CSCI567 Machine Learning (Spring 2025)

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Administration

HW1 was due yesterday. Remember: only one late day allowed

HW2 will be released next week.

Outline

1. Review of Last Lecture

2. Multiclass Classification

3. Neural Nets

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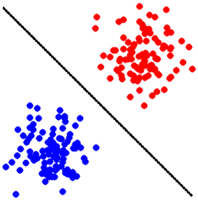
Linear classifiers

Linear models for **binary** classification:

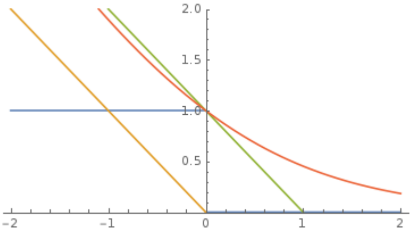
Step 1. Model is the set of **separating hyperplanes**

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



Linear classifiers

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)

Linear classifiers

Step 3. Find empirical risk minimizer (ERM):

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

using

- **GD:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta\nabla F(\boldsymbol{w})$
- **SGD:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta\tilde{\nabla} F(\boldsymbol{w})$ $\quad (\mathbb{E}[\tilde{\nabla} F(\boldsymbol{w})] = \nabla F(\boldsymbol{w}))$
- **Newton:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \left(\nabla^2 F(\boldsymbol{w})\right)^{-1} \nabla F(\boldsymbol{w})$

Convergence guarantees of GD/SGD

- GD/SGD converges to a stationary point

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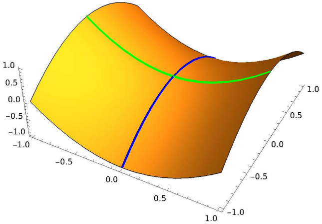
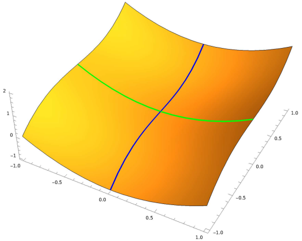
- for convex objectives, this is all we need
- for nonconvex objectives, can get stuck at local minimizers or "bad" saddle points (random initialization escapes "good" saddle points)



"good" saddle points



"bad" saddle points

Perceptron and logistic regression

Initialize $\boldsymbol{w} = \mathbf{0}$ or randomly.

Repeat:

- pick a data point $\boldsymbol{x}_n$ uniformly at random (**common trick for SGD**)

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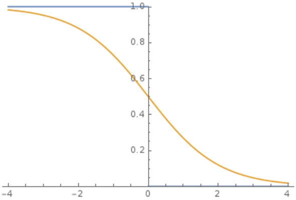
Repeat:

- pick a data point $\boldsymbol{x}_n$ uniformly at random (**common trick for SGD**)
- update parameter:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \begin{cases} \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n & \text{(Perceptron)} \\ \eta \sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n & \text{(logistic regression)} \end{cases}$$



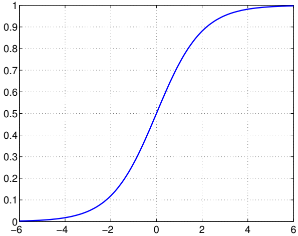
A Probabilistic view of logistic regression

Minimizing logistic loss = MLE for the sigmoid model

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

where

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



Outline

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): $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$
- 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
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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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for any $\boldsymbol{w}_1, \boldsymbol{w}_2$ s.t. $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$

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

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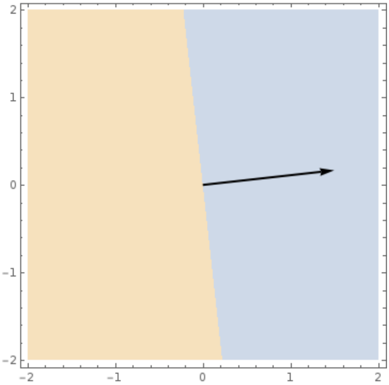

$$\boldsymbol{w} = (\tfrac{3}{2}, \tfrac{1}{6})$$

- Blue class: $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0\}$
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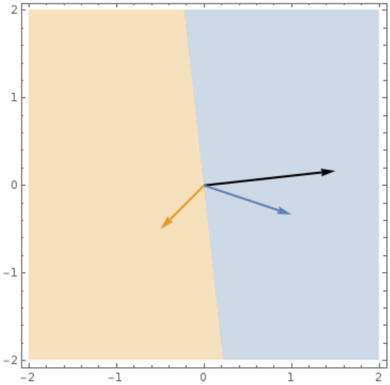
Linear models: from binary to multiclass



$\boldsymbol{w} = (\frac{3}{2}, \frac{1}{6}) = \boldsymbol{w}_1 - \boldsymbol{w}_2$
$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
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- Blue class: $\{\boldsymbol{x} : 1 = \text{argmax}_k\, \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$
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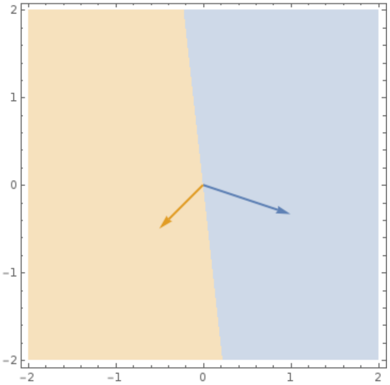

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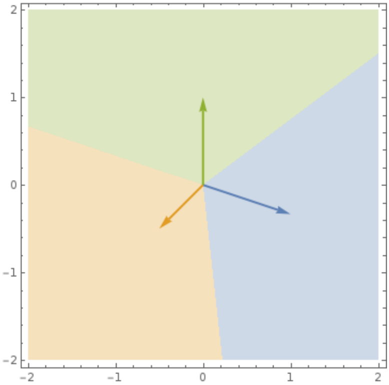

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$\boldsymbol{w}_3 = (0, 1)$

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

Linear models for multiclass classification

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

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$$
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&= \left\{ f(\boldsymbol{x}) = \underset{k \in [\mathsf{C}]}{\operatorname{argmax}} \ (\boldsymbol{W}\boldsymbol{x})_k \mid \boldsymbol{W} \in \mathbb{R}^{\mathsf{C} \times \mathsf{D}} \right\}
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Step 2: *How do we generalize perceptron/hinge/logistic loss?*

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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 $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$:

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

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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

$$F(\boldsymbol{W}) = \sum_{n=1}^{\mathsf{N}} \ln \left(\frac{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}_n}}{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}} \boldsymbol{x}_n}} \right)$$

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

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

Step 3: Optimization

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

$$F_n(\boldsymbol{W}) = \ln\left(1 + \sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}} \boldsymbol{x}_n}\right)?$$

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else:

$$\nabla_{\boldsymbol{w}_k^{\mathrm{T}}} F_n(\boldsymbol{W}) = \frac{-\left(\sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}\right)}{1 + \sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}}$$

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It's a C $\times$ D matrix. Let's focus on the k-th row:

If $k \neq y_n$:

$$\nabla_{\boldsymbol{w}_k^{\mathrm{T}}} F_n(\boldsymbol{W}) = \frac{e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}} \boldsymbol{x}_n}}{1 + \sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}} \boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} = \mathbb{P}(k \mid \boldsymbol{x}_n; \boldsymbol{W}) \boldsymbol{x}_n^{\mathrm{T}}$$

else:

$$\nabla_{\boldsymbol{w}_k^{\mathrm{T}}} F_n(\boldsymbol{W}) = \frac{-\left(\sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}} \boldsymbol{x}_n}\right)}{1 + \sum_{k' \neq y_n} e^{(\boldsymbol{w}_{k'} - \boldsymbol{w}_{y_n})^{\mathrm{T}} \boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} = \left(\mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{W}) - 1\right) \boldsymbol{x}_n^{\mathrm{T}}$$

SGD for multinomial logistic regression

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

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

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

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Think about why the algorithm makes sense intuitively.

A note on prediction

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

- make a *deterministic* prediction $\operatorname{argmax}_{k \in [\mathsf{C}]} \ \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}$

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- make a *deterministic* prediction $\operatorname{argmax}_{k\in[\mathsf{C}]}\ \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$
- make a *randomized* prediction according to $\mathbb{P}(k \mid \boldsymbol{x}; \boldsymbol{W}) \propto e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}}$

Generalization of cross-entropy loss

Given a general model class:

$$\mathcal{F} = \left\{ f(\boldsymbol{x}) = \underset{k \in [\mathsf{C}]}{\operatorname{argmax}} \; s_k(\boldsymbol{x}) \right\}$$

where s_k is the **"scoring" function** for class k.

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The cross-entropy loss of f for a training sample $(\boldsymbol{x}, y)$ is

$$-\ln\left(\frac{e^{s_y(\boldsymbol{x})}}{\sum_{k \in [\mathsf{C}]} e^{s_k(\boldsymbol{x})}}\right) = \ln\left(1 + \sum_{k \neq y} e^{s_k(\boldsymbol{x}) - s_y(\boldsymbol{x})}\right)$$

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Is there an *even more general and simpler approach* to derive multiclass classification algorithms?

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Given a binary classification algorithm (*any one*, not just linear methods), can we turn it to a multiclass algorithm, *in a black-box manner*?

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.

One-versus-all (OvA)

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Training: for each class $k \in [\mathsf{C}]$,

- relabel examples with class k as $+1$, and all others as -1
- train a binary classifier h_k using this new dataset

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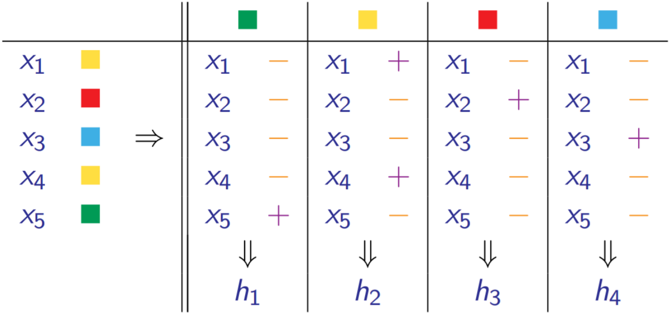

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Issue: will (probably) make a mistake *as long as one of h_k errs*.

One-versus-one (OvO)

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

One-versus-one (OvO)

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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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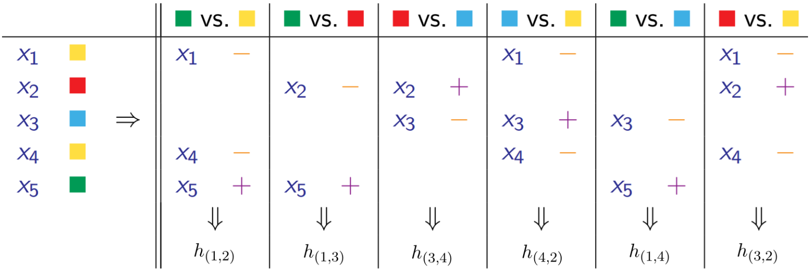

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More robust than one-versus-all, but *slower* in prediction.

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
■	+	−	+	−	+
■	−	−	+	+	+
■	+	+	−	−	−
■	+	+	+	+	−

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
[green]	+	−	+	−	+
[yellow]	−	−	+	+	+
[red]	+	+	−	−	−
[blue]	+	+	+	+	−

			1		2		3		4		5	
x_1	[yellow]		x_1	−	x_1	−	x_1	+	x_1	+	x_1	+
x_2	[red]		x_2	+	x_2	+	x_2	−	x_2	−	x_2	−
x_3	[blue]	$\Rightarrow$	x_3	+	x_3	+	x_3	+	x_3	+	x_3	−
x_4	[yellow]		x_4	−	x_4	−	x_4	+	x_4	+	x_4	+
x_5	[green]		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)

Prediction: for a new example $\boldsymbol{x}$

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

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How to design the code $\boldsymbol{M}$?

- the more *dissimilar* the codes, the more robust
  - 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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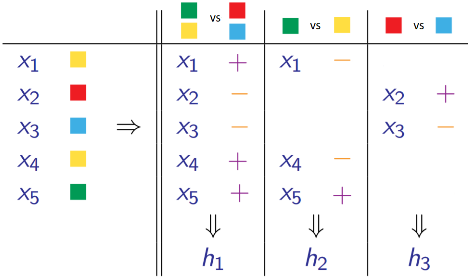
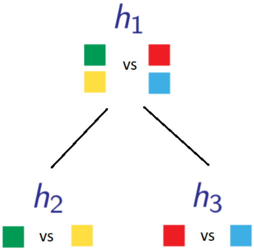
Training: see pictures

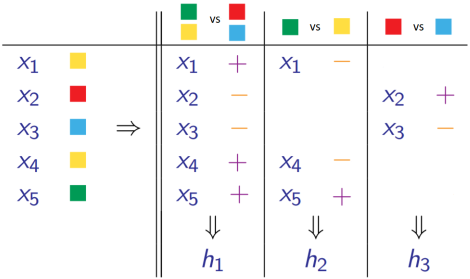


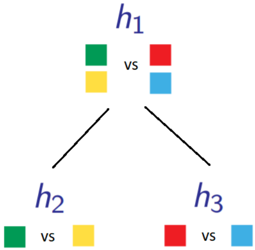


Tree based method

Idea: train ≈ C binary classifiers to learn "**belongs to which half?**".

Training: see pictures





Prediction is also natural,

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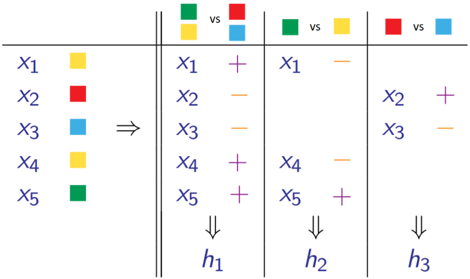

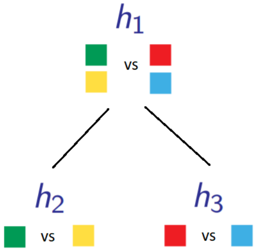

Prediction is also natural, *but is very fast!* (think ImageNet where $C \approx 20K$)

Comparisons

Reduction	**training time**	**prediction time**	**remark**

training time: how many training points are created

prediction time: how many binary predictions are made

Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA			

training time: how many training points are created

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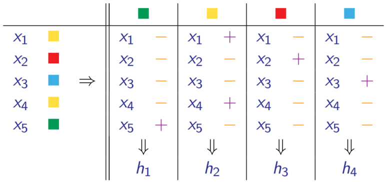
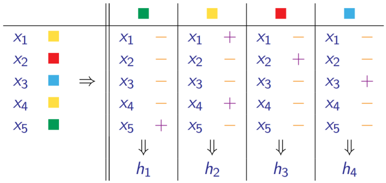


Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN		

training time: how many training points are created

prediction time: how many binary predictions are made

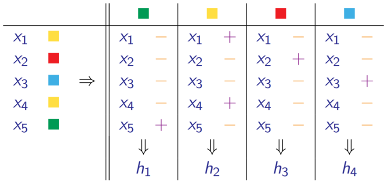


Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	

training time: how many training points are created

prediction time: how many binary predictions are made



Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	not robust

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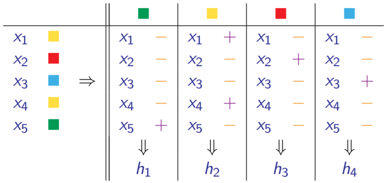

Comparisons

Reduction	training time	prediction time	remark
OvA	CN	C	not robust
OvO			

training time: how many training points are created

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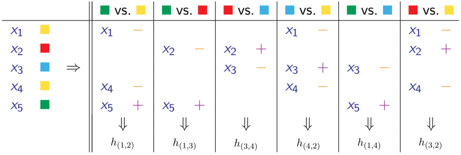

Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	not robust
OvO	$(C-1)N$		

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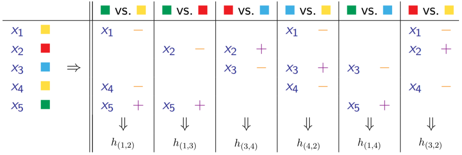

Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	not robust
OvO	$(C-1)N$	$\mathcal{O}(C^2)$	

training time: how many training points are created

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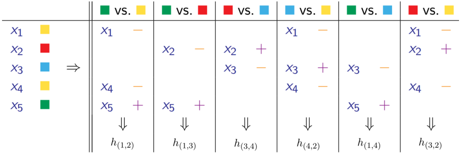

Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	not robust
OvO	$(C-1)N$	$\mathcal{O}(C^2)$	can achieve very small training error

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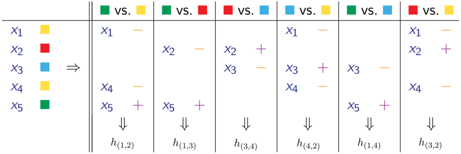

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ECOC			

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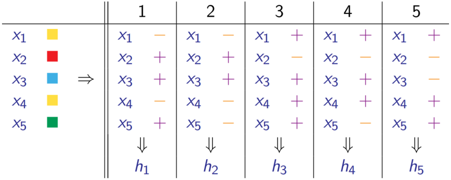

Comparisons

Reduction	**training time**	**prediction time**	**remark**
OvA	CN	C	not robust
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ECOC	LN		

training time: how many training points are created

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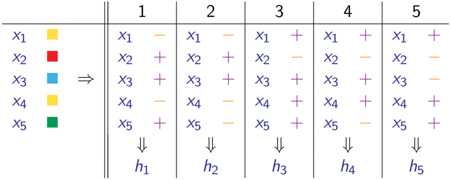

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ECOC	LN	L	

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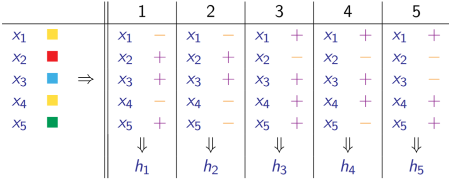

Comparisons

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OvA	CN	C	not robust
OvO	$(C-1)N$	$\mathcal{O}(C^2)$	can achieve very small training error
ECOC	LN	L	need diversity when designing code

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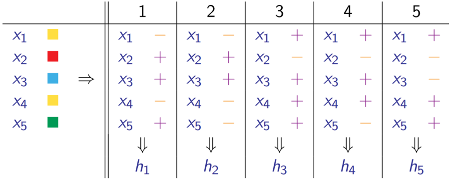

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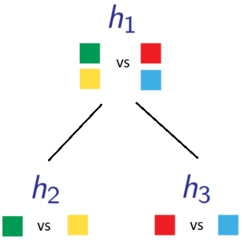
OvA	CN	C	not robust
OvO	$(C-1)N$	$\mathcal{O}(C^2)$	can achieve very small training error
ECOC	LN	L	need diversity when designing code
Tree			

training time: how many training points are created

prediction time: how many binary predictions are made



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ECOC	LN	L	need diversity when designing code
Tree	$\mathcal{O}((\log_2 C)N)$		

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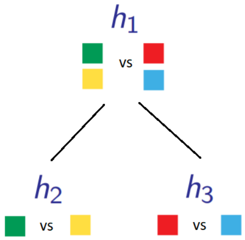

Comparisons

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OvO	$(C-1)N$	$\mathcal{O}(C^2)$	can achieve very small training error
ECOC	LN	L	need diversity when designing code
Tree	$\mathcal{O}((\log_2 C)N)$	$\mathcal{O}(\log_2 C)$	

training time: how many training points are created

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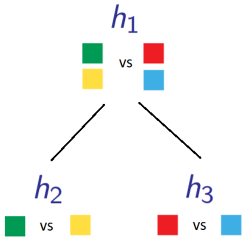

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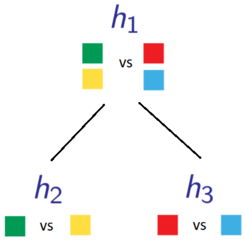
ECOC	LN	L	need diversity when designing code
Tree	$\mathcal{O}((\log_2 C)N)$	$\mathcal{O}(\log_2 C)$	good for "extreme classification"

training time: how many training points are created

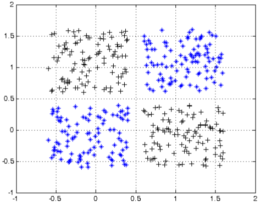
prediction time: how many binary predictions are made

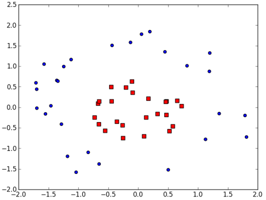


Outline

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

Linear models are not always adequate

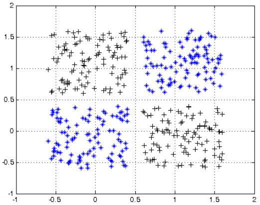


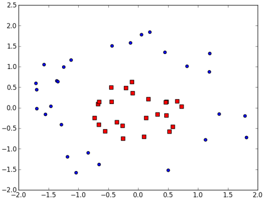


We can use a nonlinear mapping as discussed:

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

Linear models are not always adequate





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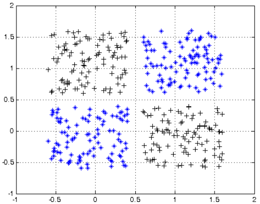

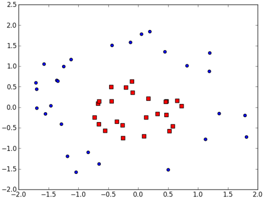

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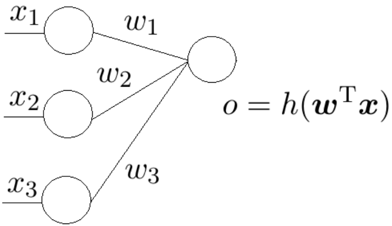
The most popular nonlinear models nowadays: **neural nets**

Linear model as a one-layer neural net



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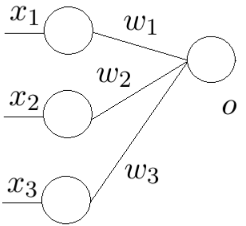
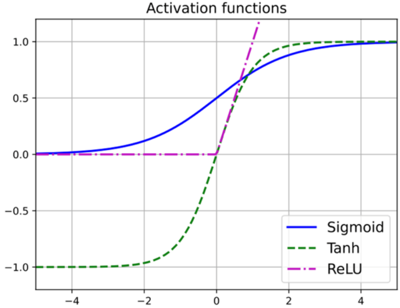


$o = h(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

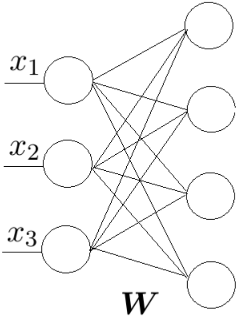
$h(a) = a$ for linear model

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



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

$\boldsymbol{W} \in \mathbb{R}^{4\times 3}$, $\boldsymbol{h} : \mathbb{R}^4 \to \mathbb{R}^4$ 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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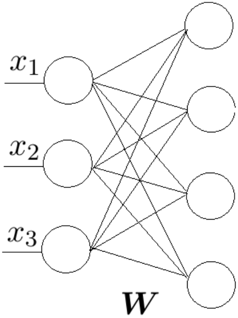

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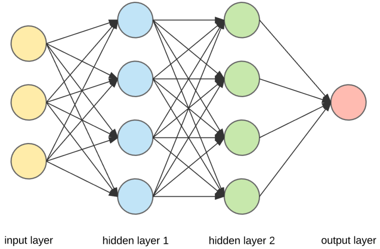
Can think of this as a nonlinear mapping: $\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$

More layers

Becomes a network:



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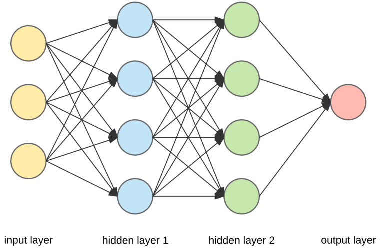

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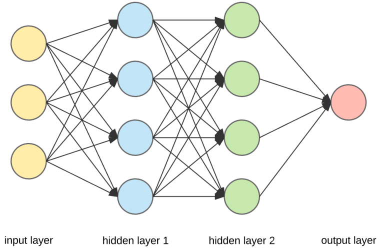

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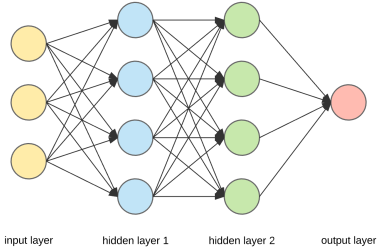

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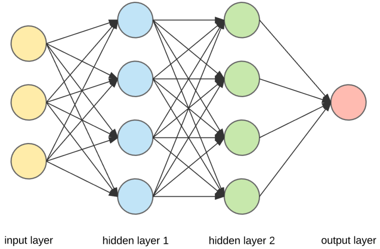

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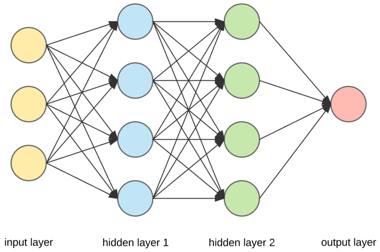

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- **deep** neural nets can have many layers and *millions* of parameters
- this is a **feedforward, fully connected** neural net, there are many variants (convolutional nets, recurrent nets, transformers, etc.)

How powerful are neural nets?

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

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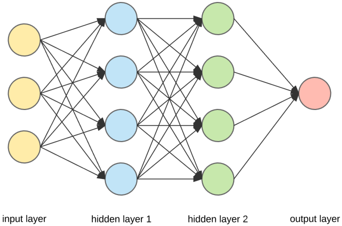
Designing network architecture is important and very complicated

- 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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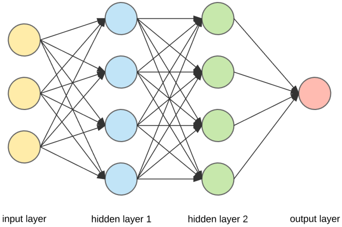

To ease notation, for a given input $\boldsymbol{x}$, define recursively

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

where

- $\boldsymbol{W}_\ell \in \mathbb{R}^{\mathsf{D}_\ell \times \mathsf{D}_{\ell-1}}$ is the weights between layer $\ell - 1$ and 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 of layer ℓ
- $\boldsymbol{h}_\ell : \mathbb{R}^{\mathsf{D}_\ell} \to \mathbb{R}^{\mathsf{D}_\ell}$ is activation functions at layer ℓ

Learning the model

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

$$F(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}) = \frac{1}{N} \sum_{n=1}^{\mathsf{N}} F_n(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L})$$

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where

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

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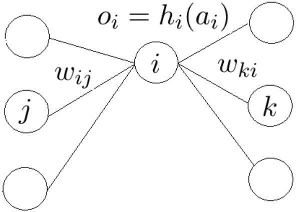
the simplest example $f(g_1(w), g_2(w)) = g_1(w)g_2(w)$

Computing the derivative

Drop the subscript ℓ for layer for simplicity.

Find the **derivative of F_n w.r.t. to w_{ij}**



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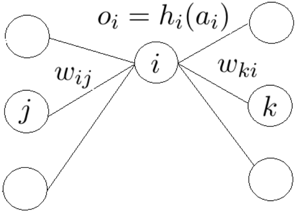

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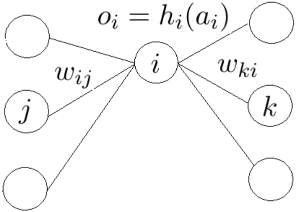

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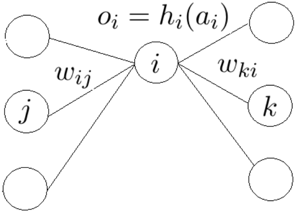

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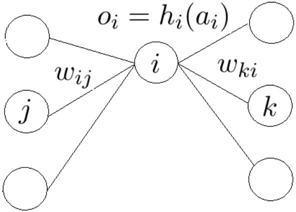

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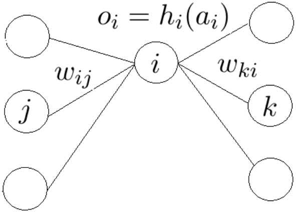

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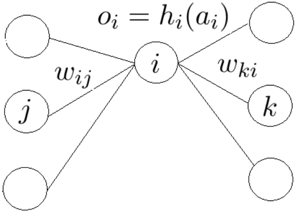

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Adding the subscript for layer:

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

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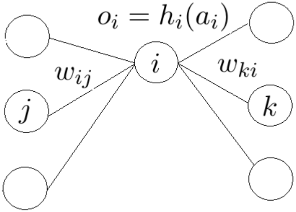

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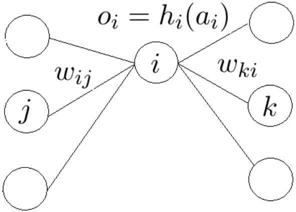

For the last layer, for square loss

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

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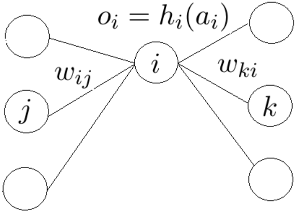

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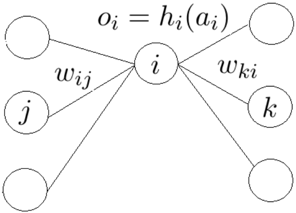

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Exercise: try to do it for cross-entropy loss yourself.

Computing the derivative

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

$$\frac{\partial F_n}{\partial \boldsymbol{W}_\ell} = \frac{\partial F_n}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathrm{T}} \in \mathbb{R}^{\mathsf{D}_\ell \times \mathsf{D}_{\ell-1}}$$

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

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 $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}$ randomly.

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2. **forward propagation**: for each layer $\ell = 1, \ldots, \mathsf{L}$
   - compute $\boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}$ and $\boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell)$ $(\boldsymbol{o}_0 = \boldsymbol{x}_n)$

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3. **backward propagation**: for each $\ell = L, \ldots, 1$
   - compute

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

   - update weights

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

Putting everything into SGD

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

Initialize $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}$ randomly. Repeat:

1. randomly pick one data point $n \in [\mathsf{N}]$
2. **forward propagation**: for each layer $\ell = 1, \ldots, \mathsf{L}$
   - compute $\boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}$ and $\boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell)$ $\qquad (\boldsymbol{o}_0 = \boldsymbol{x}_n)$
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(Important: *should $\boldsymbol{W}_\ell$ be overwritten immediately in the last step?*)

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- **momentum**: make use of previous gradients (taking inspiration from physics)
- ...

SGD with momentum (a simple version)

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

For $t = 1, 2, \ldots$

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

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Updates for first few rounds:

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Adam (most popular) $\approx$ SGD + adaptive learning rate + momentum

Overfitting

Overfitting is very likely since neural nets 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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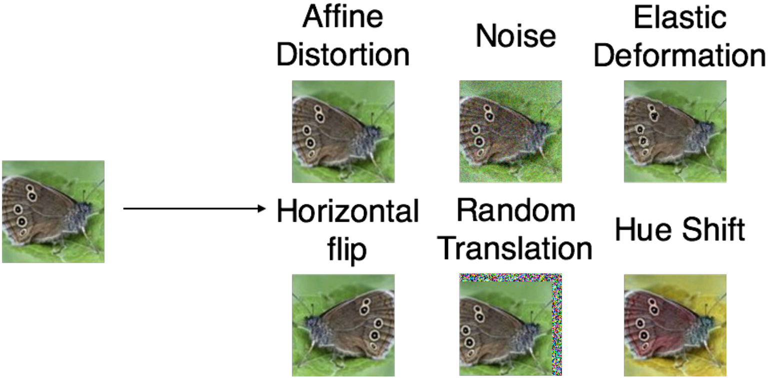
Exploit prior knowledge to add more training data



Regularization

L2 regularization: minimize

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

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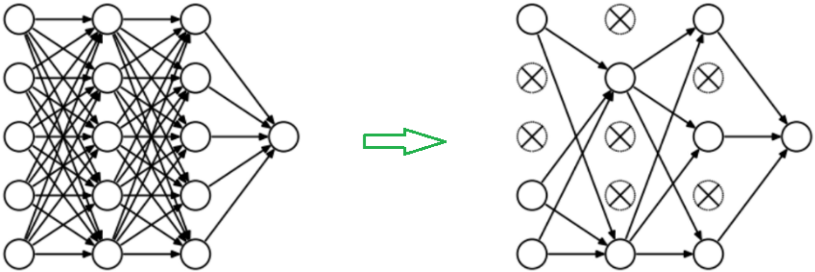
Introduce *weight decaying effect*

Dropout

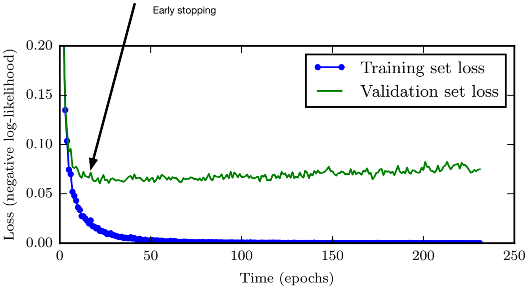
Independently delete each neuron with a fixed probability (say 0.5), during each iteration of Backprop (only for training, not for testing)



Very effective, makes training faster as well

Early stopping

Stop training when the performance on validation set stops improving



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- do need *a lot of data* to work well
- 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