CSCI567 Machine Learning (Spring 2021)

Sirisha Rambhatla

University of Southern California

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Outline

1. Logistics
2. Review of Last Lecture
3. Multiclass Classification

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Logistics

- HW 1 is due today, and HW 2 will be assigned.
- Please form the groups for the project, we'll have groups of 3 students working together. Use piazza to find group members.

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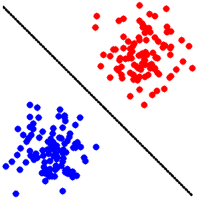
Summary

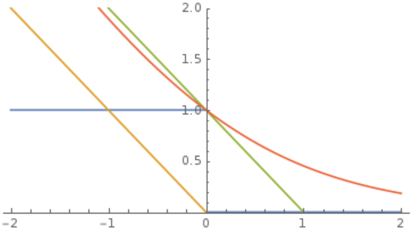
Linear models for **binary** classification:

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

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



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):

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

using

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

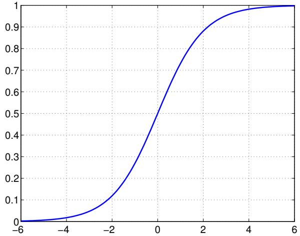
A Probabilistic view of logistic regression

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 Logistics

2 Review of Last Lecture

3 Multiclass Classification
- Multinomial logistic regression
- Reduction to binary classification

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

Step 1: *What should a linear model look like for multiclass tasks?*

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Note: a linear model for binary tasks (switching from $\{-1, +1\}$ to $\{1, 2\}$)

$$f(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0 \\ 2 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} < 0 \end{cases}$$

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can be written as

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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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$$= \operatorname*{argmax}_{k \in \{1,2\}} \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$$

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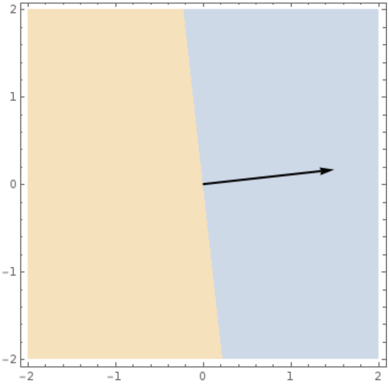
$$\begin{aligned} f(\boldsymbol{x}) &= \begin{cases} 1 & \text{if } \boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x} \geq \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x} \\ 2 & \text{if } \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x} > \boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x} \end{cases} \\ &= \operatorname*{argmax}_{k \in \{1,2\}} \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x} \end{aligned}$$

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**.

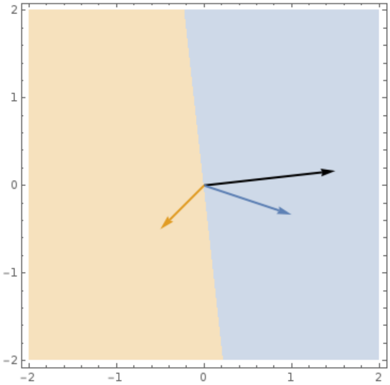
Linear models: from binary to multiclass



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

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

Linear models: from binary to multiclass



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

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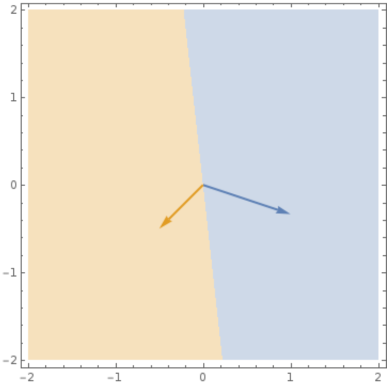

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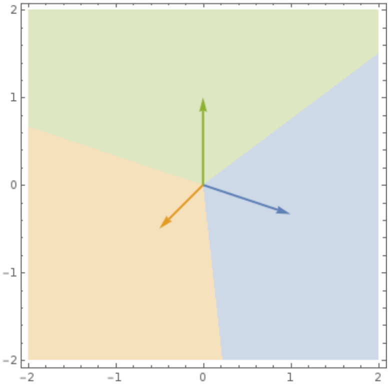

$$w_1 = (1, -\tfrac{1}{3})$$
$$w_2 = (-\tfrac{1}{2}, -\tfrac{1}{2})$$
$$w_3 = (0, 1)$$

- Blue class: $\{x : 1 = \text{argmax}_k\, w_k^T x\}$
- Orange class: $\{x : 2 = \text{argmax}_k\, w_k^T x\}$
- Green class: $\{x : 3 = \text{argmax}_k\, w_k^T x\}$

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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$$= \left\{ f(\boldsymbol{x}) = \operatorname*{argmax}_{k \in [\mathsf{C}]} (\boldsymbol{W}\boldsymbol{x})_k \mid \boldsymbol{W} \in \mathbb{R}^{\mathsf{C} \times \mathsf{D}} \right\}$$

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

Linear models for multiclass classification

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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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Naturally, for multiclass:

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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

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

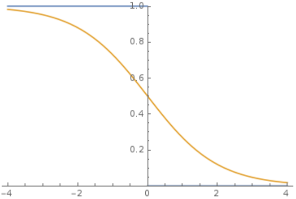
SGD for Binary Classification case (last lecture)

Recall that $\ell_{\text{logistic}}(z) = ln(1 + \exp(-z))$

$$\begin{aligned}
\boldsymbol{w} &\leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w}) \\
&= \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \qquad (n \in [N] \text{ is drawn u.a.r.}) \\
&= \boldsymbol{w} - \eta \left(\frac{\partial \ell_{\text{logistic}}(z)}{\partial z} \Big|_{z = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} - \eta \left(\frac{-e^{-z}}{1 + e^{-z}} \Big|_{z = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} + \eta \sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} + \eta \mathbb{P}(-y_n \mid \boldsymbol{x}_n; \boldsymbol{w}) y_n \boldsymbol{x}_n
\end{aligned}$$

This is a *soft version of Perceptron!*

$\mathbb{P}(-y_n | \boldsymbol{x}_n; \boldsymbol{w})$ versus $\mathbb{I}[y_n \neq \text{sgn}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)]$



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

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If $k \neq y_n$:

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

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else:

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

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else:

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

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.

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Reduce multiclass to binary

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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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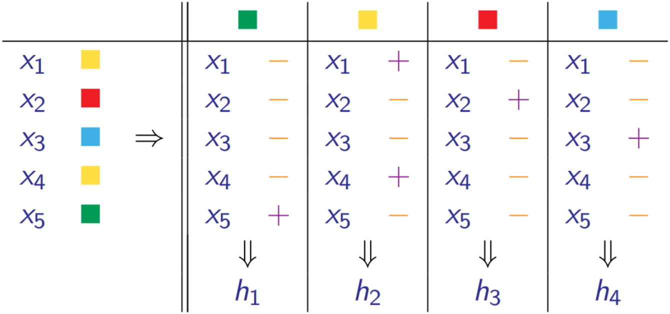

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Issue: will (probably) make a mistake *as long as one of h_k errs*.

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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- *discard all other examples*
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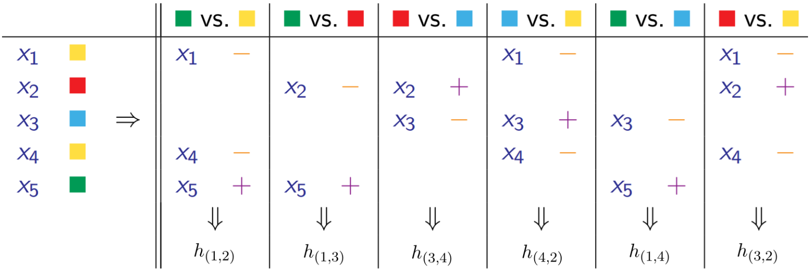

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More robust than one-versus-all, but *slower* in prediction.

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

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

- re-label 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	+
			$\Downarrow$ h_1		$\Downarrow$ h_2		$\Downarrow$ h_3		$\Downarrow$ h_4		$\Downarrow$ 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

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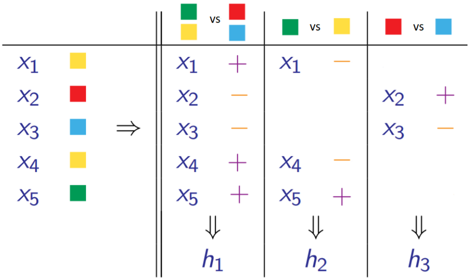
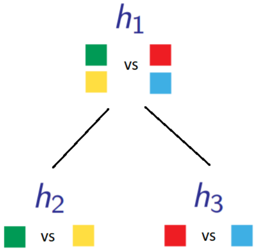
Training: see pictures





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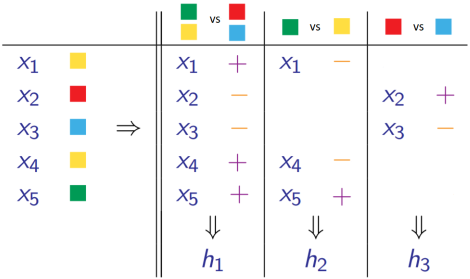

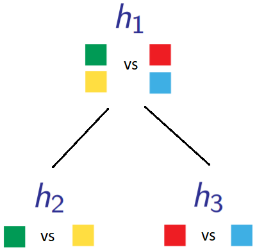

Prediction is also natural,

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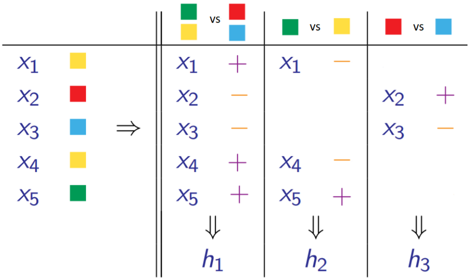

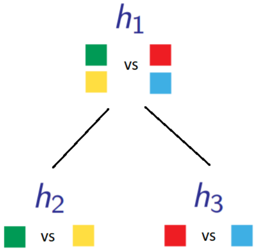

Prediction is also natural, *but is very fast!* (think ImageNet where $C \approx 20K$)

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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Tree	$(\log_2 C)N$	$\log_2 C$	good for “extreme classification”