CSCI567 Machine Learning (Spring 2023)
Week 5: Neural Networks

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Administration

Outline

1. Multiclass Classification

2. Neural Nets

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Classification

Recall the setup:

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

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Examples:

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

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Nearest Neighbor Classifier naturally works for arbitrary C.

Linear models: from binary to multiclass

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

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

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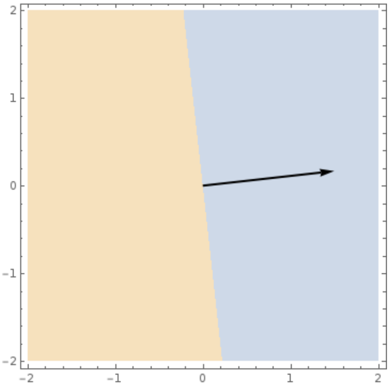

$$\boldsymbol{w} = \left(\tfrac{3}{2}, \tfrac{1}{6}\right)$$

- Blue class: $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0\}$
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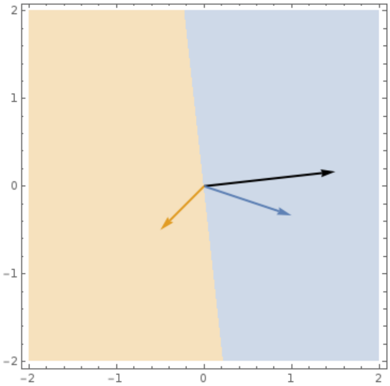

$\boldsymbol{w} = (\frac{3}{2}, \frac{1}{6}) = \boldsymbol{w}_1 - \boldsymbol{w}_2$
$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
$\boldsymbol{w}_2 = (-\frac{1}{2}, -\frac{1}{2})$

- Blue class: $\{\boldsymbol{x} : 1 = \mathrm{argmax}_k\, \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$
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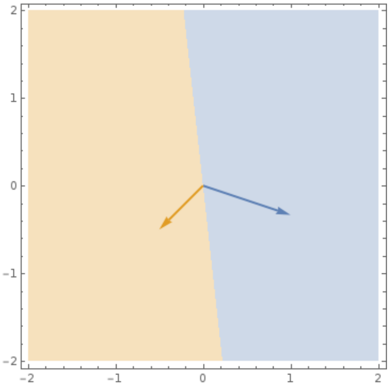

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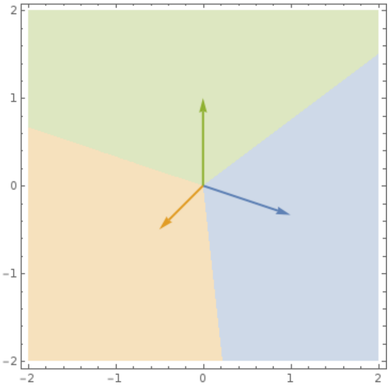

$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
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$\boldsymbol{w}_3 = (0, 1)$

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

Linear models for multiclass classification

$$\mathcal{F} = \left\{ f(\boldsymbol{x}) = \operatorname*{argmax}_{k \in [\mathsf{C}]} \ \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x} \mid \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{\mathsf{C}} \in \mathbb{R}^{\mathsf{D}} \right\}$$

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

Multinomial logistic regression: a probabilistic view

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

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

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This is called the *softmax function*.

Applying MLE again

Maximize probability of seeing labels $y_1, \ldots, y_\mathsf{N}$ given $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\mathsf{N}$

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

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

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When $\mathsf{C} = 2$, this is the same as binary logistic loss.

Optimization

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

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SGD for multinomial logistic regression

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

1. pick $n \in [\mathsf{N}]$ uniformly at random
2. update the parameters

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Think about why the algorithm makes sense intuitively.

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$$\mathbb{E}\left[\mathbb{I}[f(\boldsymbol{x}) \neq y]\right] = 1 - \mathbb{P}(y \mid \boldsymbol{x}; \boldsymbol{W})$$

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$$\mathbb{E}\left[\mathbb{I}[f(\boldsymbol{x}) \neq y]\right] = 1 - \mathbb{P}(y \mid \boldsymbol{x};\boldsymbol{W}) \leq -\ln \mathbb{P}(y \mid \boldsymbol{x};\boldsymbol{W})$$

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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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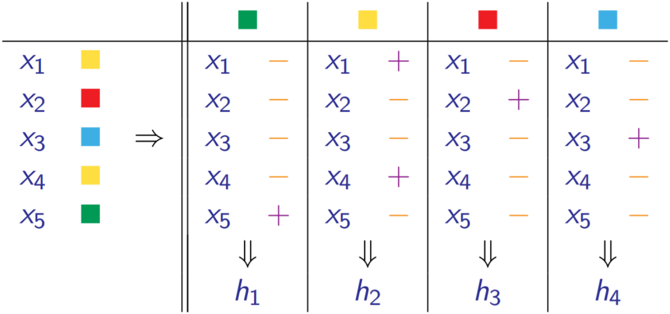

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Issue: will (probably) make a mistake *as long as one of h_k errs*.

One-versus-one (OvO)

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

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Training: for each pair (k, k'),

- relabel examples with class k as $+1$ and examples with class k' as -1
- *discard all other examples*
- train a binary classifier $h_{(k,k')}$ using this new dataset

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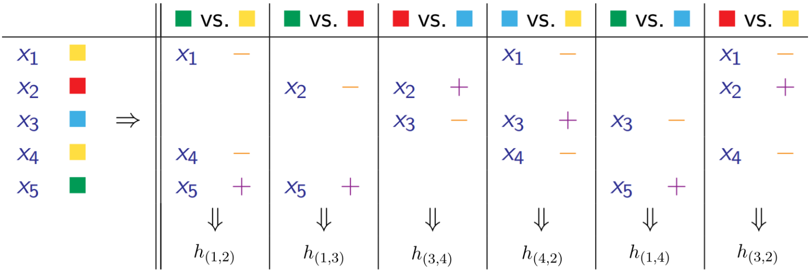

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More robust than one-versus-all, but *slower* in prediction.

Error-correcting output codes (ECOC)

(picture credit: link)

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

M	1	2	3	4	5
green	+	−	+	−	+
yellow	−	−	+	+	+
red	+	+	−	−	−
blue	+	+	+	+	−

Error-correcting output codes (ECOC) (picture credit: link)

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

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

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

M	1	2	3	4	5
🟩	+	−	+	−	+
🟨	−	−	+	+	+
🟥	+	+	−	−	−
🟦	+	+	+	+	−

			1		2		3		4		5	
x_1	🟨		x_1	−	x_1	−	x_1	+	x_1	+	x_1	+
x_2	🟥		x_2	+	x_2	+	x_2	−	x_2	−	x_2	−
x_3	🟦	$\Rightarrow$	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	

Error-correcting output codes (ECOC)

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- compute the **predicted code** $\boldsymbol{c} = (h_1(\boldsymbol{x}), \ldots, h_{\mathsf{L}}(\boldsymbol{x}))^{\mathrm{T}}$

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- *random code* is a good choice, but might create *hard* training sets

Tree based method

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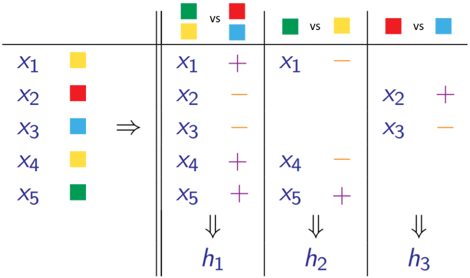
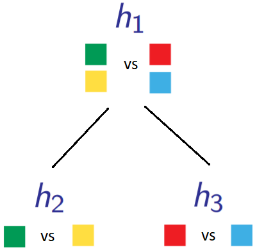
Training: see pictures





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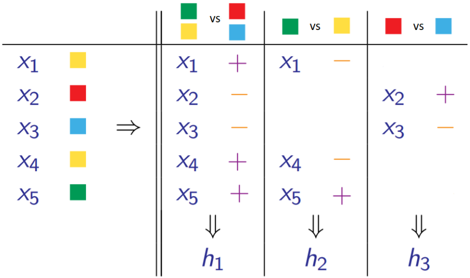

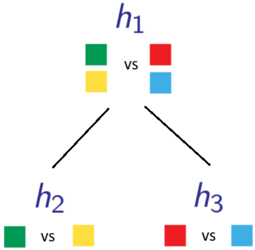

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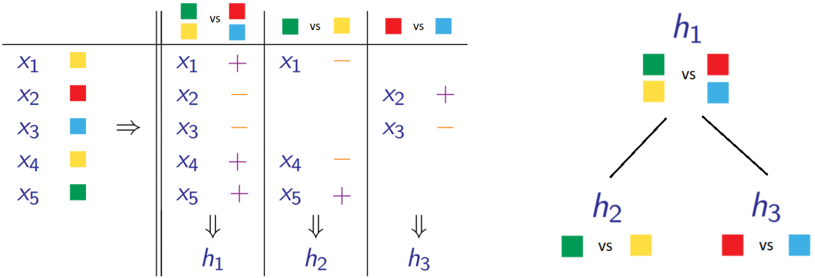

Prediction is also natural, *but is very fast!* (think ImageNet where $C \approx 20K$)

Comparisons

In big O notation,

Reduction	**#training points**	**test time**	**remark**
OvA			
OvO			
ECOC			
Tree			

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In big O notation,

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OvO			
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Reduction	**#training points**	**test time**	**remark**
OvA	CN	C	not robust
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Tree			

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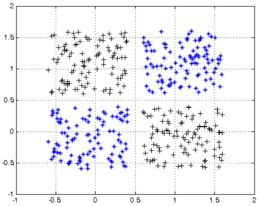
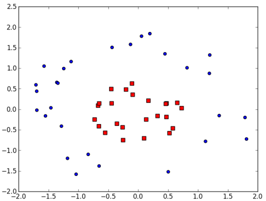
ECOC	LN	L	need diversity when designing code
Tree	$(\log_2 C)N$	$\log_2 C$	good for "extreme classification"

Outline

Linear models are not always adequate





We can use a nonlinear mapping as discussed:

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^{\mathsf{D}} \rightarrow \boldsymbol{z} \in \mathbb{R}^{\mathsf{M}}$$

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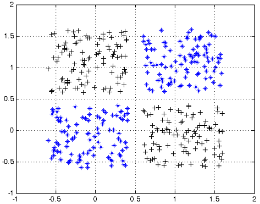

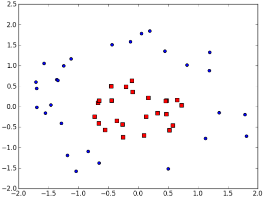

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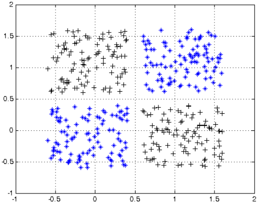

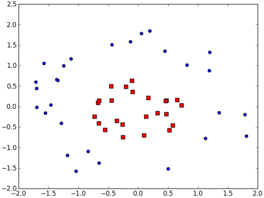

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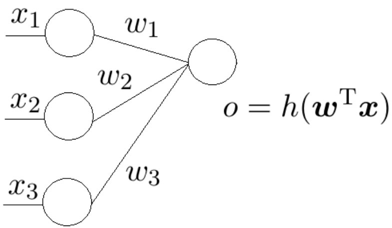
THE most popular nonlinear models nowadays: **neural nets**

Linear model as a one-layer neural net



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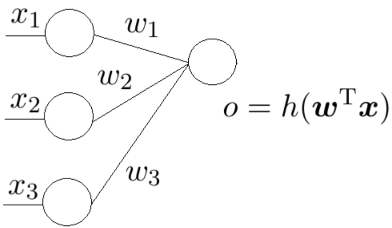

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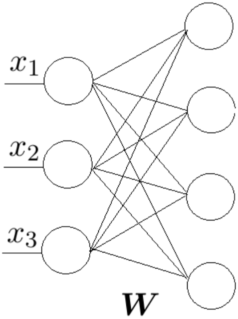
To create non-linearity, can use

- 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



$$\boldsymbol{o} = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$$

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

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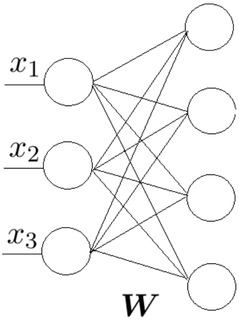

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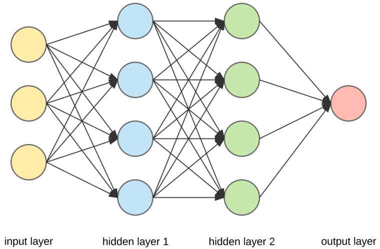
Can think of this as a nonlinear basis: $\boldsymbol{\Phi}(\boldsymbol{x}) = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$

More layers

Becomes a network:



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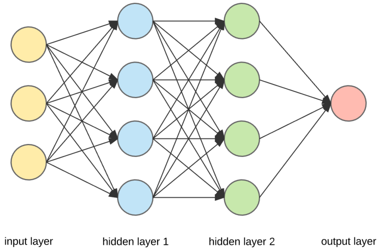

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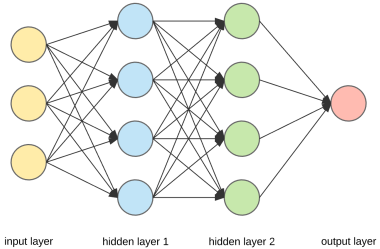

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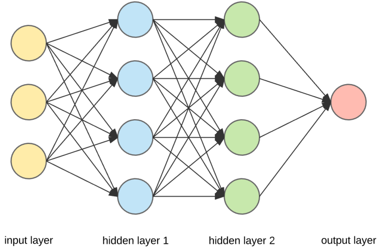

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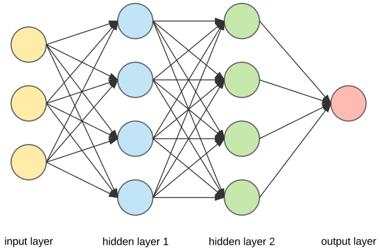

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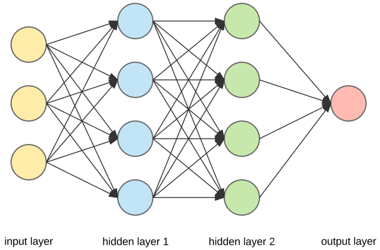

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- **deep** neural nets can have many layers and *millions* of parameters
- this is a **feedforward, fully connected** neural net, there are many variants

How powerful are neural nets?

Universal approximation theorem (Cybenko, 89; Hornik, 91):

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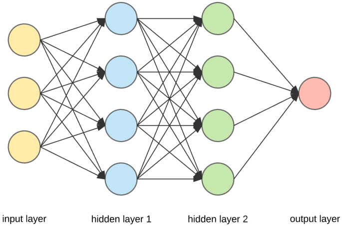
Designing network architecture is important and very complicated

- 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

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{h}_{\mathsf{L}}\left(\boldsymbol{W}_L \boldsymbol{h}_{\mathsf{L}-1}\left(\boldsymbol{W}_{L-1} \cdots \boldsymbol{h}_1\left(\boldsymbol{W}_1 \boldsymbol{x}\right)\right)\right)$$



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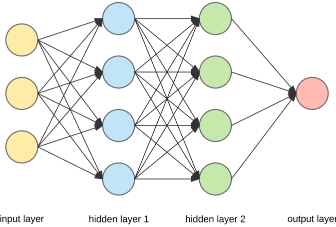

To ease notation, for a given input $\boldsymbol{x}$, define recursively

$$\boldsymbol{o}_0 = \boldsymbol{x}, \qquad \boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}, \qquad \boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell) \qquad\qquad (\ell = 1, \ldots, \mathsf{L})$$

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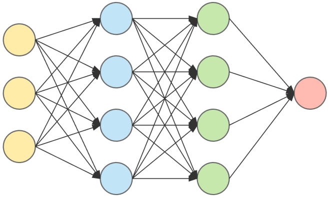

To ease notation, for a given input $\boldsymbol{x}$, define recursively

$$\boldsymbol{o}_0 = \boldsymbol{x}, \qquad \boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}, \qquad \boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell) \qquad\qquad (\ell = 1, \ldots, \mathsf{L})$$

where

- $\boldsymbol{W}_\ell \in \mathbb{R}^{\mathsf{D}_\ell \times \mathsf{D}_{\ell-1}}$ is the weights for layer ℓ
- $\mathsf{D}_0 = \mathsf{D}, \mathsf{D}_1, \ldots, \mathsf{D}_{\mathsf{L}}$ are numbers of neurons at each layer
- $\boldsymbol{a}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is input to layer ℓ
- $\boldsymbol{o}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is output to layer ℓ
- $\boldsymbol{h} : \mathbb{R}^{\mathsf{D}_\ell} \to \mathbb{R}^{\mathsf{D}_\ell}$ is activation functions at layer ℓ

Learning the model

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

$$\mathcal{E}(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}) = \sum_{n=1}^{\mathsf{N}} \mathcal{E}_n(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L})$$

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where

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

How to optimize such a complicated function?

Same thing: apply **SGD**! even if the model is *nonconvex*.

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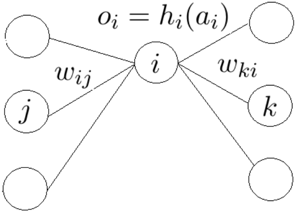
the simplest example $f(g_1(w), g_2(w)) = g_1(w)g_2(w)$

Computing the derivative

Drop the subscript ℓ for layer for simplicity.

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



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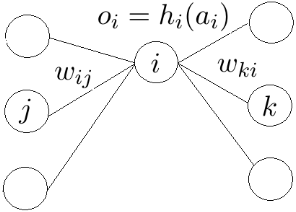

$$\frac{\partial \mathcal{E}_n}{\partial w_{ij}} = \frac{\partial \mathcal{E}_n}{\partial a_i} \frac{\partial a_i}{\partial w_{ij}}$$

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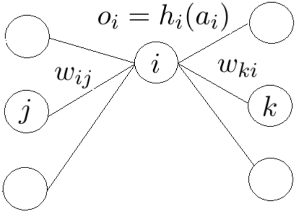

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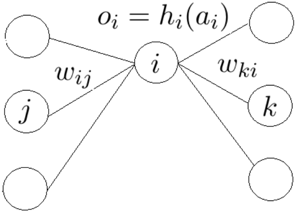

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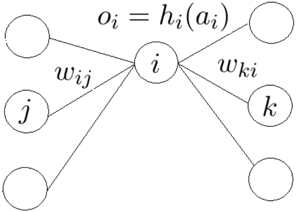

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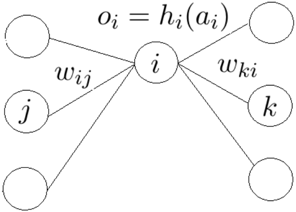

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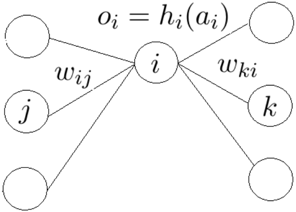

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Computing the derivative

Adding the subscript for layer:

$$\frac{\partial \mathcal{E}_n}{\partial w_{\ell,ij}} = \frac{\partial \mathcal{E}_n}{\partial a_{\ell,i}} o_{\ell-1,j}$$

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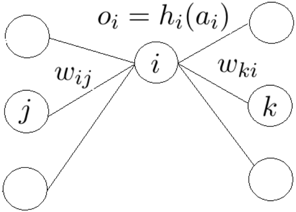

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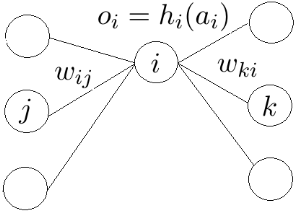

For the last layer, for square loss

$$\frac{\partial \mathcal{E}_n}{\partial a_{\mathsf{L},i}} = \frac{\partial (h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i})^2}{\partial a_{\mathsf{L},i}}$$

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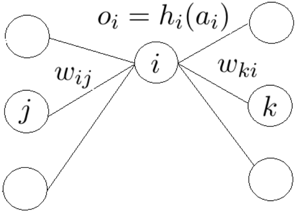

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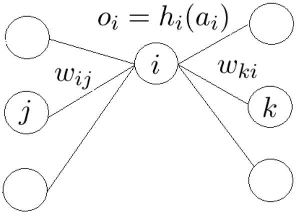

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Exercise: try to do it for logistic loss yourself.

Computing the derivative

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

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

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

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

Verify yourself!

Putting everything into SGD

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

Initialize $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}$ (all $\mathbf{0}$ or randomly). Repeat:

1. randomly pick one data point $n \in [\mathsf{N}]$

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

   - update weights

$$\boldsymbol{W}_\ell \leftarrow \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{W}_\ell} = \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathrm{T}}$$

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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**
- $\cdots$

SGD with momentum

Initialize $\boldsymbol{w}_0$ and **velocity** $\boldsymbol{v} = \boldsymbol{0}$

For $t = 1, 2, \ldots$

- form a stochastic gradient $\boldsymbol{g}_t$
- update velocity $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \eta \boldsymbol{g}_t$ for some discount factor $\alpha \in (0, 1)$
- update weight $\boldsymbol{w}_t \leftarrow \boldsymbol{w}_{t-1} + \boldsymbol{v}$

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Updates for first few rounds:

- $\boldsymbol{w}_1 = \boldsymbol{w}_0 - \eta \boldsymbol{g}_1$
- $\boldsymbol{w}_2 = \boldsymbol{w}_1 - \alpha\eta \boldsymbol{g}_1 - \eta \boldsymbol{g}_2$
- $\boldsymbol{w}_3 = \boldsymbol{w}_2 - \alpha^2\eta \boldsymbol{g}_1 - \alpha\eta \boldsymbol{g}_2 - \eta \boldsymbol{g}_3$
- $\cdots$

Overfitting

Overfitting is very likely since the models are too powerful.

Methods to overcome overfitting:

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

Data augmentation

Data: the more the better. How do we get more data?

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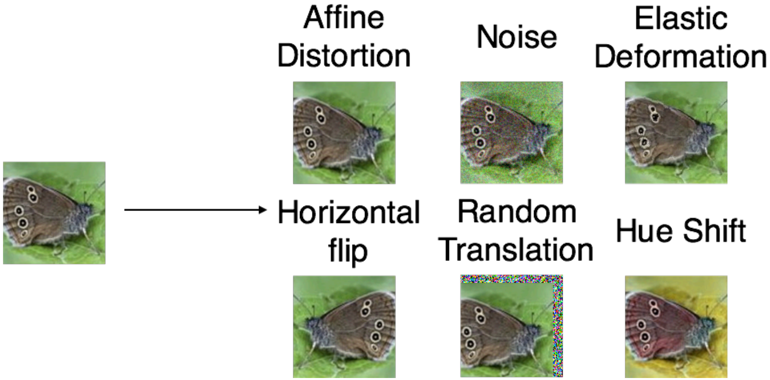
Exploit prior knowledge to add more training data



Regularization

L2 regularization: minimize

$$\mathcal{E}'(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}) = \mathcal{E}(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}) + \lambda \sum_{\ell=1}^{\mathsf{L}} \|\boldsymbol{W}_\ell\|_2^2$$

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Simple change to the gradient:

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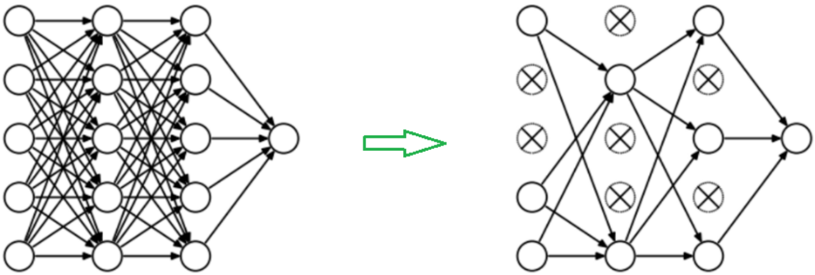
Simple change to the gradient:

$$\frac{\partial \mathcal{E}'}{\partial w_{ij}} = \frac{\partial \mathcal{E}}{\partial w_{ij}} + 2\lambda w_{ij}$$

Introduce *weight decaying effect*

Dropout

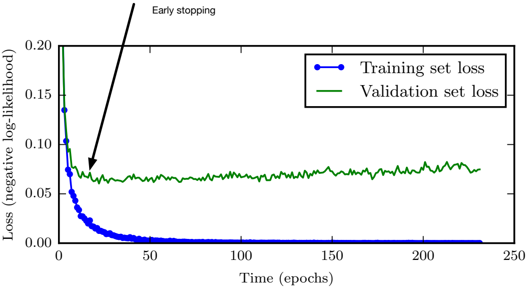
Randomly delete neurons during training



Very effective, makes training faster as well

Early stopping

Stop training when the performance on validation set stops improving



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- are hugely popular, achieving *best performance* on many problems

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- take *a lot of time* to train (need GPUs for massive parallel computing)
- take some work to select architecture and hyperparameters
- are still not well understood in theory