

# CSCI567 Machine Learning (Fall 2020)

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U of Southern California

Sep 17, 2020

# Administration

HW1 is being graded. Will discuss solutions today.

HW2 will be released after this lecture. Due on 9/29.

# Outline

- 1 Review of Last Lecture
- 2 Multiclass Classification
- 3 Neural Nets

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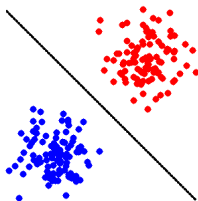
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# Summary

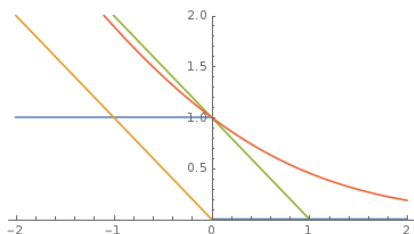
Linear models for **binary** classification:

Step 1. Model is the set of **separating hyperplanes**

$$\mathcal{F} = \{f(x) = \text{sgn}(w^T x) \mid w \in \mathbb{R}^D\}$$



## Step 2. Pick the **surrogate loss**



- **perceptron loss**  $\ell_{\text{perceptron}}(z) = \max\{0, -z\}$  (used in Perceptron)
- **hinge loss**  $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$  (used in SVM and many others)
- **logistic loss**  $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$  (used in logistic regression)

Step 3. Find empirical risk minimizer (ERM):

$$\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^D} F(\mathbf{w}) = \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^N \ell(y_n \mathbf{w}^T \mathbf{x}_n)$$

using

- **GD:**  $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla F(\mathbf{w})$
- **SGD:**  $\mathbf{w} \leftarrow \mathbf{w} - \eta \tilde{\nabla} F(\mathbf{w})$
- **Newton:**  $\mathbf{w} \leftarrow \mathbf{w} - (\nabla^2 F(\mathbf{w}))^{-1} \nabla F(\mathbf{w})$

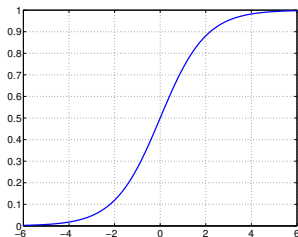
# A Probabilistic view of logistic regression

## Minimizing logistic loss = MLE for the sigmoid model

$$\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w}} \sum_{n=1}^N \ell_{\text{logistic}}(y_n \mathbf{w}^T \mathbf{x}_n) = \operatorname{argmax}_{\mathbf{w}} \prod_{n=1}^N \mathbb{P}(y_n \mid \mathbf{x}_n; \mathbf{w})$$

where

$$\mathbb{P}(y \mid \mathbf{x}; \mathbf{w}) = \sigma(y \mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-y \mathbf{w}^T \mathbf{x}}}$$





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- 1 Review of Last Lecture
- 2 Multiclass Classification
  - Multinomial logistic regression
  - Reduction to binary classification
- 3 Neural Nets

# Classification

Recall the setup:

- input (feature vector):  $\mathbf{x} \in \mathbb{R}^D$
- output (label):  $y \in [C] = \{1, 2, \dots, C\}$
- goal: learn a mapping  $f : \mathbb{R}^D \rightarrow [C]$

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## Examples:

- recognizing digits ( $C = 10$ ) or letters ( $C = 26$  or  $52$ )
- predicting weather: sunny, cloudy, rainy, etc
- predicting image category: ImageNet dataset ( $C \approx 20K$ )

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**Nearest Neighbor Classifier** naturally works for arbitrary  $C$ .

# Linear models: from binary to multiclass

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for any  $\mathbf{w}_1, \mathbf{w}_2$  s.t.  $\mathbf{w} = \mathbf{w}_1 - \mathbf{w}_2$

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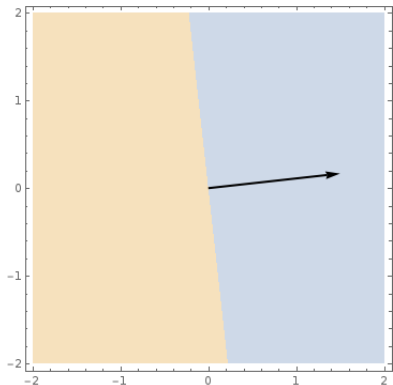
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for any  $\mathbf{w}_1, \mathbf{w}_2$  s.t.  $\mathbf{w} = \mathbf{w}_1 - \mathbf{w}_2$

Think of  $\mathbf{w}_k^T \mathbf{x}$  as **a score for class  $k$** .

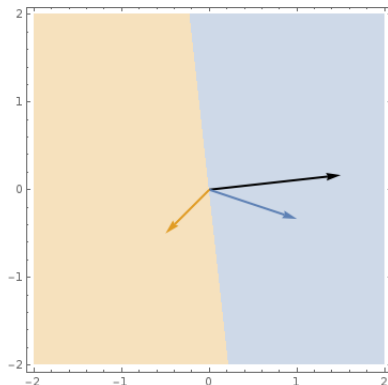
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$$w = \left(\frac{3}{2}, \frac{1}{6}\right)$$

- Blue class:  
 $\{x : w^T x \geq 0\}$
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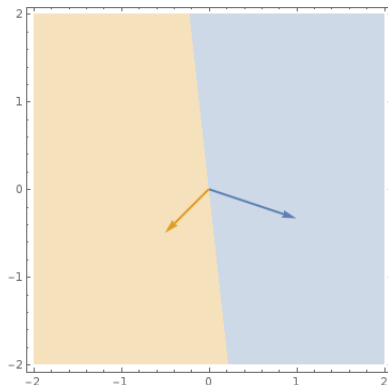
$$\mathbf{w} = \left(\frac{3}{2}, \frac{1}{6}\right) = \mathbf{w}_1 - \mathbf{w}_2$$

$$\mathbf{w}_1 = \left(1, -\frac{1}{3}\right)$$

$$\mathbf{w}_2 = \left(-\frac{1}{2}, -\frac{1}{2}\right)$$

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 $\{\mathbf{x} : 1 = \operatorname{argmax}_k \mathbf{w}_k^T \mathbf{x}\}$
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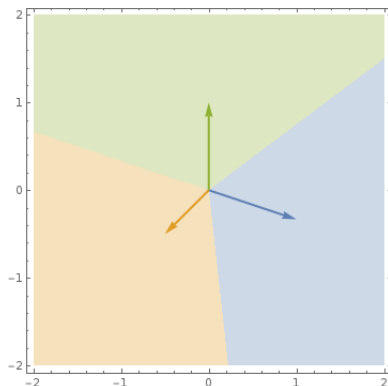


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$$\mathbf{w}_3 = (0, 1)$$

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- Orange class:  
 $\{\mathbf{x} : 2 = \operatorname{argmax}_k \mathbf{w}_k^T \mathbf{x}\}$
- Green class:  
 $\{\mathbf{x} : 3 = \operatorname{argmax}_k \mathbf{w}_k^T \mathbf{x}\}$

# Linear models for multiclass classification

$$\mathcal{F} = \left\{ f(\mathbf{x}) = \operatorname{argmax}_{k \in [C]} \mathbf{w}_k^T \mathbf{x} \mid \mathbf{w}_1, \dots, \mathbf{w}_C \in \mathbb{R}^D \right\}$$

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Step 2: *How do we generalize perceptron/hinge/logistic loss?*

This lecture: focus on the more popular **logistic loss**

# Multinomial logistic regression: a probabilistic view

Observe: for binary logistic regression, with  $\mathbf{w} = \mathbf{w}_1 - \mathbf{w}_2$ :

$$\mathbb{P}(y = 1 \mid \mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}} = \frac{e^{\mathbf{w}_1^T \mathbf{x}}}{e^{\mathbf{w}_1^T \mathbf{x}} + e^{\mathbf{w}_2^T \mathbf{x}}} \propto e^{\mathbf{w}_1^T \mathbf{x}}$$

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This is called the *softmax function*.

## Applying MLE again

Maximize probability of seeing labels  $y_1, \dots, y_N$  given  $\mathbf{x}_1, \dots, \mathbf{x}_N$

$$P(\mathbf{W}) = \prod_{n=1}^N \mathbb{P}(y_n \mid \mathbf{x}_n; \mathbf{W}) = \prod_{n=1}^N \frac{e^{\mathbf{w}_{y_n}^T \mathbf{x}_n}}{\sum_{k \in [C]} e^{\mathbf{w}_k^T \mathbf{x}_n}}$$

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By taking **negative log**, this is equivalent to minimizing

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This is the *multiclass logistic loss*, a.k.a *cross-entropy loss*.



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When  $C = 2$ , this is the same as binary logistic loss.

## Step 3: Optimization

Apply **SGD**: what is the gradient of

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# SGD for multinomial logistic regression

Initialize  $\mathbf{W} = \mathbf{0}$  (or randomly). Repeat:

- 1 pick  $n \in [N]$  uniformly at random
- 2 update the parameters

$$\mathbf{W} \leftarrow \mathbf{W} - \eta \begin{pmatrix} \mathbb{P}(y = 1 \mid \mathbf{x}_n; \mathbf{W}) \\ \vdots \\ \mathbb{P}(y = y_n \mid \mathbf{x}_n; \mathbf{W}) - 1 \\ \vdots \\ \mathbb{P}(y = C \mid \mathbf{x}_n; \mathbf{W}) \end{pmatrix} \mathbf{x}_n^T$$



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Think about why the algorithm makes sense intuitively.

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Having learned  $\mathbf{W}$ , we can either

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In either case, **(expected) mistake is bounded by logistic loss**

- deterministic

$$\mathbb{I}[f(\mathbf{x}) \neq y] \leq \log_2 \left( 1 + \sum_{k \neq y} e^{(\mathbf{w}_k - \mathbf{w}_y)^T \mathbf{x}} \right)$$

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In either case, **(expected) mistake is bounded by logistic loss**

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$$\mathbb{I}[f(\mathbf{x}) \neq y] \leq \log_2 \left( 1 + \sum_{k \neq y} e^{(\mathbf{w}_k - \mathbf{w}_y)^T \mathbf{x}} \right)$$

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## A note on prediction

Having learned  $\mathbf{W}$ , we can either

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Yes, there are in fact many ways to do it.

- **one-versus-all** (one-versus-rest, one-against-all, etc)
- **one-versus-one** (all-versus-all, etc)
- **Error-Correcting Output Codes** (ECOC)
- **tree-based reduction**

# One-versus-all (OvA)

(picture credit: [link](#))

Idea: train  $C$  binary classifiers to learn “**is class  $k$  or not?**” for each  $k$ .

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$x_1$		$x_1$ —	$x_1$ +	$x_1$ —	$x_1$ —
$x_2$		$x_2$ —	$x_2$ —	$x_2$ +	$x_2$ —
$x_3$		$x_3$ —	$x_3$ —	$x_3$ —	$x_3$ +
$x_4$		$x_4$ —	$x_4$ +	$x_4$ —	$x_4$ —
$x_5$		$x_5$ +	$x_5$ —	$x_5$ —	$x_5$ —
	$\Rightarrow$	$\Downarrow$ $h_1$	$\Downarrow$ $h_2$	$\Downarrow$ $h_3$	$\Downarrow$ $h_4$

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Issue: will (probably) make a mistake *as long as one of  $h_k$  errs*.

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(picture credit: [link](#))

Idea: train  $\binom{C}{2}$  binary classifiers to learn “**is class  $k$  or  $k'$ ?**”.

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		■ vs. ■	■ vs. ■	■ vs. ■	■ vs. ■	■ vs. ■	■ vs. ■
$x_1$	■	$x_1$ —			$x_1$ —		$x_1$ —
$x_2$	■		$x_2$ —	$x_2$ +			$x_2$ +
$x_3$	■			$x_3$ —	$x_3$ +	$x_3$ —	
$x_4$	■	$x_4$ —			$x_4$ —		$x_4$ —
$x_5$	■	$x_5$ +	$x_5$ +			$x_5$ +	
		⇓	⇓	⇓	⇓	⇓	⇓
		$h_{(1,2)}$	$h_{(1,3)}$	$h_{(3,4)}$	$h_{(4,2)}$	$h_{(1,4)}$	$h_{(3,2)}$

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**More robust** than one-versus-all, but *slower* in prediction.

# Error-correcting output codes (ECOC)

(picture credit: [link](#))

Idea: based on a code  $\mathbf{M} \in \{-1, +1\}^{C \times L}$ , train  $L$  binary classifiers to learn “**is bit  $b$  on or off**”.

<b>M</b>	1	2	3	4	5
	+	—	+	—	+
	—	—	+	+	+
	+	+	—	—	—
	+	+	+	+	—







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Training: for each bit  $b \in [L]$

- relabel example  $x_n$  as  $M_{y_n, b}$
- train a binary classifier  $h_b$  using this new dataset.

$\mathbf{M}$	1	2	3	4	5
	+	−	+	−	+
	−	−	+	+	+
	+	+	−	−	−
	+	+	+	+	−

		1	2	3	4	5
$x_1$ 	$\Rightarrow$	$x_1$ −	$x_1$ −	$x_1$ +	$x_1$ +	$x_1$ +
$x_2$ 		$x_2$ +	$x_2$ +	$x_2$ −	$x_2$ −	$x_2$ −
$x_3$ 		$x_3$ +	$x_3$ +	$x_3$ +	$x_3$ +	$x_3$ −
$x_4$ 		$x_4$ −	$x_4$ −	$x_4$ +	$x_4$ +	$x_4$ +
$x_5$ 		$x_5$ +	$x_5$ −	$x_5$ +	$x_5$ −	$x_5$ +
		$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$
		$h_1$	$h_2$	$h_3$	$h_4$	$h_5$

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  - if any two codes are  $d$  bits away, then prediction can tolerate about  $d/2$  errors
- *random code* is often a good choice

# Tree based method


















Idea: train  $\approx C$  binary classifiers to learn “**belongs to which half?**”.

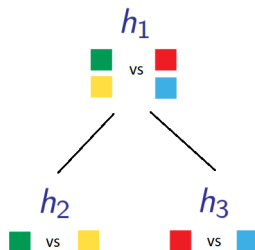


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Training: see pictures

		 vs   vs 	 vs   vs 	 vs   vs 
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		$\Downarrow$ $h_1$	$\Downarrow$ $h_2$	$\Downarrow$ $h_3$

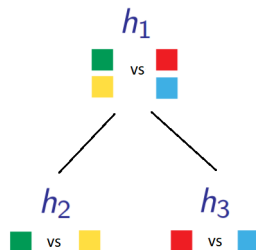


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		<div><div><div></div><div></div></div> vs <div><div><div></div><div></div></div></div></div>	<div><div><div></div><div></div></div> vs <div><div><div></div><div></div></div></div></div>	<div><div><div></div><div></div></div> vs <div><div><div></div><div></div></div></div></div>
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$x_1$	<div><div><div></div><div></div></div></div>	$x_1$	<div><div><div></div><div></div></div></div>	$x_1$
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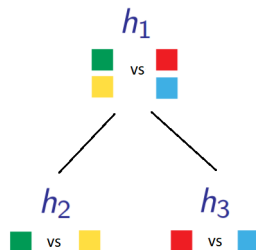
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	$\Rightarrow$	$\Downarrow$ $h_1$	$\Downarrow$ $h_2$	$\Downarrow$ $h_3$



Prediction is also natural, *but is very fast!* (think ImageNet where  $C \approx 20K$ )

# Comparisons

In big O notation,

Reduction	#training points	test time	remark
OvA			
OvO			
ECOC			
Tree			

# Comparisons

In big O notation,

Reduction	#training points	test time	remark
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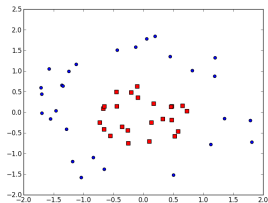
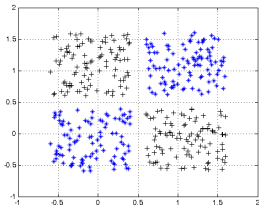
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Tree	$(\log_2 C)N$	$\log_2 C$	good for “extreme classification”



# Outline

- 1 Review of Last Lecture
- 2 Multiclass Classification
- 3 Neural Nets
  - Definition
  - Backpropagation
  - Preventing overfitting

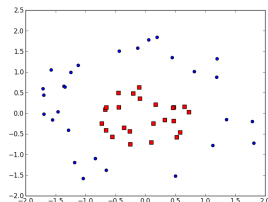
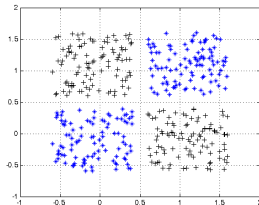
# Linear models are not always adequate



We can use a nonlinear mapping as discussed:

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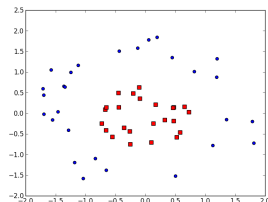
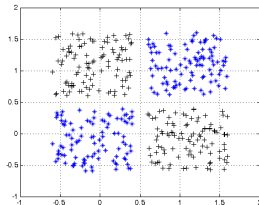


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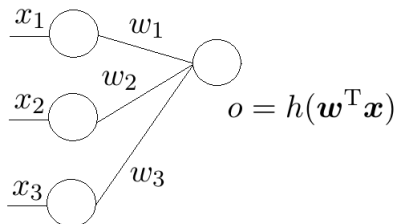
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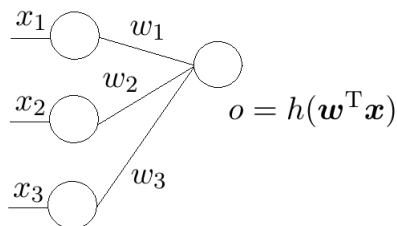
THE most popular nonlinear models nowadays: **neural nets**

# Linear model as a one-layer neural net



$$h(a) = a \text{ for linear model}$$

# Linear model as a one-layer neural net

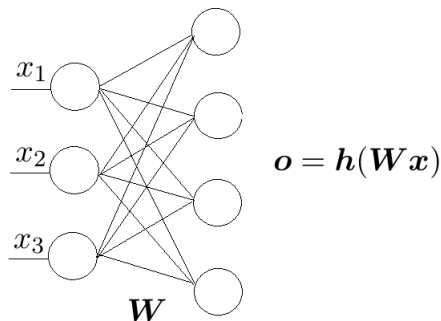


$$h(a) = a \text{ for linear model}$$

To create non-linearity, can use

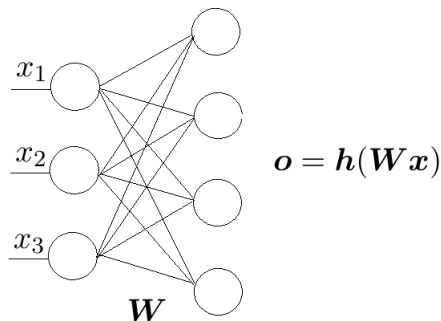
- Rectified Linear Unit (**ReLU**):  $h(a) = \max\{0, a\}$
- sigmoid function:  $h(a) = \frac{1}{1+e^{-a}}$
- TanH:  $h(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$
- many more

# More output nodes



$W \in \mathbb{R}^{4 \times 3}$ ,  $h : \mathbb{R}^4 \rightarrow \mathbb{R}^4$  so  $h(\mathbf{a}) = (h_1(a_1), h_2(a_2), h_3(a_3), h_4(a_4))$

## More output nodes



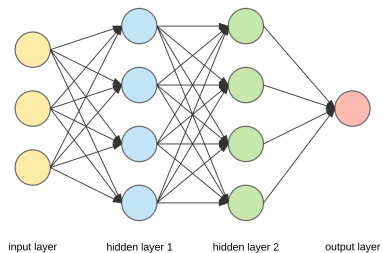
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Can think of this as a nonlinear basis:  $\Phi(\mathbf{x}) = h(W\mathbf{x})$



# More layers

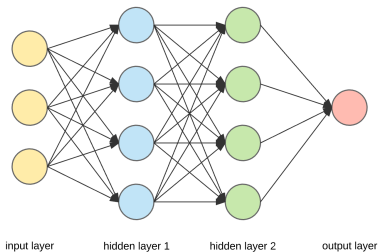
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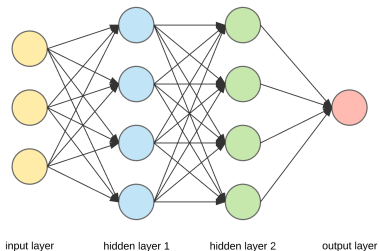
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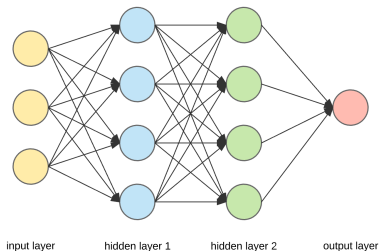
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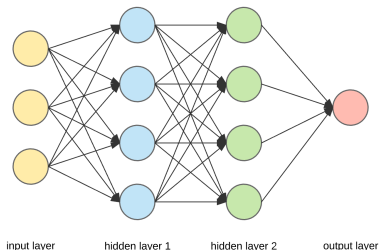
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- #layers refers to #hidden\_layers (plus 1 or 2 for input/output layers)



# More layers

Becomes a network:

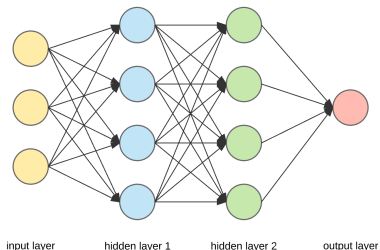
- each node is called a **neuron**
- $h$  is called the **activation function**
  - can use  $h(a) = 1$  for one neuron in each layer to *incorporate bias term*
  - output neuron can use  $h(a) = a$
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- **deep** neural nets can have many layers and *millions* of parameters
- this is a **feedforward, fully connected** neural net, there are many variants



# How powerful are neural nets?

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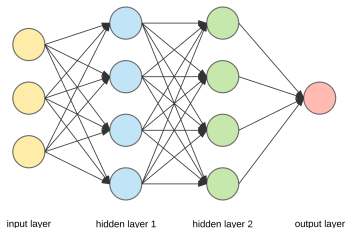
Designing network architecture is important and very complicated

- for feedforward network, need to decide number of hidden layers, number of neurons at each layer, activation functions, etc.

# Math formulation

An L-layer neural net can be written as

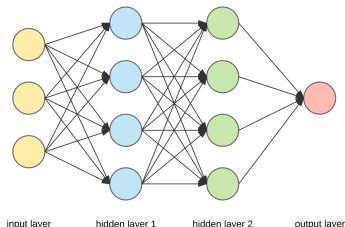
$$f(x) = h_L(W_L h_{L-1}(W_{L-1} \cdots h_1(W_1 x)))$$



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To ease notation, for a given input  $x$ , define recursively

$$o_0 = x, \quad a_\ell = W_\ell o_{\ell-1}, \quad o_\ell = h_\ell(a_\ell) \quad (\ell = 1, \dots, L)$$

where

- $W_\ell \in \mathbb{R}^{D_\ell \times D_{\ell-1}}$  is the weights between layer  $\ell - 1$  and  $\ell$
- $D_0 = D, D_1, \dots, D_L$  are numbers of neurons at each layer
- $a_\ell \in \mathbb{R}^{D_\ell}$  is input to layer  $\ell$
- $o_\ell \in \mathbb{R}^{D_\ell}$  is output to layer  $\ell$
- $h_\ell : \mathbb{R}^{D_\ell} \rightarrow \mathbb{R}^{D_\ell}$  is activation functions at layer  $\ell$

# Learning the model

*No matter how complicated the model is, our goal is the same:* minimize

$$\mathcal{E}(\mathbf{W}_1, \dots, \mathbf{W}_L) = \frac{1}{N} \sum_{n=1}^N \mathcal{E}_n(\mathbf{W}_1, \dots, \mathbf{W}_L)$$

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where

$$\mathcal{E}_n(\mathbf{W}_1, \dots, \mathbf{W}_L) = \begin{cases} \|\mathbf{f}(\mathbf{x}_n) - \mathbf{y}_n\|_2^2 & \text{for regression} \\ \ln \left( 1 + \sum_{k \neq y_n} e^{f(\mathbf{x}_n)_k - f(\mathbf{x}_n)_{y_n}} \right) & \text{for classification} \end{cases}$$

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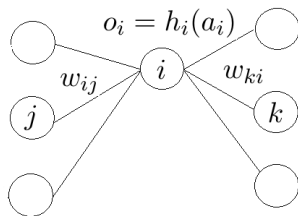
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the simplest example  $f(g_1(w), g_2(w)) = g_1(w)g_2(w)$

# Computing the derivative

Drop the subscript  $\ell$  for layer for simplicity.

Find the **derivative of  $\mathcal{E}_n$  w.r.t. to  $w_{ij}$**

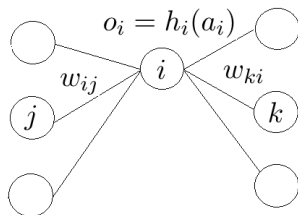


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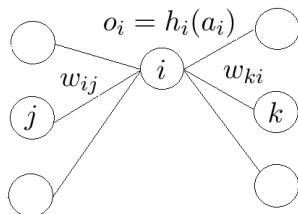
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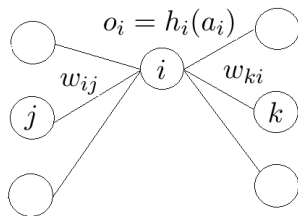


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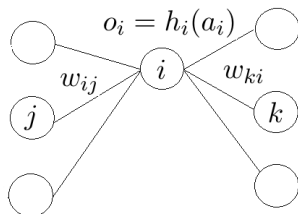


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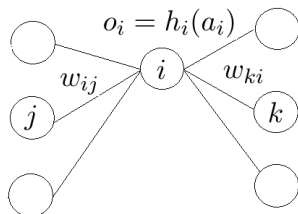
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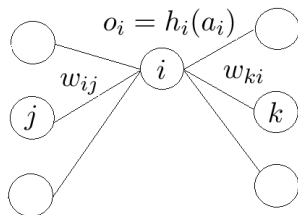
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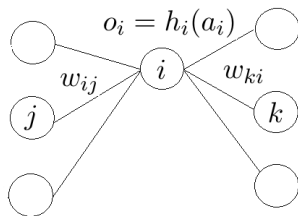
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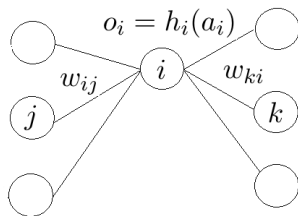
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For the last layer, for square loss

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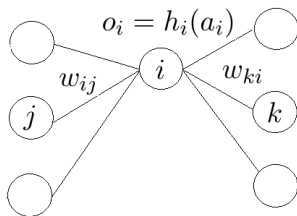


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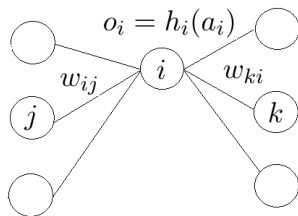
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**Exercise:** try to do it for logistic loss yourself.

## Computing the derivative

Using **matrix notation** greatly simplifies presentation and implementation:

$$\frac{\partial \mathcal{E}_n}{\partial \mathbf{W}_\ell} = \frac{\partial \mathcal{E}_n}{\partial \mathbf{a}_\ell} \mathbf{o}_{\ell-1}^T$$

$$\frac{\partial \mathcal{E}_n}{\partial \mathbf{a}_\ell} = \begin{cases} \left( \mathbf{W}_{\ell+1}^T \frac{\partial \mathcal{E}_n}{\partial \mathbf{a}_{\ell+1}} \right) \circ \mathbf{h}'_\ell(\mathbf{a}_\ell) & \text{if } \ell < L \\ 2(\mathbf{h}_L(\mathbf{a}_L) - \mathbf{y}_n) \circ \mathbf{h}'_L(\mathbf{a}_L) & \text{else} \end{cases}$$

where  $\mathbf{v}_1 \circ \mathbf{v}_2 = (v_{11}v_{21}, \dots, v_{1D}v_{2D})$  is the element-wise product (a.k.a. Hadamard product).

Verify yourself!

# Putting everything into SGD

The **backpropagation** algorithm (**Backprop**)

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*Think about how to do the last two steps properly!*

# More tricks to optimize neural nets

Many variants based on backprop

- SGD with **minibatch**: randomly sample a batch of examples to form a stochastic gradient
- SGD with **momentum**
- ...

# SGD with momentum

Initialize  $w_0$  and **velocity**  $v = 0$

For  $t = 1, 2, \dots$

- form a stochastic gradient  $g_t$
- update velocity  $v \leftarrow \alpha v - \eta g_t$  for some discount factor  $\alpha \in (0, 1)$
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Updates for first few rounds:

- $w_1 = w_0 - \eta g_1$
- $w_2 = w_1 - \alpha \eta g_1 - \eta g_2$
- $w_3 = w_2 - \alpha^2 \eta g_1 - \alpha \eta g_2 - \eta g_3$
- $\dots$

# Overfitting

**Overfitting is very likely** since the models are too powerful.

Methods to overcome overfitting:

- data augmentation
- regularization
- dropout
- early stopping
- ...

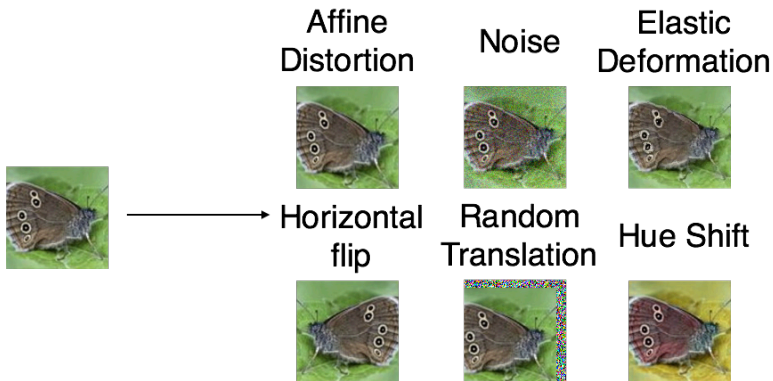
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**Exploit prior knowledge to add more training data**





# Regularization

**L2 regularization:** minimize

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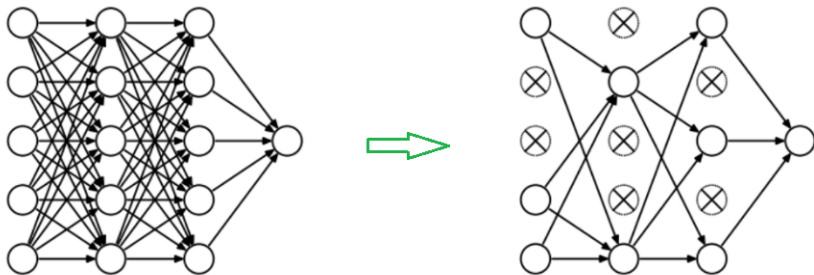
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Introduce *weight decaying effect*

# Dropout

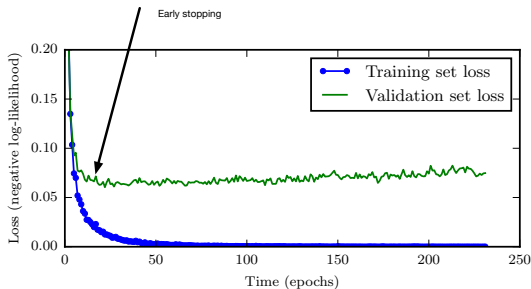
**Randomly delete neurons** during training



Very effective, makes training faster as well

# Early stopping

Stop training when the performance on validation set stops improving



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- take some work to select architecture and hyperparameters
- are still not well understood in theory