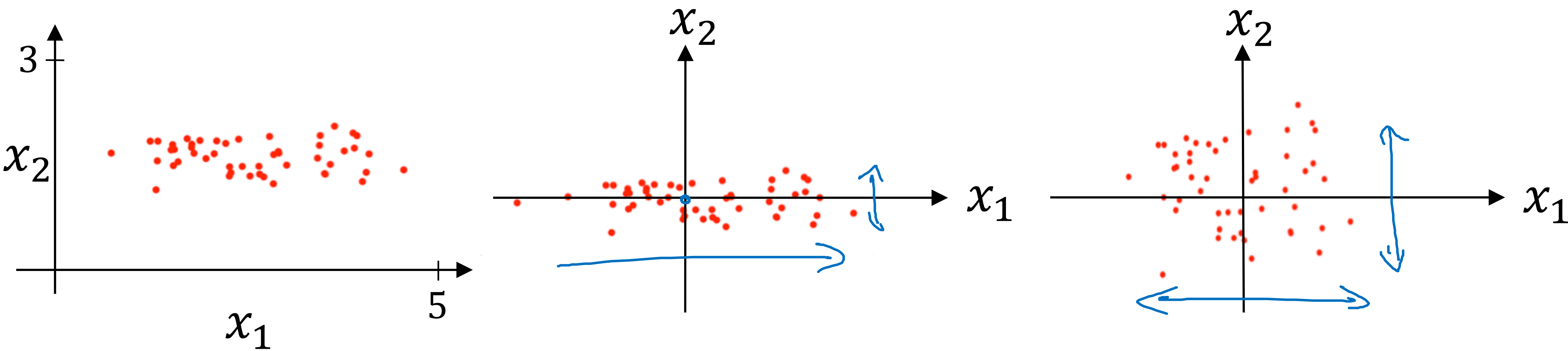
Setting up your optimization problem

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.

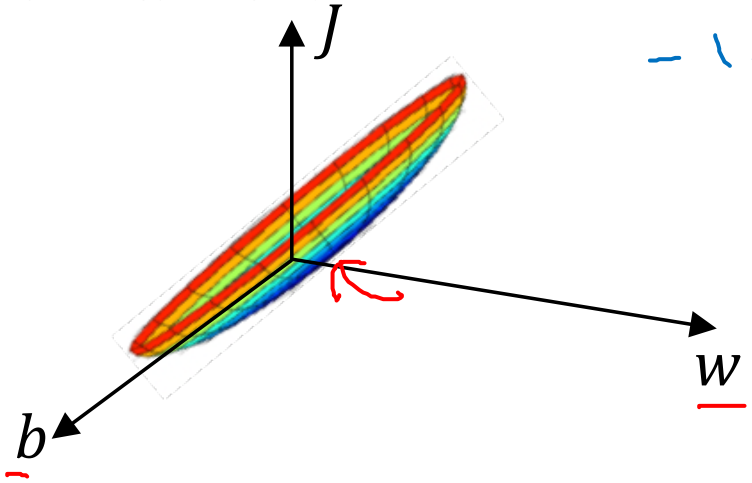
Why normalize inputs?

$w_1 \quad x_1 : \underline{1 \ldots 1000} \leftarrow$

$w_2 \quad x_2 : \underline{0 \ldots 1} \leftarrow$

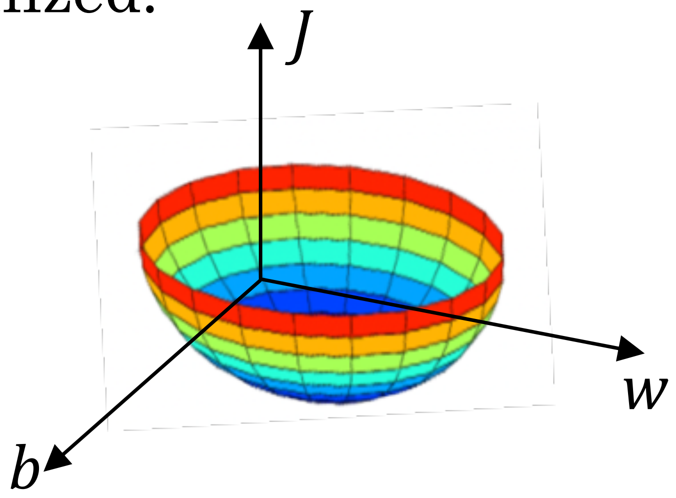
$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$

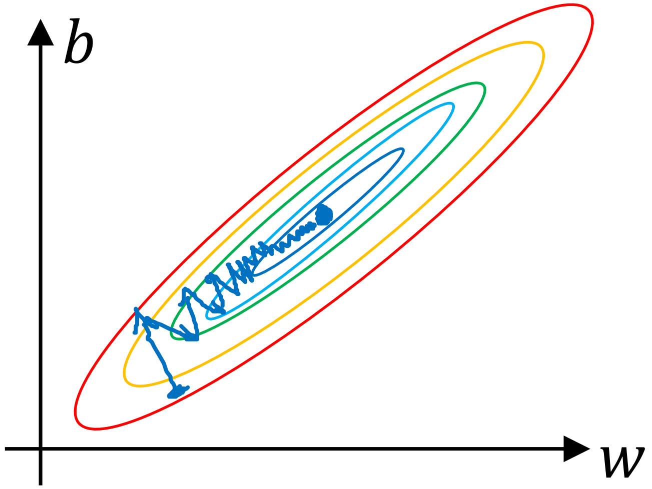
Unnormalized:



$-1 \ldots 1$

Normalized:

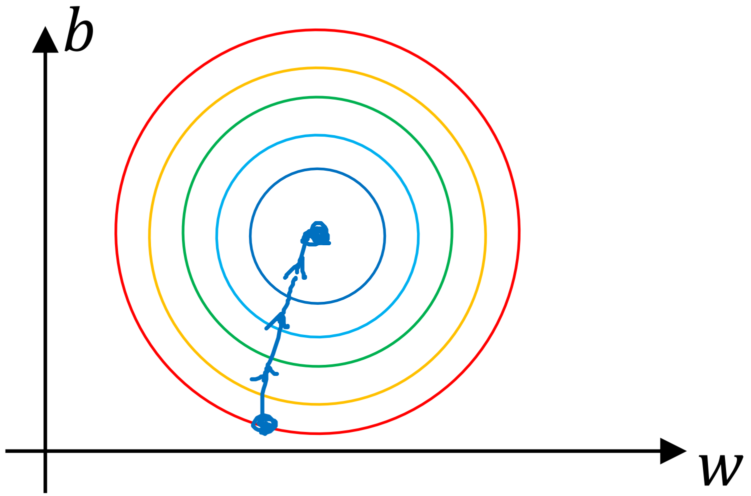




$x_1 : 0 \ldots 1$

$x_2 : -1 \ldots 1$

$x_3 : 1 \ldots 2$



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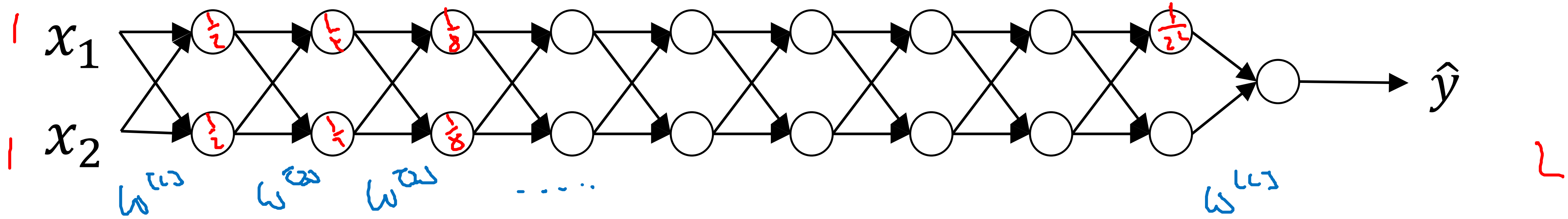
Setting up your optimization problem

Vanishing/exploding gradients

Vanishing/exploding gradients

$L = 150$



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

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

1.5^L

0.5^L

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

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

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

$W^{[l]} > I$

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

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

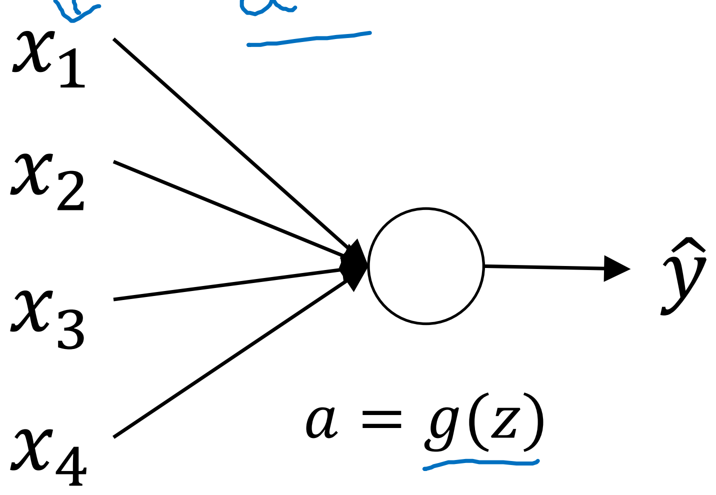
$$\hat{y} = \underbrace{W^{[L]} \begin{bmatrix} \overset{0.5}{\cancel{1.5}} & 0 \\ 0 & \underset{0.5}{\cancel{1.5}} \end{bmatrix}^{L-1}} x$$

$1.5^{L-1} x$

$0.5^{L-1} x$

Single neuron example

$a^{[l]}$



$a = g(z)$

$w^{[l]}$

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

Large n → Smaller w_i

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

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

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

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

$J \rightarrow \underline{f(\theta)} = \underline{\theta^3}$

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

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

$dw, db \rightarrow \underline{g(\theta) = 3\theta^2}.$

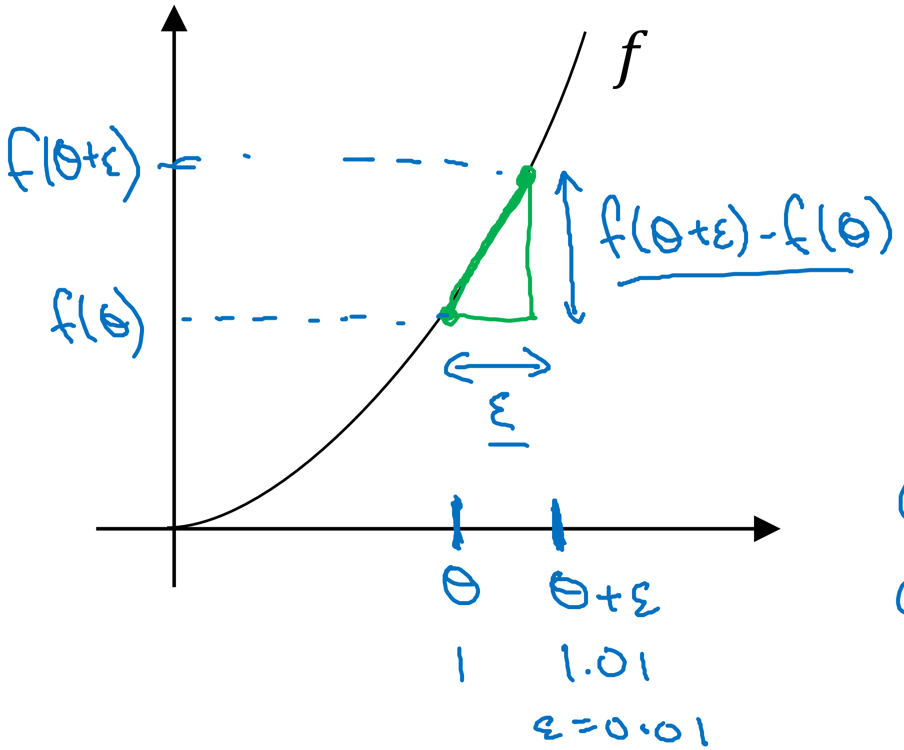
$g(\theta) = 3\cdot(1)^2 = 3$ when $\theta = 1$

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

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

$\theta = 1$

$\theta + \varepsilon = 1.01$



0.0301

3.1

3.2

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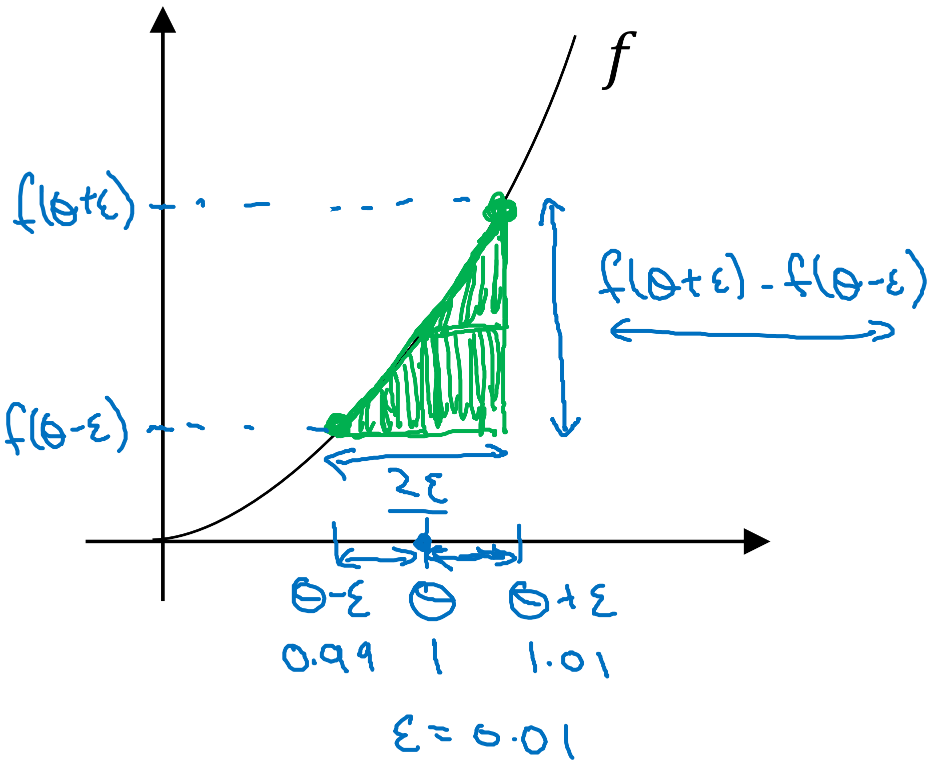
Checking your derivative computation

$\underline{f(\theta) = \theta^3}$



$$\left[\frac{f(\theta+\varepsilon)-f(\theta-\varepsilon)}{2\varepsilon} \approx \underline{g(\theta)}\right.$$

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

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

approx error: 0.0001

(prev slide: 3.0301. error: 0.03)

$$\left(f'(\theta) = \lim_{\varepsilon \to 0} \frac{f(\theta+\varepsilon)-f(\theta-\varepsilon)}{2\varepsilon} \right. \quad \underline{O(\varepsilon^2)}$$

0.01

$\underline{0.0001}$

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

0.01

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Setting up your optimization problem

Gradient Checking

Gradient check for a neural network

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

concatenate

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

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

concatenate

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

Gradient checking (Grad check)

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

for each i :

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

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

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

Check

$$\rightarrow \frac{\|d\theta_{approx} - d\theta\|_2}{\|d\theta_{approx}\|_2 + \|d\theta\|_2} \approx \boxed{10^{-7} - \text{great!}} \leftarrow$$

i

10^{-5}

$\rightarrow 10^{-3}$ – worry. $\leftarrow$

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

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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

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

$$\uparrow \quad \uparrow \qquad\qquad \uparrow$$

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

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

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

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

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