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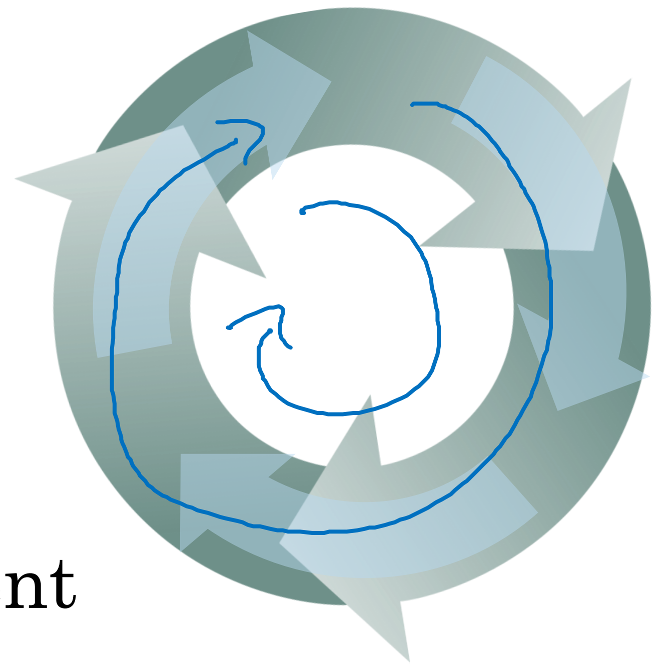
Setting up your ML application

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 logistic ....

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Train/dev/test sets

Data

training set	dev	test

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

test

Previous era:

train test

70/30%

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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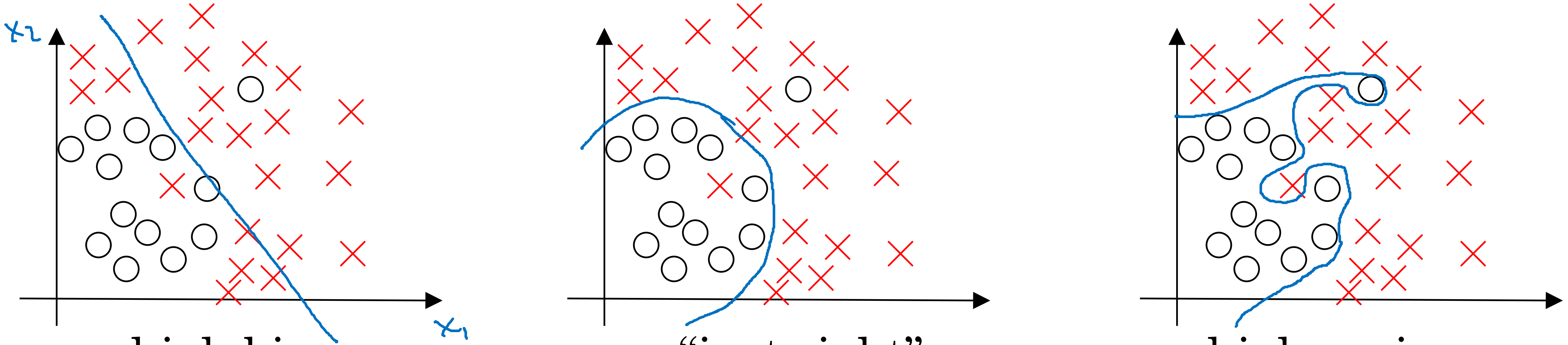
Setting up your ML application

Bias/Variance

Bias and Variance



high bias　　　　　“just right”　　　　　high variance

Underfitting　　　　　　　　　　　　　　Overfitting

Bias and Variance

Cat classification

$y=1$

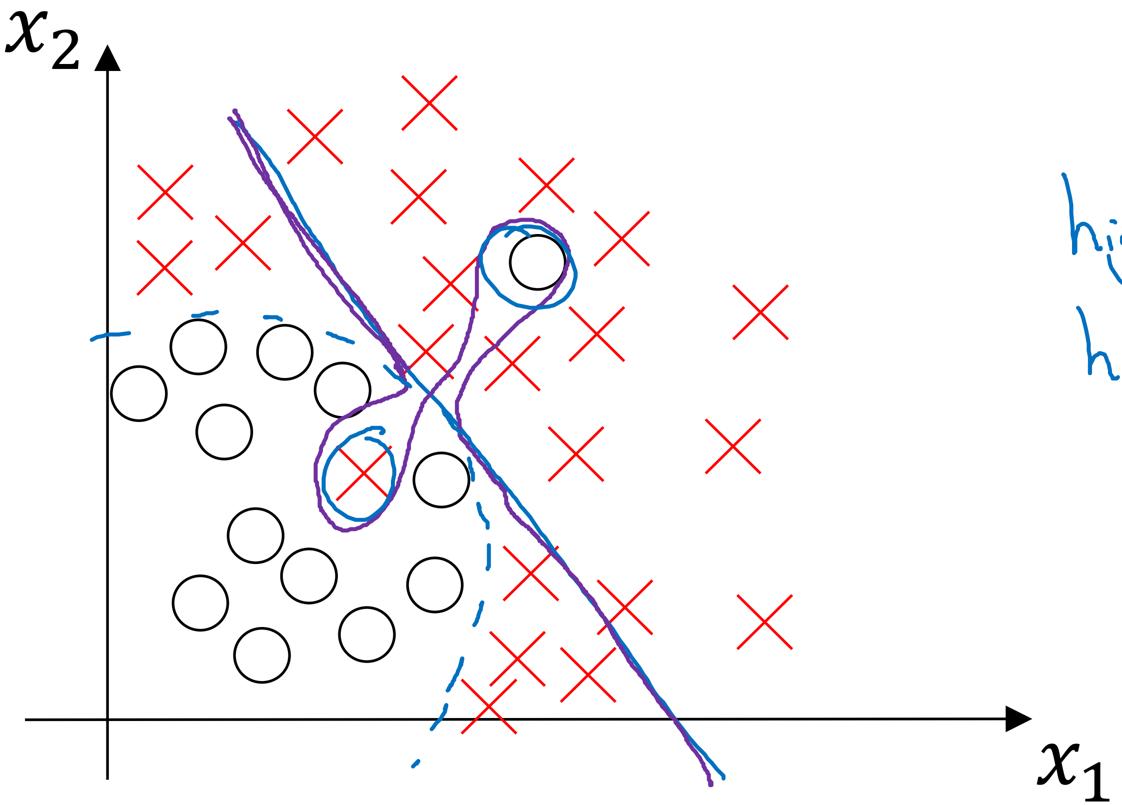
$y=0$

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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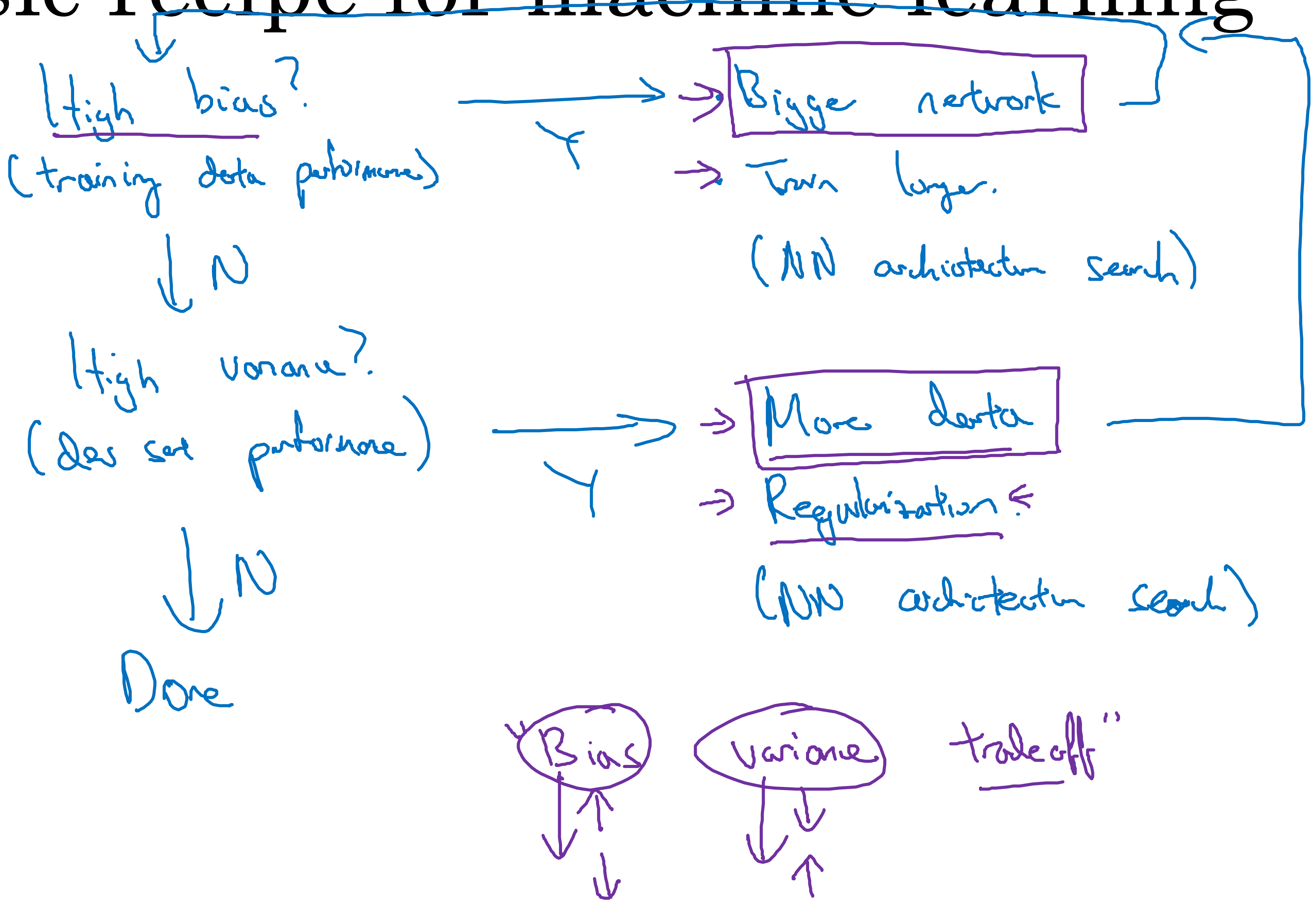
Setting up your ML application

Basic "recipe" for machine learning

Basic "recipe" for machine learning

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

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

omit

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

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

w will be sparse

Neural network

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

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

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

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

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

"Weight decay"

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

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

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

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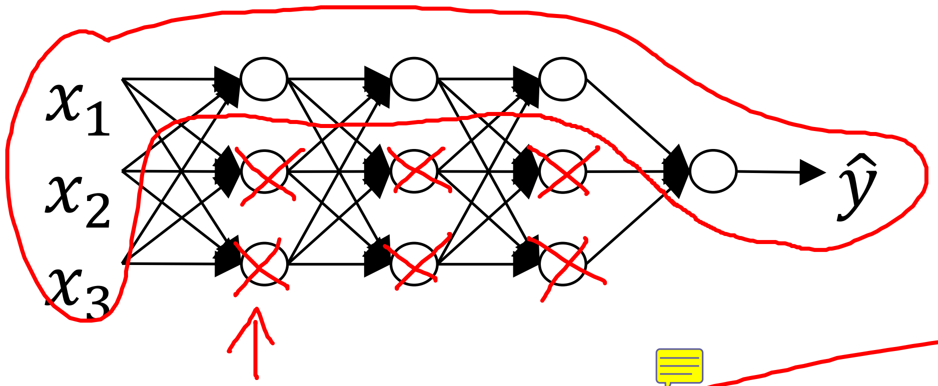
Regularizing your neural network

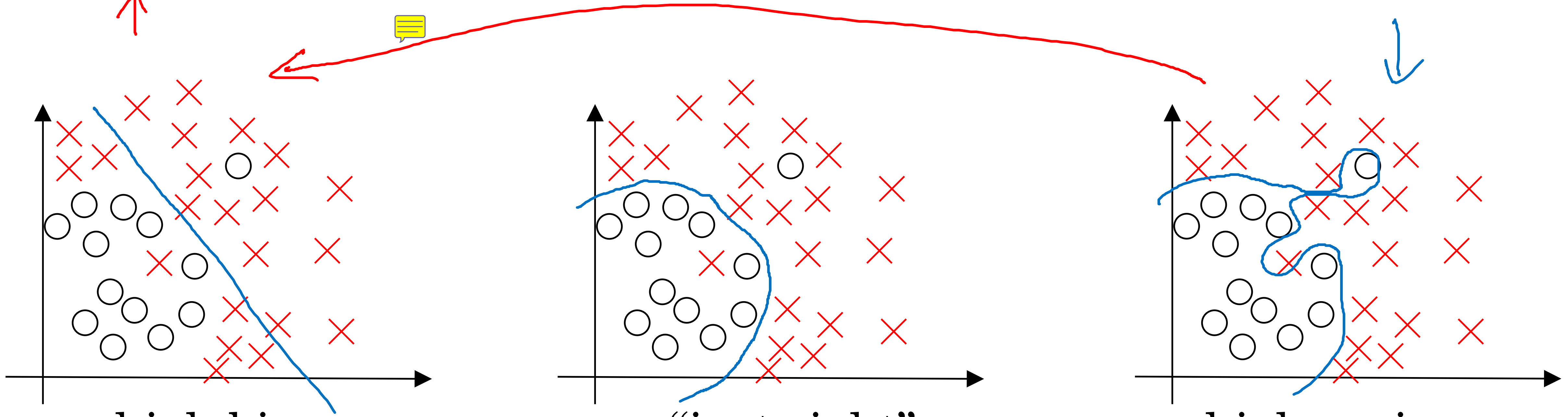
Why regularization reduces overfitting

How does regularization prevent overfitting?



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

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



high bias "just right" high variance

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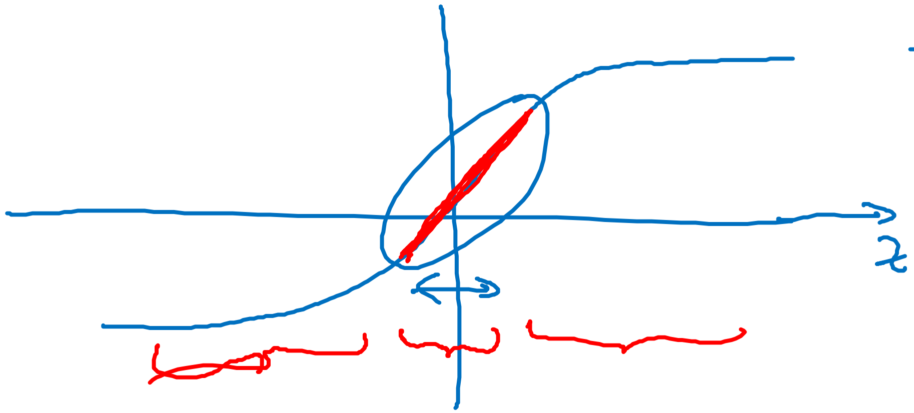
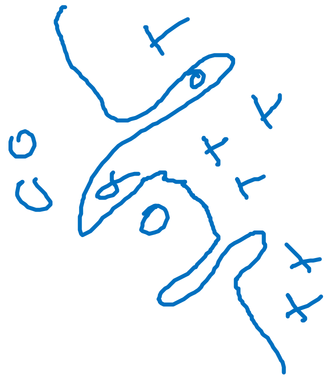
How does regularization prevent overfitting?



tanh

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

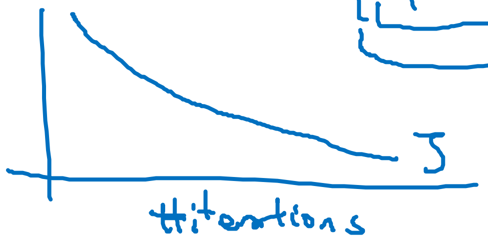


$\lambda \uparrow \qquad W^{[l]} \downarrow$

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

Every layer $\approx$ linear.

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



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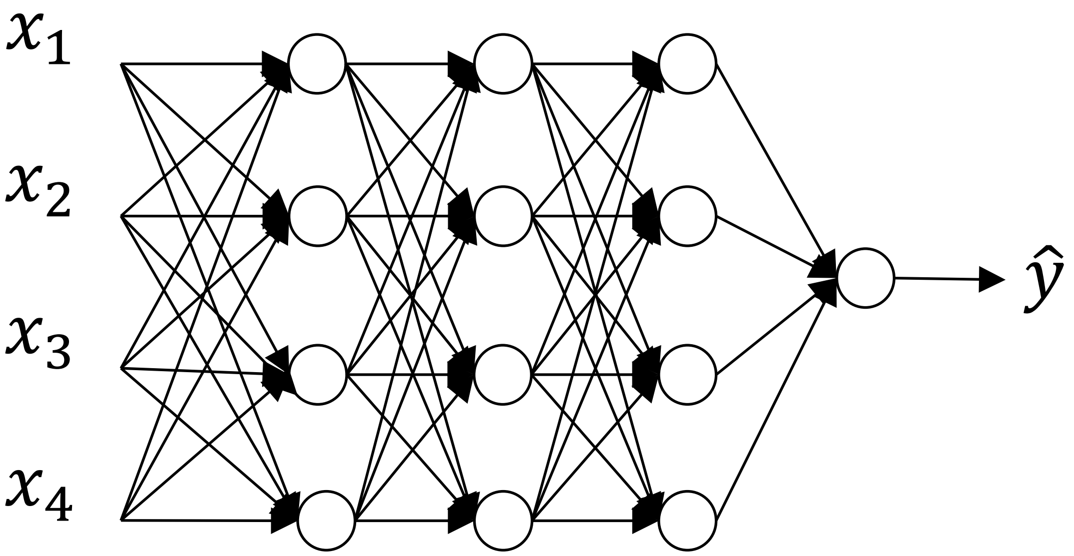
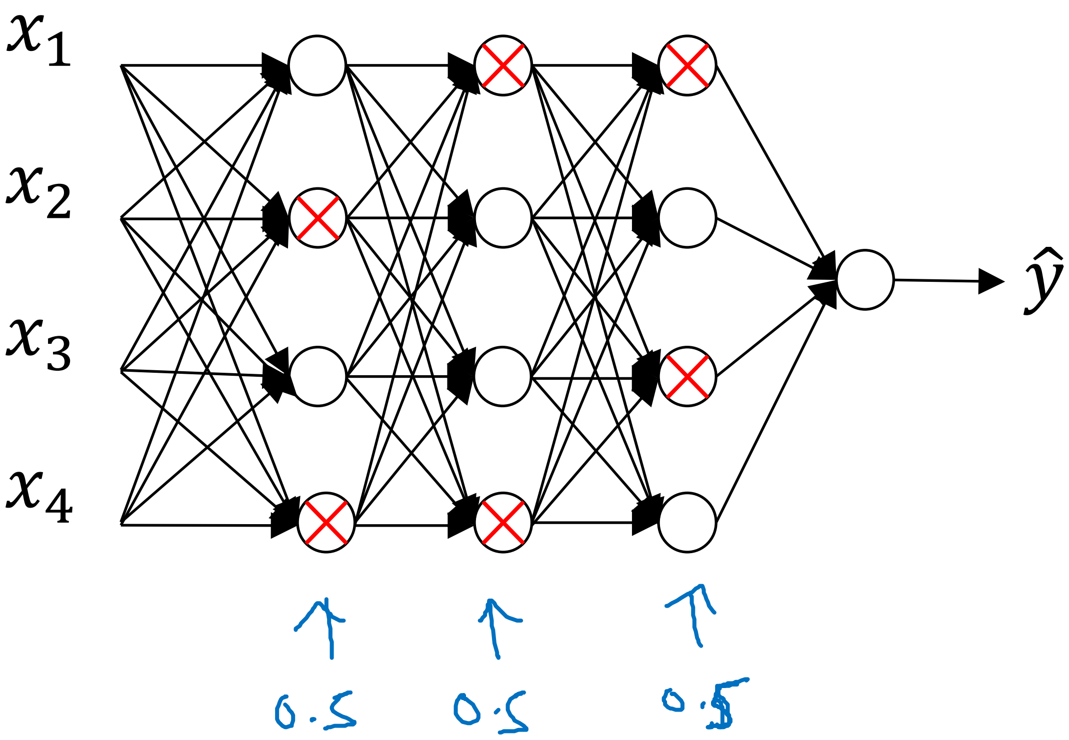
Regularizing your neural network

Dropout regularization

Dropout regularization





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Implementing dropout (~~"Inverted dropout"~~)

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

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

$\underline{a3} = \text{np.multiply(a3, d3)}$ # a3 *= d3.

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

50 units. ⤳ 10 units shut off

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

reduced by $\underline{20}\%$. Test

$/= \underline{0.8}$

Making predictions at test time

$a^{[0]} = X$

No drop out.

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

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

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

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

$\downarrow$

$\hat{y}$

/= keep-prob

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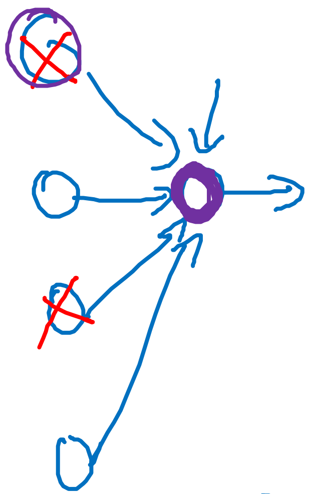
Regularizing your neural network

Understanding dropout

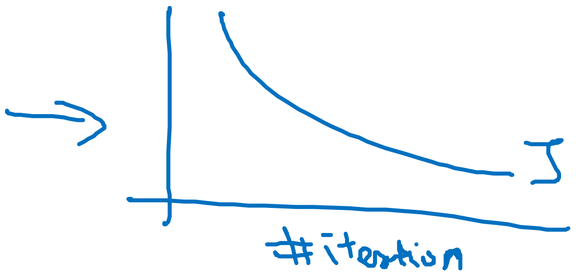
Why does drop-out work?

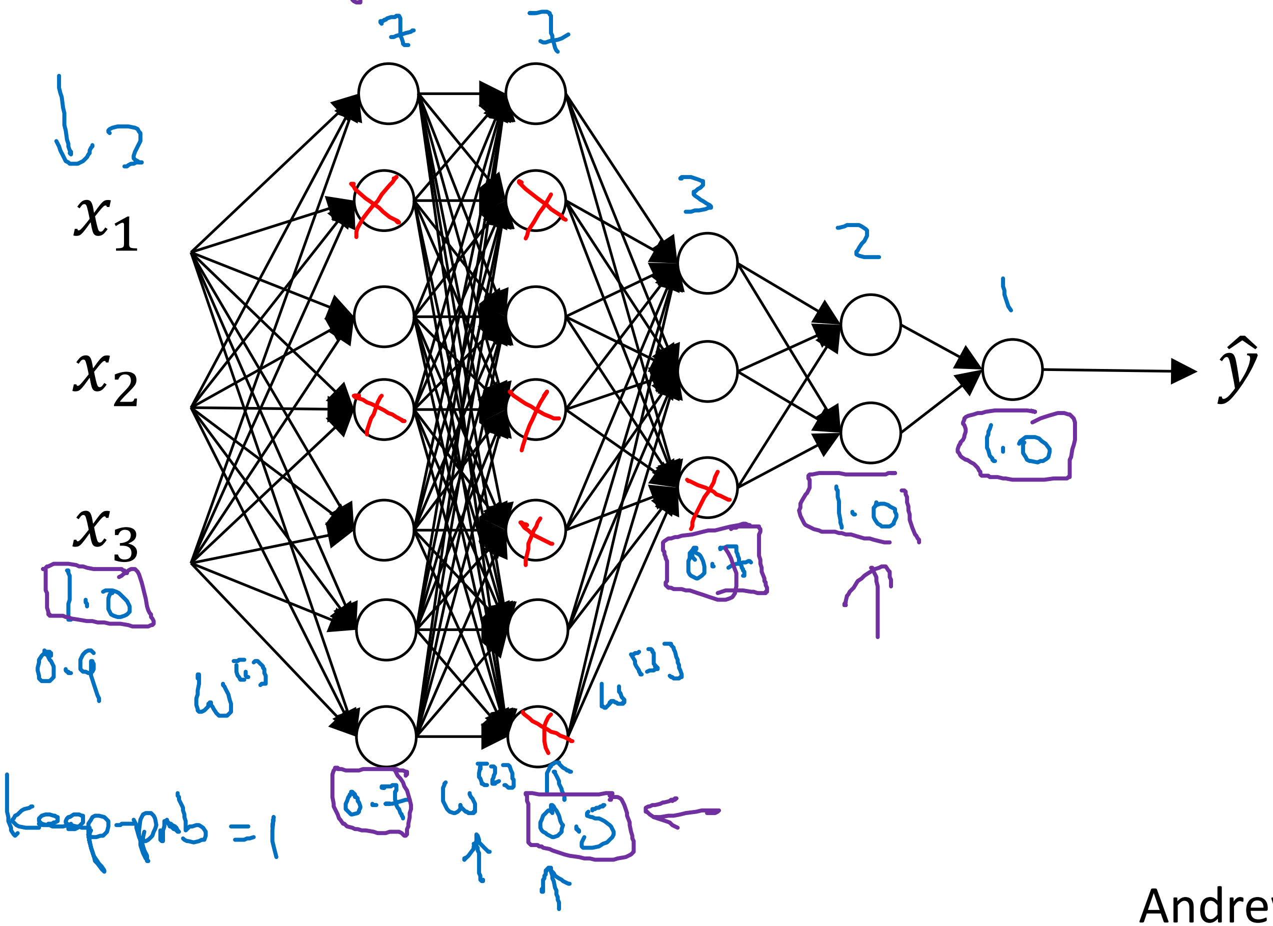
Intuition: Can't rely on any one feature, so have to spread out weights. ⇝ Shrink weights. L2



→ Computer Vision

Downside: J





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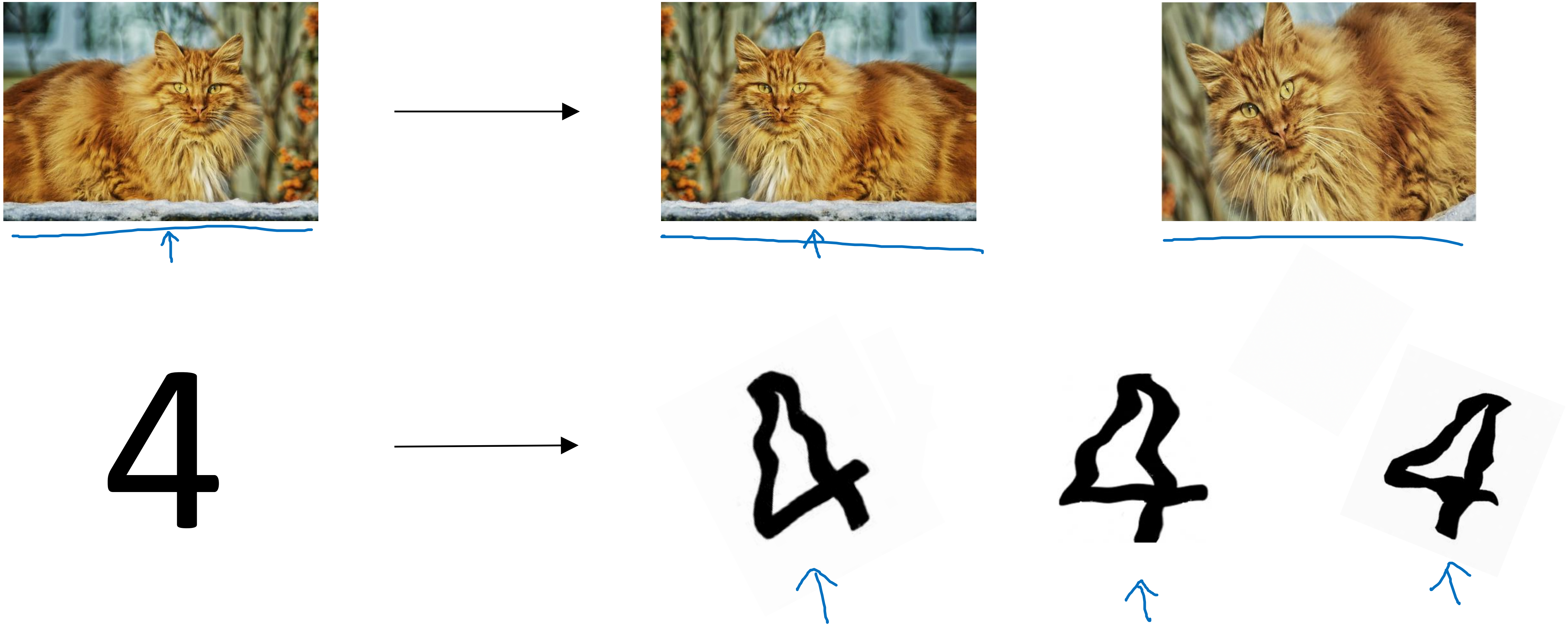
Regularizing your neural network

Other regularization methods

Data augmentation



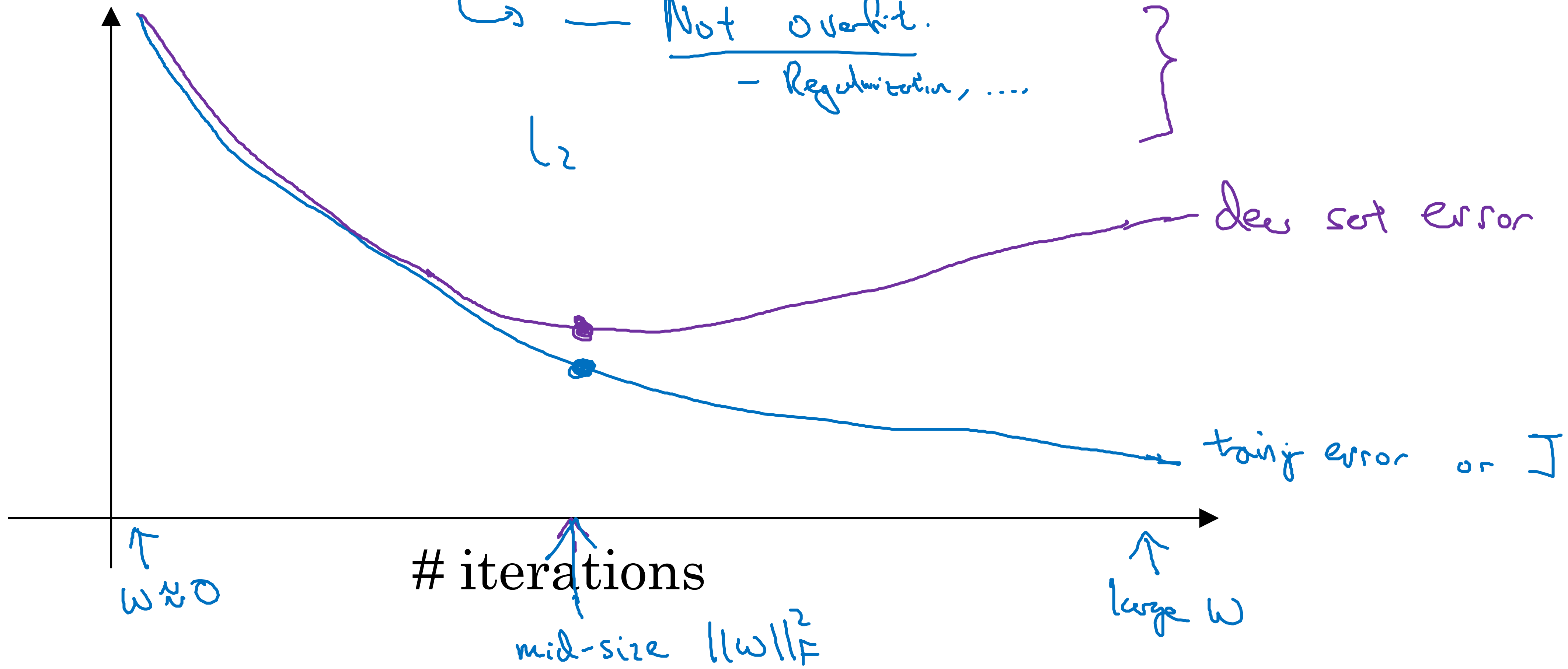
Early stopping

Orthogonalization.

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

L_2

$J(w,b)$



Setting up your optimization problem

Normalizing inputs

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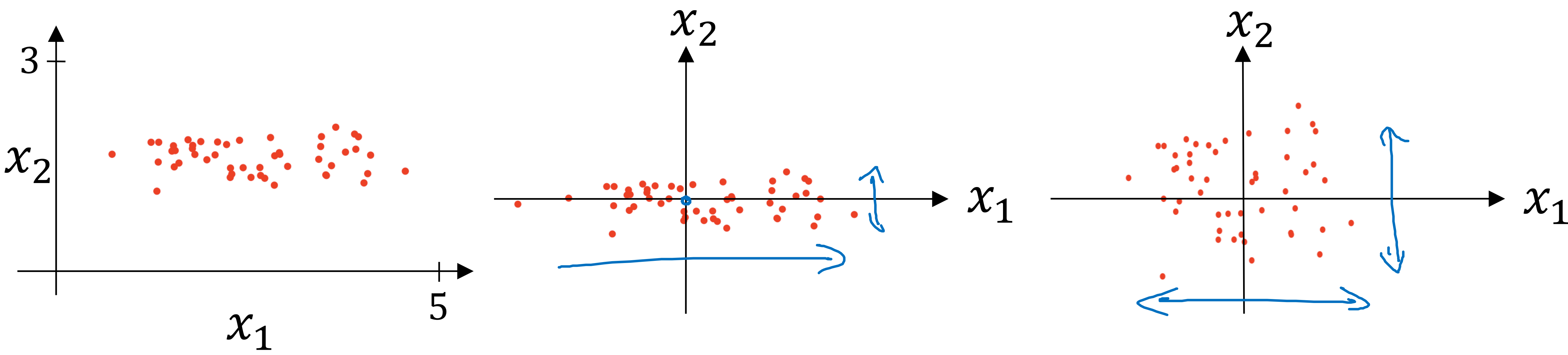
Normalizing training sets

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



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

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

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

Use same μ, σ to normalize test set.

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Why normalize inputs?

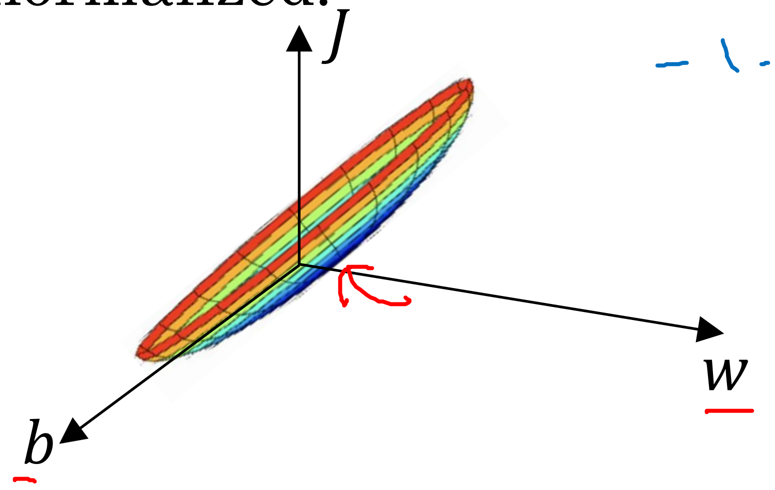
$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

w_1 x_1 : $1 \ldots 1000$ ←

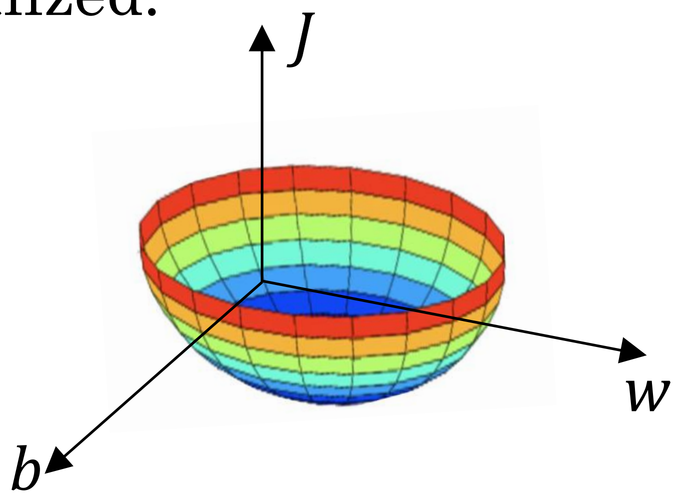
w_2 x_2 : $0 \ldots 1$ ←

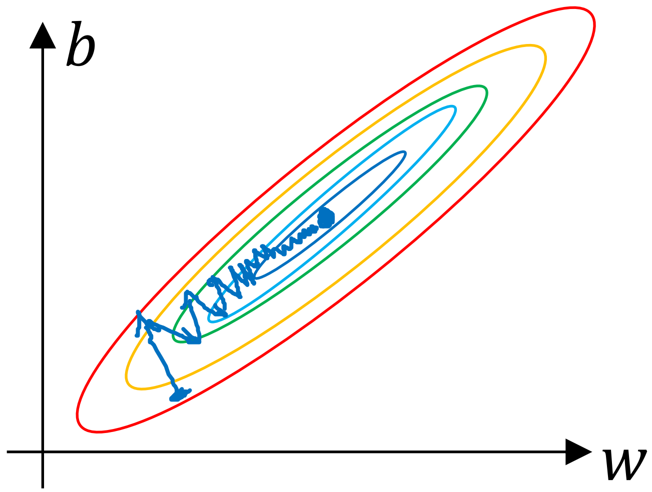
$-1 \ldots 1$

Unnormalized:



Normalized:

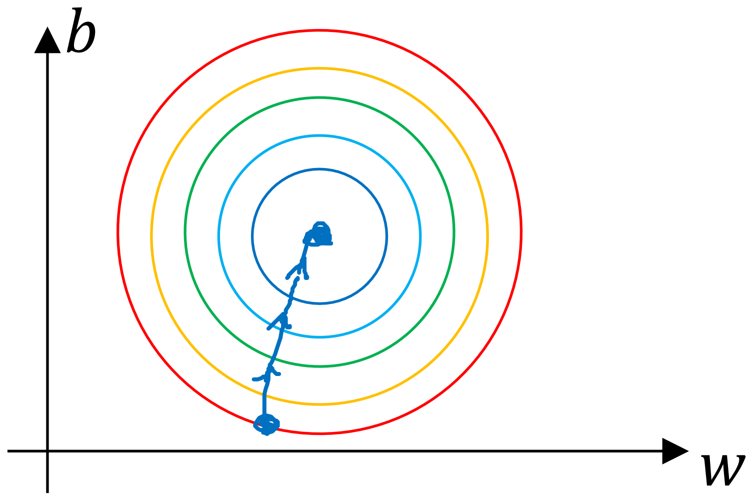




x_1 : $0 \ldots 1$

x_2 : $-1 \ldots 1$

x_3 : $1 \ldots 2$



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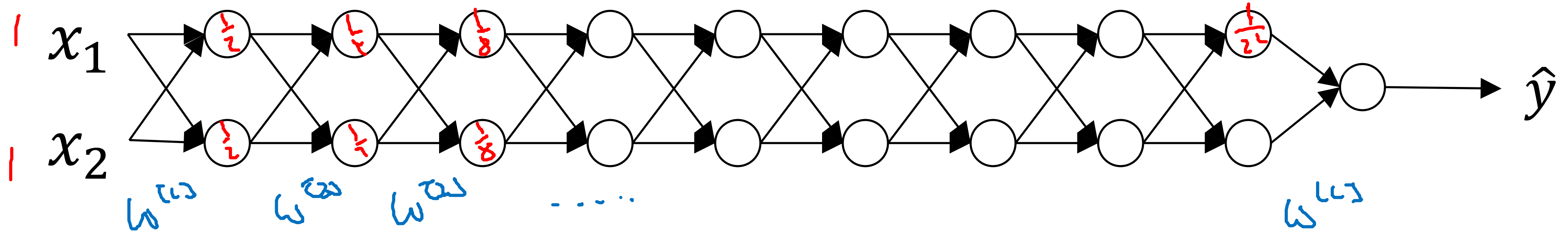
Setting up your optimization problem

Vanishing/exploding gradients

Vanishing/exploding gradients

$L = 150$



L

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

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

$a^{[3]}$

1.5^L

0.5^L

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

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

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

$W^{[l]} > I$

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

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

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

$1.5^{L-1} x$

$0.5^{L-1} x$

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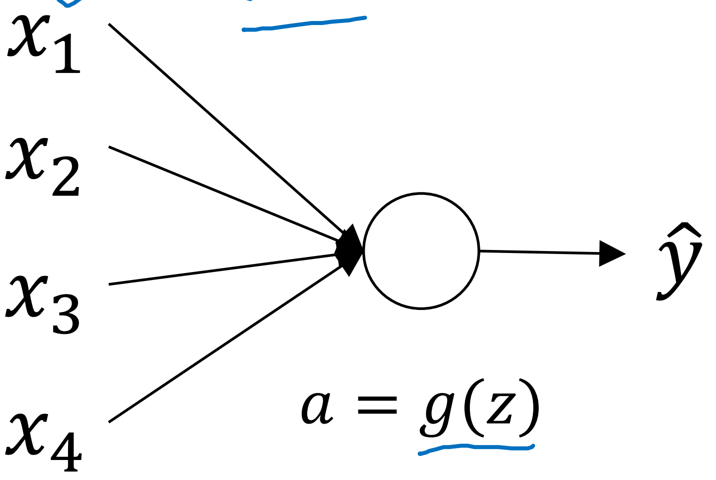
Single neuron example



$a^{[l]}$

$w^{[l]}$

$a = g(z)$

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

Large n → Smaller w_i

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

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

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

Other variants:

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

Xavier initialization

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

Setting up your optimization problem

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Numerical approximation of gradients

Checking your derivative computation

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

$\theta \in \mathbb{R}$

J

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

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

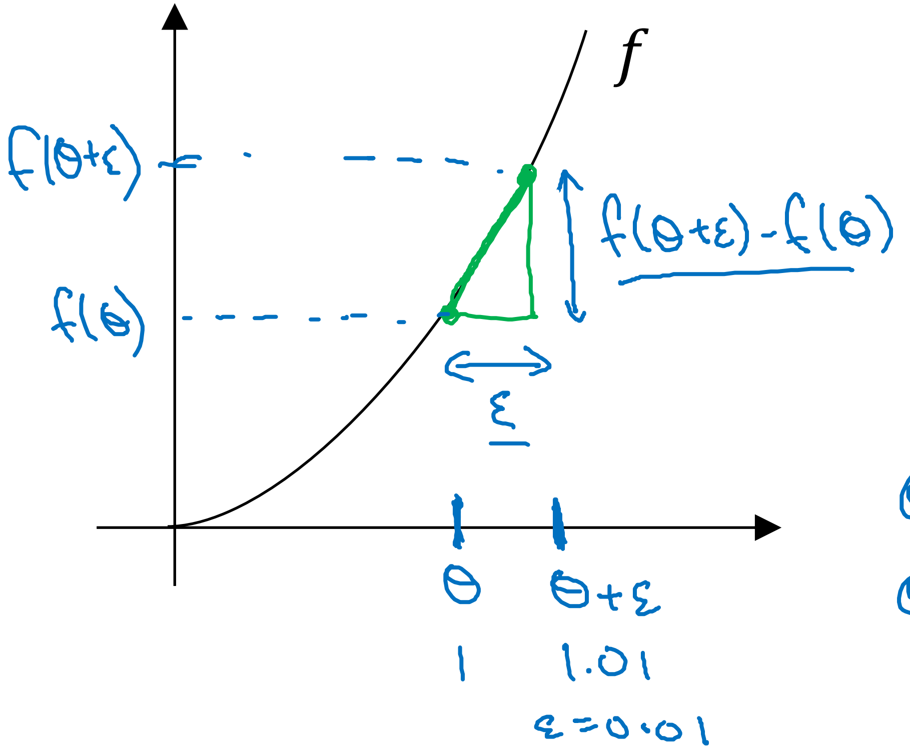
$g(\theta) = 3 \cdot (1)^2 = 3$

when $\theta = 1$

dw

db

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



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

$\theta = 1$

$\theta + \varepsilon = 1.01$

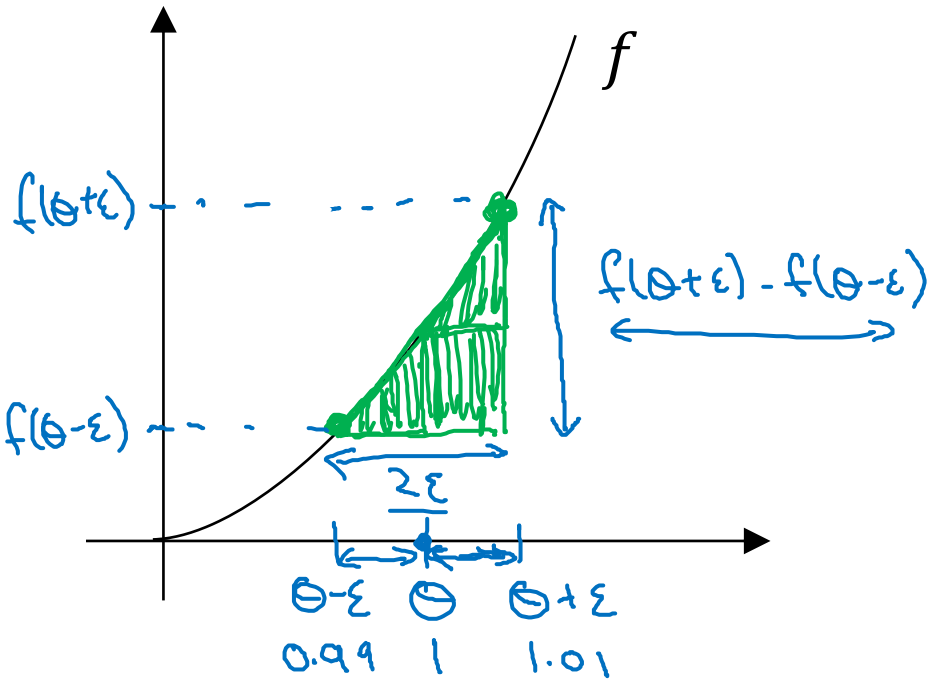
0.0301

3.1

3.2

Checking your derivative computation

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



$\varepsilon = 0.01$

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

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

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

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

Gradient checking (Grad check)

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

for each i:

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

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

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

i

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

10^{-5}

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

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

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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

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

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

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

- Remember regularization.

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

$d\theta$ = gradient of J wrt. θ

- Doesn't work with dropout.

J keep-prob = 1.0

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

$w, b \approx 0$

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